Appendix G

NUCLEAR WASTE MANAGEMENT PROCEDURE Sandia National Laboratories	**User's Manual Criteria**	**Form Number: NP 19-1-6** **Page 1 of 1**

Does the User's Manual contain as appropriate:

1. **Software Name:** BRAGFLO
2. **Software Version:** 7.00
3. **Document Version:** 7.00
4. **ERMS #:** 570275

Prior to sign-off of the User's Manual, all items shall be appropriately addressed by the code sponsor so that "**Yes**" or "**N/A**" may be checked. Include this form as part of the User's Manual.

5. A statement(s) of functional requirements (consistent with those in the RD) and system limitations? ☒ Yes
6. An explanation of the mathematical model and numerical models, where applicable as based on code functionality? ☒ Yes ☐ N/A
7. Physical and mathematical assumptions, where applicable as based on code functionality? ☒ Yes ☐ N/A
8. The capabilities and limitations inherent in the software? ☒ Yes
9. Instructions that describe the user's interaction with the software? ☒ Yes
10. The identification of input parameters, formats, and valid ranges? ☒ Yes
11. Messages initiated as a result of improper input and how the user can respond? ☒ Yes
12. The identification and description of output specifications and formats? ☒ Yes
13. A description of any required training necessary to use the software? ☒ Yes
14. The identification of components of the code that were not tested? ☒ Yes ☐ N/A

15.	Brad Day **Code Team/Sponsor** (*print*)	Signature	12/19/18 Date
16.	Todd R. Zeitler **Technical Reviewer** (*print*)	Signature	12/19/2018 Date
17.	Shelly Nielsen **QA Reviewer** (*print*)	Shelly R. Nielsen Signature	12-19-18 Date
18.	Chris Camphouse **Responsible Manager** (*print*)	Signature	1/14/19 Date
19.	Jennifer Long **SCM Coordinator** (*print*)	Jennifer Long Signature	1/15/19 Date

User's Manual

for

BRAGFLO Version 7.00

Document Version 7.00

ERMS# 570275

January 2019

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1.0 INTRODUCTION

This document serves as a User's Manual for BRAGFLO Version 7.00. As such, it describes the purpose and function of the code, the user's interaction with the code, and the models and methods employed by the code. Examples of user-accessible input and output files are included for the user's convenience.

1.1 Software Identifier

Code Name:	BRAGFLO
Version:	7.00
Platform:	Oracle SUN X4-2B, Dell PowerEdge R820, Oracle SUN X6270 M2 server / SunOS 5.11 11.3 i86pc i386 i86pc

1.2 Points of Contact

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2.0 FUNCTIONAL REQUIREMENTS

The functional requirements for BRAGFLO, Version 7.00, include two additions (R.25 and R.26) and are defined in the Requirements Document / Verification and Validation Plan / Validation Document (Day, 2018) and repeated below.

R.1 Input defining the problem to be run is read in, including mesh size, simulation time specifications, and output files to be used.

R.2 The time and/or frequency of output to each output file and the variables whose values will be output are specified in the input.

R.3 The code reads input defining the finite difference grid for the problem to be run, including values of Δx, Δy, and Δz, and elevations of grid block centers, or input parameters that allow BRAGFLO to calculate the elevations. These input parameters may also specify how the mesh is rotated or dipped relative to a reference right hand coordinate system.

R.4 The default boundary conditions are no-flow conditions. BRAGFLO also allows constant pressure (Dirichlet) boundary conditions to be applied at specified grid blocks. The Dirichlet conditions fix the brine pressure and gas saturation at their initial values.

R.5 The following initial conditions are specified on input at each grid block: brine pressure, brine saturation, iron concentration, the concentration of biodegradables and the MgO concentration.

R.6 Parameters are inputs that control the numerical behavior of BRAGFLO. These include specifications of convergence tolerances, iteration limits, upstream weighting control parameters, dependent variable increments used to calculate Jacobian element derivatives numerically, and the solver to be used. Two solvers are currently available, the original LU decomposition solver and the point successive over-relaxation (SOR) solver, and only the original LU decomposition solver will be used in WIPP compliance calculations.

R.7 Material maps at specified times are input. For each material, material properties are input, including two-phase flow parameters, intrinsic permeabilities, reference condition porosities, and compressibilities. Also specified are the relative permeability and capillary pressure model to be used for each material. Furthermore, BRAGFLO allows for the change of pressure and saturation values, as well as the capability to turn off the chemistry reactions when materials change.

R.8 Relative permeabilities and capillary pressure are calculated for each material using one of several available models including original and modified versions of the Brooks-Corey and van Genuchten-Parker empirical relations, linear models, an open cavity model, and a waste area-specific model. Also, some of the QA tests use relative permeability models that are included in BRAGFLO specifically for those tests.

R.9 A simplified rock fracture model allows the porosity and permeability to increase as pore pressure increases above a threshold value, simulating a fracture network. In the absence of fracturing, the porosity may vary slightly with pressure due to rock compressibility effects.

R.10 The Klinkenberg effect is included, allowing the gas-phase permeability to become elevated over the intrinsic brine-phase permeability at low pressures in low-permeability materials.

R.11 Brine salinity, density at reference conditions, and compressibility are specified by input values, and the density of brine varies as a function of pressure.

R.12 Gas properties are given by the Redlich-Kwong-Soave (RKS) equation of state. The WIPP compliance calculations will use a single pure gas, H_2.

R.13 Two primary chemical reactions are modeled in BRAGFLO: anoxic corrosion of iron and microbial degradation of cellulosics. Both of these reactions produce gas (H_2) and consume brine according to specified stoichiometry. Reaction rates and stoichiometry are specified for brine-inundated conditions and for humid conditions.

R.14 The effects of salt creep, whereby the surrounding halite closes in on the waste or other excavated regions, compressing them, may be simulated in BRAGFLO through the use of a closure surface input data file.

R.15 BRAGFLO numerically calculates the flow of two phases, brine and gas, in porous media as a function of time and space, using an implicit finite difference method with variable time step control.

R.16 Well models in BRAGFLO allow simulation of wells that are completed within the formations or porous media being modeled. The types of wells that can be specified/modeled are constant injection or production rate wells and constant down-hole pressure wells.

R.17 BRAGFLO simulates flow through heterogeneous as well as homogeneous porous media.

R.18 BRAGFLO writes binary and ASCII output files. These files echo much of the input file information as well as primary and secondary dependent variables at user specified frequencies or at specific times. Many output variables are user selected and defined.

R.19 BRAGFLO provides the user with an error check on the consistency with how waste regions are specified.

R.20 Six additional chemical reactions are modeled in BRAGFLO: sulfidation of iron hydroxide; sulfidation of iron; hydration of MgO; carbonation of MgO; carbonation of $Mg(OH)_2$; and conversion of hydromagnesite. Stoichiometry is specified for each reaction with all necessary parameters specified in the input.

R.21 Chemical rates of all reactions are zero below a specified cutoff value in saturation which is specified in the input.

R.22 Chemical rates of all reactions are multiplied by their respective initial concentrations if specified by a flag in the input.

R.23 BRAGFLO calculates the change in solid volume from the chemical reactions.

R.24 BRAGFLO allows for the smooth change in permeability of materials in time as specified in the input.

R.25 BRAGFLO allows for the calculation of mass for up to five radionuclides in up to two waste areas by accounting for radioactive decay.

R.26 BRAGFLO allows for the calculation of radiolysis (the radiolytic breakdown of water/brine into hydrogen and oxygen) resulting from up to five inventory radionuclides. Radiolysis can result from radionuclides dissolved in brine and, optionally, from the remaining inventory of solid (precipitated) radionuclides that are in contact with brine (wetted). The fraction of disintegration energy from the solid radionuclides that contributes to radiolysis can be specified.

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3.0 REQUIRED USER TRAINING AND/OR BACKGROUND

In order to run the BRAGFLO code successfully, the user will need a basic knowledge of

- Solaris
- Sandia's CAMDAT database, (Gilkey, 2006a).

In addition, users should also have access to the WIPP cluster of Solaris microcomputers.

To interpret the input to and results from BRAGFLO, users should have:

- knowledge of basic mathematics through calculus and computational linear algebra
- an understanding of two-phase flow in porous media.

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4.0 DESCRIPTION OF THE MODELS AND METHODS

Quantification of the effects of gas and brine flow on radionuclide transport for undisturbed and disturbed conditions requires use of a two-phase flow code. For performance assessment at the WIPP repository, the U.S. Department of Energy (DOE) uses the two-phase flow code BRAGFLO to simulate brine and gas flow. The BRAGFLO code incorporates the effects of disposal room consolidation and closure, gas generation from corrosion and biodegradation reactions, brine consumption from corrosion, and inter-bed fracturing in response to gas pressure. This section develops the governing equations for BRAGFLO, its initial and boundary conditions, and the submodels incorporated in BRAGFLO that were developed specifically for performance assessment of the WIPP.

4.1 One-Dimensional Fluid Flow in Porous Media

Historically, BRAGFLO was developed as a two-phase flow model for petroleum production applications. For this reason, BRAGFLO uses terminology common to the petroleum industry. Further details of the concepts necessary for the finite difference solution of reservoir simulation problems are available in Peaceman (1977), Aziz and Settari (1979), and Thomas (1982).

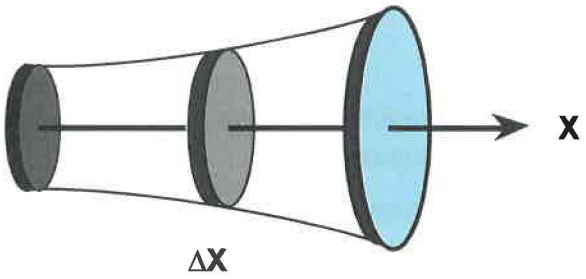


Figure 1. One dimensional reservoir with area-normal-to-flow as a function of x.

Consider now the material balance equation governing the flow of a fluid in a one-dimensional porous media. Figure 1 shows a one-dimensional reservoir with area-normal-to-flow as a function of x; area = $A(x)$. The flow streamlines will actually flare in or out due to the variable area. However, we make the assumption that density and velocity are representative of average properties over the area normal to flow. From the reservoir, select an element of volume of incremental length Δx.

Let

Q = volume flow rate [l^3/t]

ρ = fluid density [m/l^3]

q = mass flow rate [m/t]

v = flow velocity [l/t]

ϕ = porosity [pore volume/bulk volume]

A = normal cross-section area [l^2]

where the generic units are:

m = mass

l = length

t = time.

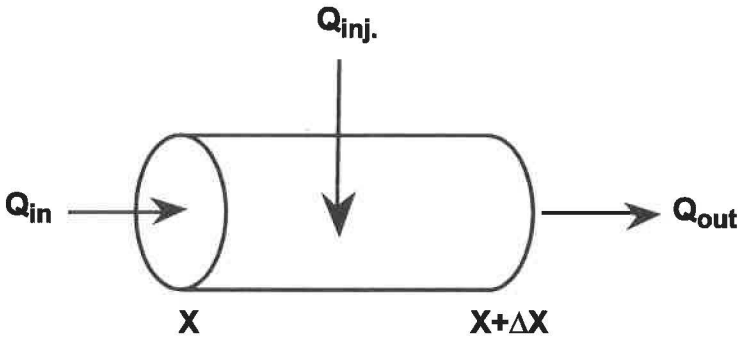


Figure 2. Element of volume of length Δx.

The mass rate and volume rate of flow are related by $q = \rho Q$. The sign convention on Q_{inj} is

$Q_{inj} > 0$, injection, (1)

$Q_{inj} < 0$, production. (2)

Also, Q_{inj} = volume rate/injected volume, which implies fluid injection is uniformly distributed over control volume $A\Delta x$. Mass balance requires that

$q_{in} - q_{out} + q_{inj} A\Delta x$ = change in fluid mass/time (3)

where

q_{inj} = mass injection rate/unit volume. (4)

Now

$q_{in} = (vA\rho)_x$ (5)

$q_{out} = (vA\rho)_{x+\Delta x}$ (6)

and

$$\text{rate of change of fluid mass} = \frac{\partial}{\partial t}(\phi A \Delta x \rho) \quad (7)$$

The mass balance is then

$$(vA\rho)_x - (vA\rho)_{x+\Delta x} + q_{inj} A\Delta x = \frac{\partial}{\partial t}(\phi A \Delta x \rho) \quad (8)$$

Express the area as $A = \alpha(x)$, then dividing by Δx yields

$$\frac{(\alpha v\rho)_x - (\alpha v\rho)_{x+\Delta x}}{\Delta x} + \alpha q_{inj} = \frac{\partial}{\partial t}(\alpha\phi\rho). \quad (9)$$

In the limit as $\Delta x \rightarrow 0$, we get the material balance equation for one-dimensional single phase flow

$$-\frac{\partial}{\partial x}(\alpha v \rho) + \alpha q_{inj} = \frac{\partial}{\partial t}(\alpha \phi \rho). \tag{10}$$

4.2 Darcy's Law

For the viscous flow of a fluid through a porous medium the flow velocity is related to the fluid potential by Darcy's Law (Darcy, 1856) a mathematical model developed from empirical data gathered in experiments using a device similar to the one illustrated in Figure 3.

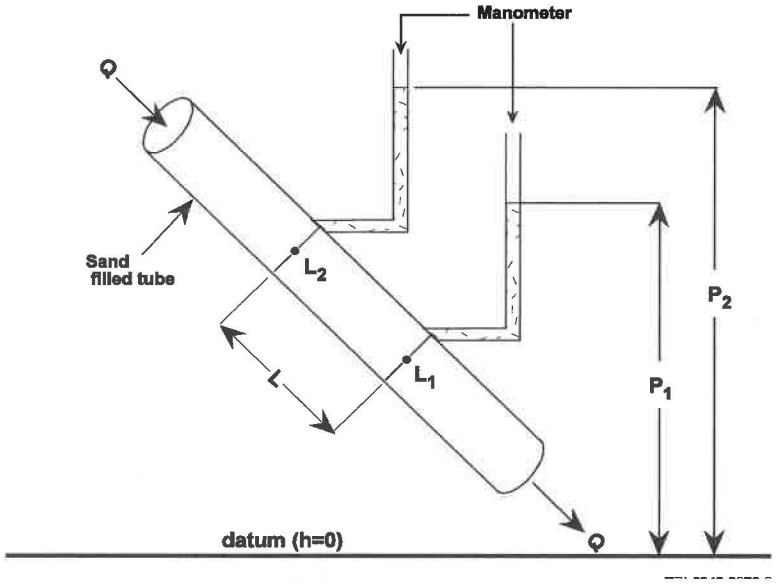


Figure 3. Experiment for illustration of Darcy's Law.

In Figure 3, Q is volumetric flow rate, and distance is measured in the positive x-direction, from L_2 to L_1, where the fluid pressure is P_2 and P_1, respectively. The height above a reference datum is h. The cross-sectional area is A, and the fluid has viscosity, μ, and density, ρ. The permeability of the porous medium is k. The differential form of Darcy's Law is:

$$Q = \frac{-kA}{\mu}\left(\frac{dP}{dx} + \rho g \frac{dh}{dx}\right). \tag{11}$$

The negative sign in Darcy's Law indicates that flow is in the direction of decreasing pressure or height above the datum.

The units used in BRAGFLO are

Q = m^3/s

k = m^2

A = m^2

$$\frac{dP}{dx} = \text{Pa/m}$$

$$\mu = \text{Pa} \cdot \text{s}$$

$$\rho = \text{kg/m}^3$$

$$\frac{dh}{dx} = \text{m/m}$$

$$g = \text{m/s}^2.$$

Velocity is given by

$$v = \frac{Q}{A} = -\frac{k}{\mu}\left(\frac{dP}{dx} + \rho g \frac{dh}{dx}\right), \tag{12}$$

where v is called the Darcy velocity or superficial flow velocity. The quantity

$$V = \frac{Q}{A\phi} = \frac{v}{\phi} = \frac{\text{bulk volume}}{\text{normal area}} \,/\, \text{time} \tag{13}$$

is called the interstitial or average linear velocity, where ϕ is the formation porosity.

The distinction between the Darcy velocity and the interstitial velocity is demonstrated in Figure 4. Assume fluid in the unit bulk volume at the left end of the reservoir is displaced by a piston over unit time into a media with porosity $\phi = 0.20$. The cubic meter of fluid will occupy 5 m^3 of the porous material and the fluid will advance to a position 5 meters from the interface. The velocity of the fluid in the bulk volume is Q/A, or the Darcy velocity, while the fluid velocity in the porous material is $Q/(A\phi)$, or the interstitial velocity. For example, if a tracer element were introduced into the porous material, it would travel at the interstitial velocity. The Darcy velocity is the rate at which the bulk volume is transported.

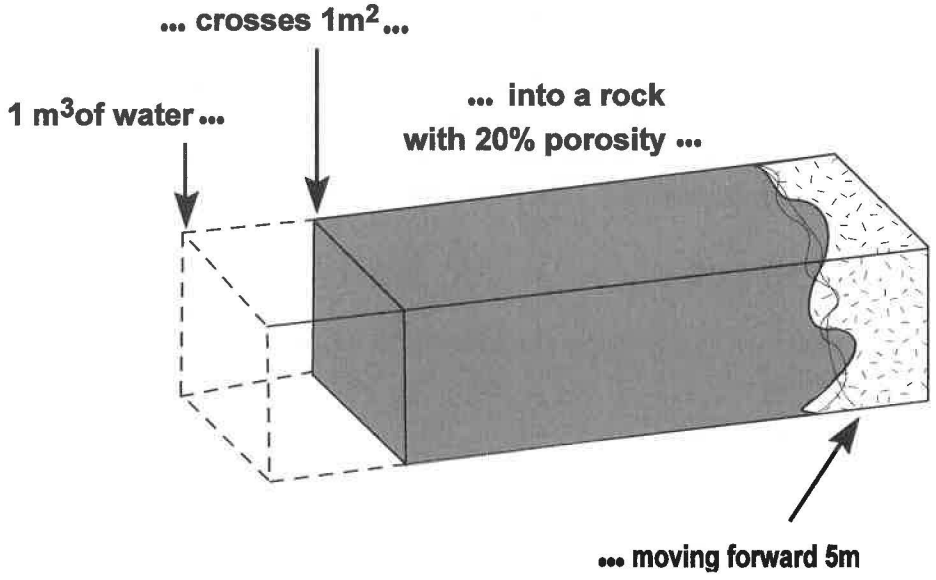


Figure 4. Volume versus porous media displacement.

4.3 Permeability Tensor, Darcy's Law, and Material Balance in Higher Dimension

The permeability of a geological formation can be direction dependent (anisotropic). For example, a sedimentary formation may consist of uniform sand or lime laminae of high permeability alternating with thin, uniform layers of silty, shaley laminae of low permeability. The large scale permeability characteristics can be approximated as uniformly anisotropic. That is, the layered system is replaced by a homogeneous system having permeability k_1 parallel to the plane of the laminae and k_2 normal to this plane. Further, the direction of the laminae may not be parallel or normal to the formation boundary as evident in a cross-bedded structure.

Figure 5 shows two Cartesian coordinate systems (ξ, η) and (x,y). Suppose the principal permeabilities are given with respect to (ξ, η) system with k_1 the permeability in the ξ direction and k_2 the permeability in the η direction. Further, assume the reservoir geometry is aligned with respect to the (x,y) system, which implies that the fluid flow equations are to be formulated with respect to the (x,y)-axes.

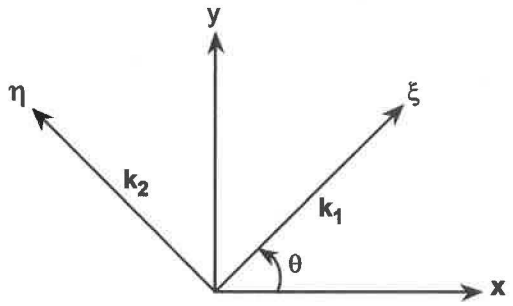


Figure 5. Permeability with anisotropic values k_1 and k_2 in direction ξ and η

The coordinate transformation from the (ξ, η) system to the (x,y) system is

$$x = \xi \cos\theta - \eta \sin\theta \qquad (14)a,b$$

$$y = \xi \sin\theta + \eta \cos\theta.$$

If $\hat{\mathbf{1}}_\xi$ and $\hat{\mathbf{1}}_\eta$ represent the unit vectors in the ξ, η-directions, respectively, then the Darcy velocity vector (ignoring gravitational effects for now) is

$$\hat{\mathbf{v}} = -\frac{k_1}{\mu}\frac{\partial P}{\partial \xi}\hat{\mathbf{1}}_\xi - \frac{k_2}{\mu}\frac{\partial P}{\partial \eta}\hat{\mathbf{1}}_\eta. \qquad (15)$$

The coordinate transformation maps the unit vectors into

$$\hat{\mathbf{1}}_\xi \rightarrow \cos\theta\hat{\mathbf{1}}_x + \sin\theta\hat{\mathbf{1}}_y \qquad (16)$$

and

$$\hat{\mathbf{1}}_\eta \rightarrow -\sin\theta\hat{\mathbf{1}}_x + \cos\theta\hat{\mathbf{1}}_y. \qquad (17)$$

The chain rule gives

$$\frac{\partial P}{\partial \xi} = \cos\theta \frac{\partial P}{\partial x} + \sin\theta \frac{\partial P}{\partial y} \tag{18}$$

and

$$\frac{\partial P}{\partial \eta} = -\sin\theta \frac{\partial P}{\partial x} + \cos\theta \frac{\partial P}{\partial y}. \tag{19}$$

Then the Darcy velocity is

$$\begin{aligned} \hat{\mathbf{v}} = & \frac{-k_1}{\mu}\left(\cos\theta \frac{\partial P}{\partial x} + \sin\theta \frac{\partial P}{\partial y}\right)\left(\cos\theta \hat{\mathbf{1}}_x + \sin\theta \hat{\mathbf{1}}_y\right) \\ & -\frac{k_2}{\mu}\left(-\sin\theta \frac{\partial P}{\partial x} + \cos\theta \frac{\partial P}{\partial y}\right)\left(-\sin\theta \hat{\mathbf{1}}_x + \cos\theta \hat{\mathbf{1}}_y\right) \end{aligned} \tag{20}$$

The vector components of the Darcy velocity are

$$v_x = \frac{-k_1}{\mu}\left(\cos^2\theta \frac{\partial P}{\partial x} + \sin\theta\cos\theta \frac{\partial P}{\partial y}\right) - \frac{k_2}{\mu}\left(\sin^2\theta \frac{\partial P}{\partial x} - \sin\theta\cos\theta \frac{\partial P}{\partial y}\right), \tag{21}$$

$$v_y = \frac{-k_1}{\mu}\left(\sin\theta\cos\theta \frac{\partial P}{\partial x} + \sin^2\theta \frac{\partial P}{\partial y}\right) - \frac{k_2}{\mu}\left(-\sin\theta\cos\theta \frac{\partial P}{\partial x} + \cos^2\theta \frac{\partial P}{\partial y}\right). \tag{22}$$

The dependence of the Darcy velocity components on pressure gradients in both x- and y-directions will add significantly to the complexity of the material balance equation in 2-dimensions. A similar analysis with more complexity could be performed in 3-dimensions.

A significant simplification occurs if the directions of the permeability tensor are aligned with the reservoir coordinate axis; that is, $\theta = 0$. If $\theta = 0$, then

$$v_x = \frac{-k_1}{\mu}\frac{\partial P}{\partial x} \quad \text{and} \quad v_y = \frac{-k_2}{\mu}\frac{\partial P}{\partial y}. \tag{23}$$

BRAGFLO makes this assumption. Thus, in three dimensions with anisotropic permeability, the components of the Darcy velocity are

$$v_x = \frac{-k_x}{\mu}\frac{\partial P}{\partial x}, \quad v_y = \frac{-k_y}{\mu}\frac{\partial P}{\partial y}, \quad v_z = \frac{-k_z}{\mu}\frac{\partial P}{\partial z} \tag{24}$$

where k_x, k_y, k_z are input permeabilities in the direction of the corresponding coordinate axes.

When the effect of gravity is included, the components of the Darcy velocity become

$$v_x = \frac{-k_x}{\mu}\left(\frac{\partial P}{\partial x} + \rho g \frac{\partial h}{\partial x}\right), \quad v_y = \frac{-k_y}{\mu}\left(\frac{\partial P}{\partial y} + \rho g \frac{\partial h}{\partial y}\right), \quad v_z = \frac{-k_z}{\mu}\left(\frac{\partial P}{\partial z} + \rho g \frac{\partial h}{\partial z}\right) \tag{25}$$

To generalize the flow equation to higher dimension, we replace the flux term with (Peaceman, 1977)

$$\begin{aligned}\nabla\bullet\left[\frac{\alpha\rho[k]}{\mu}(\nabla P+\rho g\nabla h)\right]&\\ =\left(\frac{\partial}{\partial x}\hat{\mathbf{i}}+\frac{\partial}{\partial y}\hat{\mathbf{j}}+\frac{\partial}{\partial z}\hat{\mathbf{k}}\right)\bullet\left[\frac{\alpha\rho k_x}{\mu}\left(\frac{\partial P}{\partial x}+\rho g\frac{\partial h}{\partial x}\right)\hat{\mathbf{i}}+\frac{\alpha\rho k_y}{\mu}\left(\frac{\partial P}{\partial y}+\rho g\frac{\partial h}{\partial y}\right)\hat{\mathbf{j}}+\frac{\alpha\rho k_z}{\mu}\left(\frac{\partial P}{\partial z}+\rho g\frac{\partial h}{\partial z}\right)\hat{\mathbf{k}}\right]&\\ =\frac{\partial}{\partial x}\left[\frac{\alpha\rho k_x}{\mu}\left(\frac{\partial P}{\partial x}+\rho g\frac{\partial h}{\partial x}\right)\right]+\frac{\partial}{\partial y}\left[\frac{\alpha\rho k_y}{\mu}\left(\frac{\partial P}{\partial y}+\rho g\frac{\partial h}{\partial y}\right)\right]+\frac{\partial}{\partial z}\left[\frac{\alpha\rho k_z}{\mu}\left(\frac{\partial P}{\partial z}+\rho g\frac{\partial h}{\partial z}\right)\right]&\end{aligned} \tag{26}$$

where

$[k]$ = permeability tensor,

α = area normal to flow direction in one dimension (x), or

= thickness normal to flow plane in two-dimensions (x,y), or

= 1 in three-dimensions (x,y,z).

The three-dimensional flow of a single fluid incorporating Darcy's law is

$$\frac{\partial}{\partial x}\left[\frac{\alpha\rho k_x}{\mu}\left(\frac{\partial P}{\partial x}+\rho g\frac{\partial h}{\partial x}\right)\right]+\frac{\partial}{\partial y}\left[\frac{\alpha\rho k_y}{\mu}\left(\frac{\partial P}{\partial y}+\rho g\frac{\partial h}{\partial y}\right)\right]+\frac{\partial}{\partial z}\left[\frac{\alpha\rho k_z}{\mu}\left(\frac{\partial P}{\partial z}+\rho g\frac{\partial h}{\partial z}\right)\right]+\alpha q_{inj}=\frac{\partial}{\partial t}(\alpha\phi\rho) \tag{27}$$

4.4 Equation of State

From the previous section the three dimensional flow of a single phase fluid is governed by the equation

$$\frac{\partial}{\partial x}\left[\frac{\alpha\rho k_x}{\mu}\left(\frac{\partial P}{\partial x}+\rho g\frac{\partial h}{\partial x}\right)\right]+\frac{\partial}{\partial y}\left[\frac{\alpha\rho k_y}{\mu}\left(\frac{\partial P}{\partial y}+\rho g\frac{\partial h}{\partial y}\right)\right]+\frac{\partial}{\partial z}\left[\frac{\alpha\rho k_z}{\mu}\left(\frac{\partial P}{\partial z}+\rho g\frac{\partial h}{\partial z}\right)\right]+\alpha q_{inj}=\frac{\partial}{\partial t}(\alpha\phi\rho) \tag{28}$$

This equation has two dependent variables, pressure, P, and density, ρ. Independent variables are space (x, y, z) and time (t). We must relate ρ and P and hence eliminate one of the dependent variables. This problem is generally treated over three fluid regimes:

- incompressible fluid (ρ = constant)
- slightly compressible fluid (water, oil)
- highly compressible fluid (gas)

The incompressible fluid assumption is not valid for most applications and will not be considered.

Slightly compressible fluid assumes:

$$\left(\frac{\partial\rho}{\partial P}\right)_T=c\rho, \tag{29}$$

where c is fluid compressibility. For ideal fluid c = constant. Then the differential equation can be solved as

$$\rho = \rho_o \exp\left[c\left(P - P_o\right)\right] \tag{30}$$

where ρ_o is density at reference pressure P_o. This is the equation BRAGFLO uses to evaluate brine density.

Recall the series for the exponential function

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots \tag{31}$$

and if x is close to zero

$$e^x \cong 1 + x. \tag{32}$$

Therefore, if $c(P\text{-}P_o)$ is relatively small, then

$$\rho \cong \rho_o\left[1 + c\left(P - P_o\right)\right]. \tag{33}$$

This linearization is sometimes used as an approximation to the exponential density function.

A highly compressible fluid such as gas requires a real gas equation of state

$$\rho = \rho(P,T) \tag{34}$$

which, for isothermal flow, gives density as a function of pressure. BRAGFLO uses the Redlich-Kwong-Soave equation of state to relate gas density to pressure (Walas, 1985).

The formation rock behaves as a slightly compressible material, which yields an expression for porosity analogous to the expression for brine density. In BRAGFLO the formation porosity is evaluated as

$$\phi = \phi_o \exp\left[c_\phi\left(P - P_o\right)\right] \tag{35}$$

where ϕ_o is the porosity at reference pressure P_o and c_ϕ denotes pore compressibility (note: assuming all of the change in volume during compression occurs in the pore volume, pore compressibility is approximated by the radio of bulk rock compressibility to porosity; hereafter, simply referred to as rock compressibility).

With the equation of state, the material balance equation is formulated and solved in terms of a single dependent variable, namely pressure. Note that the partial differential equation (PDE) is nonlinear. Non-linearity occurs from several sources:

- nonlinear dependence of density on pressure
- product of density and pressure gradient
- product of porosity and density in accumulation term since porosity is pressure dependent due to rock compressibility
- viscosity could be pressure dependent for gases, however, BRAGFLO treats viscosity constant for both water and gas.

For the one-dimensional case of the equation presented at the end of Section 4.3,

$$\frac{\partial}{\partial x}\left[\frac{\alpha\rho k_x}{\mu}\left(\frac{\partial P}{\partial x}+\rho g\frac{\partial h}{\partial x}\right)\right]+\alpha q_{inj}=\frac{\partial}{\partial t}(\alpha\phi\rho), \tag{36}$$

The material balance equation (PDE) requires:

Initial conditions:

$$P(x,0)=f(x),\quad 0\le x\le L \tag{37}$$

and

Boundary conditions:

$$P(0,t)=g_o(t),\quad P(L,t)=g_L(t),\quad t\ge 0 \tag{38}$$

or

$$\frac{\partial P}{\partial x}(0,t)=g_o(t),\qquad \frac{\partial P}{\partial x}(L,t)=g_L(t)\qquad t\ge 0. \tag{39}$$

The first type of boundary condition in which the solution is specified at the boundary is called a Dirichlet boundary condition. The condition in which the pressure gradient is specified is called a Neumann boundary condition. Generally, most reservoir simulations assume $\partial P/\partial x=0$ on the boundary (no-flow boundary condition). The boundary condition may be of mixed type. BRAGFLO assumes a no-flow Neumann type boundary condition at all exterior grid boundaries.

BRAGFLO has the capability of maintaining (Dirichlet condition) pressure and/or saturation at specified grid blocks. This allows the maintenance of initial conditions at far field locations in the upper formations such as the Culebra.

4.5 Finite Difference and Discretization of Material Balance Equation

Recall Taylor's formula with remainder for a function f expanded about x_o:

$$\begin{aligned} f(x)=f(x_o)+f'(x_o)(x-x_o)+\frac{f^{(2)}(x_o)}{2!}(x-x_o)^2 \\ +\ldots+\frac{f^{(n)}(x_o)}{n!}(x-x_o)^n+\frac{f^{(n+1)}(\xi)}{(n+1)!}(x-x_o)^{n+1} \end{aligned} \tag{40}$$

where ξ is the interval between x and x_o. Thus

$$f(x)\ =\ p(x)\ +\ R_n(x,x_o) \tag{41}$$

or

$$f(x)\ -\ p(x)\ =\ R_n(x,x_o), \tag{42}$$

where p(x) is a polynomial approximation to f and the remainder term is the error.

If $f^{(n+1)}$ is continuous on some interval $[a,b]$ containing, (x, x_o), then $f^{(n+1)}$ is bounded,

$$\left|f^{(n+1)}(x)\right| \leq M, \tag{43}$$

and

$$\left|f(x) - p(x)\right| \leq C\left|x - x_o\right|^{n+1} \tag{44}$$

Therefore, as $x \to x_o$, the error goes to zero like $(x - x_o)^{n+1}$. Consider the following derivative approximations. First order forward difference requires the Taylor formula:

$$f(x) = f(x_o) + f'(x_o)(x - x_o) + R_2(x, x_o) \tag{45}$$

Let $x = x_o + h$, then

$$\left|\frac{f(x_o + h) - f(x_o)}{h} - f'(x_o)\right| = \left|\frac{R_2(x, x_o)}{h}\right| \leq \frac{Ch^2}{h} = Ch. \tag{46}$$

The difference approximation

$$f'(x_o) \cong \frac{f(x_o + h) - f(x_o)}{h} \tag{47}$$

is said to be first order in h. This type of approximation is used for the time derivative.

Second order central approximation:

$$f(x_o + h) = f(x_o) + f'(x_o)h + \frac{f^{(2)}(x_o)}{2!}h^2 + R_3(x_o, x_o + h) \tag{48}$$

$$f(x_o - h) = f(x_o) - f'(x_o)h + \frac{f^{(2)}(x_o)}{2!}h^2 + R_3(x_o, x_o - h) \tag{49}$$

where subtraction yields

$$f(x_o + h) - f(x_o - h) = 2hf(x_o)' + R_3(x_o, x_o + h) - R_3(x_o, x_o - h). \tag{50}$$

This is rearranged to give:

$$\frac{f(x_o + h) - f(x_o - h)}{2h} - f'(x_o) = \frac{R_3(x_o, x_o + h) - R_3(x_o, x_o - h)}{2h} \tag{51}$$

which produces the estimate

$$\left|\frac{f(x_o + h) - f(x_o - h)}{2h} - f'(x_o)\right| \leq \frac{Ch^3}{h} = Ch^2. \tag{52}$$

Therefore, the difference approximation $\frac{f(x_o + h) - f(x_o - h)}{h}$ is a second order approximation to $f'(x_o)$.

Consider discretization of the one-dimensional material balance equation:

$$\frac{\partial}{\partial x}\left[\frac{\alpha\rho k_x}{\mu}\left(\frac{\partial P}{dx}\right)\right] + \alpha q_{inj} = \frac{\partial}{\partial t}(\alpha\phi\rho) \tag{53}$$

where we assume the gradient of the depth, dh/dx is zero.

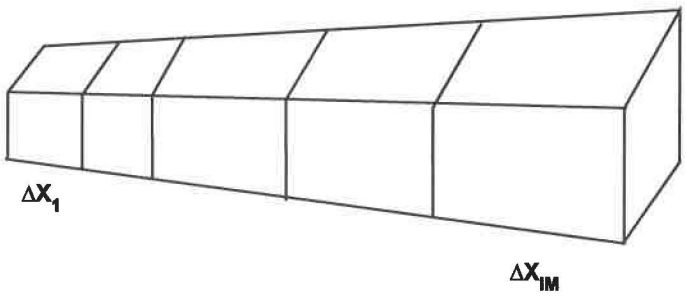


Figure 6. Partition interval [0,*L*] into IM subintervals.

Space discretization requires the partition of the interval [0,*L*] into IM subintervals with length Δx_i, i=1, 2, ..., IM, as shown in Figure 6. Consider an arbitrary grid block i and its neighbors i-1, i+1 as shown in Figure 7.

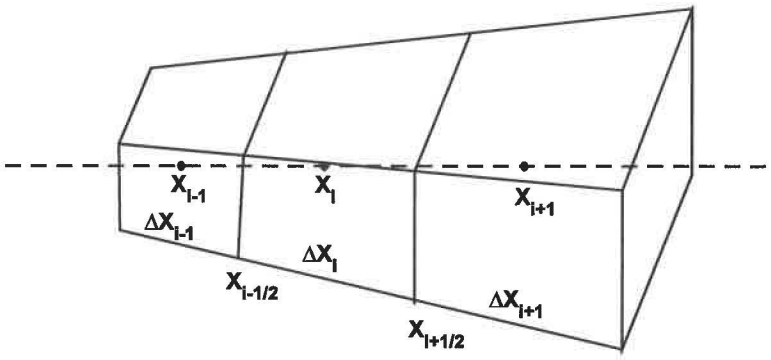


Figure 7. Depiction of arbitrary grid block.

We reference the location of the grid block interfaces as

$x_{i-1/2}$ = location of interface between i-1 and i,

$x_{i+1/2}$ = location of interface between i and i+1.

For example,

$$x_{i-1/2} = x_{i-1} + \Delta x_{i-1/2}. \tag{54}$$

On the i^{th} grid block the partial derivative in the flux term is approximated by the 2nd order correct finite difference

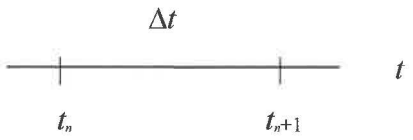
$$\frac{\partial}{\partial x}\left(\frac{\alpha k\rho}{\mu}\frac{\partial P}{\partial x}\right) \cong \frac{\left(\frac{\alpha k\rho}{\mu}\frac{\partial P}{\partial x}\right)_{i+1/2} - \left(\frac{\alpha k\rho}{\mu}\frac{\partial P}{\partial x}\right)_{i-1/2}}{\Delta x_i} \tag{55}$$

The partials are approximated at the interface by the 2nd order correct finite difference

$$\left(\frac{\alpha k\rho}{\mu}\frac{\partial P}{\partial x}\right)_{i-1/2} = \left(\frac{\alpha k\rho}{\mu}\right)_{i-1/2}\frac{P_i - P_{i-1}}{x_i - x_{i-1}}. \tag{56}$$

A similar expression exists at $i + 1/2$. If the gridding is non-uniform, then the above approximations are no longer 2nd order correct.

Time discretization is as shown below.



Assume the solution is known at time t_n, and we wish to compute a solution at time t_{n+1} with time step size $\Delta t = t_{n+1} - t_n$. The time discretization of the accumulation term in the i^{th} grid block uses the first order correct finite difference

$$\frac{\partial}{\partial t}(\alpha\phi\rho) \cong \frac{(\alpha\phi\rho)_i^{n+1} + (\alpha\phi\rho)_i^n}{\Delta t}, \tag{57}$$

where the superscript references the time index. The fully discretized system of equations can be written as

$$\begin{aligned}&\frac{(\alpha\phi\rho)_i^{n+1} - (\alpha\phi\rho)_i^n}{\Delta t} - \frac{1}{\Delta x_i}\left(\frac{\alpha k\rho}{\mu}\right)_{i+1/2}\frac{P_{i+1} - P_i}{x_{i+1} - x_i}\\ &+\frac{1}{\Delta x_i}\left(\frac{\alpha k\rho}{\mu}\right)_{i-1/2}\frac{P_i - P_{i-1}}{x_i - x_{i-1}} - \alpha_i\left(q_{inj}\right)_i = 0, \qquad i = 1, 2, \ldots, IM\end{aligned} \tag{58}$$

In this equation, the time level is not indicated on the pressure and pressure dependent variables in the flux and injection terms.

If all the pressures and pressure dependent variables in the flux and source/sink terms are evaluated at the beginning of the time step, $t = t_n$, then the formulation is called explicit. If these quantities are evaluated at the end of the time step, $t = t_{n+1}$ the formulation is called implicit.

The numerical solution of the material balance equation starts at initial time with specified initial pressures. The evaluation of the pressure solution in time requires at each time step the solution of a system of nonlinear algebraic equations for the grid block pressures. The error introduced by the discretization of the continuum equation is called truncation error. Errors will also be introduced in the nonlinear equation solver since it will not solve the system exactly (see Section 4.6, Newton-Raphson Method). Another source of error involves the choice of discretization. A numerical artifact of the solution of evolution equations is that small errors introduced at early time can either be damped with time (stable) or grow with time (unstable). The errors in an unstable solution will usually grow large enough to dominate the solution with numerical noise. The numerical stability of a discretization can sometimes depend of the size of the space discretization (Δx) relative to the time discretization (Δt). In this case, the method is said to be conditionally stable.

In the above formulations (explicit, implicit) we observe that

Formulation Advantages:

- Explicit is simplistic computationally.
- Implicit is unconditionally stable.

Formulation Disadvantages:

- Implicit is complex computationally.
- Explicit is conditionally stable.

The stability question dictates that the BRAGFLO formulation be fully implicit. The evaluation of the inter-block flux coefficients at $x \pm 1/2$ will be discussed in Section 4.8, Two Phase Flow.

4.6 Newton-Raphson Method for Solution of Nonlinear Algebraic Equations

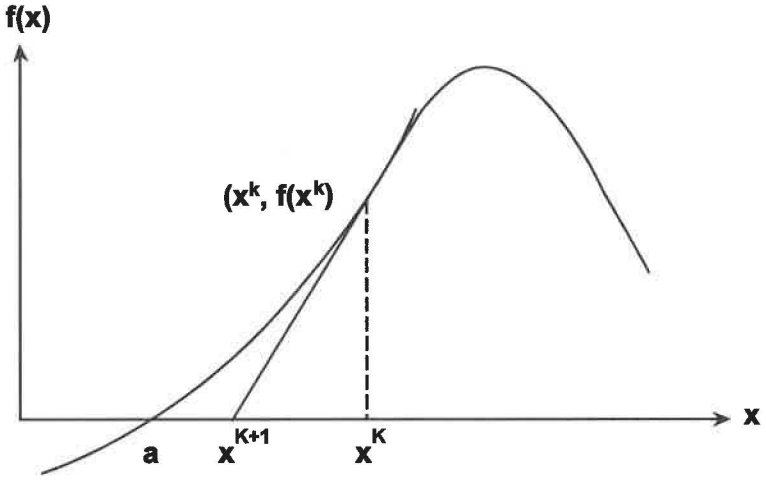


Figure 8. Newton-Raphson method.

Consider a real valued function of a real variable (scalar case). A root of f is a value $x = a$ such that $f(a) = 0$. Let x^k be an approximation to the root of f (k^{th} iterate approximation). Expand $f(x)$ in a Taylor series about x_k:

$$f(x) = f(x^k) + f'(x^k)(x - x^k) + \frac{f^{(2)}(x^k)}{2!}(x - x^k)^2 + \ldots = 0. \tag{59}$$

Replace the nonlinear root problem with the linear approximation:

$$f(x^k) + f'(x^k)(x - x^k) = 0 \tag{60}$$

with solution $x = x^{k+1}$. Define

$$\delta x^k = x^{k+1} - x^k \tag{61}$$

Then

$$\delta x^k = -\frac{f(x^k)}{f'(x^k)}, \tag{62}$$

and

$$x^{k+1} = x^k + \delta x^k. \tag{63}$$

The Newton-Raphson iteration requires an initial guess to the root. In Figure 8 it appears from the geometry that the iteration would proceed to the root of f. If the initial guess was not close to the solution, such as to the right of the maximum in Figure 8, then the iteration may not converge, or it could converge to another solution. When solving the system of nonlinear material balance equations over a time step, the solution at the beginning of the time step is used as an initial guess for the Newton-Raphson iteration.

In general, consider a system of n nonlinear equations (64) in n unknowns:

$$\begin{aligned} f_1(x_1, \ldots, x_n) &= 0 \\ f_2(x_1, \ldots, x_n) &= 0 \\ &\vdots \\ f_n(x_1, \ldots, x_n) &= 0 \end{aligned} \tag{64}$$

In vector notation, the system is written

$$\mathbf{F}(x_1, \ldots, x_n) = \begin{pmatrix} f_1(x_1, \ldots x_n) \\ \vdots \\ f_n(x_1, \ldots x_n) \end{pmatrix} = 0, \tag{65}$$

and further, if $\hat{\mathbf{x}} = (x_1, \ldots, x_n)$, then, $\mathbf{F}(\hat{\mathbf{x}}) = 0$ is equivalent to (64).

Consider Newton-Raphson for $n = 2$. Let $\left(x_1^k, x_2^k\right)$ be an approximation to the root of

$$\begin{aligned} f_1(x_1, x_2) &= 0 \\ f_2(x_1, x_2) &= 0. \end{aligned} \tag{66}$$a,b

The Taylor series through linear terms expanded about $\left(x_1^k, x_2^k\right) = \hat{\mathbf{x}}^k$ are

$$\begin{aligned} f_1(x_1, x_2) &= f_1\left(x_1^k, x_2^k\right) + \frac{\partial f_1}{\partial x_1}\left(x_1^k, x_2^k\right)\left(x_1 - x_1^k\right) + \frac{\partial f_1}{\partial x_2}\left(x_1^k, x_2^k\right)\left(x_2 - x_2^k\right) \\ f_2(x_1, x_2) &= f_2\left(x_1^k, x_2^k\right) + \frac{\partial f_2}{\partial x_1}\left(x_1^k, x_2^k\right)\left(x_1 - x_1^k\right) + \frac{\partial f_2}{\partial x_2}\left(x_1^k, x_2^k\right)\left(x_2 - x_2^k\right). \end{aligned} \tag{67}$$a,b

Replace the system of nonlinear equations in equation (66)a,b by the linear system

$$\frac{\partial f_1}{\partial x_1}\left(\hat{\mathbf{x}}^k\right)\left(x_1^{k+1} - x_1^k\right) + \frac{\partial f_1}{\partial x_2}\left(\hat{\mathbf{x}}^k\right)\left(x_2^{k+1} - x_2^k\right) = f_1\left(\hat{\mathbf{x}}^k\right)$$

$$\frac{\partial f_2}{\partial x_1}\left(\hat{\mathbf{x}}^k\right)\left(x_1^{k+1} - x_1^k\right) + \frac{\partial f_2}{\partial x_2}\left(\hat{\mathbf{x}}^k\right)\left(x_2^{k+1} - x_2^k\right) = -f_2\left(\hat{\mathbf{x}}^k\right). \qquad (68)\text{a,b}$$

Define the change in iterate values

$$\delta x_1 = x_1^{k+1} + x_1^k$$

$$\delta x_2 = x_2^{k+1} + x_2^k. \qquad (69)\text{a,b}$$

Then the above linear system is written

$$\frac{\partial f_1}{\partial x_1}\left(\hat{\mathbf{x}}^k\right)\delta x_1 + \frac{\partial f_1}{\partial x_2}\left(\hat{\mathbf{x}}^k\right)\delta x_2 = -f_1\left(\hat{\mathbf{x}}^k\right)$$

$$\frac{\partial f_2}{\partial x_1}\left(\hat{\mathbf{x}}^k\right)\delta x_1 + \frac{\partial f_2}{\partial x_2}\left(\hat{\mathbf{x}}^k\right)\delta x_2 = -f_2\left(\hat{\mathbf{x}}^k\right). \qquad (70)\text{a,b}$$

The coefficient matrix

$$\mathbf{J}(\hat{\mathbf{x}}) = \begin{pmatrix} \frac{\partial f_1}{\partial x_1}(\hat{\mathbf{x}}) & \frac{\partial f_1}{\partial x_2}(\hat{\mathbf{x}}) \\ \frac{\partial f_2}{\partial x_1}(\hat{\mathbf{x}}) & \frac{\partial f_2}{\partial x_2}(\hat{\mathbf{x}}) \end{pmatrix} \qquad (71)$$

is called the Jacobian matrix for the nonlinear system.

Then the $(k+1)^{th}$ iterative step of the Newton-Raphson method is

$$\mathbf{J}(\hat{\mathbf{x}}^k)\delta\hat{\mathbf{x}} = -\mathbf{F}(\hat{\mathbf{x}}^k) \qquad (72)$$

or

$$\delta\hat{\mathbf{x}} = -\mathbf{J}^{-1}(\hat{\mathbf{x}}^k)\mathbf{F}(\hat{\mathbf{x}}^k) \qquad (73)$$

and

$$\hat{\mathbf{x}}^{k+1} = \hat{\mathbf{x}}^k + \delta\hat{\mathbf{x}}. \qquad (74)$$

For a system of n equations in n unknowns the Jacobian matrix generalizes to

$$\mathbf{J}(\hat{\mathbf{x}}) = \begin{pmatrix} \frac{\partial f_1}{\partial x_1}(\hat{\mathbf{x}}) \cdots \frac{\partial f_1}{\partial x_n}(\hat{\mathbf{x}}) \\ \vdots \qquad\qquad \vdots \\ \frac{\partial f_n}{\partial x_1}(\hat{\mathbf{x}}) \cdots \frac{\partial f_n}{\partial x_n}(\hat{\mathbf{x}}) \end{pmatrix} \qquad (75)$$

or

$$J(\hat{\mathbf{x}})_{i,j} = \frac{\partial f_i}{\partial x_j}(\hat{\mathbf{x}}). \tag{76}$$

The computation procedure in Newton-Raphson method computes the Jacobian matrix, $\mathbf{J}(\hat{\mathbf{x}}^k)$, and the function vector, $\mathbf{F}(\hat{\mathbf{x}}^k)$. The matrix inversion is equivalent to the solution of a system of linear equations which returns the changes in iterate values. The iterates are then updated.

When analytical derivatives are not tractable, Newton-Raphson uses difference quotient approximation for partials

$$\frac{\partial f_i}{\partial x_j}(\hat{x}) = \frac{f_i(x_1, \ldots, x_j + \Delta x_j, \ldots, x_n) - f_i(x_1, \ldots, x_n)}{\Delta x_j} \tag{77}$$

The major computational effort involves the function evaluations. The above numerical approach to the Jacobian requires n^2+n evaluations of the function f.

If the Jacobian is evaluated by an analytic derivative, then any change in the formulation of properties would require significant code changes. Also, some properties, see Characteristic Curves (Section 4.9), use different model descriptions with user input control. In this case it would be difficult to implement the analytic derivative treatment. For these reasons BRAGFLO uses the difference approximation for the Jacobian evaluation.

The modified Newton-Raphson algorithm is

$$\mathbf{J}(\hat{\mathbf{x}}^1)\delta\hat{\mathbf{x}} = -\mathbf{F}(\hat{\mathbf{x}}^k), \quad k = 1,2,\ldots, \tag{78}$$

that is, the Jacobian is not updated each iteration. In BRAGFLO the user can specify from input directives the iteration frequency for the Jacobian evaluation.

Consider now the solution of the nonlinear flow equation. The i^{th} equation represents material balance in i^{th} grid block. Newton-Raphson iteration requires solution of the linear system

$$\begin{bmatrix} J_{11} & J_{12}\cdots & J_{1IM} \\ J_{21} & J_{22}\cdots & J_{2IM} \\ \vdots & & \\ J_{IM1} & J_{IM2}\cdots & J_{IMIM} \end{bmatrix} \begin{bmatrix} \delta p_1 \\ \delta p_2 \\ \vdots \\ \delta p_{IM} \end{bmatrix} = - \begin{bmatrix} F_1 \\ F_2 \\ \vdots \\ F_{IM} \end{bmatrix} \tag{79}$$

and $p_i^{(k+1)} = p_i^{(k)} + \delta p_i$ where Jacobian and right hand side are evaluated at k^{th} iteration pressures. If the Newton-Raphson iteration converges then

$$\lim_{k\to\infty} p_i^{(k)} = p_i^{n+1}. \tag{80}$$

When testing for convergence during the Newton-Raphson iteration, the following test criteria are applied uniformly over all grid blocks:

- Test gas saturation and brine pressure for physically real values.
- Test if the change in gas saturation over an iteration is sufficiently small.

- Test if the gas material balance equation is satisfied.
- Test if the change in brine pressure over an iteration is sufficiently small.
- Test if the brine material balance equation is satisfied.
- Test if the changes in gas saturation and brine pressure over the time step are sufficiently small.

See Section 7.2.7 for input parameters that specify when convergence has been obtained or that affect the rate of convergence.

From the one-dimensional flow equations, we note the Jacobian matrix has a tridiagonal structure

$$\begin{bmatrix} J_{11} & J_{12} & 0 & \cdots & \cdots & \cdots & \cdots & 0 \\ J_{21} & J_{22} & J_{23} & & & & & \\ & \ddots & \ddots & \ddots & & & & \\ 0 & \cdots & J_{i\,i-1} & J_{i\,i} & J_{i\,i+1} & \cdots & \cdots & 0 \\ & & & \ddots & \ddots & \ddots & & \\ 0 & \cdots & \cdots & & J_{\mathrm{IM\ IM-1}} & J_{\mathrm{IM\ IM}} & & \end{bmatrix} \begin{bmatrix} \delta p_1 \\ \delta p_2 \\ \vdots \\ \delta p_i \\ \vdots \\ \delta p_{\mathrm{IM}} \end{bmatrix} = - \begin{bmatrix} F_1 \\ F_2 \\ \vdots \\ F_i \\ \vdots \\ F_{\mathrm{IM}} \end{bmatrix} \tag{81}$$

For both storage and computational considerations, the linear equation solver should take advantage of the banded structure. This is true for the BRAGFLO direct solvers.

4.7 Discretization in Two-Dimensions

Consider the two-dimensional flow equation with gravitational effects neglected:

$$\frac{\partial}{\partial x}\left(\frac{\alpha k_x \rho}{\mu}\frac{\partial p}{\partial x}\right) + \frac{\partial}{\partial y}\left(\frac{\alpha k_y \rho}{\mu}\frac{\partial p}{\partial y}\right) + \alpha q_{inj} = \frac{\partial}{\partial t}(\alpha\phi\rho) \tag{82}$$

Discretized equation in 2-dimensions with implicit treatment of the well and flux terms is

$$\begin{aligned} &-\frac{(\alpha\phi\rho)_{i,j}^{n+1} - (\alpha\phi\rho)_{i,j}^{n}}{\Delta t} + \frac{1}{\Delta x_i}\left(\frac{\alpha k_x \rho}{\mu}\right)_{i+1/2,j}^{n+1} \frac{p_{i+1,j}^{n+1} - p_{i,j}^{n+1}}{x_{i+1} - x_i} \\ &-\frac{1}{\Delta x_i}\left(\frac{\alpha k_x \rho}{\mu}\right)_{i-1/2,j}^{n+1} \frac{p_{i,j}^{n+1} - p_{i-1,j}^{n+1}}{x_i - x_{i-1}} + \frac{1}{\Delta y_j}\left(\frac{\alpha k_y \rho}{\mu}\right)_{i,j+1/2}^{n+1} \frac{p_{i,j+1}^{n+1} - p_{i,j}^{n+1}}{y_{j+1} - y_j} \\ &-\frac{1}{\Delta y_j}\left(\frac{\alpha k_y \rho}{\mu}\right)_{i,j-1/2}^{n+1} \frac{p_{i,j}^{n+1} - p_{i,j-1}^{n+1}}{y_j - y_{j-1}} + \alpha_{i,j}\left(q_{inj}\right)_{i,j} = 0. \end{aligned} \tag{83}$$

A typical two-dimensional grid is shown in Figure 9.

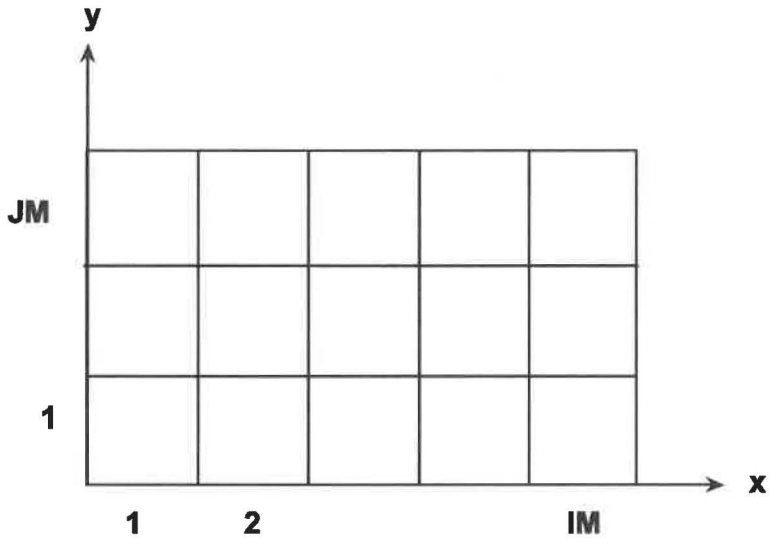


Figure 9. 2-dimensional grid.

A computational molecule or stencil is shown in Figure 10 and the stencil shows the indices of the pressures which appear in the material balance equation for the (i,j) grid block.

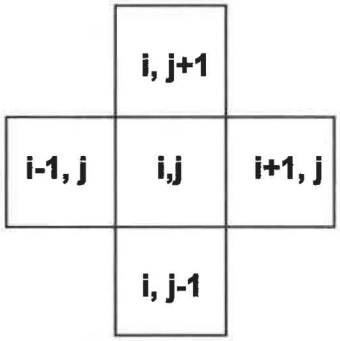


Figure 10. Computational molecule (or stencil).

With IM=5 and JM=3 in Figure 9, the number of equations is NEQ = IM × JM = 5 × 3 = 15. Suppose the equations or grid blocks are sequentially indexed as in Figure 11.

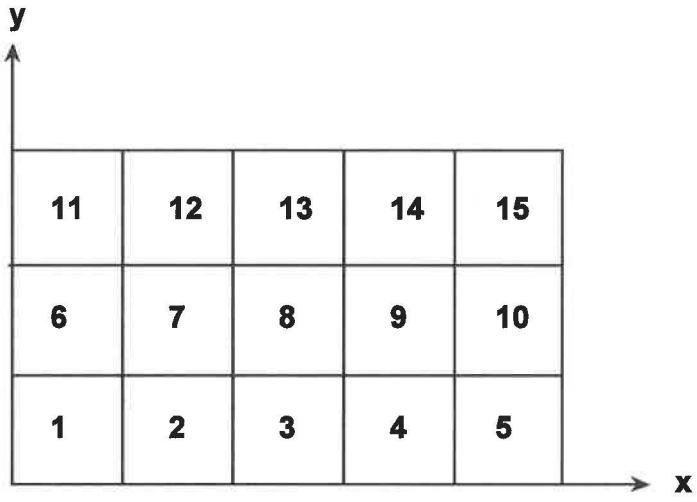


Figure 11. Sequential indexing of equations.

Then the Jacobian matrix has the structure shown in Figure 12 where * entries are the only nonzero values. This is said to have pentadiagonal band structure, with bandwidth = IBW = 2 × IM + 1 (for the example, IBW=11).

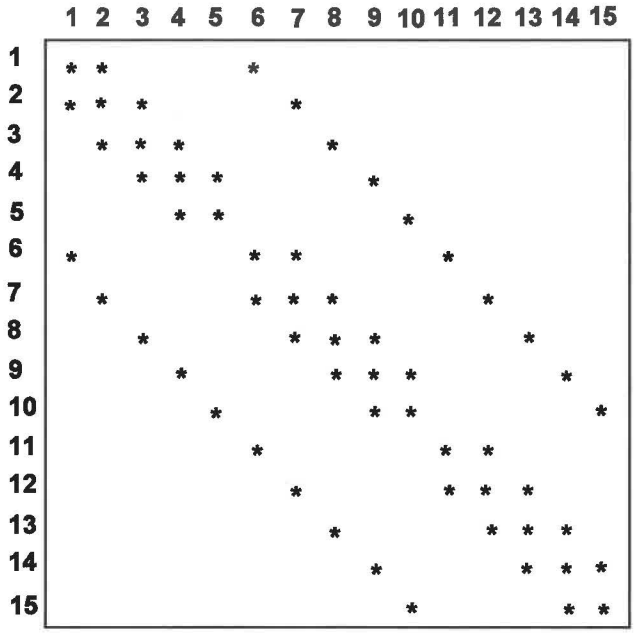


Figure 12. Jacobian matrix.

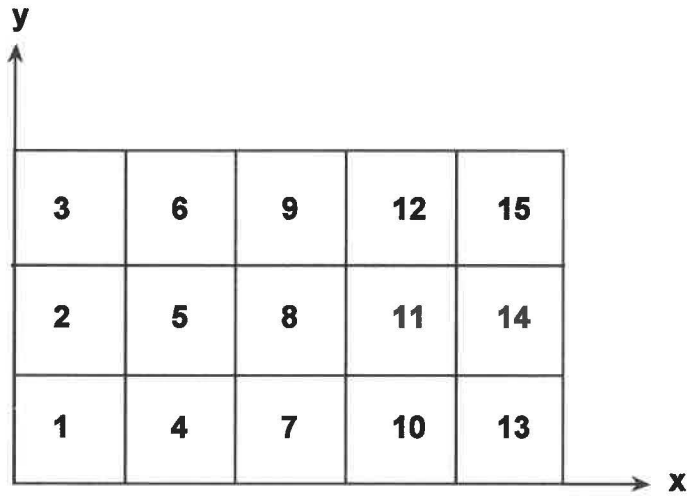


Figure 13. A different sequential indexing.

Suppose the grid is indexed as in Figure 13. Then IBW = 2 × JM + 1 (for the example, IBW=7).

Therefore, to minimize the bandwidth, BRAGFLO orders the grid blocks so that sequential indexing proceeds first in the shortest grid direction, then in the longest grid direction. In this case

IBW = 2 × min (IM, JM) + 1.

Storage requirements are as follows:

Full matrix storage = $(IM \times JM)^2$ words of memory

Band matrix storage = IM × JM × IBW words of memory

If IM ≤ JM then

$$\frac{Band\ storage}{Full\ matrix\ storage} = \frac{(2 \times IM + 1) \times IM \times JM}{(IM \times JM)^2} = \frac{2 \times IM + 1}{IM \times JM} \simeq \frac{2}{JM}$$

For various values of JM, storage ratios are given by:

JM	Storage ratio
5	0.4 (40%)
10	0.2 (20%)
50	0.04 (4%)
100	0.02 (2%)

To determine the required computational effort, assume the major effort is the multiplication/division.

Banded structure:

multiplication/division $\cong$ NEQ $\times$ IB $\times$ IB, where IB is the half bandwidth,

IB = min (IM,JM).

Full matrix:

multiplication/division $\cong$ 1/3 NEQ^3

A typical performance assessment grid is

IM = 33

JM = 31

NEQ = 31(33) = 1023

IBW = 2(31) + 1 = 63

IB = 31

Computational effort

banded matrix structure	=	1023 (31 $\times$ 31)	= 983,103
full matrix structure	=	1/3 $(1023)^3$	$\cong 3.57 \times 10^8$.

The disparity in storage and computation between a band matrix solver and a full matrix solver is greater in two-dimensions than in one dimension. Of course, when solving 3-dimensional problems this disparity becomes even greater.

Although the equation solver is a major part of the time step calculation, other calculations involve evaluation of pressure dependent functions, coefficient generation, reporting and other overhead. However, the equation solver is a good indication of the computational effort for the time step solution. If the multiplication/division count of NEQ $\times$ IB $\times$ IB is used as a measure of equation solver speed, then a grid refinement for which the number of grid blocks is doubled in both the *x*- and *y*-direction (2-dimensional) would result in an increase in the number of equations by a factor of 4 and an increase in the half bandwidth by a factor of 2. Therefore, the computational effort would increase by a factor of 16. This estimate should warn the user that when attempting a grid refinement, the computation (and also storage) does not depend linearly on the grid size.

4.8 Two-Phase Flow

BRAGFLO assumes a water/gas system. Immiscible fluids are not capable of mixing and have interfaces across which pressure discontinuities exist. This interfacial tension effect produces a capillary pressure between phases. In BRAGFLO fluids are assumed to be immiscible.

Phase saturation is the fraction of the pore space occupied by the fluids in a given phase. The notation is

S_w = water saturation,

S_g = gas saturation.

For example, the volume occupied by water within a bulk volume V with porosity ϕ is $V\phi S_w$.

The saturation constraint for fully saturated media is

$$S_w + S_g = 1. \tag{84}$$

Capillary pressure is defined by

$$P_c = P_g - P_w = P_c(S_w). \tag{85}$$

For a water wetting phase, $P_c \geq 0$.

The ability of a fluid to flow is affected by the presence of another fluid. The relative permeability is the ratio of the effective permeability of a given fluid phase to the permeability at 100% saturation. This is written as

$$k_{rl} = \frac{k_l}{k} \tag{86}$$

where k is the formation or absolute permeability, k_l is the effective permeability of phase l, and k_{rl} is the relative permeability of phase l. We observe that $0 \leq k_{rl} \leq 1$ and k_{rl} will be dependent on the phase saturation.

Typical relative permeability curves are shown in Figure 14, where S_{wr} is the residual water saturation. For water saturation at or below S_{wr}, water will not flow.

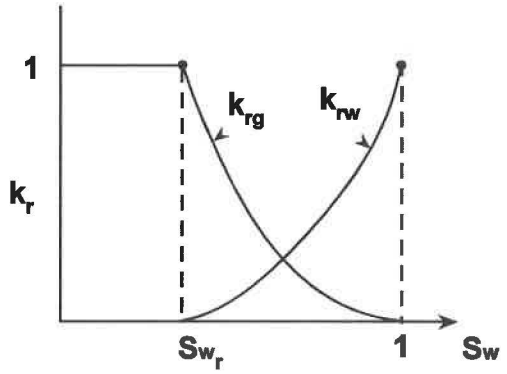


Figure 14. Typical relative permeability curve.

Darcy's Law extended to multiphase flow replaces absolute permeability with an effective permeability

$$\hat{\mathbf{q}}_l = -\frac{kk_{rl}\rho}{\mu}\left(\nabla P + \rho g \nabla h\right). \tag{87}$$

The following system of two mass balance equations and two constraint equations is the BRAGFLO description of the two-phase flow within a repository site:

Gas Mass Balance:

$$\nabla \bullet \left[\frac{\alpha \rho_g [k] k_{rg}}{\mu_g} \left(\nabla P_g + \rho_g g \nabla h \right) \right] + \alpha q_g + \alpha q_{rg} = \alpha \frac{\partial \left(\phi \rho_g S_g \right)}{\partial t} \tag{88}$$

Brine Mass Balance:

$$\nabla \bullet \left[\frac{\alpha \rho_w [k] k_{rw}}{\mu_w} \left(\nabla P_w + \rho_w g \nabla h \right) \right] + \alpha q_w + \alpha q_{rw} = \alpha \frac{\partial \left(\phi \rho_w S_w \right)}{\partial t} \tag{89}$$

Saturation Constraint:

$$S_g + S_w = 1. \tag{90}$$

Capillary Pressure Constraint:

$$P_c = P_g - P_w. \tag{91}$$

Additional terms include:

q_{rg} = rate of gas production (or consumption, if negative) due to chemical reaction.

q_{rw} = rate of water production (or consumption, if negative) due to chemical reaction.

The above system of four equations describes the time and space behavior of the four variables S_g, S_w, P_g, P_w. The finite difference method requires the introduction of a grid in one, two, or three dimensions and then a discretization of the gas and brine mass balance equations with respect to this grid and with respect to time. The resulting system of nonlinear algebraic equations is solved over a time step by the Newton-Raphson method.

The discretization of the gas mass balance equation in two dimensions (x,y) is given by

$$\begin{aligned}
&\frac{1}{\Delta x_i} \left\{ \frac{(k_{rg})^{n+1}_{i+1/2,j}}{x_{i+1} - x_i} \left[\frac{\alpha \rho_g k_x}{\mu_g} \right]^{n+1}_{i+1/2,j} \left(\Phi^{x-}_{g_{i+1,j}} - \Phi^{x+}_{g_{i,j}} \right)^{n+1} - \frac{(k_{rg})^{n+1}_{i-1/2,j}}{x_i - x_{i-1}} \left[\frac{\alpha \rho_g k_x}{\mu_g} \right]^{n+1}_{i-1/2,j} \left(\Phi^{x-}_{g_{i,j}} - \Phi^{x+}_{g_{i-1,j}} \right)^{n+1} \right\} \\
&+ \frac{1}{\Delta y_j} \left\{ \frac{(k_{rg})^{n+1}_{i,j+1/2}}{y_{j+1} - y_j} \left[\frac{\alpha \rho_g k_y}{\mu_g} \right]^{n+1}_{i,j+1/2} \left(\Phi^{y-}_{g_{i,j+1}} - \Phi^{y+}_{g_{i,j}} \right)^{n+1} - \frac{(k_{rg})^{n+1}_{i,j-1/2}}{y_j - y_{j-1}} \left[\frac{\alpha \rho_g k_y}{\mu_g} \right]^{n+1}_{i,j-1/2} \left(\Phi^{y-}_{g_{i,j}} - \Phi^{y+}_{g_{i,j-1}} \right)^{n+1} \right\} \\
&+ \alpha_{i,j} q^{n+1}_{wg_{i,j}} + \alpha_{i,j} q^{n+1}_{rg_{i,j}} - \frac{\left(\alpha \phi \rho_g S_g \right)^{n+1}_{i,j} - \left(\alpha \phi \rho_g S_g \right)^{n}_{i,j}}{\Delta t} = 0,
\end{aligned} \tag{92}$$

where Φ represents the phase potentials:

$$\begin{aligned}
\Phi^{x+}_{g_{i,j}} &= P_{g_{i,j}} + \rho_{g_{i+1/2,j}} g h_{i,j} \\
\Phi^{x-}_{g_{i,j}} &= P_{g_{i,j}} + \rho_{g_{i-1/2,j}} g h_{i,j}
\end{aligned} \tag{93}$$

and

$$\Phi^{y+}_{g_{i,j}} = P_{g_{i,j}} + \rho_{g_{i,j+1/2}} g\, h_{i,j}$$
$$\Phi^{y-}_{g_{i,j}} = P_{g_{i,j}} + \rho_{g_{i,j-1/2}} g h_{i,j}. \quad (94)$$

Subscripts denote:

i = x-direction grid index,

j = y-direction grid index,

$i\pm1/2$ = x-direction grid block interface,

$j\pm1/2$ = y-direction grid block interface,

and superscripts denote:

n = index in the time discretization, known solution time level,

$n+1$ = index in the time discretization, unknown solution time level.

The inter-block densities are defined by:

$$\rho_{g_{i+1/2,j}} = \frac{\Delta x_{i+1,j}}{\Delta x_{i,j} + \Delta x_{i+1,j}} \rho_{g_{i,j}} + \frac{\Delta x_{i,j}}{\Delta x_{i,j} + \Delta x_{i+1,j}} \rho_{g_{i+1,j}}$$
$$\rho_{g_{i-1/2,j}} = \frac{\Delta x_{i,j}}{\Delta x_{i-1,j} + \Delta x_{i,j}} \rho_{g_{i-1,j}} + \frac{\Delta x_{i-1,j}}{\Delta x_{i-1,j} + \Delta x_{i,j}} \rho_{g_{i,j}} \quad (95)$$

and

$$\rho_{g_{i,j+1/2}} = \frac{\Delta y_{i,j+1}}{\Delta y_{i,j} + \Delta y_{i,j+1}} \rho_{g_{i,j}} + \frac{\Delta y_{i,j}}{\Delta y_{i,j} + \Delta y_{i,j+1}} \rho_{g_{i,j+1}}$$
$$\rho_{g_{i,j-1/2}} = \frac{\Delta y_{i,j}}{\Delta y_{i,j-1} + \Delta y_{i,j}} \rho_{g_{i,j-1}} + \frac{\Delta y_{i,j-1}}{\Delta y_{i,j-1} + \Delta y_{i,j}} \rho_{g_{i,j}}. \quad (96)$$

Similar equations for the brine mass balance are obtained by replacing the subscript for gas (g) with the subscript for brine (w). Note that the flux and rate terms are evaluated at time level $n+1$, where the solution is not yet known. Therefore, the formulation is fully implicit.

Evaluation at grid block interfaces (*i.e.*, at $i\pm1/2$ and $j\pm1/2$) of mobility $\left[\frac{\alpha \rho_g k_{x \text{ or } y}}{\mu_g}\right]$, using harmonic averaging, and relative permeabilities (k_{rg}), using upstream weighting, will be discussed later.

For each grid block there are two material balance equations. The saturation constraint is used to eliminate brine saturation and the capillary pressure equation is used to eliminate the gas pressure. The remaining unknowns for each grid block are gas saturation, S_g, and brine pressure, P_w. Consequently, at each time step it is necessary to solve 2 × NX × NY equations for 2 × NX × NY unknowns, where NX and NY are the number of grid blocks in the x- and y-directions, respectively.

In order to investigate the Jacobian matrix structure, assume for sake of argument that NY < NX. In this case the grid indexing moves most rapid in the *y*-direction and then in the *x*-direction. If the number of grid blocks is denoted NGB, then NGB = NX × NY. In BRAGFLO the equation indexing is first with respect to the gas equation, then the brine equation and outer most indexing with respect to the grid block. For example, the equation ordering is as follows:

equation index	equation
1	gas equation in grid block 1
2	brine equation in grid block 1
3	gas equation in grid block 2
4	brine equation in grid block 2
•	
•	
•	
2 × NGB-1	gas equation in grid block NGB
2 × NGB	brine equation in grid block NGB

The unknowns are gas saturation and brine pressure. The unknowns are ordered by gas saturation, then brine pressure and then with respect to grid block. The unknown indexing is:

unknown index	unknown
1	gas saturation in grid block 1
2	brine pressure in grid block 1
3	gas saturation in grid block 2
4	brine pressure in grid block 2
•	
•	
•	
2 × NGB-1	gas saturation in grid block NGB
2 × NGB	brine pressure in grid block NGB

Information at the i,j grid block and its neighboring grid blocks will use the compass notation:

P corresponds to information with respect to grid block i,j

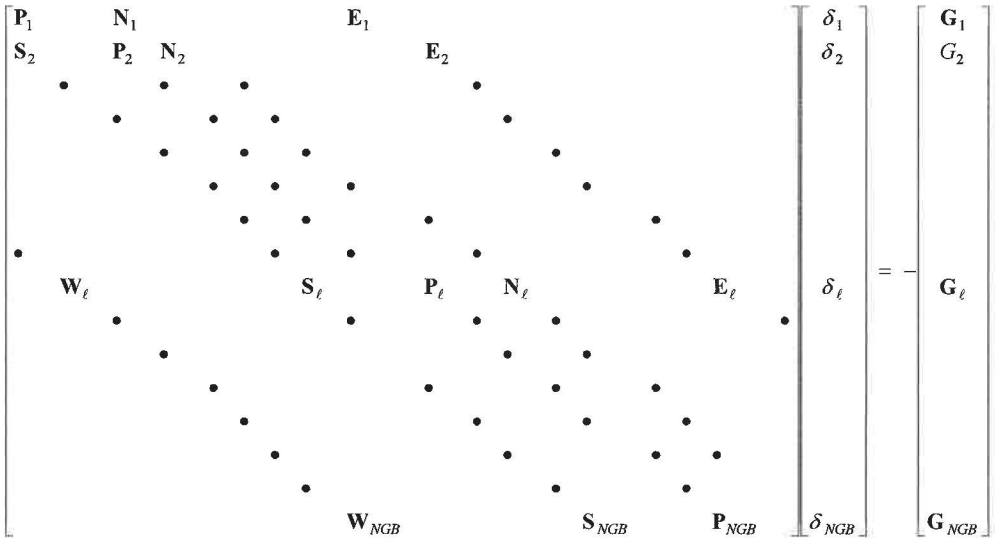
E corresponds to information with respect to grid block i+1,j

W corresponds to information with respect to grid block i-1,j

N corresponds to information with respect to grid block i,j+1

S corresponds to information with respect to grid block i,j-1.

Assume that the i,j grid block has sequential index ℓ. Then the Jacobian matrix has a 2×2 block pentadiagonal structure and the resulting linear system in the Newton-Raphson iteration step can be represented as follows



(97)

The 2 × 2 block matrices in the Jacobian are defined by

$$\mathbf{P}_\ell = \begin{pmatrix} \dfrac{\partial F_1(i,j)}{\partial S_g(i,j)} & \dfrac{\partial F_1(i,j)}{\partial P_w(i,j)} \\ \dfrac{\partial F_2(i,j)}{\partial S_g(i,j)} & \dfrac{\partial F_2(i,j)}{\partial P_w(i,j)} \end{pmatrix} \tag{98}$$

$$\mathbf{E}_\ell = \begin{pmatrix} \dfrac{\partial F_1(i,j)}{\partial S_g(i+1,j)} & \dfrac{\partial F_1(i,j)}{\partial P_w(i+1,j)} \\ \dfrac{\partial F_2(i,j)}{\partial S_g(i+1,j)} & \dfrac{\partial F_2(i,j)}{\partial P_w(i+1,j)} \end{pmatrix} \qquad \mathbf{W}_\ell = \begin{pmatrix} \dfrac{\partial F_1(i,j)}{\partial S_g(i-1,j)} & \dfrac{\partial F_1(i,j)}{\partial P_w(i-1,j)} \\ \dfrac{\partial F_2(i,j)}{\partial S_g(i-1,j)} & \dfrac{\partial F_2(i,j)}{\partial P_w(i-1,j)} \end{pmatrix} \tag{99}$$

$$\mathbf{N}_\ell = \begin{pmatrix} \dfrac{\partial F_1(i,j)}{\partial S_g(i,j+1)} & \dfrac{\partial F_1(i,j)}{\partial P_w(i,j+1)} \\ \dfrac{\partial F_2(i,j)}{\partial S_g(i,j+1)} & \dfrac{\partial F_2(i,j)}{\partial P_w(i,j+1)} \end{pmatrix} \qquad \mathbf{S}_\ell = \begin{pmatrix} \dfrac{\partial F_1(i,j)}{\partial S_g(i,j-1)} & \dfrac{\partial F_1(i,j)}{\partial P_w(i,j-1)} \\ \dfrac{\partial F_2(i,j)}{\partial S_g(i,j-1)} & \dfrac{\partial F_2(i,j)}{\partial P_w(i,j-1)} \end{pmatrix} \tag{100}$$

The block vectors in the unknown solution vector are

$$\delta_\ell = \begin{pmatrix} \delta S_g(i,j) \\ \delta P_w(i,j) \end{pmatrix}. \tag{101}$$

The block vectors in the equation vector are

$$\mathbf{G}_\ell = \begin{pmatrix} F_1(i,\ j) \\ F_2(i,\ j) \end{pmatrix}. \tag{102}$$

In the above, F_1 denotes the left-hand side of the gas mass balance equation, and F_2 denotes the left-hand side of the brine mass balance equation.

An inspection of the above discretized gas mass balance equation shows that the flux between neighboring grid blocks involves inter-block flow terms evaluated at grid block interfaces, such as i+1/2, i-1/2, j+1/2 and j-1/2. It is necessary to discuss how BRAGFLO evaluates these inter-block flow terms.

Consider the following term in the brine equation for flow in the x-direction between grid blocks i and i+1, with gravitational effects neglected to simplify the discussion:

$$\frac{(k_{rw})_{i+1/2}}{\Delta x_i (x_{i+1} - x_i)} \left(\frac{\alpha \rho_w k_x}{\mu_w} \right)_{i+1/2} \left(P_{w_{i+1}} - P_{w_i} \right). \tag{103}$$

Since pressure and saturation are determined at grid block centers x_i and x_{i+1}, the question remains as to how to evaluate the interface term at $x_{i+1/2}$.

First, we define the harmonic average, H, of a_1, a_2, as

$$\frac{1}{H} = \frac{1}{2} \left(\frac{1}{a_1} + \frac{1}{a_2} \right) \tag{104}$$

or

$$H = \frac{2 a_1 a_2}{a_1 + a_2}. \tag{105}$$

Further, the harmonic weighted-average of a_1, a_2 is

$$\frac{1}{H} = \frac{w_1}{a_1} + \frac{w_2}{a_2} \tag{106}$$

or

$$H = \frac{a_1 a_2}{w_2 a_1 + w_1 a_2}, \tag{107}$$

where the weights satisfy $w_1 + w_2 = 1$. Now introduce the shorthand notation

$$\tau_{i+1/2} = \left(\frac{\alpha \rho_w k_x}{\mu_w} \right)_{i+1/2}. \tag{108}$$

At the i+1/2 interface, assume the mass flux is continuous

$$\bar{q}_{i+1/2} = q^{-}_{i+1/2} = q^{+}_{i+1/2} \tag{109}$$

where

$\bar{q}_{i+1/2}$ is average flow between x_i and x_{i+1},

$q^{-}_{i+1/2}$ is flow to the left of interface,

$q^{+}_{i+1/2}$ is flow to the right of interface.

From Darcy's Law, neglecting gravitational effects,

$$\bar{q}_{i+1/2} = \tau_{i+1/2}(k_{rw})_{i+1/2}\frac{P_{i+1} - P_i}{x_{i+1} - x_i} \tag{110}$$

or

$$\bar{q}_{i+1/2} = \tau_{i+1/2}(k_{rw})_{i+1/2}\frac{P_{i+1} - P_i}{1/2(\Delta x_i - \Delta x_{i+1})} \tag{111}$$

This yields

$$P_{i+1} - P_i = \frac{\bar{q}_{i+1/2}\dfrac{1}{2}(\Delta x_i + \Delta x_{i+1})}{\tau_{i+1/2}(k_{rw})_{i+1/2}} \tag{112}$$

Similarly,

$$q^{-}_{i+1/2} = \tau_i(k_{rw})_{i+1/2}\frac{(P_{i+1/2} - P_i)}{\dfrac{1}{2}\Delta x_i} \tag{113}$$

$$q^{+}_{i+1/2} = \tau_{i+1}(k_{rw})_{i+1/2}\frac{(P_{i+1} - P_{i+1/2})}{\dfrac{1}{2}\Delta x_{i+1}} \tag{114}$$

Pressure drop is then written as

$$P_{i+1} - P_i = P_{i+1} - P_{i+1/2} + (P_{i+1/2} - P_i)\,. \tag{115}$$

Then

$$\bar{q}_{i+1/2}\frac{\dfrac{1}{2}(\Delta x_i + \Delta x_{i+1})}{\tau_{i+1/2}(k_{rw})_{i+1/2}} = q^{+}_{i+1/2}\frac{\dfrac{1}{2}\Delta x_{i+1}}{\tau_{i+1}(k_{rw})_{i+1/2}} + q^{-}_{i+1/2}\frac{\dfrac{1}{2}\Delta x_i}{\tau_i(k_{rw})_{i+1/2}}\,. \tag{116}$$

Solving for $\tau_{i+1/2}$ yields

$$\tau_{i+1/2} = \frac{\tau_i\tau_{i+1}}{\dfrac{\Delta x_{i+1}}{\Delta x_i + \Delta x_{i+1}}\tau_i + \dfrac{\Delta x_i}{\Delta x_i + \Delta x_{i+1}}\tau_{i+1}}\,. \tag{117}$$

This is the harmonic mean of τ_i, τ_{i+1}, weighted with respect to the distance to the interface.

The inter-block relative permeability is evaluated by upstream weighting:

$$\left(k_{rw}\right)_{i+1/2} = \begin{cases} k_{rw_{i+1}}, & P_{w_i} < P_{w_{i+1}} \\ k_{rw_i}, & \text{otherwise.} \end{cases} \tag{118}$$

The following process typical in performance assessment analysis justifies this treatment of the interblock flow term. Assume gas is generated and is displacing water from the left to the right as in Figure 15. At the gas front, the gas pressure, P_g, is highest in the i^{th} grid block. Therefore, gas wants to flow from i to i+1 grid block. Although the gas is mobile ($k_{rg} > 0$) in the i^{th} block, it is immobile ($k_{rg} = 0$) in the i+1th block. If the relative permeability is included in the inter-block harmonic averaging, then $\tau_{i+1/2}$ is zero and no gas is transported. By upstream weighting the gas relative permeability we allow the mobile gas to flow from i to i+1 block.

$S_g > S_{g_r}$	$S_g \le S_{g_r}$
P_{gi}	P_{gi+1}
x_i	x_{i+1}

i+1/2

Figure 15. Gas displacement front.

Another treatment of relative permeability is to evaluate it as an arithmetic average of the two adjacent relative permeabilities.

$$\left(k_{rw}\right)_{i+1/2} = w_i k_{rw_i} + w_{i+1} k_{rw_{i+1}} \tag{119}$$

where the weights sum to 1. The arithmetic average of inter-block relative permeability does not correctly treat the following case. Suppose water is displaced from left to right in Figure 16:

$S_w \le S_{wr}$	$S_w > S_{wr}$
P_{wi}	P_{wi+1}
x_i	x_{i+1}

Figure 16. Displacement of immobile water.

with pressure satisfying $P_{wi} > P_{wi+1}$. The pressure tries to move water from i to i+1 block. Since $k_{rw_i} = 0$ and $k_{rw_{i+1}} > 0$, the inter-block relative permeability by arithmetic averaging is greater than zero and the immobile water would be transported from the i^{th} block. Upstream weighting would yield inter-block relative permeability of zero with no water transported. Thus, the upstream weighting prevents immobile fluid from being transported. The upstream weighting of relative permeability is controlled by input parameters.

4.9 Characteristic Curves

Relative permeability and capillary pressure are computed from several different empirical relations (Brooks, 1964; van Genuchten, 1978; WIPP PA, 1992a). Input directives control choice of the characteristic curves.

The original van Genuchten-Parker model determines

Capillary Pressure:

$$P_c = \begin{cases} P_o\left(S_{e_1}^{-1/m}-1\right)^{1-m} & \text{if } S_{e_1}<1 \\ 0 & \text{otherwise} \end{cases} \quad \text{if } S_w > S_{wr} \qquad \text{otherwise: } 0 \tag{120}$$

where P_o is a constant determined by equating the original van Genuchten-Parker capillary pressure with the 2nd modified Brooks-Corey capillary pressure (discussed below) at $S_{e_2} = 0.5$.

Relative Permeabilities:

$$k_{rw} = \begin{cases} S_{e_1}^{1/2}\left(1-\left(1-S_{e_1}^{1/m}\right)^m\right)^2 & \text{if } S_{e_1}<1 \\ 1 & \text{otherwise} \end{cases} \quad \text{if } S_w > S_{wr} \qquad \text{otherwise: } 0 \tag{121}$$

$$k_{rg} = \begin{cases} \left(1-S_{e_1}\right)^{1/2}\left(1-S_{e_1}^{1/m}\right)^{2m} & \text{if } S_{e_1}<1 \\ 0 & \text{otherwise} \end{cases} \quad \text{if } S_w > S_{wr} \qquad \text{otherwise: } 1 \tag{122}$$

where the effective saturations are

$$S_{e_1} = \frac{S_w - S_{wr}}{1 - S_{wr}} \tag{123}$$

and

$$S_{e_2} = \frac{S_w - S_{wr}}{1 - S_{gr} - S_{wr}}. \tag{124}$$

In the original van Genuchten-Parker model, the effective saturation is associated with a residual gas saturation, S_{gr}, equal to zero. BRAGFLO has the capability of using nonzero residual gas saturation in the calculation of S_{e_2} for the modified van Genuchten-Parker relations (presented below).

The parameter m is related to the pore size distribution parameter, λ, by

$$m = \frac{\lambda}{1+\lambda}. \tag{125}$$

The P_o constant used in the original van Genuchten-Parker capillary pressure equation is related to the threshold pressure, P_t, by

$$P_o = P_t 2^{1/\lambda}\left(\left[\frac{0.5(1-S_{gr}-S_{wr})}{1-S_{wr}}\right]^{-1/m}-1\right)^{m-1}, \tag{126}$$

where threshold pressure is given as a function of intrinsic permeability k and linear, a, and exponential, η, constants

$$P_t = ak^{\eta}. \tag{127}$$

Typical characteristic curves using the original van Genuchten-Parker model and specified parameters are shown in Figure 17.

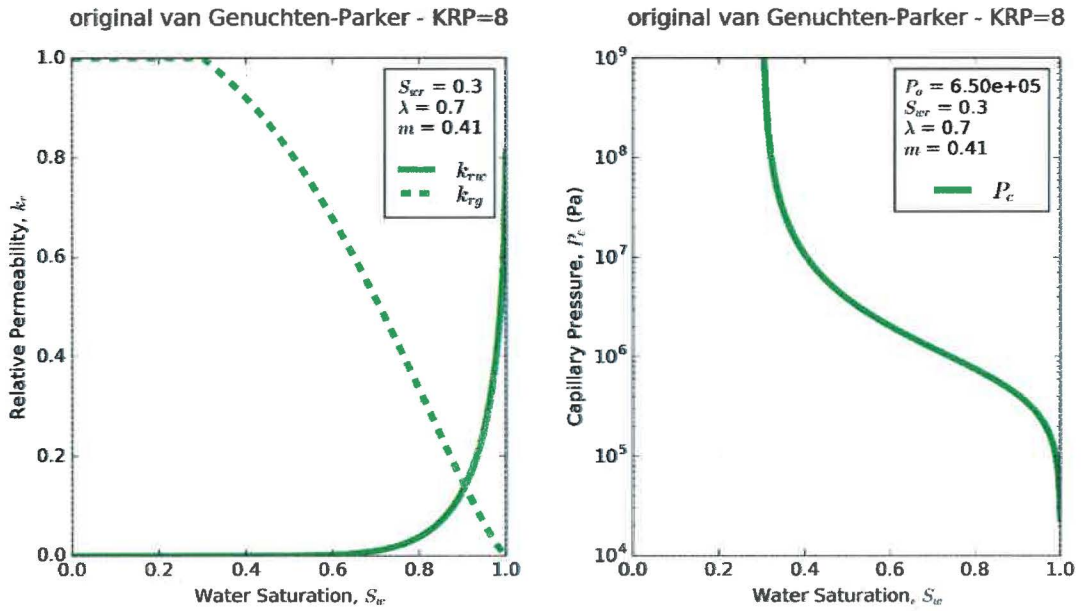


Figure 17. Relative permeabilities for the original van Genuchten-Parker model (left plot) and capillary pressure for the original van Genuchten-Parker model (right plot).

The modified van Genuchten-Parker model includes residual gas saturation in the calculation of effective saturation (S_{e_2}) applied to the capillary pressure and gas phase relative permeability.

The modified van Genuchten-Parker model determines

Capillary Pressure:

$$P_c = \begin{cases} P_o\left(S_{e_2}^{-1/m} - 1\right)^{1-m} & \text{if } S_g \le S_{gr} \\ P_o\left(S_{e_2}^{-1/m} - 1\right)^{1-m} & \text{if } S_w > S_{wr} \\ 0 & \text{otherwise} \end{cases} \tag{128}$$

Relative Permeabilities:

$$k_{rw} = \begin{cases} S_{e_1}^{1/2}\left(1-\left(1-S_{e_1}^{1/m}\right)^m\right)^2 & \text{if } S_g \le S_{gr} \\ S_{e_1}^{1/2}\left(1-\left(1-S_{e_1}^{1/m}\right)^m\right)^2 & \text{if } S_w > S_{wr} \\ 0 & \text{otherwise} \end{cases} \tag{129}$$

$$k_{rg} = \begin{cases} 0 & \text{if } S_g \le S_{gr} \\ \left(1-S_{e_2}\right)^{1/2}\left(1-S_{e_2}^{1/m}\right)^{2m} & \text{if } S_w > S_{wr} \\ 1 & \text{otherwise} \end{cases} \tag{130}$$

Typical characteristic curves using the modified van Genuchten-Parker model and specified model parameters are shown in Figure 18.

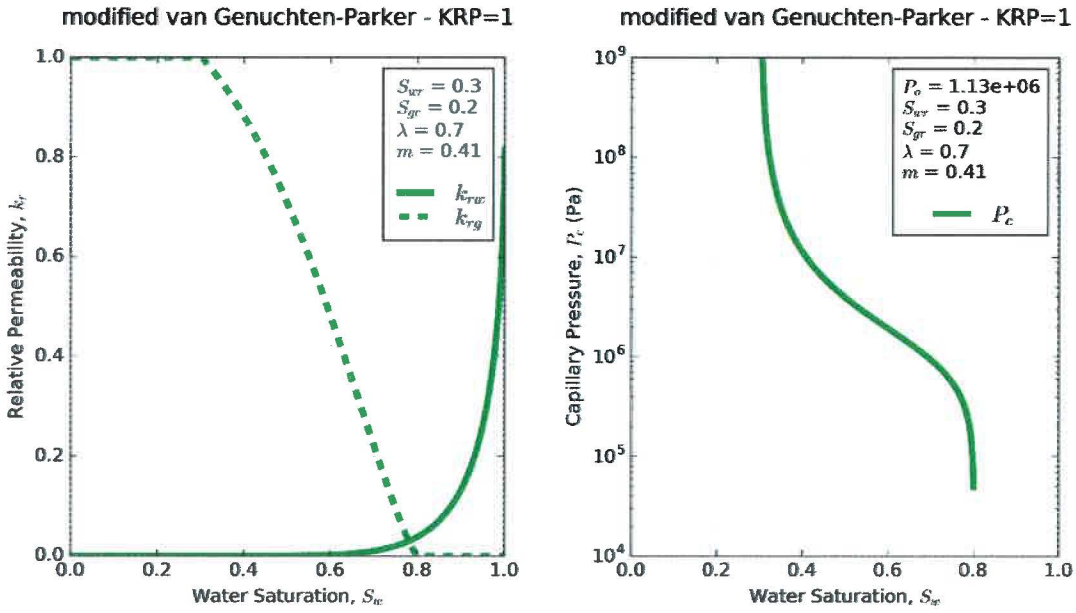


Figure 18. Relative permeabilities for the modified van Genuchten-Parker model (left plot) and capillary pressure for the modified van Genuchten-Parker model (right plot).

The original Brooks-Corey model determines

Capillary Pressure:

$$P_c = \begin{cases} 0 & \text{if } S_w \le S_{wr} \\ \dfrac{P_t}{S_{e_1}^{1/\lambda}} & \text{otherwise} \end{cases} \tag{131}$$

Relative Permeabilities:

$$k_{rw} = \begin{cases} 0 & \text{if } S_w \le S_{wr} \\ S_{e_1}^{(2+3\lambda)/\lambda} & \text{otherwise} \end{cases} \tag{132}$$

$$k_{rg} = \begin{cases} 1 & \text{if } S_w \le S_{wr} \\ \left(1-S_{e_1}\right)^2\left(1-S_{e_1}^{(2+\lambda)/\lambda}\right) & \text{otherwise} \end{cases}. \tag{133}$$

Note that if this option is used with $P_t = 0$, then P_c is identically zero.

Typical characteristic curves using the original Brooks-Corey model and specified model parameters are shown in Figure 19.

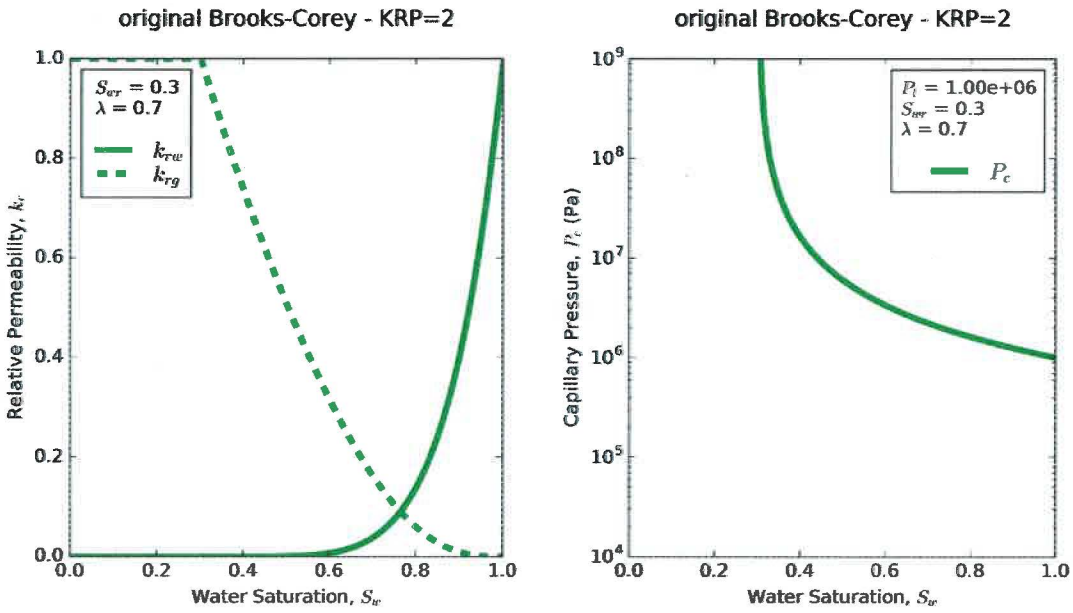


Figure 19. Relative permeabilities for the original Brooks-Corey model (left plot) and capillary pressure for the original Brooks-Corey model (right plot).

Two modifications of the Brooks-Corey model are available which differ in the treatment of the effective saturation, S_e. The 1st modified Brooks-Corey model uses an effective saturation, S_{e_2}, in the calculation of capillary pressure and relative permeability.

The 1st modified Brooks-Corey model determines

Capillary Pressure:

$$P_c = \begin{cases} P_t & \text{if } S_g \le S_{gr} \\ \dfrac{P_t}{S_{e_2}^{1/\lambda}} & \text{if } S_w > S_{wr} \\ 0 & \text{otherwise} \end{cases} \tag{134}$$

Relative Permeabilities:

$$k_{rw} = \begin{cases} 1 & \text{if } S_g \le S_{gr} \\ S_{e_2}^{(2+3\lambda)/\lambda} & \text{if } S_w > S_{wr} \\ 0 & \text{otherwise} \end{cases} \tag{135}$$

$$k_{rg} = \begin{cases} 0 & \text{if } S_g \le S_{gr} \\ \left(1-S_{e_2}\right)^2 \left(1-S_{e_2}^{(2+\lambda)/\lambda}\right) & \text{if } S_w > S_{wr} \\ 1 & \text{otherwise} \end{cases} \tag{136}$$

Typical characteristic curves using the 1st modified Brooks-Corey model and specified model parameters are shown in Figure 20.

Note that for $S_w \geq 1\text{-}S_{gr}$, gas is immobile and water has 100% mobility. Also, note that the capillary pressure curve assumes the threshold capillary pressure at $S_w = 1\text{-}S_{gr}$.

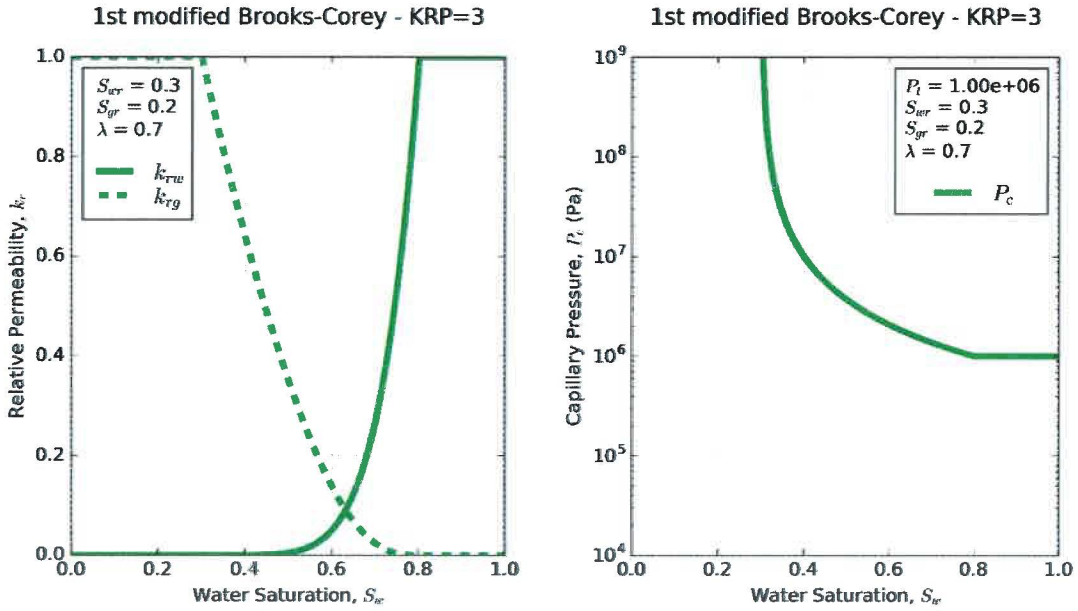


Figure 20. Relative permeabilities for 1st modified Brooks-Corey model (left plot) and capillary pressure for 1st modified Brooks-Corey model (right plot).

The second modified Brooks-Corey model includes residual gas saturation in the calculation of effective saturation (S_{e_2}) applied to the capillary pressure and gas phase relative permeability.

The 2nd modified Brooks-Corey model determines

Capillary Pressure:

$$P_c = \begin{cases} \dfrac{P_t}{S_{e_2}^{1/\lambda}} & \text{if } S_g \leq S_{gr} \\ \dfrac{P_t}{S_{e_2}^{1/\lambda}} & \text{if } S_w > S_{wr} \\ 0 & \text{otherwise} \end{cases} \tag{137}$$

Relative Permeabilities:

$$k_{rw} = \begin{cases} S_{e_1}^{(2+3\lambda)/\lambda} & \text{if } S_g \le S_{gr} \\ S_{e_1}^{(2+3\lambda)/\lambda} & \text{if } S_w > S_{wr} \\ 0 & \text{otherwise} \end{cases} \tag{138}$$

$$k_{rg} = \begin{cases} 0 & \text{if } S_g \le S_{gr} \\ \left(1 - S_{e_2}\right)^2 \left(1 - S_{e_2}^{(2+\lambda)/\lambda}\right) & \text{if } S_w > S_{wr} \\ 1 & \text{otherwise} \end{cases} \tag{139}$$

Typical characteristic curves using the 2nd modified Brooks-Corey model and specified model parameters are shown in Figure 21.

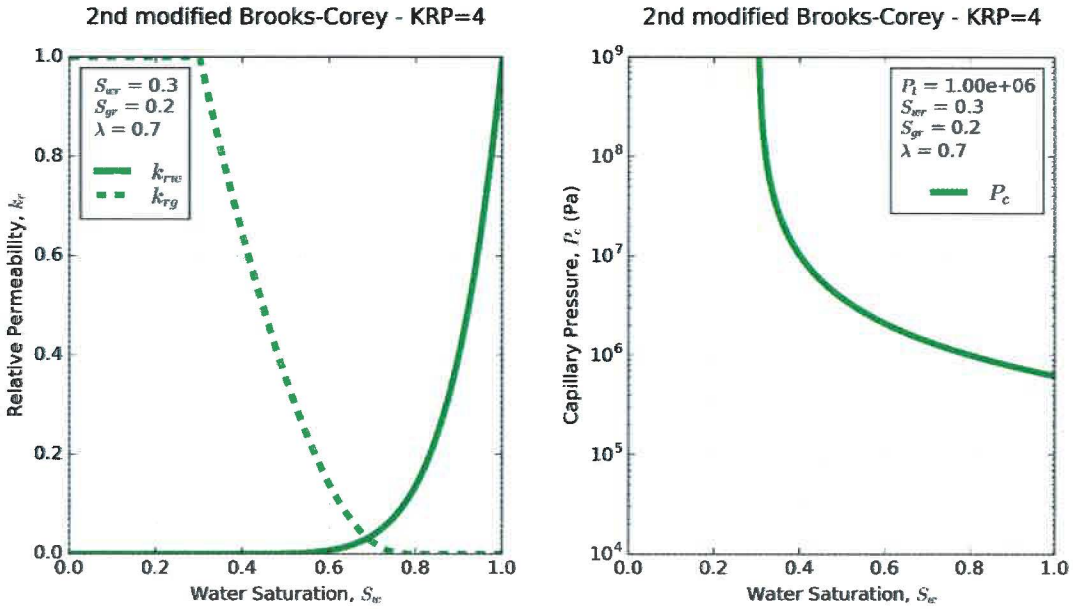


Figure 21. Relative permeabilities for 2nd modified Brooks-Corey model (left plot) and capillary pressure for 2nd modified Brooks-Corey model (right plot).

For both the van Genuchten-Parker and the Brooks-Corey models, the capillary pressure function is unbounded from the right ($S_w = S_{wr}^{+}$). An option is available which truncates the capillary pressure function at the PCMAX value. The capillary pressure curve with this option and PCMAX = 1.0×10^8 Pa is shown in Figure 22 (left plot) for the modified van Genuchten-Parker model and in Figure 22 (right plot) for the 2nd modified Brooks-Corey model.

The dependence of the characteristic curves for both the modified van Genuchten-Parker and 2nd modified Brooks-Corey models on the pore size distribution parameter λ is shown in Figure 23 and Figure 24.

When the Jacobian is calculated, derivatives with respect to saturation are taken so as not to cross residual brine saturation, where the capillary pressure is either discontinuous or has discontinuous derivatives, depending on which option is chosen to model capillary pressure.

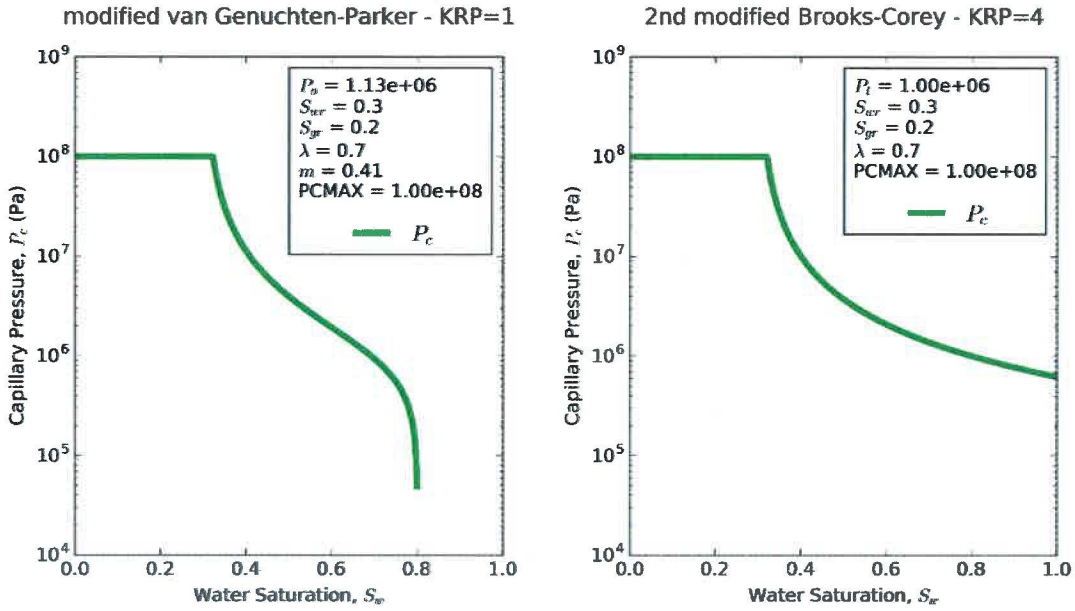


Figure 22. Capillary pressure for modified van Genuchten-Parker model (left plot) and 2nd modified Brooks-Corey model (right plot).

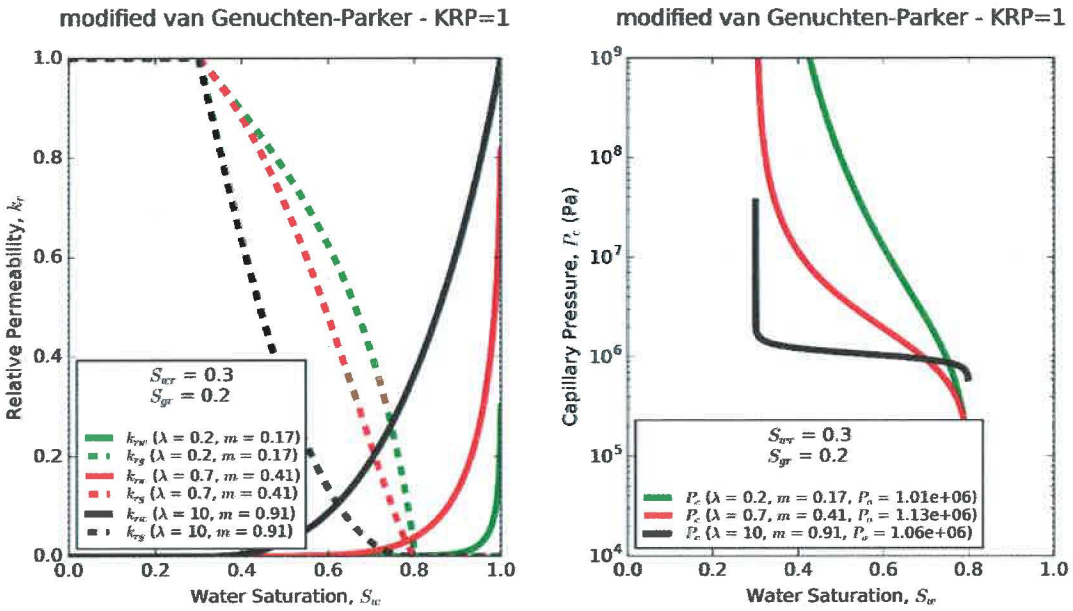


Figure 23. Relative permeabilities for modified van Genuchten-Parker model, effect of parameter *m* (left plot) and capillary pressure for modified van Genuchten-Parker model, effect of parameter *m* (right plot).

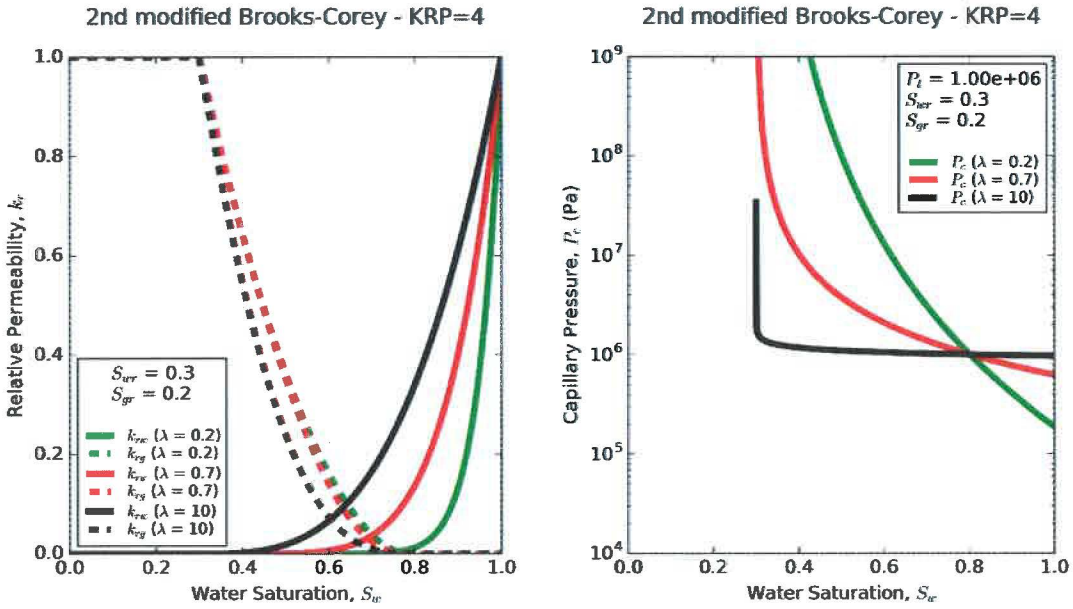


Figure 24. Relative permeabilities for 2nd modified Brooks-Corey model effect of pore size distribution parameter (left plot) and capillary pressure for 2nd modified Brooks-Corey model effect of pore size distribution parameter (right plot).

Three linear models (A, B, and D), give relative permeability and capillary pressure. The linear model A determines

Capillary Pressure:

$$P_c = \begin{cases} P_{c\max} & \text{if } S_w \le S_{wr} \\ P_t & \text{if } S_g \le S_{gr} \\ (P_t - P_{c\max})S_{e_2} + P_{c\max} & \text{otherwise} \end{cases} \tag{140}$$

Relative Permeabilities:

$$k_{rw} = \begin{cases} 0 & \text{if } S_w \le S_{wr} \\ 1 & \text{if } S_g \le S_{gr} \\ S_{e_2} & \text{otherwise} \end{cases} \tag{141}$$

$$k_{rg} = \begin{cases} 1 & \text{if } S_w \le S_{wr} \\ 0 & \text{if } S_g \le S_{gr} \\ 1 - S_{e_2} & \text{otherwise} \end{cases}. \tag{142}$$

Typical characteristic curves using the linear model A and specified model parameters are shown in Figure 25, where $P_{c\max} = \text{PCMAX}$.

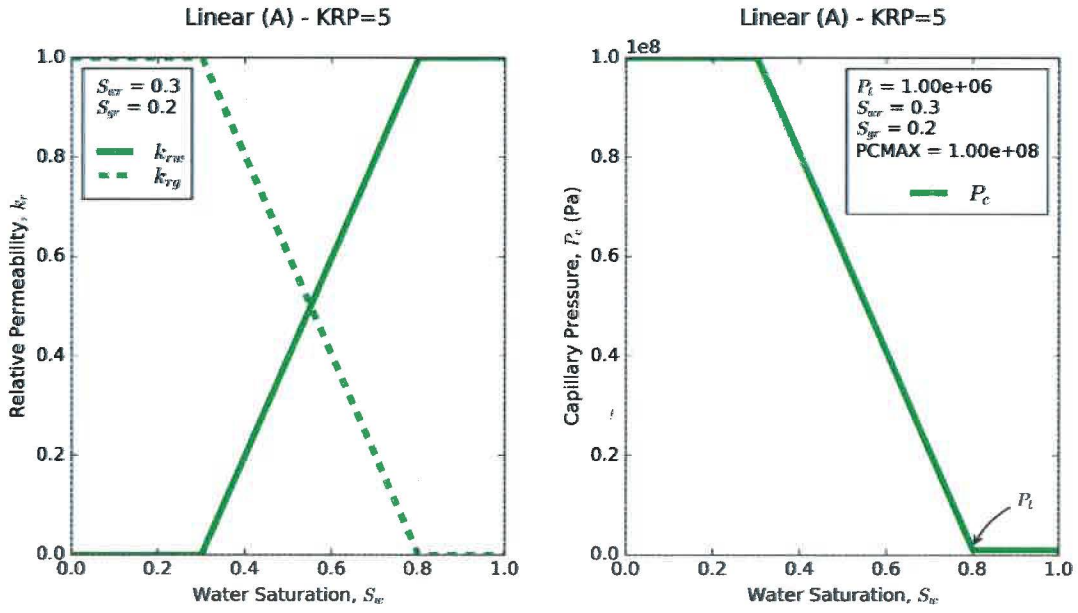


Figure 25. Relative permeabilities for linear model A (left plot) and capillary pressure for linear model A (right plot).

The linear B model determines

Capillary Pressure:

$$P_c = \begin{cases} P_{c\max} & \text{if } S_w \le S_{wr} \\ P_t & \text{if } S_g \le S_{gr} \\ (P_t - P_{c\max})S_{e_2} + P_{c\max} & \text{otherwise} \end{cases} \tag{143}$$

Relative Permeabilities:

$$k_{rw} = \begin{cases} 0 & \text{if } S_w \le S_{wr} \\ S_{e_1} & \text{if } S_g \le S_{gr} \\ S_{e_1} & \text{otherwise} \end{cases} \tag{144}$$

$$k_{rg} = \begin{cases} 1 & \text{if } S_w \le S_{wr} \\ 0 & \text{if } S_g \le S_{gr} \\ 1 - S_{e_2} & \text{otherwise} \end{cases}. \tag{145}$$

Typical characteristic curves using the linear model B and specified model parameters are shown in Figure 26.

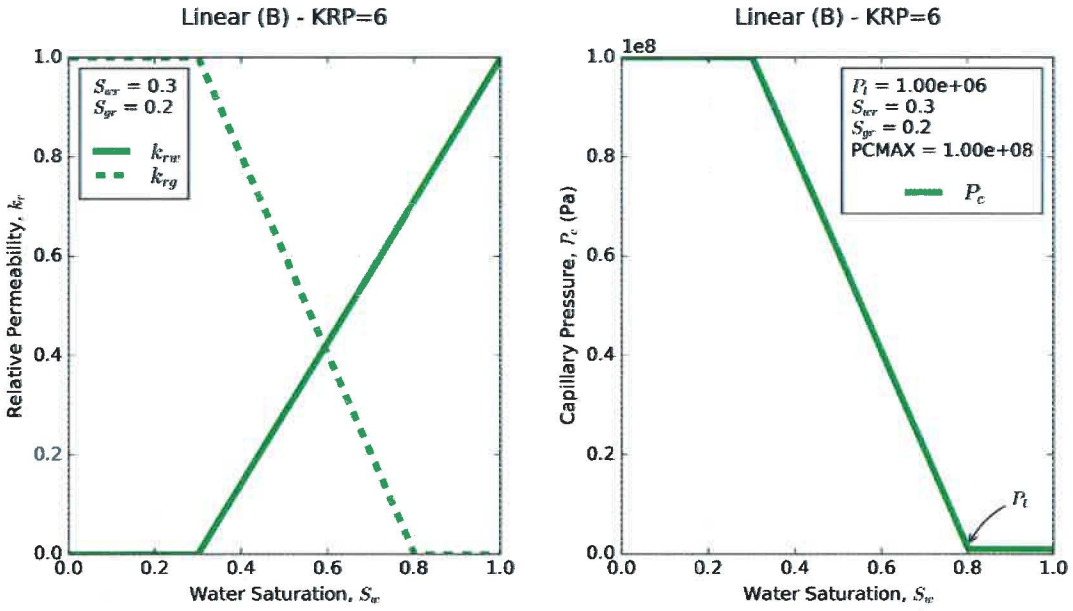


Figure 26. Relative permeabilities for linear model B (left plot) and capillary pressure for linear model B (right plot).

The linear D model determines

Capillary Pressure:

$$P_c = P_t \tag{146}$$

Relative Permeabilities:

$$k_{rw} = \begin{cases} 0 & \text{if } S_w \le S_{wr} \\ 1 & \text{if } S_g \le S_{gr} \\ 1 & \text{otherwise} \end{cases} \tag{147}$$

$$k_{rg} = \begin{cases} 1 & \text{if } S_w \le S_{wr} \\ 0 & \text{if } S_g \le S_{gr} \\ 1 & \text{otherwise} \end{cases}. \tag{148}$$

Typical characteristic curves using the linear model D and specified model parameters are shown in Figure 27.

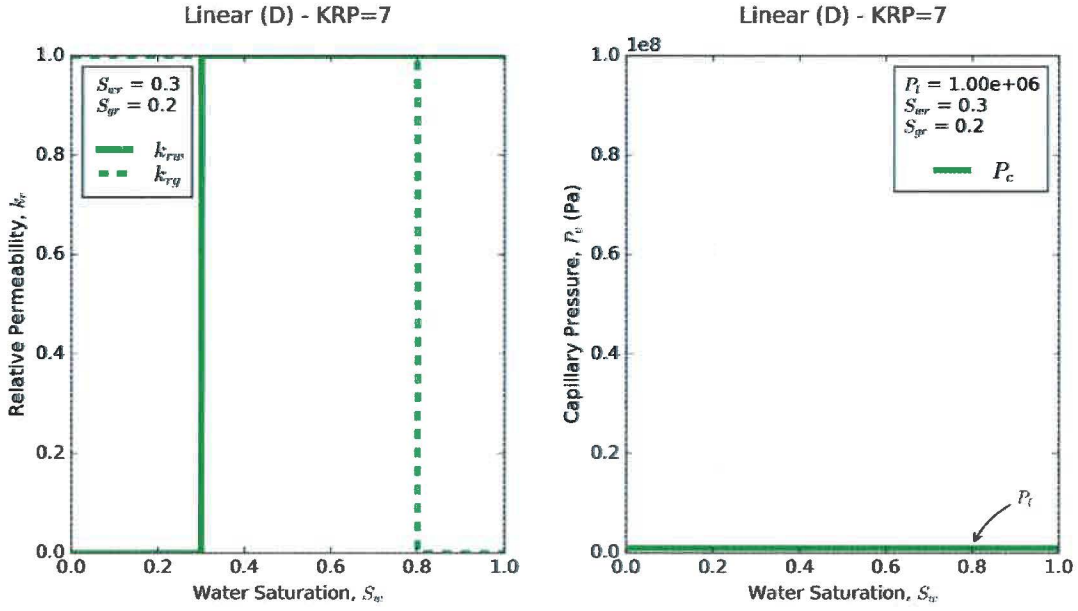


Figure 27. Relative permeabilities for linear model D (left plot) and capillary pressure for linear model D (right plot).

In running BRAGFLO, the capillary pressure-saturation relationships were typically turned off in waste-filled regions because they caused the solver to take very small time steps around $S_w \sim S_{wr}$. When the Jacobian is calculated, derivatives with respect to saturation are taken so as not to cross residual brine saturation. Nonetheless the Newton-Raphson solver can have difficulty finding a solution around the discontinuous derivative in capillary pressure when capillary pressure is capped at PCMAX. In past calculations this problem occurred when iron

corrosion (which consumes water) reduced the saturation below residual saturation in the waste-filled regions.

To remedy the numerical problem due to the discontinuity in capillary-pressure, an additional Brooks-Corey model modification for waste areas is implemented in BRAGFLO. In this model, the capillary pressure is calculated using a modified saturation,

$$S_{e_{21}} = \max\left[\min\left[\frac{S_w - \left(S_{\min} - S_{eff\,\min}\right)}{1 - \left(S_{\min} - S_{eff\,\min}\right)}, 1\right], S_{eff\,\min}\right], \tag{149}$$

where $S_{\min}$ is a cut off in saturation that is considered numerically dry (see Section 4.13.1) and $S_{eff\,\min}$ is a small tolerance which pushes the singularity in the capillary pressure equation to a saturation slightly below $S_{\min}$.

The waste area modification model determines

Capillary Pressure:

$$P_c = \frac{P_t}{S_{e_{21}}^{1/\lambda}} \tag{150}$$

Relative Permeabilities:

$$k_{rw} = \begin{cases} S_{e_1}^{(2+3\lambda)/\lambda} & \text{if } S_g \le S_{gr} \\ S_{e_1}^{(2+3\lambda)/\lambda} & \text{if } S_w > S_{wr} \\ 0 & \text{otherwise} \end{cases} \tag{151}$$

$$k_{rg} = \begin{cases} 0 & \text{if } S_g \le S_{gr} \\ \left(1 - S_{e_2}\right)^2 \left(1 - S_{e_2}^{(2+\lambda)/\lambda}\right) & \text{if } S_w > S_{wr} \\ 1 & \text{otherwise} \end{cases} \tag{152}$$

where the effective saturations are restricted as

$$S_{e_1} = \max\left[\min\left[\frac{S_w - S_{wr}}{1 - S_{wr}}, 1\right], 0\right] \tag{153}$$

and

$$S_{e_2} = \max\left[\min\left[\frac{S_w - S_{wr}}{1 - S_{gr} - S_{wr}}, 1\right], 0\right] \tag{154}$$

Typical characteristic curves using the waste area model and specified model parameters are shown in Figure 28.

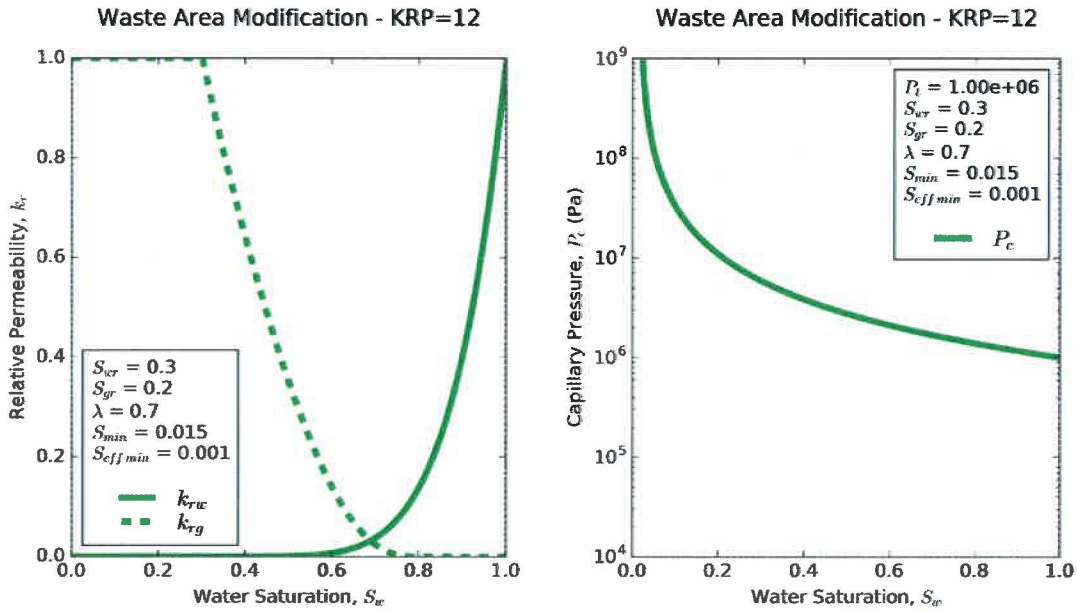


Figure 28. Relative permeabilities for waste area model (left plot) and capillary pressure for waste area model (right plot).

Previously, in BRAGFLO, an inconsistency occurred during the -5 to 0 year operational period during which BRAGFLO is run. During this period the operational areas were modeled as open-completely-saturated cavities with porosity equal to 1. If capillary pressure were turned on during this period, the model would predict significant capillary-pressure effects on the relative permeabilities, although the open repository is not completely saturated and does not have significant capillary pressure effects on pressure or permeability. A model to remove capillary-pressure effects from the relative permeabilities for open cavities is implemented in BRAGFLO. In this model, the capillary pressure is set to zero and the relative permeabilities decrease from 1 to zero linearly between the residual saturations (brine and gas) and the residual saturation plus a tolerance.

The open cavity modification model determines

Capillary Pressure:

$$P_c = 0 \tag{155}$$

Relative Permeabilities:

$$k_{rw} = \begin{cases} 0 & \text{if } S_w \le S_{wr} \\ 1 & \text{if } S_g \le S_{gr} \\ \dfrac{S_w - S_{wr}}{S_{tol}} & \text{if } S_w \le S_{wr} + S_{tol} \\ 1 & \text{if } S_g \le S_{gr} + S_{tol} \\ 1 & \text{otherwise} \end{cases} \tag{156}$$

$$k_{rg} = \begin{cases} 1 & \text{if } S_w \le S_{wr} \\ 0 & \text{if } S_g \le S_{gr} \\ 1 & \text{if } S_w \le S_{wr} + S_{tol} \\ \dfrac{S_g - S_{gr}}{S_{tol}} & \text{if } S_g \le S_{gr} + S_{tol} \\ 1 & \text{otherwise} \end{cases} \tag{157}$$

where S_{tol} is given below and tol is a tolerance over which the relative permeability changes linearly from zero to 1,

$$S_{tol} = \text{tol}(1 - S_{gr} - S_{wr}). \tag{158}$$

Typical characteristic curves using the waste area model and specified model parameters are shown in Figure 29.

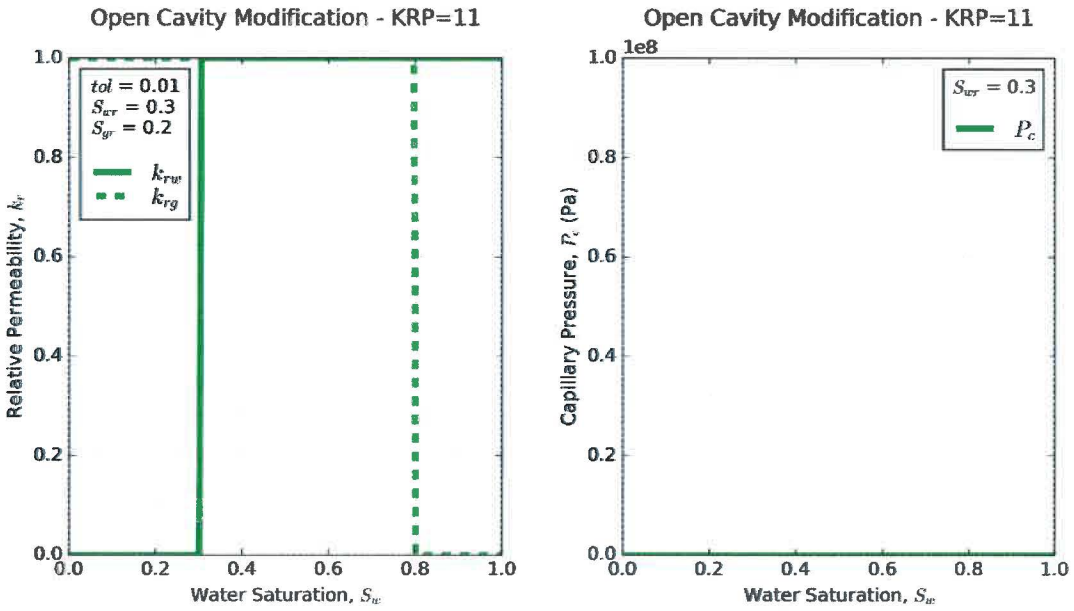


Figure 29. Relative permeabilities for open cavity model (left plot) and capillary pressure for open cavity model (right plot).

4.10 Pressure-Induced Fracture Treatment

Most fluid flow models for porous media, such as BRAGFLO, allow for coupling to the mechanical system (rock matrix) through the introduction of pore compressibility (*i.e.*, bulk rock compressibility / porosity; hereafter, referred to as rock compressibility), which is defined as the relative rate of change of porosity with respect to pressure

$$C = \frac{1}{\phi}\frac{d\phi}{dP} \tag{159}$$

where

C = rock compressibility,

ϕ = porosity,

P = pore pressure.

For constant compressibility, porosity can be expressed as a function of pressure

$$\phi = \phi_o \exp\left[C\left(P - P_o\right)\right] \tag{160}$$

where ϕ_o is the porosity at reference pressure, P_o.

The fracture treatment in BRAGFLO (Key, 1994) allows for pressure induced alterations to the porosity by introducing a pressure-dependent porosity. Figure 30 shows the piecewise linear rock compressibility function. Below an initiating pressure, P_i, compressibility is a constant intact value, C_i. For pressures above P_i, the compressibility increases linearly to a fully altered compressibility, C_a, at the fully altered pressure, P_a. For pressures above P_a no further alteration occurs, which implies that $C = 0$.

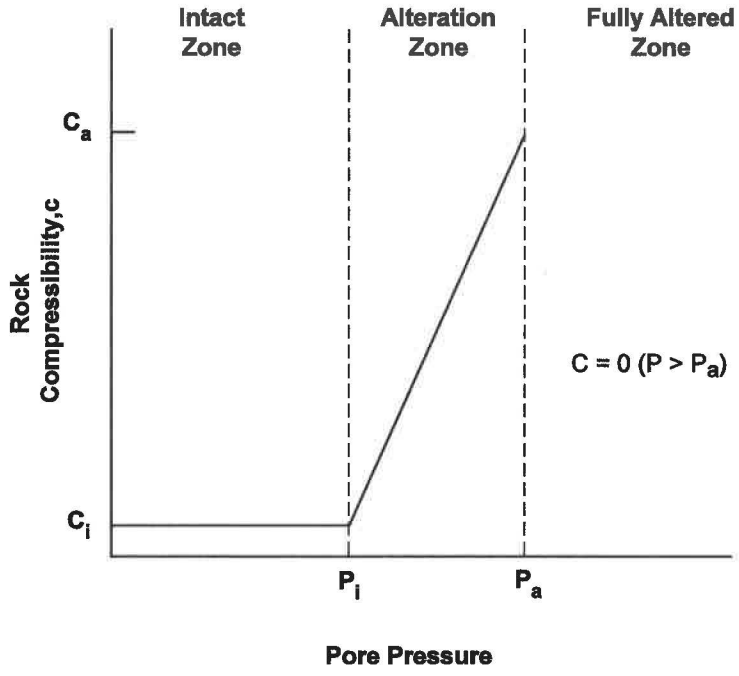


Figure 30. Pressure dependent compressibility.

The porosity can now be computed from the compressibility definition giving

$$\phi = \begin{cases} \phi_0 \exp\left[C_i (P - P_0)\right] & P \le P_i \\ \phi_0 \exp\left\{C_i (P - P_o) + \dfrac{(C_a - C_i)}{(P_a - P_i)} \dfrac{(P - P_i)^2}{2}\right\} & P_i < P < P_a \\ \phi_a & P_a \le P \end{cases} \tag{161}$$

BRAGFLO input requires the pressures P_i and P_a and the porosity at the fully altered conditions, ϕ_a be specified. From this information, the fully altered compressibility, C_a, is determined as

$$C_a = C_i \left[1 - 2\frac{(P_a - P_o)}{P_a - P_i}\right] + \frac{2}{(P_a - P_i)} \ln\left(\frac{\phi_a}{\phi_o}\right). \tag{162}$$

The BRAGFLO fracture treatment further allows for change in the fracture material permeability. The often-used parallel plate analogy for flow in fractured rock suggests the form

$$\frac{k}{k_i} = \left[\frac{\phi}{\phi_i}\right]^n \tag{163}$$

where

k = permeability of altered material,

k_i = permeability of intact material,

ϕ = porosity of altered material,

ϕ_i = porosity of intact material,

n = an empirical parameter.

The altered permeability model requires as input n. Also, the anisotropic nature of permeability is specified for the fracture materials.

A geometric realization of the pressure-dependent porosity and permeability within a fracture material is shown in Figure 31.

In a system where gas is displacing water, the fracture treatment can influence the gas migration distance. At elevated pressure, the increased porosity will produce more storage with corresponding shorter gas migration distance, while the increase in permeability will enhance the fluid mobility with resulting longer gas migration. The net effect will depend on the relative magnitudes of the storage and permeability effects.

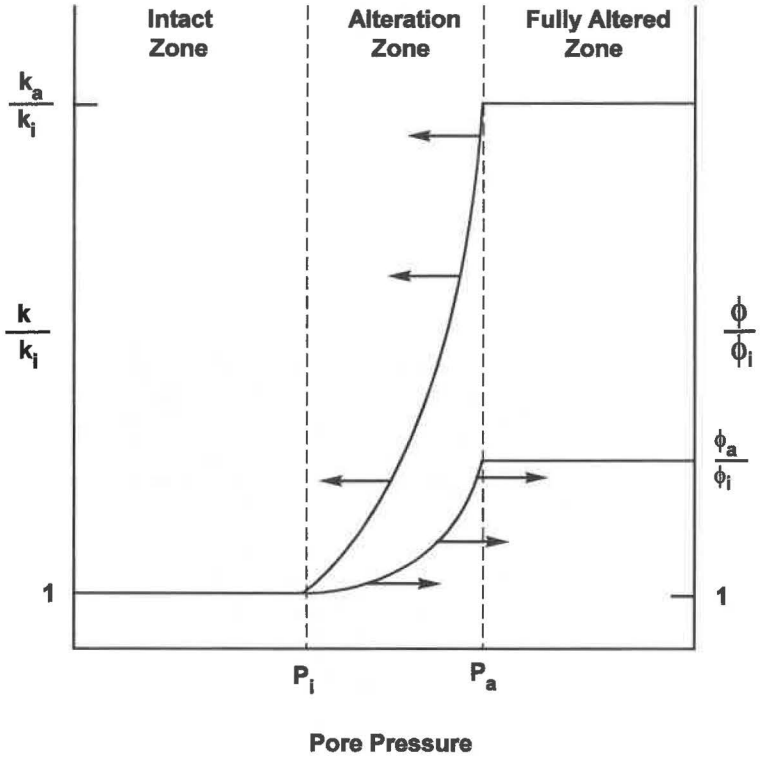


Figure 31. Pressure dependent porosity and permeability.

4.11 Creep Closure

The excavation of the WIPP will result in the plastic deformation of the salt material (creep) and resultant closure (creep closure) of excavated areas. The principal effect of this closure for performance assessment is its effect on repository pressure due to the reduction in void volume accompanying creep closure. Accordingly, creep closure is represented in BRAGFLO by changing the porosity of the waste disposal area in a manner consistent with expectations developed from detailed modeling studies. Detailed modeling studies used the code SANCHO (Butcher et al., 1995), and more recently, SANTOS (Park and Hansen, 2003), to develop time- and pressure-dependent predictions of waste disposal area void volume. Pressure variation was consistent with variation in the gas generation rates possible in the waste disposal areas. The results were used to develop a look-up table of porosity as a function of time and waste disposal area pressure that is used in BRAGFLO to vary waste disposal area porosity. Essential features of the look-up table (porosity surface) are shown in Figure 32.

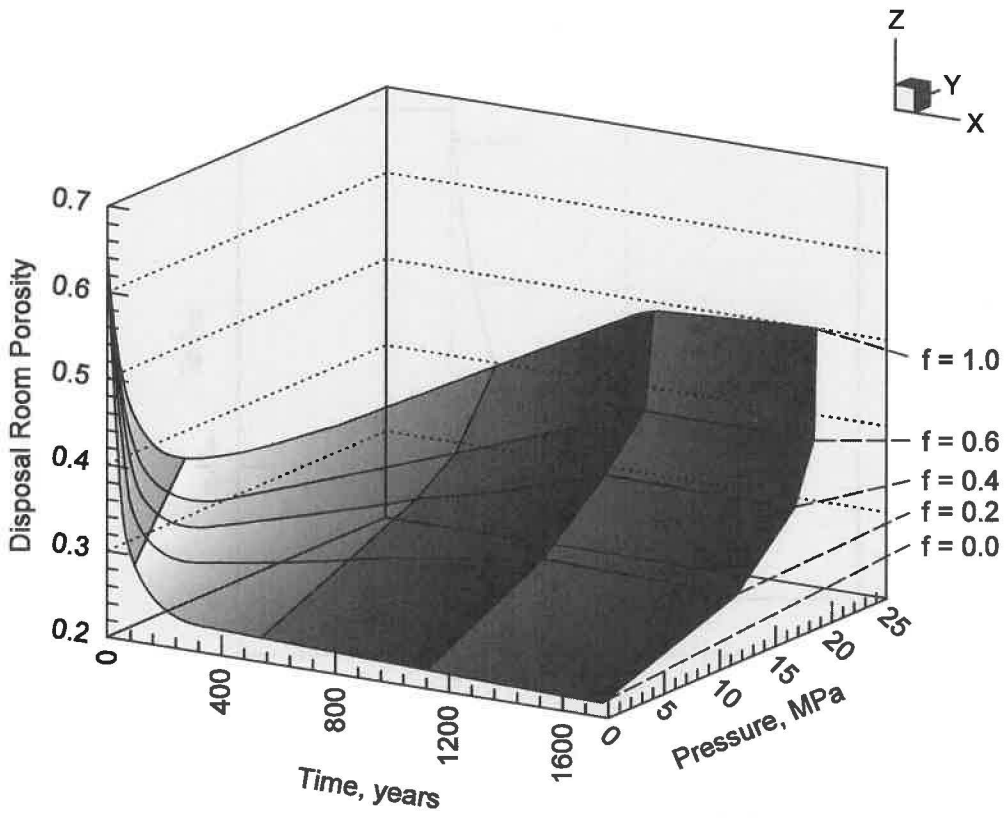


Figure 32. Pressure driven porosity function generated from SANTOS structural mechanics code.

The surface is generated by a family of f factors which is representative of the level of gas generation. The value of $f = 1.0$ corresponds to 2 moles of gas per drum per year for 550 years, 1 mole per drum per year from 550 to 1050 years, and zero gas generation after 1050 years. For each f factor the above rates are scaled by f. Four porosity surfaces or "look-up" tables are available as discussed in the Section 7.2.11. For compliance calculations the porosity "look-up" is done on a grid block scale and uses grid block pressure.

4.12 Klinkenberg Effect

For gases in a tight porous material at low pressures the boundary condition of zero gas velocity at the solid surface is not satisfied (Klinkenberg, 1941; Corey, 1990; WIPP PA, 1992a). This phenomenon has been called gas slippage and results in a larger gas velocity. This slipping of the gas flow contributes to an apparent pressure-dependent increase in permeability, which was originally observed by Klinkenberg. A correction to the formation permeability to the gas phase is related to pressure by

$$k_g = k_w\left(1 + b\, k_w^{-a} / P\right) \tag{164}$$

where

k_g = formation permeability to gas [m^2],

k_w = formation permeability to water [m^2],

a,b = formation dependent constants,

P = pressure [Pa].

The constants a,b are input. The recommended values found in the BRAGFLO User's Manual are from a tight gas/sand correlation. Figure 33 shows the gas phase permeability as a function of pressure for a family of k_w with $a = 0.33$ and $b = 0.98$.

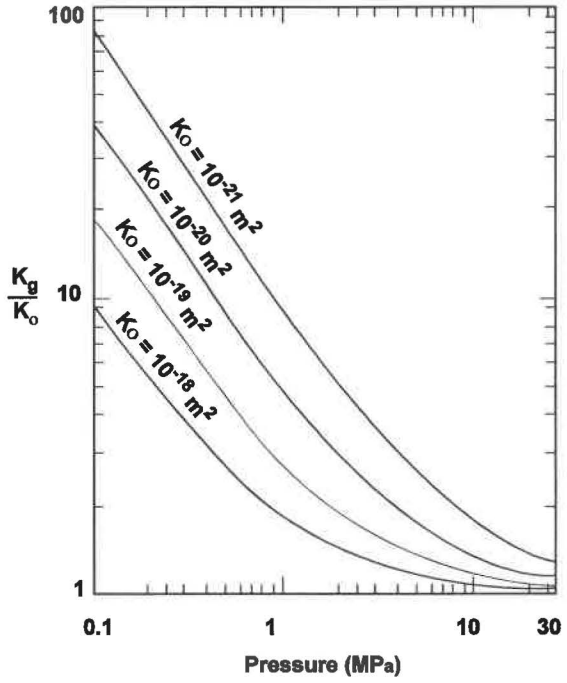


Figure 33. Increase in gas phase permeability due to Klinkenberg effect.

4.13 Chemistry Model

Within BRAGFLO there are chemical reactions (Table 1) with the effect of consuming/producing brine and gas. In BRAGFLO, the kinetics of most chemical reactions are assumed to be zero'th order.

4.13.1 Wicking and the Effective Saturation

Brine-consuming reactions such as anoxic iron corrosion and MgO hydration tend to dry out the waste-filled regions of the repository. MgO hydration tends to dry out the repository quickly because the rate of hydration far exceeds the rate of brine inflow. The BRAGFLO code and the underlying models (being a two-phase porous media flow code) cannot simulate completely dry ($S_w = 0$) cells. Furthermore, there is no reason to believe that MgO hydration will stop at the residual brine saturation since MgO hydrates under humid and inundated conditions. Thus, to

accommodate MgO hydration and allow the code to run, a lower cut off in saturation S_{min} in the waste filled areas that is considered numerically dry is implemented. This cut off is to be chosen small enough such that the amount of water in the waste filled areas at the cut off is small, but large enough to prevent numerical difficulties. Below this saturation MgO hydration, biodegradation, and iron corrosion ceases. The parameter S_{min} shows up in the subroutines PROPS and PROPS1, which calculate the properties of the grid or a single cell, respectively. In these routines an effective saturation S_{eff} is calculated and sent to each of the chemistry routines which calculate the rates of reactions, based on the effective saturation (not the actual saturation). The effective saturation is calculated from,

$$S_{eff} = \mathrm{Max}\left[\mathrm{Min}\left(S_w - S_{min} + S_{wick}\left\{1-\exp\left[200\alpha\left(\mathrm{Max}\left(S_w - S_{min}, 0\right)\right)^2\right]\right\}, 1\right), 0\right], \qquad (165)$$

where factor α is ALPHARXN, and S_{wick} is SATWICK.

The value of S_{eff} goes to zero as S_w approaches S_{min}. The factor of 200 in the exponential function was chosen to make the difference small away from $S_{eff} = 0$. The term $(S_w - S_{min})^2$ insures that the value and first derivative of S_{eff} are continuous around $S_{eff} = 0$. The parameter S_{min} is also used in determining the capillary pressure in the waste filled areas, as described above in Section 4.9. The parameter S_{min} enters BRAGFLO through the input file as SOCMIN. Equation (165) and its derivative are illustrated in Figure 34.

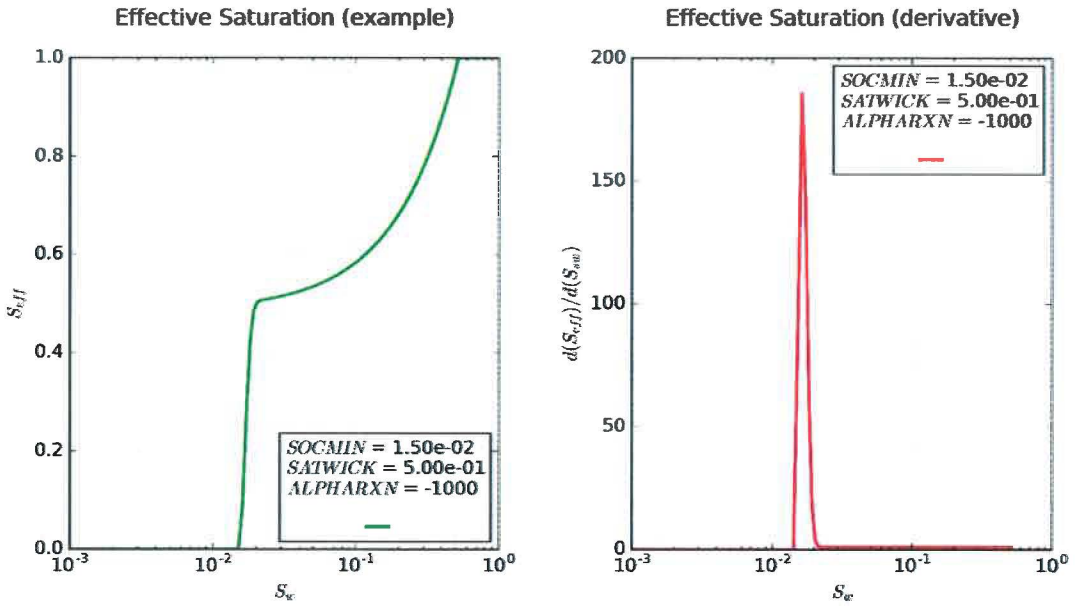


Figure 34. Effective saturation (left plot) and derivative (right plot).

4.13.2 Stoichiometry Matrix

In BRAGFLO Version 6.0 and above the stoichiometric coefficients for the chemical reactions have been reorganized into a single matrix S(I,J); stoichiometric coefficients are dimensionless. This matrix is organized as follows: I represents the reaction and J represents the individual

compound, which are given below in Table 1 and Table 2. A positive value of S(I,J) represents production, and negative represents consumption.

Table 1. Stoichiometric matrix S(I,J) row number I and corresponding reaction

Index (I)	Reaction
1	Anoxic corrosion of iron
2	Microbial gas generation
3	Iron hydroxide sulfidation
4	Metallic iron sulfidation
5	MgO hydration
6	Magnesium hydroxide (brucite) carbonation
7	MgO carbonation
8	Hydromagnesite conversion

Table 2. Stoichiometric matrix S(I,J) column number J and corresponding compound

Index (J)	Compound
1	H_2
2	H_2O
3	Fe
4	Cellulosics
5	$Fe(OH)_2$
6	FeS
7	MgO
8	$Mg(OH)_2$
9	Hydromagnesite
10	$MgCO_3$

The individual reactions are described below.

4.13.3 Iron Corrosion

In WIPP PA, the anoxic iron corrosion reaction is modeled as:

$$Fe(s) + 2\ H_2O(g,l) \rightarrow H_2(g) + Fe(OH)_2(s) \qquad (166)$$

In order to account for the material balance of brine and gas, the rate of reaction must be specified. BRAGFLO assumes iron corrosion reaction rates are zero order (constant). However, BRAGFLO recognizes a different reaction rate if the steel is in contact with liquid brine (inundated condition) or if the steel reacts with brine in the gas phase (humid condition). The input directives describing the two reaction rates are

RK(1) = brine inundated corrosion reaction rate [gm-mol Fe/m^3/s],

HF(1) = factor multiplying RK(1) to get humid corrosion reaction rate.

We introduce the notation

K_{CI} = RK(1), inundated reaction rate,

K_{CH} = HF(1) × RK(1), humid reaction rate.

The portion of steel in contact with brine is assumed to react at the inundated rate, while the portion of steel in contact with gas reacts at the humid rate as long as some liquid phase brine is present to be in equilibrium with the brine in the gas phase. The fraction of steel in contact with brine in a grid block is assumed equal to the volume fraction of brine in the pore space, S_w. Similarly, the fraction of steel in contact with gas is equal to the volume fraction of gas, $(1\text{-}S_w)$. Thus, the effective corrosion reaction rate becomes

$$K_C = K_{CI} S_w + K_{CH} (1 - S_w). \quad (167)$$

4.13.4 Microbial Gas Generation

In BRAGFLO, the biodegradation reaction assumes microbial consumption of cellulose, $C_6H_{10}O_5$, with hydrogen gas as a product

$$C_6H_{10}O_5(s) + \text{microbes} \rightarrow H_2(g) + \text{unknowns}, \quad (168)$$

The major pathways for biodegradation include the following reactions:

$$C_6H_{10}O_5(s) + 4.8\ H^+(aq) + 4.8\ NO_3^-(aq) \rightarrow 7.4\ H_2O(l) + 6\ CO_2(g) + 2.4\ N_2(g) \quad (169)$$

$$C_6H_{10}O_5(s) + 6\ H^+(aq) + 3\ SO_4^{2-}(aq) \rightarrow 5\ H_2O(l) + 6\ CO_2(g) + 3\ H_2S(g) \quad (170)$$

$$C_6H_{10}O_5(s) + H_2O(g,l) \rightarrow 3\ CH_4(g) + 3\ CO_2(g) \quad (171)$$

These reactions are assumed to proceed sequentially, consuming the limited amount of nitrate (NO_3^-) and sulfate (SO_4^{2-}) in the repository. Currently, it is assumed that there is sufficient sulfate in the surrounding rock to consume all the cellulose, and hence reaction (171) is not used.

Reaction rates for biodegradation are analogous to the iron corrosion reaction rates; that is, rates are specified for both inundated and humid conditions. The input directives describing the two reaction rates are

RK(2) = brine inundated biodegradation rate [gm-mol [$C_6H_{10}O_5$]/6 /m^3/s]

HF(2) = factor multiplying RK(2) to get humid biodegradation rate

and are used to determine the overall biodegradation rate K_B in the same way RK(1) and HF(1) are used to determine the overall corrosion rate,

$$K_B = K_{BI} S_w + K_{BH} (1\text{-}S_w), \quad (172)$$

where

K_{BI} = RK(2), inundated reaction rate,

K_{BH} = HF(2) × RK(2), humid reaction rate,

and S_{eff} from equation (165) is sent to the subroutines BIOSAT and BIOHUM as S_w.

When cellulosics are degraded by sulfate reduction, hydrogen sulfide (H_2S) is produced. The reactions of iron and its corrosion products with H_2S are modeled as,

$$Fe(s) + H_2S(g) \rightarrow FeS(s) + H_2(g), \quad (173)$$

$$Fe(OH)_2(s) + H_2S(g) \rightarrow FeS(s) + 2\ H_2O(l). \quad (174)$$

The effective rates of iron sulfidation are calculated by the subroutine BIOFES. It is assumed that these reactions are much faster than the biodegradation and effectively happen instantaneously such that the rate is calculated as the biodegradation rate multiplied by a factor,

$$K_{FeS} = RXH2S\ K_B, \quad (175)$$

where the factor *RXH2S* is the ratio of moles of H_2S produced per mole of carbon generated by the biodegradation. For example, with no nitrate in the repository, only reaction (170) would be used and *RXH2S* would be calculated as 0.5. It is assumed that reaction (174) kinetically dominates reaction (173) if iron hydroxide is available. If iron hydroxide is not available, it is assumed that equation (174) occurs. This is rarely used since iron corrosion is generally faster than biodegradation but is included for completeness.

4.13.5 MgO Hydration and Carbonation

In BRAGFLO the subroutine CORMGO calculates the effective rate of MgO hydration to form brucite, $Mg(OH)_2$, under inundated and humid conditions

$$MgO(s) + H_2O(g,l) \rightarrow Mg(OH)_2(s). \quad (176)$$

This routine takes as input the base rates of hydration of MgO under humid (*BRUCITEH*) and inundated (*BRUCITEI*) conditions, which enter BRAGFLO through the input file. If water is present, the humidity of WIPP is an assumed constant at 70% relative humidity (see Section 1.10.3 of Brush, 1990). The rate of MgO hydration is calculated analogously to the previously discussed chemistry rates under inundated and humid conditions,

$$K_{Mg(OH)2} = BRUCITEI\ S_w + BRUCITEH\ (1\text{-}S_w), \quad (177)$$

where S_{eff} from equation (165) is sent to the subroutine CORMGO as S_w.

The subroutine BIOMGO has been added to calculate the rate of brucite carbonation to hydromagnesite, $Mg_5(CO_3)_4(OH)_2{:}4H_2O$,

$$5\ Mg(OH)_2(s) + 4\ CO_2(g,aq) \rightarrow Mg_5(CO_3)_4(OH)_2{:}4H_2O(s). \quad (178)$$

It is assumed that this reaction is much faster than the biodegradation and so it effectively happens instantaneously such that the rate is calculated as the biodegradation rate multiplied by a factor,

$$K_{HYDRO} = RXCO2\ K_B, \quad (179)$$

where the factor *RXCO2* is the ratio of moles of CO_2 produced per mole of carbon generated by the biodegradation. For example, using reactions (169) and (170) gives a *RXCO2* of 1.0. In the event that there is production of CO_2, but no brucite available, the BIOMGO subroutine will convert MgO directly to magnesite. This is rarely used since MgO hydration is generally faster than biodegradation but is included for completeness.

Since hydromagnesite is not thermodynamically stable under repository conditions, it is expected to dehydrate to form magnesite. The subroutine HYDROCONV calculates the rate of hydromagnesite conversion to magnesite, $MgCO_3$,

$$Mg_5(CO_3)_4(OH)_2{:}4\ H_2O(s) \rightarrow 4\ MgCO_3(s) + Mg(OH)_2(s) + 4\ H_2O(l). \quad (180)$$

This routine takes as input the intrinsic rate of hydromagnesite conversion (*HYMAGCON*), which enters BRAGFLO through the input file. The rate of hydromagnesite conversion is calculated as the product of the intrinsic rate and the hydromagnesite concentration, C_{HYDRO},

$$K_{MgCO3} = HYMAGCON\ C_{HYDRO}, \quad (181)$$

4.13.6 Rate Smoothing and Tapering

In BRAGFLO, an additional smoothing is performed on the total (inundated+hydrated) rates of all chemical reactions,

$$K_{smoothed} = K\left(1 - Exp\left(\alpha\, C / C_i\right)\right), \quad (182)$$

where K is the unsmoothed rate of a reaction described in Subsections 4.13.3-4.13.5, C is the concentration of the species being produced (or destroyed) by the reactions described in Subsections 4.13.3-4.13.5, C_i is a initial concentration of a relevant compound, and α is described in Section 4.13.1. For all MgO reactions (hydration and carbonation) the initial concentration of MgO is used for C_i. For all iron reactions the initial concentration of iron is used for C_i. For all biodegradation reactions the initial concentration of cellulosics is used for C_i. This smoothing prevents a discontinuity in the first derivative of the rates when a reaction runs out of a reactant (other than water which is handled by equation (165). This is necessary because most of the reactions in BRAGFLO are assumed to be zero'th order and some reactions will continuously have and run out of reactants, such as brucite carbonation, and sulfidation of iron hydroxide.

In BRAGFLO, the initial concentrations of cellulosics, iron, and MgO, are stored on a cell by cell basis in the arrays CONCBIOI, CONCFEI, and CONCMGI respectively. This is accomplished in the subroutine STOREINT. The initial concentrations enter BRAGFLO through the input file.

In BRAGFLO, all of the chemistry rates are tapered in the event that a reaction will run out of a reactant (other than water) in the middle of a time step. If given the current time step and current concentrations, a reactant will be used up in the current time step, the rate is adjusted so that the reactant will have zero concentration at the end of the time step.

4.13.7 Solids Production

In BRAGFLO, the volume of solids produced (or consumed) from the chemical reactions discussed in Section 4.13.3 through 4.13.5 are calculated.

The total volume of solids produced (or consumed), as normalized by cell volume, is calculated from the concentrations of species 3 through 10 in Table 2 and the concentration of salt produced by dehydrating brine minus the initial concentrations

$$\Delta V = \sum_{i=1}^{9} \Delta V_i \quad , \tag{183}$$

where

$$\Delta V_i = (C_{i,t} - C0_i) / DEN(i) \quad , \tag{184}$$

$C_{i,t}$ is the concentration of species i at time t (in kg/m^3), $C0_i$ is the initial concentration of species i, and $DEN(i)$ the density of species i, which is part of the RXN common block. The index and identity of the species in this subroutine is given in Table 3.

Table 3. Index and corresponding compound in density array DEN

Index	Compound
1	Fe
2	$Fe(OH)_2$
3	FeS
4	cellulosics
5	MgO
6	$Mg(OH)_2$
7	Hydromagnesite
8	$MgCO_3$
9	Salts

4.13.8 Reaction Path Model

Another gas generation model is the reaction path model. This model considers a much larger number of possible reactions that could take place within the WIPP repository. Although it is still an equilibrium reaction model, it can account for the different paths that a sequence of reactions could follow. Input and output for the model is implemented, together with a multi-component gas transport scheme (see Section 7.2.13), but the reaction path model has not been validated and will not be used in compliance calculations.

4.14 Linear Equation Solver

Each iteration step in the Newton-Raphson method requires the solution of a system of linear equations. Linear equation solvers fall into two general categories: direct or elimination type solvers and iterative solvers. Algorithms for direct solvers involve a finite number of arithmetic steps to produce the solution. Solution error in a direct solver occurs from round-off error in the

arithmetic operations, which is a result of the finite word length representation of any number on a computer. BRAGFLO is written with double precision word length which produces floating point number representation of 64 bits or approximately 15 significant digits on a single word length machine. BRAGFLO has a direct solver available which uses LU-decomposition.

For large-scale problems, accumulation of round-off error in a direct solver can swamp the true solution. Also, storage and computation time may become prohibitive for direct solvers. Iterative solvers are generally advantageous over direct solvers when the problem size becomes large. There are many iterative solvers found in the numerical literature. BRAGFLO includes a successive over relaxation (SOR) solver. Iterative solvers have the disadvantage that the solution depends on the convergence of an iterative procedure. For this reason, direct solvers are more simplistic in concept and application.

For performance assessment work, the original LU-decomposition method is used exclusively. It has been found from experience that the iterative solver (SOR) is not robust enough to successfully solve many of the performance assessment problems.

A description of the LU-decomposition algorithm will be presented. The method will be demonstrated with a small (4 × 4 matrix) example. The objective is to write the coefficient matrix (Jacobian matrix) as a product of two matrices,

$$\mathbf{LU} = \mathbf{A} \tag{185}$$

where **L** is lower triangular (has non-zero elements only on the main diagonal and below) and **U** is upper triangular (has non-zero elements only on the main diagonal and above). It is further possible to require the diagonals of **L** to be equal to one. If $\mathbf{A} = (a_{ij})$, $\mathbf{L} = (\alpha_{ij})$ and $\mathbf{U} = (\beta_{ij})$, then for the case of a 4 × 4 matrix the decomposition would look like

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ \alpha_{21} & 1 & 0 & 0 \\ \alpha_{31} & \alpha_{32} & 1 & 0 \\ \alpha_{41} & \alpha_{42} & \alpha_{43} & 1 \end{bmatrix} \begin{bmatrix} \beta_{11} & \beta_{12} & \beta_{13} & \beta_{14} \\ 0 & \beta_{22} & \beta_{23} & \beta_{24} \\ 0 & 0 & \beta_{33} & \beta_{34} \\ 0 & 0 & 0 & \beta_{44} \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} \tag{186}$$

For example, it can be checked by matrix multiplication that the following is an LU-decomposition of the given 4 × 4 matrix:

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ -2 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 3 & 3 & 3 \\ 0 & 0 & -2 & -2 \\ 0 & 0 & 0 & 4 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ -2 & 1 & 1 & 1 \\ 0 & 3 & 1 & 1 \\ 1 & 4 & 2 & 6 \end{bmatrix}$$

If the LU-decomposition of the matrix **A** is known then the solution of the system of equations **Ax** = **b** can be written as

$$\mathbf{Ax} = \mathbf{(LU)x} = \mathbf{L(Ux)} = \mathbf{b}. \tag{187}$$

The solution is obtained by solving for the vector **y** such that

$$\mathbf{Ly} = \mathbf{b} \tag{188}$$

and then solving

$$\mathbf{Ux} = \mathbf{y}. \tag{189}$$

The advantage of decomposing one linear set of equations into two successive sets of equations is that the solution of a triangular set of equations is an easy substitution calculation. Recall for the Modified Newton-Raphson method the Jacobian matrix is not updated every iteration; while, the right-hand side of the system of equations is recalculated each iteration. Once the LU-decomposition of the Jacobian matrix is obtained, the Newton-Raphson iteration step is accomplished by solving the system $\mathbf{Ly} = \mathbf{b}$ with updated right-hand side vector $\mathbf{b}$ by applying the forward substitution algorithm

$$y_1 = \frac{b_1}{\alpha_{11}} \tag{190}$$

$$y_i = \frac{1}{\alpha_{ii}}\left[b_i - \sum_{j=1}^{i-1} \alpha_{ij} y_j\right] \qquad i = 2,3, \ldots, N \tag{191}$$

and then solving the system $\mathbf{Ux} = \mathbf{y}$ with the back substitution algorithm

$$x_N = \frac{y_N}{\beta_{NN}} \tag{192}$$

$$x_i = \frac{1}{\beta_{ii}}\left[y_i - \sum_{j=i+1}^{N} \beta_{ij} x_j\right] \quad i = N-1, N-2, \ldots, 1. \tag{193}$$

Given the coefficient matrix $\mathbf{A}$ consider the computation of the decomposition matrices $\mathbf{L}$ and $\mathbf{U}$. The (i,j)th entry in matrix $\mathbf{A}$ will be the inner product of the ith row of $\mathbf{L}$ with the jth column of $\mathbf{U}$. If the triangular structure of $\mathbf{L}$ and $\mathbf{U}$ are considered, then the resulting product is described by the two cases,

$$\sum_{k=1}^{i} \alpha_{ik}\beta_{kj} = a_{ij} \qquad i = 1, \ldots, j \tag{194}$$

$$\sum_{k=1}^{j} \alpha_{ik}\beta_{kj} = a_{ij} \qquad i = j+1, \ldots, N \tag{195}$$

Crout's algorithm (Maron, 1982) solves the equations for the α's and β's by arranging the equations in a certain order. The algorithm is sequential over columns from 1 to N. For the jth column the β_{1j} to β_{jj} are computed from linear system (194) by

$$\beta_{ij} = a_{ij} - \sum_{k=1}^{i-1} \alpha_{ik}\beta_{kj} \qquad \text{for } i = 1, \ldots, j \tag{196}$$

followed by the solution of α_{j+1j} to a_{Nj} from linear system (195) by

$$\alpha_{ij} = \frac{1}{\beta_{jj}}\left(a_{ij} - \sum_{k=1}^{j-1} \alpha_{ik}\beta_{kj}\right) \qquad \text{for } i = j+1, \ldots, N. \tag{197}$$

The following example will demonstrate that the α's and β's that occur on the right-hand side of equations (196) and (197) are already determined by the time they are needed.

Within BRAGFLO the LU-decomposition is done within the band structure of the Jacobian matrix. This is crucial for efficient computation. Therefore, the above algorithms must be modified to work only within the bandwidth of the Jacobian matrix. Further, only the band structure is stored in the BRAGFLO treatment. This allows considerable saving in the storage requirement. Finally, BRAGFLO implements a partial pivoting (row interchanges) which reduces the round-off errors in the arithmetic and is essential for the numerical stability of Crout's method.

Now consider the example with

$$\mathbf{A} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ -2 & 1 & 1 & 1 \\ 0 & 3 & 1 & 1 \\ 1 & 4 & 2 & 6 \end{bmatrix} \tag{198}$$

Starting with the first column we solve for $\beta_{11} = 1$ from equation (196) where the sum is taken to mean zero. Equation (197) is then used to solve sequentially for $\alpha_{21} = -2$, $\alpha_{31} = 0$, and $\alpha_{41} = 1$. We now proceed to the second column and from equation (196) compute sequentially $\beta_{12} = 1$, $\beta_{22} = 3$. Now from equation (197) we compute $\alpha_{32} = 1$ and $\alpha_{42} = 1$. This procedure is continued for the 3rd and 4th columns with the resulting **L** and **U** given by the example stated earlier in this section.

Now suppose the solution of the system $\mathbf{Ax} = \mathbf{b}$ is required given right-hand side vector $\mathbf{b} = (4, 1, 5, 13)^T$. We first solve the system $\mathbf{Ly} = \mathbf{b}$ by the forward substitution algorithm. The system is

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ -2 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix} = \begin{bmatrix} 4 \\ 1 \\ 5 \\ 13 \end{bmatrix}$$

Forward substitution from the first equation to the fourth equation yields $\mathbf{y} = (4, 9, -4, 4)^T$. We then solve the system $\mathbf{Ux} = \mathbf{y}$. The system is

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 3 & 3 & 3 \\ 0 & 0 & -2 & -2 \\ 0 & 0 & 0 & 4 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 4 \\ 9 \\ -4 \\ 4 \end{bmatrix}$$

Back substitution from the fourth equation to the first equation yields $\mathbf{x} = (1, 1, 1, 1)^T$.

4.15 Model Geometry

The mesh used in the BRAGFLO simulations incorporates radial flow phenomena at large distances from the repository and includes the full accessible volume available for multiphase

flow. Time and cost constraints currently preclude a full three-dimensional representation of the repository and surrounding strata, so a two-dimensional approximation to the actual geometry is made, as described in WIPP PA Department (1992b).

4.16 Well Models

Well behavior is described by an inflow performance relation:

$$q_l = -\frac{(PI)\rho_l k_{rl}}{\mu_l}\left(P_l - P_{wf}\right), \tag{199}$$

where

l = phase index ($l = w,g$),

q_l = phase mass flow rate [kg/s],

P_l = phase pressure [Pa],

P_{wf} = flowing wellbore pressure [Pa],

PI = well productivity index [m^3],

ρ_l = phase density [kg/m^3],

μ_l = phase viscosity [Pa s],

k_{rl} = phase relative permeability.

The material balance requires the mass rate for each phase. If a well is operated as rate-specified, the inflow performance equation determines the flowing wellbore pressure, although BRAGFLO does not do this calculation. For this reason, BRAGFLO does not use the PI and P_{wf} values for rate-specified wells, although values are required on input. If the well is operated as pressure-specified, the rate is computed from the inflow performance relation. The required input parameters for either a rate- or pressure-specified well is found in the Section 7.2.5.

The well type as specified in the input file determines the well operation. The operation by well type is as follows:

INJQ: The well injects ($q_l > 0$) or produces ($q_l < 0$) at a specified rate.

INJP: The well injects at a specified flowing wellbore pressure. If the inflow performance relation predicts $q_l < 0$, then the rate is set to zero.

PROD: The well produces at a specified flowing wellbore pressure. If the inflow performance relation predicts $q_l > 0$, then the rate is set to zero.

BRAGFLO does not allow a well with completion in multiple grid blocks. However, BRAGFLO does allow multiple wells in a single grid block. The information describing well location, number of wells in a grid block, and the time period over which each well is in operation is specified in the input file.

4.17 Special Materials

BRAGFLO has four special material types that have unique capabilities. These have evolved to handle situations encountered in modeling the WIPP, so they have names that apply to regions included in models of the WIPP, but actually have fairly general applicability. The materials are referred to as:

- Waste,
- DRZ (Disturbed Rock Zone),
- Reset
- Borehole.

4.17.1 Waste Material

In Waste materials, and only in Waste, can chemical reactions take place. Another special capability unique to Waste is simulation of creep closure, in which the porosity decreases over time, the rate depending on the rate of gas production and the pressure within the Waste. Porosity can change in any material as a result of pressure-dependent compressibility, but the change is generally quite small. In contrast, the porosity change resulting from creep closure of the Waste can be very large; for example: changing from an initial 66% porosity to 9% porosity. Only in Waste can there be an *initial* mass of radionuclides, the transport and decay of which can be modeled in any region as long as there was some amount initialized in the Waste. Finally, during the operational period in the WIPP when excavations are open to the atmosphere and any brine seepage is removed by means of ventilation or pumping, the initial brine pressure and saturation in the Waste can be specified to be different from the initial conditions. Then, at some later time the conditions in the Waste can be reset to the specified initial conditions.

4.17.2 Disturbed Rock Zone (DRZ) Material

Certain materials and flow conditions are required to be reset at the time the repository obtains closure. In the DRZ material, if the porosity has increased at the time the initial conditions are reset, the brine volume is assumed to remain fixed over that change and the brine saturation is adjusted to account for the increased pore volume. Gas is assumed to fill the additional pore space. The gas appears instantaneously, *i.e.*, it does not flow from any other cell, is not introduced by well injection, and is not created by way of chemical reaction. The pressure in this material at reset time is specified by input. This material arose from a need to simulate the disturbed rock zone surrounding excavations. The time-dependent behavior of disturbed halite is not well understood, but it is considered likely that the porosity will be greater by the time the repository is filled and sealed. This behavior is currently modeled very simply as an instantaneous increase in porosity with the additional pore space filled with gas that, in reality, would have flowed in from the adjacent excavated regions through cracks and borings. More than one DRZ material can be used, each with a different reset pressure. In modeling the WIPP the pressure is reset to1 atm (101.325 kPa), the same as in the Waste so that the newly-introduced gas in the DRZ does not expand and unrealistically flow into the Waste.

4.17.3 "Reset" Material

In this material, conditions will be reset to the initial conditions. This differs from DRZ material in that both saturation and pressure are reset. In contrast, in DRZ material, the saturation is adjusted to maintain a fixed brine volume and the pressure is reset to a specified value, rather than to the initial pressure. These materials allow the simulation of backfilled regions, which are initially excavations, but become backfill. Because the backfilled and sealed regions may cover a large number of grid blocks, these new conditions are most easily provided with the original initial conditions.

4.17.4 Borehole Material

In BRAGFLO, the subroutine RESETMID resets the saturation, pressure, and concentrations in a material at the time of a material change. This routine was designed for the Borehole material at the time of an intrusion but can be used on other materials as well. The input parameters for this subroutine are read in through the input file, in the subroutine READMAT.

In the BRAGFLO main program at the completion of a time step, BRAGFLO checks to see whether the current time is equal to a time (TIMEBORE) at which the saturation, pressure and concentrations are supposed to be reset. If yes, then the subroutine RESETMID is called; RESETMID is called before the material change is made in the subroutine MATERIALS. The subroutine RESETMID then checks each block to determine if its material is a material (MATBORE) to be reset at the current time. If yes, then the pressure is reset to PORESET and the saturation is reset to SORESET. If the flag ICHEM is set equal to one (in the input file) then all concentrations of CPR, iron, iron corrosion products, and MgO products are set equal to zero in that material. Finally, the capillary pressure, relative permeability, gas pressure, and dissolved gas terms are reset based on the new saturation and pressure.

In this material, the solute concentration and solute mass are also reset to zero when an intrusion borehole opens. This simulates the removal of radionuclides in both solid and dissolved phases when a drill cuts through the waste. This occurs only when nuclide transport is activated, but nuclide transport is not qualified for use in WIPP compliance calculations and is not tested.

4.18 Smooth Transition during Material Changes

By default, material changes such as drilling intrusions into the waste area are treated as instantaneous changes in the grid materials. This is equivalent to restarting the code at the time of the material change, but with initial conditions that were equal to the state of the previous material at the time immediately before the material change. Although certain material changes occur over very short time-scales, such as an intrusion, options exist to expand the material changes over some finite time.

BRAGFLO has a subroutine SMOOTHPERM which smoothly changes the permeability, and thus the capillary pressure with time during a material change. In the input file, the user chooses the initial material number (contained in the array MATSP), a final material number (contained in the array MATSPF), a time at which the material change ends (contained in the array TEND), and the time over which the material change occurs (contained within the array TCHANGE). The user also inputs the coefficients a_i of the polynomial used to smooth transitions

$$\ln(k) = \ln(k_i) + \left[\ln(k_f) - \ln(k_i)\right]\sum_{j=0}^{7} a_j \left(\frac{t - t_i}{\Delta t}\right)^j \quad \text{for} \quad t_i \le t \le t_f, \tag{200}$$

where k_i is the initial permeability at time t_i = TEND - TCHANGE, k_f is the final permeability, and Δt = TCHANGE is the time over which the change occurs.

4.19 Gas Dissolution Models

Dissolution of gas in brine can be modeled in BRAGFLO. A bubble point tracking treatment is available but is untested and its use is not recommended. A Henry's law treatment is also available. Additional details and input for these models are described in Section 7.2.9. Gas dissolution will not be included in the WIPP certification compliance calculations.

4.20 Radionuclide Decay and Radiolysis

The total quantity of each radionuclide resulting from radionuclide decay, $M(t)$ [mol], is a function of the radionuclide radioactive decay constant, λ, the initial inventory equally distributed in the waste material, M_o [mol], and the elapsed time, t [sec], for which the amount of decay is determined, where the radionuclide decay constant, λ, is a function of the radionuclide half-life, $T_{1/2}$ [sec], as follows:

$$\lambda = \left(\frac{\ln(2)}{T_{1/2}}\right) \tag{201}$$

$$M(t) = M_o \times e^{-\lambda t} \tag{202}$$

The radionuclide decay implementation in BRAGFLO is obtained in a manner equivalent to that defined in PANEL which allows for up to 4-generations of decay (Sarathi, 2019). BRAGFLO utilizes a closed-form analytical solution of the Bateman equations to determine the decay and ingrowth for radionuclides and their associated daughters.

BRAGFLO has the capability to model the production of hydrogen due to the dissociation of brine via radiolysis. The total radiolytic H_2 generation rate (and brine consumption rate) is due to contributions from one or more decaying radionuclides in the waste area. The amount of each radionuclide contributing to radiolysis is both from the amount of each radionuclide in solution and the remaining amount of each radionuclide in solid form that is wetted by brine. The radionuclide mobilization potential, S_{sol} [mol/m^3], is defined on an elemental basis such that the calculation of the quantity of dissolved and sorbed radionuclide in solution, $M(t)_{sol}$ [mol] is a function of the brine volume (i.e., waste volume, V_{waste} [m^3], the porosity of the waste, ϕ, the brine saturation of the waste, S_w), and the mole fraction of that radionuclide with respect to other radionuclides of the same element, mf, as follows:

$$M(t)_{sol,i} = V_{waste} \times \phi \times S_w \times S_{sol,i} \times mf_i \tag{203}$$

and

$$mf_i = \frac{M(t)_i}{\sum_{j=1}^{n} M(t)_j}, \tag{204}$$

where

i = index of radionuclides in the inventory

j = index of radionuclides of a particular element in the inventory

n = total number of radionuclides of a particular element in the inventory

In cases where the quantity of radionuclide in solution determined in equation (203) is limited by the quantity of radionuclide in the total inventory, the quantity of radionuclide in solution is set equal to the quantity of radionuclide in the total inventory.

The quantity of wetted solid radionuclide, $M(t)_{wet}$ [mol], is the difference between the total inventory and the inventory in solution multiplied by the brine saturation as follows:

$$M(t)_{wet,i} = \left(M(t)_i - M(t)_{sol,i}\right) \times S_w \tag{205}$$

Thus, the hydrogen generation rate, R_{H2} [mol/sec], due to brine radiolysis from radionuclides in solution and due to a fractional contribution from the wetted solid form of the radionuclides is defined as follows:

$$R_{H_2,i} = \left(M(t)_{sol,i} + M(t)_{wet,i} \times P_{dep}\right)\left(\lambda_i \times E_{dis,i} \times G(H_2)_{avg}\right) \tag{206}$$

where

P_{dep} = energy deposition probability for wetted solids (GDEPFAC)

$E_{dis,i}$ = disintegration energy of radionuclide [eV], i
(note that the disintegration energy is specified in units of MeV and BRAGFLO converts from MeV to eV internally)

$G(H_2)_{avg}$ = average "G" value for H_2 [molecule/eV] (GH2AVG)

When radiolysis dissociates brine (water) into H_2 and O_2, the O_2 can be treated (through a stoichiometric coefficient) as an additional contributor by assuming that the O_2 is inert (SRADO2 = 0.5) or ignored (SRADO2 = 0.0) by assuming that the O_2 instantaneously reacts with other materials. See Section 7.2.12 for additional information.

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5.0 USER INTERACTIONS WITH THE SOFTWARE

BRAGFLO Version 7.00 executes on a Solaris platform. To execute BRAGFLO, the program executable name (bragflo) must be in the user's current PATH or referenced by its path name.

BRAGFLO expects a number of command line arguments. The program arguments may either be positional (provided in order) or flagged (preceded by the appropriate flag). Flags always start with "–"; they may be abbreviated. All positional arguments must be listed before any flagged arguments. The only difference between using positional and flagged arguments is that optional arguments may be omitted for flagged arguments. The user should enter "CANCEL" for a positional optional argument that is not provided.

Interactive users may request that the program prompt for any missing command line arguments by appending "?" to the command line.

BRAGFLO expects the following command line arguments (file extensions are examples):

1. –input — The BRAGFLO input control (.inp) file for the sampled vector. This required file is the ASCII input file that controls BRAGFLO; it is generated by PREBRAG, the code immediately upstream from BRAGFLO.
2. –csd — The input file containing the closure surface data (.csd). This optional ASCII file is read by BRAGFLO if creep closure is to be simulated (i.e. CLOSURE = T on Line 10.2 of the input control file). If creep closure is not to be simulated, this file does not need to be provided. The user is responsible for the creation of the .csd file. It is not generated by PREBRAG.
3. –binary — The BRAGFLO binary output (.xbin) file for the sampled vector. This file is the primary results file that is converted by POSTBRAG into standard CAMDAT format. This optional file is only generated if LWBIN = T on Line 1.3 of the input control file.
4. –output — The BRAGFLO ASCII output (.xout) file for the sampled vector. This optional file echoes input and provides user-readable output and QA information. This optional file is only generated if LWASC = T on Line 1.3 of the input control file.
5. –summary — The BRAGFLO summary (.sum) file for the sampled vector. This file contains a limited amount of summary information on results at each time step. This optional file is only generated if LWSUM = T on Line 1.3 of the input control file.
6. –rout — The BRAGFLO restart output (.xrot) file for the sampled vector. Enough information is stored in this binary file to permit restarting BRAGFLO if execution is halted. This optional file is only generated if LWRST = T on Line 1.3 of the input control file.
7. –rin — The BRAGFLO restart input (.xrin) file for the sampled vector. This binary file, a copy of the .xrot file, is read at the beginning of a restart run. This optional file is only read if LRRST = T on Line 1.3 of the input control file.

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6.0 CAPABILITIES AND LIMITATIONS OF THE SOFTWARE FOR THE WIPP APPLICATION

BRAGFLO is the two-phase (brine and gas) finite difference program used to study the fluid flow within the WIPP repository site. The BRAGFLO code is an essential part of the probabilistic modeling necessary for performance assessment of the WIPP site. BRAGFLO Version 7.00 has more capabilities than are necessary for the WIPP PA application. The implementation of BRAGFLO Version 7.00 for the WIPP PA has the following capabilities and limitations:

1. The WIPP PA implementation of BRAGFLO assumes two fluid phases: a liquid phase (brine) and a gas phase (H2) (Section 4.8).
2. In the WIPP PA implementation of BRAGFLO fluid phases are assumed to be immiscible. (Section 4.8).
3. In the WIPP PA implementation of BRAGFLO the liquid phase consists of one component, brine. Dissolution of gas in the brine phase is not considered.
4. In the WIPP PA implementation of BRAGFLO the gas phase consists of one component, H2. Water vapor in the gas phase is not considered. The primary component of the gas generation process is H2 (Section 4.13)
5. The WIPP PA implementation of BRAGFLO has the capability of computing relative permeability and capillary pressure using several different empirical relations. Choice of the characteristic curves is controlled by the user (Section 4.9).
6. The WIPP PA implementation of BRAGFLO allows for coupling to the mechanical system (rock matrix) through the introduction of a variable rock compressibility (Section 4.10).
7. The fracture treatment in the WIPP PA implementation of BRAGFLO allows for pressure induced alterations to the porosity by introducing a pressure-dependent porosity (Section 4.10).
8. In the WIPP PA implementation of BRAGFLO fracture treatment further allows for change in the fracture material permeability (Section 4.10).
9. Representation of the creep closure within the WIPP PA implementation of BRAGFLO is accomplished by a change in the formation porosity. This porosity function or porosity surface will be time dependent and is also driven by pressure. The resulting closure information comes from a geomechanical simulation using the structural mechanics code SANTOS (Section 4.11).
10. The WIPP PA implementation of BRAGFLO corrects gas permeability for the Klinkenberg effect (Section 4.12).
11. Well models in the WIPP PA implementation of BRAGFLO allow simulation of gas or brine injection or production (Section 4.16).
12. Within the WIPP PA implementation of BRAGFLO there are chemical reactions which consume brine and generate gas. The WIPP PA implementation of BRAGFLO accounts

for these reactions by using the Average Stoichiometry Model, which, assumes that all reaction rates are zero order (independent of reactant or product concentration). However, the WIPP PA implementation of BRAGFLO recognizes a different reaction rate if the solid reactant is in contact with liquid brine (inundated condition) or if the solid reacts with brine in the gas phase (humid condition) (Section 4.13).

13. Within the WIPP PA implementation of BRAGFLO there are radiolytic reactions which consume brine and generate gas. The WIPP PA implementation of BRAGFLO accounts for the dissociation of molecules by ionizing radiation due to radioactive decay of up to 5 different radionuclides in the waste. The radioactive decay and ingrowth of radionuclides is evaluated using a close-form solution of the Bateman equations (Section 4.20).
14. The WIPP PA implementation of BRAGFLO assumes that the directions of the permeability tensor are aligned with the reservoir coordinate axis; that is, $\theta = 0$ (Section 4.3).
15. The WIPP PA implementation of BRAGFLO evaluates brine density assuming its fluid compressibility is constant (Section 4.4).
16. The WIPP PA implementation of BRAGFLO uses the Redlich-Kwong-Soave equation of state to relate gas density to pressure (Section 4.4).
17. The WIPP PA implementation of BRAGFLO treats viscosity constant for both water and gas (Section 4.4).
18. The WIPP PA implementation of BRAGFLO assumes a no-flow Neumann type boundary condition at all exterior grid boundaries (Section 4.4).
19. The WIPP PA implementation of BRAGFLO uses a fully implicit formulation to solve the material balance equations (Section 4.5).
20. The WIPP PA implementation of BRAGFLO uses a first order difference quotient approximation for the Jacobian evaluation (Section 4.6).
21. In the WIPP PA implementation of BRAGFLO the user can specify from input directives the frequency of the Jacobian evaluation in the Newton-Raphson iteration (Section 4.6).
22. For both storage and computational considerations, the linear equation solver should take advantage of the banded structure. The WIPP PA implementation of BRAGFLO uses the banded LU solver (Section 4.14).
23. To minimize the bandwidth, the WIPP PA implementation of BRAGFLO orders the grid blocks so that sequential indexing proceeds first in the shortest grid direction, then in the longest grid direction (Section 4.7).
24. The WIPP PA implementation of BRAGFLO is written with double precision word length which produces floating point number representation of 64 bits or approximately 15 significant digits. The only qualified solver is the LU-decomposition (Section 4.14).
25. The WIPP PA implementation of BRAGFLO implements a partial pivoting (row interchanges) which reduces the roundoff errors in the arithmetic and is essential for the numerical stability of Crout's method (Section 4.14).

7.0 DESCRIPTION OF INPUT FILES

BRAGFLO has up to two user specified input files. The first input file is the BRAGFLO input control file (required). This input file is described in detail in Section 7.2. The second input file is the creep closure look-up table data input file (required only if closure is activated). This input file is described in detail in Section 7.4.

7.1 Parameter Statement

BRAGFLO uses one INCLUDE file, params.inc, containing a single PARAMETER statement that sets dimensions on many of the arrays used in BRAGFLO at compile time. (Where the term "PARAMETER statement" is used in this manual, it refers to the statement in params.inc.) An example of the INCLUDE file follows:

```
C
C     NOTE:  Value of MDIM = 3*{NEQ*[MIN(MX*MY,MX*MZ,MY*MZ)+1]-1}+1
C            Value of IBWM = 3*MAX(MX*MY,MX*MZ,MY*MZ)+1
C
      INTEGER
     1   MX          , MY          , MZ          , MG          ,
     2   NEQ         , MGNEQ       , MDIM        , NPHASE      ,
     3   NWTIME      , NW          , NWPERGRID   , MMAT        ,
     4   NPINT       , NCOMP       , MGAS        , MRAD        ,
     5   MRXYZ       , MAXPRNTASC  , MAXPRNTBIN  , MAXPRNTRST
C
      INTEGER
     1   MAXMATTIMES, NWTIMEP     , NDTFIXMAX   , MAXMATTIMP  ,
     2   NDTFIXMAXP , NSDATA      , NTDATA      , MKLOS       ,
     3   MMON        , MWST        , MDRZ        , NVPR        ,
     4   MXHIV       , MVHIV       , IBWM        , MRWXYZ      ,
     5   MWXYZ       , MGVAR       , MSPEC       , NDIRMAX
C
      PARAMETER(MX=140,MY=80,MZ=1,MG=MX*MY*MZ,NEQ=2,MGNEQ=MG*NEQ,
     1          MDIM=244,NPHASE=2,NWTIME=10,NW=50,NWPERGRID=2,MMAT=80,
     2          NPINT=10000,NCOMP=3,MGAS=6,MRAD=5,MRXYZ=MRAD*MG,
     3          MAXPRNTASC=100,MAXPRNTBIN=100,MAXPRNTRST=100,
     4          MAXMATTIMES=20,NWTIMEP=NWTIME+1,NDTFIXMAX=50,
     5          MAXMATTIMP=MAXMATTIMES+1,NDTFIXMAXP=NDTFIXMAX+1,
     6          NSDATA=13,NTDATA=214,MKLOS=4,MMON=9,MWST=2,MDRZ=1,
     7          NVPR=115+(MWST*MRAD),MXHIV=15000,MVHIV=MG,IBWM=8401,
     8          MRWXYZ=MRAD*MWST*MG,MWXYZ=MWST*MG,MGVAR=10,MSPEC=23,
     9          NDIRMAX=204)
```

The parameters that can be changed by the user are listed here. Note that all of these parameters are maximum values. They can be set to be larger than required for the problem being run, but to minimize memory requirements, the smallest values needed to run the problem should be used. No values less than one should be used.

Table 4. Variables used in params.inc

Parameter	Description
MX	Maximum number of grid blocks in the *x*-direction; can be greater than the actual number of grid blocks in the problem to be run.
MY	Maximum number of grid blocks in the *y*-direction; can be greater than the actual number of grid blocks in the problem to be run.
MZ	Maximum number of grid blocks in the *z*-direction; can be greater than the actual number of grid blocks in the problem to be run.
MDIM	Minimum bandwidth of the Jacobian matrix; the value should be calculated using the formula: MDIM = 3* (NEQ* [MIN (MX*MY, MX*MZ, MY*MZ) + 1] -1) +1
NWTIME	Maximum number of times that well properties will be changed.
NW	Maximum number of wells to be specified at any given time.
NWPERGRID	Maximum number of wells in any grid block.
NMAT	Maximum number of materials regions.
MRAD	Maximum number of radionuclides allowed in the transport, decay, and radiolysis calculation.
MAXPRNTASC	Maximum number of times at which an ASCII output dump can be specified.
MAXPRNTBIN	Maximum number of times at which a binary output dump can be specified.
MAXPRNTRST	Maximum number of times at which a restart can be specified.
MAXMATTIMES	Maximum number of times at which a new material map can be specified.
NDTFIXMAX	Maximum number of times that the time step can be fixed.
MMON	Maximum number of monitor grid blocks that can be specified.
MWST	Maximum number of waste regions allowed.
MDRZ	Maximum number of DRZ regions allowed.
MXHIV	Maximum total number of history variables allowed. Includes 10 time- and performance-related history variables; therefore, must be ≥ 10.
MVHIV	Maximum number of history variables per output distribution (*e.g.*, brine pressure or gas saturation).

Parameter	Description
IBWM	Maximum bandwidth for Jacobian used in solution of multi-component gas transport model within BRAGFLO; value to be used is computed from the formula: IBWM = 3 *MAX (MX*MY, MX*MZ, MY*MZ) + 1 If gas transport is not being modeled, IBWM should be set to 1 to save large amounts of storage.
NDIRMAX	Maximum number of grid blocks in which Dirichlet boundary conditions can be specified.

Several parameters are set in the PARAMETER statement that should not or cannot be changed. These are described below so the user will know why they should not be altered, and, if they are inadvertently changed, how they can be reset to their correct values.

Table 5. Constants for params.inc

Parameter	Required Value	Description
NEQ	2	Number of equations being solved in BRAGFLO.
NPHASE	2	Number of immiscible fluid phases.
NPINT	10000	Number of pressure intervals at which gas density is evaluated when using the look-up table to obtain gas density.
NCOMP	3	Number of components in all phases. Includes gas, brine, and gas dissolved brine.
MGAS	6	Number of gases for which equation of state parameters are included in BRAGFLO (H_2, CO_2, CH_4, N_2, O_2, and H_2S).
NSDATA	13	Number of gas-generation-rate entries in creep closure surface data.
NTDATA	214	Number of time entries in creep closure surface data.
MKLOS	4	Number of creep closure surfaces available in BRAGFLO.
MGVAR	10	Number of "global" variables printed out to binary and ASCII output files.
MSPEC	23	Maximum number of species to be used in the reaction path model.

7.2 Input Control File

As is explained in Section 5.0, the input control file for BRAGFLO is created by PREBRAG based on user inputs to PREBRAG. Even though the input control file for BRAGFLO is not technically user-specified, it is still important to understand and is therefore explained in detail in this user's manual.

The input file is composed of several sections, each dealing with different types of input. Within each section, input parameters control specific areas of the simulation. Input generally consists of a line of description or informative comments followed, on the next line, by one or more parameter values. The descriptive line can be any 132 characters. It is intended solely to make the input file easier to read and be understood by the user. None of the information on any of these descriptive lines is used for program control. The content of these lines is entirely at the discretion of the user and will have no effect whatsoever on how the program runs. The line can even be blank, if the user wishes, but there must be a line, informative or blank, and only one line, everywhere that one is indicated. An example input file is provided in Appendix A: Sample BRAGFLO Input Control File.

The order of the input is fixed, *i.e.*, each line of input must appear in exactly the order described in below. Any deviation from this order will cause BRAGFLO to abort or run incorrectly.

Many input values have units associated with them, examples being time and initial pressures. BRAGFLO generally allows input to be in either of two systems of units: SI or English. The choice is up to the user, but one system must be used consistently for all input parameters that have units. The description of each input parameter includes in brackets the units that can be used for that parameter, with the SI units given first and the English units second. If the parameter has no units, none is shown. In a few instances, only SI units are allowed. If no English units are mentioned in the description of the parameter, then English units are not allowed for that particular parameter. Further details concerning units are given in Section 7.2.3.

The input control file consists of the following sections, each dealing with different types of inputs:

1. startup and time control
2. output control parameters
3. mesh description parameters
4. well parameters and boundary conditions
5. initial conditions
6. numerical control parameters
7. material maps and material properties
8. fluid properties
9. chemical reaction parameters
10. creep closure parameters
11. radionuclide transport, radiolysis, and decay parameters (Transport not used or qualified)
12. multi-component gas transport parameters (Not used or qualified).

7.2.1 PREBRAG QA Information

BRAGFLO optionally allows QA information on PREBRAG to be placed into the .CDB file that is created when POSTBRAG processes the BRAGFLO output. This is accomplished by including this information in the BRAGFLO input file created by PREBRAG. If PREBRAG is used to set up the BRAGFLO input file, this information is written automatically to the BRAGFLO input file.

Line 0.1. PREBRAG QA flag.

If PREBRAG QA information is to follow, then the first nonblank characters on this line must be the character string:

```
**QA**
```

Any number of blanks (up to 125) may precede this character string, and the rest of the line (up to 132 characters) can be blank or contain any characters or descriptions that the user wishes to use; but none of the information on this line will be saved and this line serves only as a flag.

If the characters '`**QA**`' are not the first nonblank characters on this line, then it is assumed that PREBRAG QA information does not follow, and this line is assumed to be the title of the run, Line 1.1 (see Section 7.2.2). In this case, no more input from this section can follow, or BRAGFLO will abort.

Line 0.2. Name of program.

The first nonblank characters on this line should be the string:

```
PREBRAG
```

Any number of blanks (up to 125) may precede this character string, and the rest of the line (to a total of 132 characters) can be blank or may contain any characters or descriptions that the user wishes to use, but none of that information will be saved; only the string '`PREBRAG`' will be written to output files.

If the characters '`PREBRAG`' are not the first nonblank characters on this line, then it is assumed that the input in this section is not PREBRAG QA information, and no PREBRAG QA information will be written to the output files. However, it is still necessary to include all of the lines in this section (Lines 0.1 - 0.6). If any of Lines 0.2 - 0.6 is completely blank, BRAGFLO will abort.

If this line does begin with '`PREBRAG`', then the information on the next four lines will be written to the BRAGFLO output files.

Line 0.3. PREBRAG version number.

The first 8 characters starting with the first nonblank character must be the version number of PREBRAG used to set up the input file, *e. g.*, '`6.00`'. If this line is blank, BRAGFLO will abort. Leading blanks and trailing blanks or nonblank characters are permitted, but only the eight characters starting with the first nonblank character will be written to the BRAGFLO output files.

Line 0.4. PREBRAG revision date.

The first 8 characters starting with the first nonblank character must be the revision date of PREBRAG used to set up the input file, *e. g.*, '01/19/96.' If this line is blank, BRAGFLO will abort. Leading blanks and trailing blanks or nonblank characters are permitted, but only the eight characters starting with the first nonblank character will be written to the BRAGFLO output files.

Line 0.5. PREBRAG run date.

The first 8 characters starting with the first nonblank character must be the date on which PREBRAG was run to set up the input file, *e. g.*, '01/25/96'. If this line is blank, BRAGFLO will abort. Leading blanks and trailing blanks or nonblank characters are permitted, but only the eight characters starting with the first nonblank character will be written to the BRAGFLO output files.

Line 0.6. PREBRAG run time.

The first 8 characters starting with the first nonblank character must be the time at which PREBRAG was run to set up the input file, *e. g.*, '11:13:44'. If this line is blank, BRAGFLO will abort. Leading blanks and trailing blanks or nonblank characters are permitted, but only the eight characters starting with the first nonblank character will be written to the BRAGFLO output files.

The first 7 lines of the input file will typically appear as in the following example:

```
**QA**
PREBRAG     -- Program name
8.02  -- PREBRAG version number
11/29/12    -- PREBRAG revision date
11/30/12    -- PREBRAG run date
11:13:44    -- PREBRAG run time
Title of the run (Line 1.1)
```

7.2.2 Startup and Time Control

In this section, parameters that initialize the size of the problem and control the simulation time are input.

Line 1.1. Title of run.

This is a descriptive title for the simulation being run. This title is saved and printed to the output files, but otherwise has no effect on the performance of BRAGFLO.

Line 1.2. Descriptor. Logical flags indicating files to be used.

One-line (up to 132 characters) descriptor for the following parameters:

Line 1.3. LWASC, LWBIN, LWSUM, LWRST, LRRST.

Input each flag in free format as a T, .TRUE., F, or .FALSE., separated by one or more spaces or by commas.

LWASC: Flag indicating whether an ASCII output file is to be written.

LWBIN: Flag indicating whether a binary output file is to be written.

LWSUM: Flag indicating whether an ASCII summary output file is to be written.

LWRST: Flag indicating whether a binary restart output file is to be written.

LRRST: Flag indicating whether a binary restart input file is to be read. If this flag is .TRUE., then a restart input file for this run must exist in the same directory as the input [.inp] file. This file is created by copying a restart output [.xrot] file from an initial run into a [.xrin] file having the same root name as the input file used in the restart run. (Although it is best for traceability reasons for all files used in both initial runs and in restart runs to have the same root name, it is not necessary in order for the restart to run correctly.)

NOTE: Restart capability is not QA'd or used for WIPP Compliance Calculations.

Line 1.4. Descriptor. Model type and grid size parameter.

One-line (up to 132 characters) descriptor for the following parameters:

Line 1.5. MODTYPE, NX,NY,NZ.

MODTYPE: Number of dimensions being used for this run. Although BRAGFLO is a fully three-dimensional code, many shortcuts are taken that speed up execution if the problem being run is only one-dimensional (NY = NZ = 1) or two-dimensional (NZ = 1). MODTYPE is given a value of 1, 2, or 3, depending on whether the problem is 1-, 2-, or 3-dimensional, respectively. If a value less than 1 or greater than 3 is input, the program will abort with the following message printed to the screen:

```
*** MODTYPE Error in READSTARTUP ***
```

The ASCII output file provides additional information:

```
**FATAL ERROR in Input:  MODTYPE = <input value>
**MODTYPE must be 1, 2, or 3.
```

NX: Number of grid blocks in the *x*-direction.

NY: Number of grid blocks in the *y*-direction.

NZ: Number of grid blocks in the *z*-direction. NX, NY, and NZ must be less than or equal to MX, MY, and MZ, respectively, (these are specified in the PARAMETER statement), and they must all be greater than zero. If not, BRAGFLO will abort with the following message printed to the screen:

```
*** Size error in READSTARTUP; invalid NX, NY, or NZ
```

The ASCII output file provides additional information:

```
** FATAL ERROR in Input:          NX,NY,NZ = <input values>
** Maximum values dimensioned:   MX,MY,MZ = <values set in
PARAMETER statement>
** Minimum values allowed:      MX,MY,MZ =      1      1      1
```

BRAGFLO uses a right-handed coordinate system in which the origin is at the front lower left corner of the region being modeled. In this system, the x-direction increases to the right, the y-direction increases into the page, and the z-direction increases upward. Gravity acts in the negative z-direction. The grid can be reoriented (for example, to make the y-direction vertical) with input described in Section 7.2.4 (Mesh Parameters). This will be discussed in more detail in Section 7.2.4.

Line 1.6. Descriptor. Simulation time limits.

One-line (up to 132 characters) descriptor for the following parameters:

Line 1.7. START, FINISH, MAXITF,YRSEC,SECYR.

START: Start time for the simulation [s or days]. START can be negative; if so, certain special material properties can be changed at time zero. More details can be found in Section 7.2.8 (Material Properties).

FINISH: End time for the simulation [s or days].

MAXITF: Maximum number of time steps allowed in this run. This is the only means for limiting how long the simulation will run. WIPP Performance Assessment simulations typically require about 1000 time steps to complete a 10,000-yr simulation, depending on convergence criteria selected (Section 7.2.7). On a few occasions, more than 10,000 steps have been required. A value of MAXITF = 10000 is normally used; if more steps are required, the run can be restarted from where it ended at the 10000th step, because a restart record is always written at the end of a run, provided that LWANS = .TRUE. In a restart run that is to continue from the MAXITFth step, the new input file must have a value for MAXITF that is greater than the MAXITF in the original input file.

YRSEC: Year-to-seconds conversion factor (optional, default = 3.15569259747E7).

SECYR: Seconds-to-year conversion factor (optional, default = 1/YRSEC).

Line 1.8. Descriptor. Time step controls.

One-line (up to 132 characters) descriptor for the following parameters:

Line 1.9. DELT, DELTMIN, DELTMAX, DTIMEMAX, ITIMECNTRL, TSWITCH.

DELT: Initial time step [s or days]. Recommended value: 864. s (1/10 day).

DELTMIN: Minimum time step allowed [s or days]. Recommended value: 864. s (1/10 day).

DELTMAX: Maximum time step allowed [s or days]. Recommended value: 1.728×10^9 s (20,000 days or about 55 yr.).

DTIMEMAX: Maximum fractional increase in time step that will be allowed when auto time step control is used [dimensionless]. A value of 1.0 would, in effect, turn off auto time step control. No check is made to ensure that a value greater than 1.0 is used. A value too close to 1.0, *e.g.*, 1.1, is generally inefficient, not taking full advantage of the tendency for pressures and flows eventually to equilibrate and thereby allow larger time steps. A value that is too large, greater than 2.0, is also inefficient because the solution will fail to converge much more frequently, resulting in wasted calculations as the time step size must be reduced and the time step repeated. The value used for DELTFACTOR (Section 7.2.7, Line 6.24) should be taken into consideration in selecting a value for DTIMEMAX. Recommended value: 1.5.

ITIMECNTRL: Flag for automatic time step control . Recommended value: 1.

= 0: A fixed time step of DELT will be used throughout the simulation.

= 1: Auto time step control will be used. Variable changes vary greatly throughout a typical simulation. Auto time step control allows large time steps to be taken when little is happening but forces small steps to be used when rapid changes are occurring.

TSWITCH: Value of gas saturation that determines when to switch from relative to absolute change in gas saturation for calculating time step size when auto time step control is used (ITIMECNTRL=1). When the current value of gas saturation is greater than TSWITCH, the time step algorithm uses the relative change in saturation over the previous time step; otherwise, it uses the absolute change in gas saturation. Valid range of input value: 0 - 1. Recommended value: 0.01. In some instances, BRAGFLO will run faster when TSWITCH is turned off by using an input value of TSWITCH = 1.

Line 1.10. Descriptor. Time step changes.

One-line (up to 132 characters) descriptor for the following parameters:

Line 1.11. NDTFIX.

NDTFIX: Number of times at which the time step will be reset to a specified value, overriding the time step computed by the auto time step control. This feature allows computing time to be saved when major changes in material properties at some point in simulation time are likely to cause the auto time step control to cut back the time step repeatedly. By reducing the time step manually, fewer unsuccessful calculations will be performed. If the auto time step control is not being used (ITIMECNTRL = 0), this capability is not used, but some value must still be input for NDTFIX; a value of 0 is recommended. If NDTFIX < 0, BRAGFLO will behave as though NDTFIX = 0. If NDTFIX > NDTFIXMAX (set in params.inc), the run will abort with a message printed to the screen:

```
*** ERROR in READSTARTUP:  NDTFIXMAX needs to be larger;
     NDTFIX = <input value>
*** NDTFIX error in READSTARTUP ***
```

The next line (1.12) is repeated NDTFIX times, each line with two numbers. If NDTFIX = 0, no lines are input for these two parameters. If ITIMECNTRL = 0 (*i.e.*, no auto time step control), but NDTFIX > 0, then NDTFIX lines of TIMEDTFIX and DTFIX must still be input, even though they will not be used.

Line 1.12. TIMEDTFIX(K), DTFIX(K).

TIMEDTFIX: Simulation time at which the time step will be reset [s or days].

DTFIX: New time step size to be used in the first time step after TIMEDTFIX is exceeded [s or days].

7.2.3 Output Control Parameters

This section describes input that controls output to the three output files: ASCII, binary, and restart files.

Line 2.1. Descriptor. Output interval specification; units used in input and output.

One-line (up to 132 characters) descriptor for the following parameters:

Line 2.2. IPRTYPEASC, IPRTYPEBIN, IPRTYPERST, UNITSI, UNITSO.

IPRTYPEASC: ASCII output control option.

IPRTYPEBIN: Binary output control option.

IPRTYPERST: Restart output control option.

Three options are available. Additional input is required for each option, and the type of additional input for each option differs.

= 0: Output at first, last, and fixed frequency of time steps.

= 1: Output at first and last time step and at fixed time intervals.

= 2: Output at specified times.

Printing at a fixed frequency of time steps (option 0) offers the advantage of more frequent output over a given time span when rapid changes are occurring and less output when changes are slower. This results when auto time step control is in effect, and the time step is small when changes are rapid and large when changes are small. This option is generally used only for output to the binary output file. Specifying output at selected times (option 2) or at fixed time intervals (option 1) is useful when comparisons of different runs will be made. These two options are usually used for the ASCII and restart output, where less frequent output is desired. The binary output file is intended to be the primary repository for results because more data can be stored more compactly than in the ASCII output. An important output feature in BRAGFLO is that whenever any results are printed to the ASCII file or to the restart file, they are also

printed at the same time to the binary output file. Thus, the binary file contains the complete record of all results that have been printed to any output file.

UNITSI: Units used in the input (CHARACTER*8 variable). Options are: 'SI' or 'ENGLISH'. Recommended: 'SI'. The input is read in free format, so the input character string must be enclosed in tick marks.

UNITSO: Units used in the output (CHARACTER*8 variable). Options are: 'SI' or 'ENGLISH'. Recommended: 'SI'. The input character string must be enclosed in tick marks.

The same system of units must be used consistently throughout the input. Only the units listed in Table 6 can be used in the input.

Subsequent input for output control depends on the input value selected for IPRTYPEASC, IPRTYPEBIN, and IPRTYPERST. ASCII output is dealt with first.

Table 6. Conversion factors.

Quantity	SI units	English units	Conversion Factor (multiply by value in English units to obtain value in SI units)
Length	m	ft	0.3048
Mass	kg	lb	0.4535237
Time	s	day	86400
Temperature	K	°R	5/9
Amount of substance	gm-mol (mol)	lbmol	$2.2049564333683113 \times 10^{-3}$
Area	m^2	ft^2	0.09290304
Volume	m^3	ft^3	0.028316846592
Pressure	Pa	psi	6894.757293168362
Mass flow rate	kg/s	lb/day	$5.2499116898148148 \times 10^{-6}$
Concentration rate change	$kg/(s \cdot m^3)$	$lb/(day \cdot ft^3)$	0.018539888164305717
Density or concentration	kg/m^3	lb/ft^3	16.01846337396014
Velocity	m/s	ft/day	$3.527777777777778 \times 10^{-6}$
Volumetric rate	m^3/s	ft^3/day	3.2774128×10^{-7}
Viscosity	Pa·s	cP	0.001
Productivity index	m^3	bbl · cP/ (day · psi)	$2.6688839796530887 \times 10^{-13}$
Slope of solution gas-brine ratio *vs.* pressure	Pa^{-1}	$ft^3/(bbl \cdot psi)$	$2.5832324345269173 \times 10^{-5}$
Slope of viscosity *vs.* pressure	s	cP/psi	$1.4503773773020921 \times 10^{-7}$
Permeability	m^2	darcy	$9.8692326671601282 \times 10^{-13}$

7.2.3.1 ASCII Output Controls.

Line 2.3. Descriptor. ASCII output time or frequency control parameters.

One-line (up to 132 characters) descriptor for the following parameters:

Line 2.4. IPRNTASC.

If IPRTYPEASC (Line 2.2) = 0 (output at fixed time step frequency):

IPRNTASC: ASCII output time step frequency.

Line 2.4. TMEINTASC, SPTMEASC, FPTMEASC.

If IPRTYPEASC (Line 2.2) = 1 (output at fixed time interval):

TMEINTASC: Time interval [s or days]

SPTMEASC: Starting output time [s or days]

FPTMEASC: Final output time [s or days]

Line 2.4. NPTMEASC.

If IPRTYPEASC (Line 2.2) = 2 (output at specified times):

NPTMEASC: Number of specified times.

Line 2.4.1: Descriptor. User requested printout times.

One-line (up to 132 characters) descriptor for the following parameters:

Line 2.4.2: TIMESASC (NPTMEASC values).

TIMESASC: Specified output times [s or days]

7.2.3.2 Binary output controls.

Line 2.5. Descriptor. Binary output time or frequency control parameters.

One-line (up to 132 characters) descriptor for the following parameters:

Line 2.6. IPRNTBIN.

If IPRTYPEBIN (Line 2.2) = 0 (output at fixed time step frequency):

IPRNTBIN: Binary output time step frequency.

Line 2.6. TMEINTBIN, SPTMEBIN, FPTMEBIN.

If IPRTYPEBIN (line 2.2) = 1 (output at fixed time intervals):

TMEINTBIN: Binary output time interval [s or days].

SPTMEBIN: Starting time for binary output [s or days].

FPTMEBIN: Final output time for binary output [s or days].

Line 2.6. NPTMEBIN.

If IPRTYPEBIN (Line 2.2) = 2 (output at specified times):

NPTMEBIN: Number of output times specified.

Line 2.6.1. Descriptor. Output times.

One-line (up to 132 characters) descriptor for the following parameters:

Line 2.6.2. TIMESBIN (NPTMEBIN values).

TIMESBIN: Specified binary output times [s or days]

7.2.3.3 Restart Output Controls.

The restart capability in BRAGFLO enables a run to be restarted from the point where the restart output is written. This feature is useful when debugging a case that is known to run into problems after much computing time has elapsed. It is also useful when conditions are changed part way through a base case; then, the base case can be run all the way to completion, with restarts written at specified times, and sub-cases can then be run starting from the restarts, rather than starting from the beginning, thereby saving much computing time. The restart file contains only enough information to enable BRAGFLO to resume from where the restart was written, including values of the dependent variables, certain cumulative variables, and current settings for flags that get changed over the course of a run. A regular input file is still needed to provide all the information normally obtained from an input file. The restart capability is discussed in detail in Section 7.3.

NOTE: Restart capability is not QA'd or used for WIPP Compliance Calculations.

Line 2.7. Descriptor. Restart output time or frequency control parameters.

One-line (up to 132 characters) descriptor for the following parameters:

Line 2.8. IPRNTRST.

If IPRTYPERST (Line 2.2) = 0 (restart output at fixed time step frequency):

IPRNTRST: Restart output time step frequency.

Line 2.8. TMEINTRST, SPTMERST, FPTMERST.

If IPRTYPERST (Line 2.2) = 1 (restart output at fixed time intervals):

TMEINTRST: Restart output time interval [s or days]

SPTMERST: Starting time for restart output [s or days]

FPTMERST: Final time for restart output [s or days]

Line 2.8. NPTMERST.

If IPRTYPERST (Line 2.2) = 2 (restart output at specified times):

NPTMERST: Number of times to specify restart output.

Line 2.8.1. Descriptor. Restart output times.

One-line (up to 132 characters) descriptor for the following parameters:

Line 2.8.2. TIMESRST (NPTMERST values).

TIMESRST: Specified restart output times [s or days].

7.2.3.4 Element Variables.

The next inputs are the ASCII and binary print control flags. These flags indicate which of at least 115 element variables are printed to the output files. Element variables are defined as any variable that has a time-varying value at each grid block. These are listed in Table 7. The number of element variables available to be printed out depends on the maximum number of waste regions (defined in Section 7.2.8) and the maximum number (if any) of radionuclides being tracked in the radiolysis and radionuclide decay calculations. There are 115 element variables that are always available. Of these 115 variables, 45 (numbers 69-113) are associated with the reaction-path gas-generation model, which has been partially implemented but is not available for use in the current version of BRAGFLO. Any of the reaction path model variables can be printed out, but their values are all zero. The total number available is NVPR = 115 + MWST × MRAD, where MWST is the number of waste regions, and MRAD is the number of radionuclides involved in radiolysis and decay. With MWST = 2 and MRAD = 5 in the current version of BRAGFLO, 10 additional isotope amount element variables are available for output.

Line 2.9. Descriptor. ASCII print flags.

One-line (up to 132 characters) descriptor for the following parameters:

Line 2.10. NPRNTA (NVPR values).

NPRNTA: Flag to indicate output of element variables to the ASCII output file.

= 0: Do *not* print this element variable to the ASCII output file.

= 1: *Do* print this element variable to the ASCII output file.

Line 2.11. Descriptor. Binary print flags.

One-line (up to 132 characters) descriptor for the following parameters (cannot be blank):

Line 2.12. NPRNTB (NVPR values).

NPRNTB: Flag to indicate output of element variables to the binary output file.

= 0: Do *not* print this element variable to the binary output file.

= 1: *Do* print this element variable to the binary output file.

Table 7. Element variables available for printout in BRAGFLO.

No.[2]	CAMCON Element Variable Name	Description	SI Unit
1	PRESBRIN	Brine pressure	Pa
2	PRESGAS	Gas pressure	Pa
3	POTO	Brine density × g × potentiometric head	Pa
4	POTG	Gas density × g × potentiometric head	Pa
5	PBUB	Brine bubble pressure	Pa
6	POROS	Porosity	m^3 void/m^3 rock
7	RELPERMB	Relative permeability to brine	dimensionless
8	RELPERMG	Relative permeability to gas	dimensionless
9	DENBRINE	Brine density	kg/m^3
10	DENGAS	Gas density	kg/m^3
11	PERMBRX	Permeability to brine, x-direction	m^2
12	PERMBRY	Permeability to brine, y-direction	m^2
13	PERMBRZ	Permeability to brine, z-direction	m^2
14	PERMGASX	Permeability to gas, x-direction	m^2
15	PERMGASY	Permeability to gas, y-direction	m^2
16	PERMGASZ	Permeability to gas, z-direction	m^2
17	SATBRINE	Brine saturation	fraction void volume
18	SATGAS	Gas saturation	fraction void volume
19	CBRBR	Brine component of brine phase	mass frac brine phase
20	CGASBR	Gas component of brine phase	mass frac brine phase
21	WELLBRIN	Time-averaged well brine flow rate	m^3/s (@ ref. conds)
22	WELLGAS	Time-averaged well gas flow rate	m^3/s (@ ref. conds)
23	CWELLBR	Cumulative well brine flow	m^3/s (@ ref. conds)
24	CWELLGAS	Cumulative well gas flow	m^3/s (@ ref. conds)
25	VELDBRX	Time-avg. brine Darcy velocity, x-direction	m/s
26	VELDBRY	Time-avg. brine Darcy velocity, y-direction	m/s
27	VELDBRZ	Time-avg. brine Darcy velocity, z-direction	m/s
28	VELDGASX	Time-avg. gas Darcy velocity, x-direction	m/s
29	VELDGASY	Time-avg. gas Darcy velocity, y-direction	m/s
30	VELDGASZ	Time-avg. gas Darcy velocity, z-direction	m/s

No.[2]	CAMCON Element Variable Name	Description	SI Unit
31	FLOWBRX	Time-avg. inter-block brine flow, *x*-direction	m^3/s (@ ref. conds)
32	FLOWBRY	Time-avg. inter-block brine flow, *y*-direction	m^3/s (@ ref. conds)
33	FLOWBRZ	Time-avg. inter-block brine flow, *z*-direction	m^3/s (@ ref. conds)
34	FLOWGASX	Time-avg. inter-block gas flow, *x*-direction	m^3/s (@ ref. conds)
35	FLOWGASY	Time-avg. inter-block gas flow, *y*-direction	m^3/s (@ ref. conds)
36	FLOWGASZ	Time-avg. inter-block gas flow, *z*-direction	m^3/s (@ ref. conds)
37	MASSBALB	Relative Brine mass balance	dimensionless
38	MASSBALG	Relative Gas mass balance	dimensionless
39	CORRATI	Inundated corrosion rate–simple model	gm-mol/s
40	CORRATH	Humid corrosion rate–simple model	gm-mol/s
41	BIORATI	Inundated biodegradation rate–simple model	gm-mol/s
42	BIORATH	Humid biodegradation rate–simple model	gm-mol/s
43	FEOH2_SR	$Fe(OH)_2$ sulfidation rate-simple model	gm-mol/s
44	FE_SR	Fe sulfidation rate-simple model	gm-mol/s
45	MGO_HR	MgO hydration rate-simple model	gm-mol/s
46	MGOH2_CR	$Mg(OH)_2$ carbonation rate-simple model	gm-mol/s
47	MGO_CR	MgO carbonation rate-simple model	gm-mol/s
48	HYMAG_CR	Hydromagnesite conversion rate-simple model	gm-mol/s
49	H2RATE	H_2 generation rate–simple model	$kg/(s \cdot m^3)$
50	BRINRATE	Brine consumption rate–simple model	$kg/(s \cdot m^3)$
51	FERATE	Fe consumption rate–simple model	$kg/(s \cdot m^3)$
52	CELLRATE	Biodegrad consumption rate–simple model	$kg/(s \cdot m^3)$
53	FEOH2R	$Fe(OH)_2$ generation rate–simple model	$kg/(s \cdot m^3)$
54	FESR	FeS generation rate–simple model	$kg/(s \cdot m^3)$
55	MGOR	MgO generation rate–simple model	$kg/(s \cdot m^3)$
56	MGOH2R	$Mg(OH)_2$ generation rate–simple model	$kg/(s \cdot m^3)$
57	HYMAGR	Hydromagnesite generation rate-simple model	$kg/(s \cdot m^3)$
58	MGCO3R	$MgCO_3$ generation rate–simple model	$kg/(s \cdot m^3)$
59	FECONC	Fe concentration–simple model	kg/m^3
60	CELLCONC	Biodegradables concentration–simple model	kg/m^3

No.[2]	CAMCON Element Variable Name	Description	SI Unit
61	FEOH2C	$Fe(OH)_2$ concentration–simple model	kg/m^3
62	FESC	FeS concentration–simple model	kg/m^3
63	MGOC	MgO concentration–simple model	kg/m^3
64	MGOH2C	$Mg(OH)_2$ concentration–simple model	kg/m^3
65	HYMAGC	Hydromagnesite concentration-simple model	kg/m^3
66	MGCO3C	$MgCO_3$ concentration–simple model	kg/m^3
67	SALTC	Salt concentration–simple model	kg/m^3
68	PORSOLID	Volume fraction of generated solids	dimensionless
69	H2_R[1]	H_2 generation rate–reaction path model	$kg/(s \cdot m^3)$
70	CO2_R[1]	CO_2 generation rate–reaction path model	$kg/(s \cdot m^3)$
71	CH4_R[1]	CH_4 generation rate–reaction path model	$kg/(s \cdot m^3)$
72	N2_R[1]	N_2 generation rate–reaction path model	$kg/(s \cdot m^3)$
73	H2S_R[1]	H_2S generation rate–reaction path model	$kg/(s \cdot m^3)$
74	O2_R[1]	O_2 generation rate–reaction path model	$kg/(s \cdot m^3)$
75	H2O_R[1]	H_2O generation rate–reaction path model	$kg/(s \cdot m^3)$
76	H2SO4_R[1]	H_2SO_4 generation rate–reaction path model	$kg/(s \cdot m^3)$
77	HNO3_R[1]	HNO_3 generation rate–reaction path model	$kg/(s \cdot m^3)$
78	CELL_R[1]	Biodegrad consumption rate–reaction path model	$kg/(s \cdot m^3)$
79	FE_R[1]	Fe generation rate–reaction path model	$kg/(s \cdot m^3)$
80	FES2F_R[1]	FeS_2 generation rate–reaction path model	$kg/(s \cdot m^3)$
81	FES20_R[1]	FeS_2 generation rate–reaction path model	$kg/(s \cdot m^3)$
82	FECO3F_R[1]	$FeCO_3$ generation rate–reaction path model	$kg/(s \cdot m^3)$
83	FECO3O_R[1]	$FeCO_3$ generation rate–reaction path model	$kg/(s \cdot m^3)$
84	FEOH2_R[1]	$Fe(OH)_2$ generation rate–reaction path model	$kg/(s \cdot m^3)$
85	FEOOH_R[1]	FeO(OH) generation rate–reaction path model	$kg/(s \cdot m^3)$
86	FE304_R[1]	Fe_3O_4 generation rate–reaction path model	$kg/(s \cdot m^3)$
87	FES_R[1]	FeS generation rate–reaction path model	$kg/(s \cdot m^3)$
88	CAO_R[1]	CaO generation rate–reaction path model	$kg/(s \cdot m^3)$
89	CAOH2_R[1]	$Ca(OH)_2$ generation rate–reaction path model	$kg/(s \cdot m^3)$
90	CACO3_R[1]	$CaCO_3$ generation rate–reaction path model	$kg/(s \cdot m^3)$

No.[2]	CAMCON Element Variable Name	Description	SI Unit
91	H2_RAD_R	H_2 generation rate–radiolysis	kg/(s·m^3)
92	H2_C[1]	H_2 concentration–reaction path model	kg/(s·m^3)
93	CO2_C[1]	CO_2 concentration–reaction path model	kg/m^3
94	CH4_C[1]	CH_4 concentration–reaction path model	kg/m^3
95	N2_C[1]	N_2 concentration–reaction path model	kg/m^3
96	H2S_C[1]	H_2S concentration–reaction path model	kg/m^3
97	O2_C[1]	O_2 concentration–reaction path model	kg/m^3
98	H2O_C[1]	H_2O concentration–reaction path model	kg/m^3
99	H2SO4_C[1]	H_2SO_4 concentration–reaction path model	kg/m^3
100	HNO3_C[1]	HNO_3 concentration–reaction path model	kg/m^3
101	CELL_C[1]	Biodegradables concentration–reaction path model	kg/m^3
102	FE_C[1]	Fe concentration–reaction path model	kg/m^3
103	FES2F_C[1]	FeS_2 concentration–reaction path model	kg/m^3
104	FES2O_C[1]	FeS_2 concentration–reaction path model	kg/m^3
105	FECO3F_C[1]	$FeCO_3$ concentration–reaction path model	kg/m^3
106	FECO3O_C[1]	$FeCO_3$ concentration–reaction path model	kg/m^3
107	FEOH2_C[1]	$Fe(OH)_2$ concentration–reaction path model	kg/m^3
108	FE3O4_C[1]	Fe_3O_4 concentration–reaction path model	kg/m^3
109	FES_C[1]	FeS concentration–reaction path model	kg/m^3
110	FEOOH_C[1]	FeO(OH) concentration–reaction path model	kg/m^3
111	CAO_C[1]	CaO concentration–reaction path model	kg/m^3
112	CAOH2_C[1]	$Ca(OH)_2$ concentration–reaction path model	kg/m^3
113	CACO3_C[1]	$CaCO_3$ concentration–reaction path model	kg/m^3
114	H2_RAD_C	H_2 concentration–radiolysis	kg/m^3
115	H2OFLOWI[1]	Water inflow rate	kg/s
116	SM1AM241[2]	Amount of isotope 1 from Waste Region 1	gm-mol
117	SM2AM241[2]	Amount of isotope 1 from Waste Region 2	gm-mol
118	SM1PU238[2]	Amount of isotope 2 from Waste Region 1	gm-mol
119	SM2PU238[2]	Amount of isotope 2 from Waste Region 2	gm-mol
120	SM1PU239[2]	Amount of isotope 3 from Waste Region 1	gm-mol
121	SM2PU239[2]	Amount of isotope 3 from Waste Region 2	gm-mol

No.[2]	CAMCON Element Variable Name	Description	SI Unit
122	SM1PU240[2]	Amount of isotope 4 from Waste Region 1	gm-mol
123	SM2PU240[2]	Amount of isotope 4 from Waste Region 2	gm-mol
124	SM1PU242[2]	Amount of isotope 5 from Waste Region 1	gm-mol
125	SM2PU242[2]	Amount of isotope 5 from Waste Region 2	gm-mol

1) Not Used or QA'd for WIPP compliance calculations.

2) Variables 1 - 115 are, by default, available in any run. Variables 116 and greater depend on the values of MWST and MRAD. This list is for MWST = 2, MRAD = 5 (using the following radionuclides to produce the example CAMCON element variable names: Am241, Pu238, Pu239, Pu240, Pu242), which results in a total of NVPR = 115 + MWST × MRAD = 125 element variables.

7.2.3.5 History Variables.

For purposes of the BRAGFLO input, a history variable is defined as any variable listed in Table 7, at a specified grid block location. History variables are printed at every time step, unlike the rest of the ASCII and binary printout, which is generally not printed at every time step, but rather at multiple time steps or at intervals specified in the input, as described above. History variables are printed only to the binary output file, never to the ASCII output file. The purpose for history variables is to allow accurate post-processing. For example, integration of brine flow past some boundary can be done in post-processing to give cumulative flows that are as accurate as if they were computed internally to BRAGFLO. Earlier versions of BRAGFLO performed some of this integration, but, without extremely complex input, it was not possible to keep the code general and not specific to a particular mesh. Without history variables, post-processing can only be done using the element variables, which are usually output at multi-step intervals. Then, variables that change rapidly over a short period of time cannot be integrated accurately.

Line 2.13. Descriptor. History variables.

One-line (up to 132 characters) descriptor for the following parameters (cannot be blank):

Line 2.14. NHIV.

NHIV: Total number of element variables (from the list in Table 7) that will be printed as history variables. This is the number of sets of variables to be read from input.

= 0: no history variables will be printed out, and no more history variable input will be read from input.

> 0: then read NHIV sets of lines 2.15 and 2.16.

Line 2.15. LH, NGBHIV, Text Label (i.e. NAME=BRINE PRESUURE).

LH: Element variable number from Table 7.

NGBHIV: Number of grid blocks to be printed as history variables for variable number LH.

Line 2.16. IIHIV, JJHIV, KKHIV (NGBHIV sets).

IIHIV: I-index for grid block location for the history variable.

JJHIV: J-index for grid block location for the history variable.

KKHIV: K-index for grid block location for the history variable.

7.2.3.6 Monitor Blocks.

BRAGFLO prints out certain summary data to the screen and to the .sum file at each time step to provide the user with continuous information on the how the run is progressing. This summary includes two lines showing simulation time along with time step and global mass balance information (described more fully in Section 9.3). In addition, the summary allows the user to monitor values of certain element variables at specified grid blocks. These monitor blocks are intended solely to monitor progress, rather than to provide data for post-processing or other later use, so only a few grid blocks should be selected where significant changes are likely to occur or where the behavior is representative of an entire region. Typically, one to three monitor blocks are selected. Because this information is printed both to the screen (or to a .xlog file if run in batch) and to the .sum file at every time step, the amount of information printed out can become large in a long run if too many monitor blocks are selected. The maximum number of blocks allowed is MMON, which is set in the PARAMETER statement.

Line 2.17. Descriptor. Monitor block parameters.

One-line (up to 132 characters) descriptor for the following parameters:

Line 2.18. MONITOR.

MONITOR: LOGICAL Flag for monitoring key parameters at a specified grid block.

= F: no monitor blocks will be printed out, and no more monitor block input will be read.

= T: read lines 2.19, 2.20, and 2.21 and then line 2.22 (NMON times)

Line 2.19. Descriptor. Number of monitor blocks.

One-line (up to 132 characters) descriptor for the following parameters:

Line 2.20. NMON.

NMON: Number of monitor blocks to be specified. NMON should be less than 100, because the monitor block number printout is formatted I2. If NMON > MMON (where MMON is set in the PARAMETER statement), BRAGFLO will abort with a message is printed to the screen:

```
*** ERROR:  Too many Monitor Blocks in Input:
    Specified: NMON = <NMON input value>
    Maximum:   MMON = <MMON value set in PARAMETER
statement>
*** Monitor error in READPRTYPE ***
```

Line 2.21. Descriptor. Monitor block locations.

One-line (up to 132 characters) descriptor for the following parameters:

Line 2.22. IMONITOR, JMONITOR, KMONITOR

IMONITOR: I-index of grid block to be monitored.

JMONITOR: J-index of grid block to be monitored.

KMONITOR: K-index of grid block to be monitored.

7.2.4 Mesh Description Parameters

BRAGFLO provides several options for inputting the mesh. With these options, a simple mesh can be easily set up with very little input, yet very complex meshes can still be specified, with correspondingly more detailed input. BRAGFLO uses a rectilinear grid; defining the mesh requires specifying the Δx (DXGRID), Δy (DYGRID), and Δz (DZGRID), and the elevation (DEPTH) for each grid block. How much of this information has to be input depends on which input option is selected.

Line 3.1. Descriptor. Grid data flags.

One-line (up to 132 characters) descriptor for the following parameters:

Line 3.2. IDXFLAG, IDYFLAG, IDZFLAG, IDEPTHFLAG.

IDXFLAG: Specifies how grid block width Δx (DXGRID) is to be read.

= 0: DXGRID does not vary; input one value of DXGRID.

= 1: DXGRID varies in I-direction; input NX values of DXGRID.

IDYFLAG: Specifies how grid block width Δy (DYGRID) is to be read.

= 0: DYGRID does not vary; input one value of DYGRID.

= 1: DYGRID varies in I-direction; input NX values of DYGRID.

= 2: DYGRID varies in J-direction; input NY values of DYGRID.

IDZFLAG: Specifies how grid block width Δz (DZGRID) is to be read.

= 0: DZGRID does not vary; input one value of DZGRID.

= 1: DZGRID varies in I-direction; input NX values of DZGRID.

= 2: DZGRID varies in J-direction; input NY values of DZGRID.

= 3: DZGRID varies in K-direction; input NZ values of DZGRID.

= 4: DZGRID varies in I- and J-directions; input NX x NY values of DZGRID.

IDEPTHFLAG: Specifies how grid block elevations (DEPTH) are to be read.

= 0: Elevation does not vary; input one value of DEPTH.

= 1: Elevation varies in I-direction; input NX values of DEPTH.

= 2: Elevation varies in J-direction; input NY values of DEPTH.

= 3: Elevation varies in K-direction; input NZ values of DEPTH.

= 4: Elevation varies in I- and J-directions; input NX x NY values of DEPTH.

= 5: Elevation varies in I- and K-directions; input NX x NZ values of DEPTH.

= 6: Elevation varies in J- and K-directions; input NY x NZ values of DEPTH.

= 7: Elevation varies in I-, J-, and K-directions; input NX x NY x NZ values of DEPTH.

= -1: Elevation varies in I-direction; have BRAGFLO calculate values of DEPTH.

= -2: Elevation varies in J-direction; have BRAGFLO calculate values of DEPTH.

= -3: Elevation varies in K-direction; have BRAGFLO calculate values of DEPTH.

= -4: Elevation varies in I- and J-directions; have BRAGFLO calculate values of DEPTH.

= -5: Elevation varies in I- and K-directions; have BRAGFLO calculate values of DEPTH.

= -6: Elevation varies in J- and K-directions; have BRAGFLO calculate values of DEPTH.

= -7: Elevation varies in I-, J-, and K-directions; have BRAGFLO calculate values of DEPTH.

If the input value for any of these flags is outside the range listed above, BRAGFLO will abort, with messages printed to the screen indicating what the problems are. The final messages printed are:

```
Number of FATAL errors in READMESH = <number of errors>
*** FATAL geometry input errors in READMESH ***
```

Subsequent input depends on the values of the geometry flags. There are four sets of input, one each for inputting DXGRID, DYGRID, DZGRID, and DEPTH.

7.2.4.1 DXGRID input

Line 3.3. Descriptor. DXGRID input.

One-line (up to 132 characters) descriptor for the following parameters:

Line 3.4. DXCONST.

If IDXFLAG (Line 3.2) = 0:

DXCONST: Uniform grid block Δx-dimension [m or ft].

Line 3.4. (DXGRID(I,1,1), I=1, NX).

If IDXFLAG (Line 3.2) = 1:

DXGRID(I,1,1): Grid block Δx-dimensions, varying in the I-direction [m or ft].

BRAGFLO does not allow DXGRID to vary in the J- or K-directions; thus, only values for DXGRID in the I-direction need (and can) be input.

7.2.4.2 DYGRID input

Line 3.5. Descriptor. DYGRID input.

One-line (up to 132 characters) descriptor for the following parameters:

Line 3.6. DYCONST.

If IDYFLAG (Line 3.2) = 0:

DYCONST: Uniform grid block Δy-dimension [m or ft].

Line 3.6. (DYGRIDI(I), I=1, NX).

If IDYFLAG (Line 3.2) = 1:

DYGRIDI(I): Grid block Δy-dimensions, varying only in the I-direction [m or ft].

Line 3.6. (DYGRIDJ(J), J=1, NY).

If IDYFLAG (Line 3.2) = 2:

DYGRIDJ(J): Grid block Δy-dimensions, varying only in the J-direction [m or ft].

BRAGFLO does not allow Δy to vary in the K-direction, nor in the I- and J-directions simultaneously.

7.2.4.3 DZGRID input.

Line 3.7. Descriptor. DZGRID input.

One-line (up to 132 characters) descriptor for the following parameters:

Line 3.8. DZCONST.

If IDZFLAG (Line 3.2) = 0:

DZCONST: Uniform grid block Δz dimensions [m or ft].

Line 3.8. (DZGRIDI(I), I=1, NX).

If IDZFLAG (Line 3.2) = 1:

DZGRIDI(I): Grid block Δz-dimensions, varying only in the I-direction [m or ft].

Line 3.8. (DZGRIDJ(J), J=1, NY).

If IDZFLAG (Line 3.2) = 2:

DZGRIDJ(J): Grid block Δz-dimensions, varying only in the J-direction [m or ft].

Line 3.8. (DZGRIDK(K), K=1, NZ).

If IDZFLAG (Line 3.2) = 3:

DZGRIDK(K): Grid block Δz-dimensions, varying only in the K-direction [m or ft].

Line 3.8. ((DZGRIDIJ(I,J), I=1, NX), J=1, NY).

If IDZFLAG (Line 3.2) = 4:

DZGRIDIJ(I,J): Grid block dimensions, varying in both I- and J-directions [m or ft].

BRAGFLO does not allow DZGRID to vary simultaneously in all three directions.

7.2.4.4 IDEPTHFLAG input

Line 3.9. Descriptor. IDEPTHFLAG input.

One-line (up to 132 characters) descriptor for the following parameters:

Input values are elevations above the origin to the center of grid blocks. Positive values increase with elevation, indicating grid block center elevations above the elevation of the origin. If IDEPTHFLAG is greater than zero, user-specified values of DEPTH are entered. If IDEPTHFLAG is less than zero, elevations will be calculated from input inclinations.

Line 3.10. DEPTHCONST.

If IDEPTHFLAG (Line 3.2) = 0:

DEPTHCONST: Uniform elevation in all I-, J-, and K-directions [m or ft]. Using a value for IDEPTHFLAG of zero is physically realistic only if the problem is one- or two-dimensional, and NX, NY, or NZ, or two of these, is 1. However, a uniform elevation can be specified for a fully three-dimensional problem or for a two-dimensional problem with a vertical cross-section. The effect, which is sometimes desired, is to "turn off" gravity because there is no difference in elevation between any adjacent layers in the mesh.

Line 3.10: (DEPTHI(I), I=1, NX).

If IDEPTHFLAG (Line 3.2) = 1:

DEPTHI(I): Elevations to grid block centers, varying only in the I-direction [m or ft].

Line 3.10. (DEPTHJ(J), J=1, NY).

If IDEPTHFLAG (Line 3.2) = 2:

DEPTHJ(J): Elevations to grid block centers, varying only in the J-direction [m or ft].

Line 3.10. (DEPTHK(K), K=1, NZ).

If IDEPTHFLAG (Line 3.2) = 3:

DEPTHK(K): Elevations to grid block centers, varying only in the K-direction [m or ft].

Line 3.10. ((DEPTHIJ(I,J), I=1, NX), J=1, NY).

If IDEPTHFLAG (Line 3.2) = 4:

DEPTHIJ(I,J): Elevations to grid block centers, varying in both I- and J-directions [m or ft].

Line 3.10. ((DEPTHIK(I,K), I=1, NX), K=1, NZ).

If IDEPTHFLAG (Line 3.2) = 5:

DEPTHIK(I,K): Elevations to grid block centers, varying in both I- and K-directions [m or ft].

Line 3.10. ((DEPTHJK(J,K), J=1, NY), K=1, NZ).

If IDEPTHFLAG (Line 3.2) = 6:

DEPTHJK(J,K): Elevations to grid block centers, varying in both J- and K-directions [m or ft].

Line 3.10. (((DEPTH(I,J,K), I=1, NX), J=1, NY), K=1, NZ).

If IDEPTHFLAG (Line 3.2) = 7:

DEPTH(I,J,K): Elevations to grid block centers, varying in all three directions [m or ft].

Line 3.10. IORIG, JORIG, KORIG, ZERODEPTH, THETAX, THETAY, THETAZ.

IORIG: I-index of origin block.

JORIG: J-index of origin block.

KORIG: K-index of origin block.

ZERODEPTH: Elevation of origin block [m or ft].

THETAX: Angle of positive right-handed rotation about the *x*-axis [degrees].

THETAY: Angle of positive right-handed rotation about the *y*-axis [degrees].

THETAZ: Angle of positive right-handed rotation about the *z*-axis [degrees].

If IDEPTHFLAG (Line 3.2) < 0: Elevations will be calculated from inclination input. Certain rules must be carefully followed to achieve the proper orientation of the mesh. Start with a right-handed coordinate system, with the origin at $(x,y,z) = (0,0,0)$ in the center of the front lower left corner block. The *x*-direction increases to the right; the *y*-direction increases into the page; and the *z*-direction increases upward. Translate the mesh so that the new origin is at the center of grid block (IORIG, JORIG, KORIG). Next, set the elevation at the center of this grid block to ZERODEPTH. Finally, rotate the mesh about the axes in the following order: 1) Positive rotation about the original *x*-axis; 2) Positive rotation about the original *y*-axis; 3) Positive rotation about the original *z*-axis.

The "original" axes are the axes as they exist after the elevation is set to ZERODEPTH; in other words, the axes of rotation do not change after each rotation.

If IDEPTHFLAG (Line 3.2) = -1: Elevation varies only in I-direction; there must be only one layer in the K-direction. In this case, BRAGFLO allows only rotation about the original *y*-axis. The only value used from Line 3.10 is THETAY; all other inputs are ignored, but appropriate placeholder values (three integers and four real numbers) must be input.

If IDEPTHFLAG (Line 3.2) = -2: Elevation varies only in J-direction; there must be only one layer in the K-direction. BRAGFLO allows only rotation about the original *x*-axis. The only value used from Line 3.10 is THETAX; all other inputs are ignored, but appropriate placeholder values (three integers and four real numbers) must be input.

If IDEPTHFLAG (Line 3.2) < -2: Elevation can vary in all three directions. This is the most general case, and it is used whenever IDEPTHFLAG < -2. Other specialized cases, for IDEPTHFLAG = -3 to -6, analogous to IDEPTHFLAG = +3 to +6, are not yet implemented in BRAGFLO, so any value of IDEPTHFLAG between -3 and -7, inclusive, is treated as IDEPTHFLAG = -7.

7.2.5 Well Parameters and Boundary Conditions

BRAGFLO is capable of simulating wells that are completed within the formations or porous media being modeled. A well is either an injection well or a production (or withdrawal) well. Each type of well can be treated as a constant-pressure well or as a constant flow rate well.

In a constant-pressure well, fluids (gas and brine) are injected or produced at whatever rate is necessary to maintain the specified pressure. The amount of each phase that is injected or produced is proportional to the saturation of each phase in the grid block containing the well.

A constant-pressure well is useful for simulating constant-pressure boundary conditions, and, in earlier versions of BRAGFLO, this was the only means of maintaining a truly fixed boundary pressure. In the current version, constant-pressure boundary conditions can be specified directly, so wells are no longer used for that purpose.

In a constant-flow injection or production well, the rate of injection or production of each phase is specified, and the pressure in the grid block containing the well fluctuates accordingly. Injection and production wells are useful for simulating sources and sinks, for example, generation of gas by a chemical reaction.

In BRAGFLO, a well exists only in a single grid block. In reality, a well might be completed (*i.e.*, open to the surrounding formation) over a range of depths, which might encompass more than one grid block in the mesh. To simulate such a well using BRAGFLO, multiple wells must be used, one for each grid block in which the well is completed. More than one well may exist in a grid block. Each well in a grid block must be specified individually in the input. All wells are assumed to be located at the center of the grid block. (In fact, BRAGFLO, as a cell-centered finite difference code, considers all properties and influences as occurring at the centers of grid blocks.) It is currently not possible in BRAGFLO for wells to interact directly; for example, fluids withdrawn from one well cannot be injected in another well. Furthermore, injection and production rates are fixed over the specified time period; they cannot be varied over time, except in finite increments as specified explicitly in the input, and they cannot be made to vary as a

function of any other rates or processes simulated in BRAGFLO. They depend solely, although implicitly, on the brine pressure and gas saturation within the grid block in which the wells are completed.

Specified well conditions remain in effect only until the next time at which conditions in any well are changed. For example, suppose two constant-pressure wells are specified initially, and a third well, a constant-flow well, is to be added after 1000 years. If only the third well is specified at 1000 years, the two constant-pressure wells will be turned off at 1000 years. If these two wells are to continue to be in effect after 1000 years, their conditions must be specified at 1000 years (along with the third well) as well as at the start of the run. Wells are turned off simply by specifying another time when conditions go into effect, but without specifying any conditions for those wells.

Constant-pressure (Dirichlet) boundary conditions can be specified directly, instead of being simulated by means of constant-pressure wells. BRAGFLO assumes all external mesh boundaries to be no-flow boundaries. Although constant-pressure wells can usually hold the pressure constant in any grid cell where they are applied, numerical problems are sometimes encountered. Using wells also requires that productivity indexes (PIWELL-Line 4.6) be judiciously chosen. If PIWELL is too small, the pressure will not be held exactly constant; if PIWELL is too big, numerical difficulties are exacerbated. When gas dissolution is being simulated, constant-pressure wells may not work at all. Specifying Dirichlet boundary conditions can eliminate these problems. The user has the option of fixing either the brine pressure or the gas saturation, or both, in any grid block in the mesh.

Dirichlet boundary conditions are in effect during the entire run. They cannot be turned on or off at various times the way wells can.

Line 4.1. Descriptor. Well parameters.

One-line (up to 132 characters) descriptor for the following parameters:

Line 4.2. NWELLTIMES.

NWELLTIMES: Number of times to specify well conditions. If NWELLTIMES is greater than NWTIME (which is set in the PARAMETER statement in params.inc), BRAGFLO will abort with the message:

```
In READWELL, NWTIME needs to be larger.
NWELLTIMES = <NWELLTIMES input value>
*** Well time errors in READWELL ***
```

The next line (4.3) is repeated NWELLTIMES times.

Line 4.3. WELLTIME, NWELLS.

WELLTIME: Time when conditions go into effect [s or days]. Conditions specified at this time remain in effect only until the next WELLTIME. In order for a well to remain in effect after the next WELLTIME, the description and conditions for that well (Lines 4.4, 4.5, and 4.6) must be repeated at the next WELLTIME. If this information is *not* repeated at the next WELLTIME, the well is, in effect, turned off at that time.

NWELLS: Number of grid blocks containing wells at this WELLTIME.

The next line (4.4) is repeated NWELLS times.

Line 4.4. IWELLNODE, JWELLNODE, KWELLNODE, NWELLSPERGRID.

IWELLNODE: I-index of grid block containing the well(s).

JWELLNODE: J-index of grid block containing the well(s).

KWELLNODE: K-index of grid block containing the well(s).

NWELLSPERGRID: Number of wells that exist in this grid block.

The next line (4.5) is repeated NWELLSPERGRID times.

Line 4.5. WELLTYPE.

WELLTYPE: Type of well. This is a CHARACTER*4 variable. It is input in free format, with *no* enclosing tick marks and any number of leading spaces, in contrast to earlier versions of BRAGFLO, which used a formatted read statement. The available options are:

= INJP: Pressure-controlled (or constant-pressure) injection well.

= INJQ: Flow-rate-controlled injection well.

= PROD: Production well.

= NONE: None of the above. This is the initial value for WELLTYPE; if not changed by an input value, a well that is otherwise fully specified by input will be ignored and has no effect.

Line 4.6. QGWELL, QOWELL, PIWELL, PW.

QGWELL: Gas mass flow rate [kg/s or lb/day].

QOWELL: Brine mass flow rate [kg/s or lb/day].

PIWELL: Injectivity or productivity index [m^3 or (bbl cP)/(day psi)]. Recommended value: 1.0×10^{-6} m^3, to achieve constant pressure (PO = PW), as when wells are used to maintain a specified boundary condition.

PW: Flowing down-hole well bore pressure [Pa or psi].

The productivity index, PIWELL, is a function of grid block dimensions, permeability, and borehole diameter that allows accurate simulation of well behavior when a small-diameter borehole is completed within a large grid block. To simulate the pressure drop from the formation immediately surrounding a borehole into the borehole, the productivity index must be calibrated to actual measurements of pressure and flow rates. In the WIPP PA, wells are generally used only to maintain fixed pressures at the boundaries of a mesh, rather than to simulate the actual behavior of a well. (Since Dirichlet boundary conditions were implemented, wells are now seldom used at all.) In this case, accurate simulation of the pressure behavior in the vicinity of the well is unimportant, and a large productivity index (say, 1.0×10^{-6} m^3) is used so that the pressure in the grid block is the same as specified for the borehole. Because the productivity index is dependent on grid block dimensions, a "large" value in one grid block

may not be large enough in another. However, for grid blocks as large as 15 km × 60 km × 100 m, a productivity index of 1.0×10^{-6} m^3 [3.7×10^{12} bbl cP/(day psi)] provides the desired equal pressures in the well borehole and the grid block.

Line 4.7. Descriptor. Constant brine pressure and gas saturation boundary conditions.

One-line (up to 132 characters) descriptor for the following parameters:

Line 4.8. DIRICHLET, NO_DIRGRID.

DIRICHLET: Logical flag (T or F) indicating that Dirichlet boundary conditions will be used.

NO_DIRGRID: Number of grid blocks in which Dirichlet boundary conditions will be applied.

If DIRICHLET is .FALSE., no additional well or boundary condition data are input.

If DIRICHLET is .TRUE., the following line (4.9) is repeated NO_DIRGRID times.

Line 4.9. IR,JR,KR,DIRGRIDP,DIRGRIDS,DIR_PRES,DIR_SATB.

IR: I-index of grid block in which Dirichlet boundary conditions are applied.

JR: J-index of grid block in which Dirichlet boundary conditions are applied.

KR: K-index of grid block in which Dirichlet boundary conditions are applied.

DIRGRIDP: Logical flag (T or F) indicating that a constant brine pressure is to be used.

DIRGRIDS: Logical flag (T or F) indicating that a constant gas saturation is to be used.

DIR_PRES: Brine pressure specified to be constant [Pa].

DIR_SATB: Brine saturation specified to be constant. Because BRAGFLO solves for gas saturation, it is actually the gas saturation that will be held constant. However, to be consistent with the initial condition input, where brine saturation is input, brine saturation is specified here, rather than gas saturation.

DIR_PRES and DIR_SATB must be identical to the initial values, PIINIT (IR,JR,KR) and SOINIT (IR,JR,KR), respectively (see next subsection). Otherwise, BRAGFLO will run incorrectly. BRAGFLO does not check to be sure that DIR_PRES and DIR_SATB are the same as the initial; it is up to the user to ensure that this is true.

7.2.6 Initial Conditions

Initial conditions must be input for brine pressure, brine saturation, iron concentration, and cellulosics concentration.

Line 5.1. Descriptor. Brine pressure initial conditions.

One-line (up to 132 characters) descriptor for the following parameters:

Line 5.2. (((PINIT(I,J,K), I=1, NX), J=1, NY), K=1, NZ).

PINIT: Initial brine pressure [Pa or psi].

Line 5.3. Descriptor. Brine saturation initial conditions.

One-line (up to 132 characters) descriptor for the following parameters:

Line 5.4. (((SOINIT(I,J,K), I=1, NX), J=1, NY), K=1, NZ).

SOINIT: Initial brine saturation [dimensionless].

Line 5.5. Descriptor. Iron concentration initial conditions.

One-line (up to 132 characters) descriptor for the following parameters:

Line 5.6. (((CONCFE(I,J,K), I=1, NX), J=1, NY), K=1, NZ).

CONCFE: Initial iron concentration [kg/m^3 or lb/ft^3].

Line 5.7. Descriptor. Cellulosics concentration initial conditions.

One-line (up to 132 characters) descriptor for the following parameters:

Line 5.8. (((CONCBIO(I,J,K), I=1, NX), J=1, NY), K=1, NZ).

CONCBIO: Initial cellulosics concentration [kg/m^3 or lb/ft^3].

Line 5.9. Descriptor. MgO concentration initial conditions.

One-line (up to 132 characters) descriptor for the following parameters:

Line 5.10. (((CONCMGO(I,J,K), I=1, NX), J=1, NY), K=1, NZ).

CONCMGO: Initial magnesium oxide concentration [kg/m^3 or lb/ft^3].

It is sometimes desirable to calculate, rather than input, certain initial conditions, an example being the initial brine pressure distribution in formations surrounding the WIPP repository. In this example, other initial conditions, such as the brine pressure within the repository and initial concentrations of reactants (iron and cellulosics), still need to be specified in the input, even though pressures outside the repository are calculated. BRAGFLO accommodates this need to calculate initial conditions of only some variables in only part of the mesh by means of a somewhat convoluted interaction between special materials specifications and starting times.

If a run begins at time START >= TIMEICRESET (described in Section 7.2.8, Line 7.24; generally, TIMEICRESET = 0.), BRAGFLO uses only the initial conditions specified in Lines 5.1-5.10 above. This use of initial conditions is straightforward and uncomplicated, being the obvious way that initial conditions are expected to be used.

If a run begins at time START < TIMEICRESET, only some of the initial conditions are used at time START, while other initial conditions from Lines 5.1-5.10 are used at time TIMEICRESET. In this case, initial pressures, PINIT, will be used in all regions *except Waste regions* at time START. Initial brine saturations, SOINIT, will also be used in all regions *except Waste regions* at time START. Reactant concentrations, CONCFE, CONCBIO and CONCMGO are not used until after TIMEICRESET; furthermore, reactions that affect the values of CONCFE, CONCBIO and CONCMGO occur only in Waste regions, which are undefined prior to TIMEICRESET.

At TIMEICRESET, brine pressures *only in Reset Material regions* are set to PINIT. At the same time, brine saturations *only in Reset Material regions* are set to SOINIT. Because CONCFE,

CONCBIO, and CONCMGO are unaffected before TIMEICRESET, both of these variables have initial values as specified in Lines 5.6 and 5.8 at time START as well as at time TIMEICRESET.

7.2.7 Numerical Control Parameters

Parameters input in this section allow the user to control the numerical behavior of BRAGFLO. These parameters affect the accuracy of solutions and can have major effects on computing time. The equations solved in BRAGFLO are highly nonlinear, and the discretized equations are solved using an iterative Newton-Raphson technique. The control parameters govern the rate of convergence of the solution procedure, as well as the degree of precision to be achieved in the solution. The Newton-Raphson procedure involves computing a Jacobian matrix, which is the most computationally intensive step in the solution. The control parameters allow the user to specify the frequency at which the Jacobian is recalculated. The Jacobian is always computed at the beginning of each time step. It can be calculated as frequently as each iteration within a time step (at great computational expense), or after every so many iterations.

Line 6.1. Descriptor. Physical realism constraints.

One-line (up to 132 characters) descriptor for the following parameters:

Line 6.2. DEPLIMIT(1), DEPLIMIT(2), SATLIMIT.

DEPLIMIT(1): Limit allowed on gas saturation outside the physically realistic range of 0.0 to 1.0. The solution will not be rejected provided: 1.0 + DEPLIMIT(1) > S_g > -DEPLIMIT(1). Otherwise, the time step size will be reduced and the time step will be repeated. Note that this is only the first of several criteria that must be met before a solution is finally accepted. "Slightly unrealistic" values of gas saturation can (and generally must) be tolerated; if DEPLIMIT(1) is too small, or zero, BRAGFLO will likely struggle excessively (and consume large amounts of computing time) without appreciably improving the solution. Recommended value: DEPLIMIT(1) = 0.2.

DEPLIMIT(2): Lower limit allowed on brine pressure [Pa or psi]; primarily intended to catch large negative values of pressure. The solution will be accepted provided: PO > DEPLIMIT(2). If PO ≤ DEPLIMIT(2), the time step size will be reduced and the time step will be repeated. As with DEPLIMIT(1), DEPLIMIT(2) should not be set too stringently. These two limits are intended simply to reject the solutions that are beyond hope before any more computational effort is expended on them. Recommended value: -1.0×10^8 Pa.

SATLIMIT: Limit on gas saturation solution beyond which a solution will not be accepted; inter-step iterations will continue using the same Δt (*i.e.*, the solution is not accepted, but Δt is not reduced) even if DEPLIMIT(1) is satisfied if: 1.0 + SATLIMIT > S_g > -SATLIMIT provided that DEPLIMIT(1) > SATLIMIT. Non-convergence occurs once S_g violates the SATLIMIT constraint. This is intended to be a more stringent limit than DEPLIMIT(1), but it is up to the user to ensure that DEPLIMIT(1) > SATLIMIT. Recommended value: 1.0×10^{-3}.

Line 6.3. Descriptor. Limits on variable changes for auto time step control.

These parameters are used in the auto time step control algorithm. They affect the efficiency of BRAGFLO by allowing larger time steps when the variables (gas saturation and brine pressure) are changing slowly. If auto time step is turned off, these parameters are not used, but they must still be input.

One-line (up to 132 characters) descriptor for the following parameters:

Line 6.4. DELTADEPNORM(1), DELTADEPNORM(2).

DELTADEPNORM(1): Relative change in gas saturation across a time step; used to control size of next time step. Input value is the largest relative change in gas saturation in the time step just completed such that the new time step will be the same as the current time step. Using a smaller input value will cause smaller increases in the new time step for a given relative change in gas saturation or reduce the relative change in gas saturation that will be allowed in order to achieve a given increase in time step size. Using a larger input value will have the opposite effect. Recommended value: 0.3.

DELTADEPNORM(2): Absolute change in brine pressure across a time step [Pa or psi]; used to control size of next time step. Input value is the largest absolute change in brine pressure in the time step just completed such that the new time step will be the same as the current time step. Using a smaller input value will cause smaller increases in the new time step for a given absolute change in brine pressure or reduce the absolute change in brine pressure that will be allowed in order to achieve a given increase in time step size. Using a larger input value will have the opposite effect. Recommended value: 5.0×10^5 Pa.

Line 6.5. Descriptor. Maximum absolute variable changes.

One-line (up to 132 characters) descriptor for the following parameters:

Line 6.6. DDEPMAX(1), DDEPMAX(2).

DDEPMAX(1): Maximum absolute gas saturation change allowed over a time step. If a greater change in gas saturation occurs, the time step is repeated using a smaller time step. Recommended value: 1.0. (This allows gas saturation to change from 0.0 to 1.0 in a single step, the most that is physically possible, in effect turning off this control except when unphysical gas saturations are obtained.)

DDEPMAX(2): Maximum absolute pressure change allowed over a time step. If a greater change in brine pressure occurs, the time step is repeated using a smaller time step [Pa or psi]. Recommended value: 1.0×10^7 Pa.

Line 6.7. Descriptor. Newton-Raphson normal convergence criteria.

One-line (up to 132 characters) descriptor for the following parameters:

Line 6.8. ICONVTEST.

ICONVTEST: Flag specifying whether *either* or *both* convergence criteria must be satisfied before a solution is considered to have converged. Recommended value: 1. requiring both convergence criteria to be met should result in a more accurate solution. However, prohibitively small time steps are sometimes required because the convergence tests tend to over-emphasize the importance of small grid blocks in which small changes can result in relatively large mass balance errors. To get BRAGFLO to run to completion when such problems occur, it may be necessary to relax one of the criteria that must be met. Generally, this has been found to have little impact on gross results. However, in some instances, important short-lived transient results can differ greatly depending on whether either or both convergence criteria are met. Therefore, whenever possible, ICONVTEST = 1 should be used.

= 0: Satisfy *either* EPSNORM or FTOLNORM. (described next, on Lines 6.10 and 6.14).

= 1: Satisfy *both* EPSNORM and FTOLNORM. (described next, on Lines 6.10 and 6.14).

Line 6.9. Descriptor. Maximum change in variables for normal convergence.

One-line (up to 132 characters) descriptor for the following parameters:

Line 6.10. EPSNORM(1), EPSNORM(2).

EPSNORM(1): Number of digits of accuracy to the right of the decimal in the change in gas saturation. This parameter limits the change in gas saturation when saturations are very small, in which case DDEPMAX(1) is too easily satisfied. Recommended value range: 2 to 5 with a best estimate of 3.

EPSNORM(2): Maximum *relative* change in brine pressure allowed over a time step. This parameter provides control over brine pressure changes when the pressure is small and DDEPMAX(2) (the maximum *absolute* change) is too easily satisfied. Recommended value range: 1.0×10^{-5} to 1.0×10^{-2} with a best estimate of 1.0×10^{-3}.

Line 6.11. Descriptor. Loosened Newton-Raphson convergence criteria.

Occasionally, BRAGFLO encounters great difficulty in converging to a solution. If a solution has not been obtained at a particular time step after numerous time step reductions, it is quite likely that further time step reductions will not improve the solution sufficiently to satisfy the normal convergence criteria, EPSNORM(1) and EPSNORM(2). One option at this point is for BRAGFLO to abort. The user would then rerun the problem after adjusting one or more of the control parameters and hope for better results. However, it is often the case that BRAGFLO's difficulties are temporary, and that if it can get past the trouble spot, it will complete the run without further major difficulties. Thus, a second option has been built into BRAGFLO to handle those occasions when repeated time step reductions fail to provide convergence: The convergence criteria are temporarily relaxed. These relaxed criteria are applied after user-specified

IJACSWITCH time step reductions have occurred, and they continue to be applied only until convergence is obtained at that time step. After IJACRESET time steps, and at all subsequent time steps, the normal convergence criteria are used. This capability makes BRAGFLO a little more robust, enabling it to complete runs that would otherwise abort and require input modifications before rerunning, at only a minor cost in overall accuracy. This feature becomes important when carrying out large number of runs in automated batch systems. It can be turned off by setting all input values of the loosened criteria equal to the normal criteria. Caution is advised when using this feature because large mass balance errors can be introduced which may not be apparent in a cursory examination of the results.

NOTE: Loosened tolerance capability is not QA'd or used for WIPP Compliance Calculations. Set EPSLOOSE ≥ EPSNORM to disable.

One-line (up to 132 characters) descriptor for the following parameters:

Line 6.12. EPSLOOSE(1), EPSLOOSE(2).

EPSLOOSE(1): Same meaning as EPSNORM(1); used after IJACSWITCH time step reductions have occurred. Recommended value range: 1 to 4 with a best estimate of 2.

EPSLOOSE(2): Same meaning as EPSNORM(2); used after IJACSWITCH time step reductions have occurred. Recommended value range: 1.0×10^{-1} to 1.0×10^{-4} with a best estimate of 1.0×10^{-2}.

Line 6.13. Descriptor. Normal right-hand-side function (or residual) criteria.

BRAGFLO solves a pair of simultaneous mass balance equations: F1 = 0 (gas mass balance), and $F_2 = 0$ (brine mass balance). Because the nonlinear equations are solved numerically and iteratively, F_1 and F_2 are generally not zero. The deviation from zero is the residual, or mass balance error. Ideally, iterations will continue until the residuals are zero, but, in practice, the best that can be hoped for is to get "close" to zero. Discretization errors, round-off errors, discontinuous functional dependencies, property functions with discontinuous derivatives, and non-linearities all contribute to making convergence to truly zero residuals unattainable. The degree of closeness of the residuals to zero that is acceptable is input as the tolerances FTOLNORM(1) and FTOLNORM(2).

One-line (up to 132 characters) descriptor for the following parameters:

Line 6.14. FTOLNORM(1), FTOLNORM(2).

FTOLNORM(1): [kg gas in residual/kg gas in grid block]. For gas saturation, the value of the residual is normalized by dividing by the amount of gas present in the grid block, $\phi(\rho_g S_g + C_{gb}\rho_b S_b)$, where ϕ is the porosity, ρ_g and ρ_b are the gas and brine densities at local conditions, S_g and S_b are the gas and brine saturations, and C_{gb} is the mass fraction of gas in the brine phase ($C_{gb} = 0.0$ if no dissolved gas is present). The minimum of this normalized residual value is compared with FTOLNORM(1). If ICONVTEST = 0 and the normalized residual is less than FTOLNORM(1), convergence is accepted regardless of EPSNORM(1). If ICONVTEST = 1, the normalized residual

must be less than FTOLNORM(1) and EPSNORM(1) must be satisfied in order for the solution to be accepted. Recommended value range: 1.0×10^{-1} to 1.0×10^{-6} with a best estimate of 1.0×10^{-2}.

FTOLNORM(2): [kg brine in residual/kg brine in grid block]. For brine pressure, the value of the residual is normalized by dividing by the amount of brine present in the grid block, $\phi C_{bb} \rho_b S_b$, where ϕ is the porosity, C_{bb} is the mass fraction of brine in the brine phase ($C_{bb} = 1.0$ if no dissolved gas is present), ρ_b is the brine density at local conditions, and S_b is the brine saturation. The minimum of this normalized minimum residual value is compared with FTOLNORM(2). If ICONVTEST = 0 and the normalized residual is less than FTOLNORM(2), convergence is accepted regardless of EPSNORM(2). If ICONVTEST = 1, the normalized residual must be less than FTOLNORM(2) and EPSNORM(2) must be satisfied in order for the solution to be accepted. Recommended value range: 1.0×10^{-1} to 1.0×10^{-6} with a best estimate of 1.0×10^{-2}.

Line 6.15. Descriptor. Loosened right-hand-side function criteria.

NOTE: Loosened tolerance capability is not QA'd or used for WIPP Compliance Calculations. Set FTOLLOOSE ≥ FTOLNORM to disable.

One-line (up to 132 characters) descriptor for the following parameters:

Line 6.16. FTOLLOOSE(1), FTOLLOOSE(2).

FTOLLOOSE(1): Relaxed value of normalized residual for gas saturation below which convergence is accepted regardless of EPSLOOSE(1); used after IJACSWITCH time step reductions have occurred [kg gas in residual/kg gas in grid block]. Recommended value range: 1.0×10^{-1} to 1.0×10^{-5} with a best estimate of 1.0×10^{-1}.

FTOLLOOSE(2): Relaxed value of normalized residual for brine pressure below which convergence is accepted regardless of EPSLOOSE(2); used after IJACSWITCH time step reductions have occurred [kg brine in residual/kg brine in grid block]. Recommended value range: 1.0×10^{-1} to 1.0×10^{-5} with a best estimate of 1.0×10^{-1}.

Line 6.17. Descriptor. Multi-component gas constituent transport convergence tolerances.

One-line (up to 132 characters) descriptor for the following parameters:

Line 6.18. EPSGAS(1), EPSGAS(2), EPSGAS(3), EPSGAS(4).

EPSGAS(1): Smallest negative value allowed in the amount of each gas component in a grid block [gm-mol]. If input as a positive number, BRAGFLO sets it negative.

EPSGAS(2): Largest change in a molar concentration of a gas component that is allowed over a Newton-Raphson iteration [gm-mol/m^3].

EPSGAS(3): Smallest value of molar concentration that is considered to be nonzero. Used to ensure that, in calculating the relative change in molar concentration, a zero or essentially zero value is not used [gm-mol/m^3].

EPSGAS(4): Maximum relative change in gas component molar concentration allowed over a Newton-Raphson iteration [dimensionless].

Line 6.19. Descriptor. Equation solver selection.

One-line (up to 132 characters) descriptor for the following parameters:

Line 6.20. CHSOLVER.

CHSOLVER: This is a CHARACTER*3 variable indicating the solver to be used. It is input in free format, with *no* enclosing tick marks and any number of leading spaces. The available options are:

= LU: Original LU-decomposition solver, a direct (non-iterative) solver. This is the solver most frequently used in WIPP PA work. Its principal advantage is its great robustness: unless the Jacobian matrix is truly singular (which generally indicates flawed input or a conceptual model error), a solution (*i.e.*, inversion of the given Jacobian) is virtually guaranteed. The main disadvantages are large storage requirements and slow speed, which makes large meshes (such as realistic three-dimensional problems) impractical.

= LP: Another LU-decomposition solver from Linpack, a non-proprietary package of linear algebra routines. Essentially identical to the original LU solver, this solver first calculates a condition number, which indicates the degree of singularity of the Jacobian. If the condition number is too small, the LP solver concludes that the matrix is singular and aborts the run, in contrast to the original LU solver, which will continue with the solution unless the Jacobian determinant is exactly zero. It is currently disabled in BRAGFLO because the massive Jacobian array is rewritten into another array, nearly doubling the memory required to run BRAGFLO. It may be reactivated easily in future versions. If the LP solver is selected, the program will abort with a message printed to the screen:

```
*** Abort in READCNTRL; LP solver not available.
```

= MG: A multigrid iterative solver. In addition to speed (compared to direct solvers), this solver has the advantage of all iterative solvers in that the storage requirements are far less than for direct solvers, making large three-dimensional simulations possible. The multigrid solver originally implemented in BRAGFLO was limited to two dimensions and suffered from a lack of robustness. This option is currently not available, pending development of a robust three-dimensional multigrid solver. The shell for selecting this solver has been retained for possible future use. If it is selected, the program will abort with a message printed to the screen:

```
*** Abort in READCNTRL; MG solver not available.
```

= LSOR: A point successive over-relaxation (SOR) solver. This is another iterative solver, which, like the multigrid solver, lacks robustness. It should work on simple problems or large problems using uniform grid blocks and smoothly varying material properties.

NOTE: LP, MG, and LSOR solvers are either unavailable or not QA'd nor used for WIPP Compliance Calculations.

Line 6.21. Descriptor. Iteration limits; scaling options.

One-line (up to 132 characters) descriptor for the following parameters:

Line 6.22. ITMAX, IRESETMAX, IJACINPUT, LSCALE, P_SCALE, LVARSWTCH.

ITMAX: Maximum number of Newton-Raphson iterations per time step. Recommended value: 10.

IRESETMAX: Maximum number of time step size reductions allowed at any time step should non-convergence problems be encountered. If this number is exceeded, the run is aborted; this is the only way a BRAGFLO run will cleanly abort (aside from input errors). Note that the time steps obtained as a result of time step reductions following non-convergence are not restricted in size by the input parameter DELTMIN (Line 1.9). It is possible for a time step smaller than DELTMIN to be obtained that results in convergence after fewer than IRESETMAX time step reductions. This can only occur when non-convergence causes time steps to be reduced below DELTMIN. In this case, the next time step will automatically be reset to DELTMIN. Convergence requiring time steps smaller than DELTMIN may occur repeatedly and has the potential for causing BRAGFLO to stall out, consuming great quantities of computing time using impracticably small time steps by sidestepping the normal time step minimum through this one loophole. However, it has been found that when BRAGFLO has difficulties resulting in repeated use of time steps smaller than DELTMIN, either these problems are resolved by taking just a couple of time steps smaller than DELTMIN, or they cause IRESETMAX to be exceeded. Recommended value: 40.

IJACINPUT: Default iteration interval frequency for updating the Jacobian. The Jacobian is always evaluated at the start of each time step. Reevaluating the Jacobian at each Newton-Raphson iteration within a time step will, at least in theory, result in the fastest convergence to a solution. However, in some instances, convergence may be just as fast even when the Jacobian is evaluated only before the first iteration. Because evaluating the Jacobian is the most computationally intensive step in the solution, it is highly desirable to do this as infrequently as possible. On the other hand, reevaluating every iteration is more likely to give a solution, especially in difficult problems, whereas doing this, say, just once each time step (every 40 iterations), can sometimes cause the solution to diverge, resulting in

more computational effort than simply reevaluating every iteration. Recommended value: 1.

LSCALE: Logical flag specifying whether to scale the Jacobian and the right hand side. Scaling may reduce round-off errors that cause numerical problems when working with near-singular matrices, which is often the case in WIPP PA. Recommended value: T.

P_SCALE: When LSCALE = T, the Jacobian and right hand side are divided by P_SCALE to reduce the singularity of the Jacobian when the degree of singularity is exacerbated by round-off errors. Whether LSCALE = T or F, a value must be input here; when LSCALE = F, P_SCALE is read in but is not used. Recommended value: 1.0×10^7 Pa.

LVARSWTCH: Logical flag specifying whether variable switching will be allowed. This flag can be set to T only if dissolved gas is being modeled and Henry's law is to be used (IDGAS = 2). The gas solubility options are described in Section 7.2.9. When Henry's law gas solubility is used, LVARSWTCH *should* be set to T; this is not a requirement, but BRAGFLO may not run well or at all if variable switching is not allowed (set to F) when IDGAS = 2. When LVARSWTCH = T, the dependent variables may be automatically changed when the gas phase disappears, from the normal set of gas saturation and brine pressure (S_g and P_o) to P_a and P_o. P_a is the equilibrium Henry's law gas pressure, defined as the gas pressure that would exist if a gas phase were present given the mole fraction of gas that is currently dissolved in the brine. Because gas can dissolve in brine, it is possible for the gas phase to disappear, but a gas component will remain in the liquid phase. When this happens, it is no longer possible to keep track of the amount of gas dissolved in brine because the dissolved gas is no longer in equilibrium with gas in the (nonexistent) gas phase. Instead of solving two equations (gas mass balance and brine mass balance) for two unknowns (S_g and P_o), BRAGFLO will be trying unsuccessfully to solve just one equation, the brine mass balance, for two unknowns, since the gas mass balance is identically zero as a result of S_g being zero. This will cause the run to abort or to flounder, struggling hopelessly by cutting back time steps. The solution to this difficulty is to change the dependent variable from gas saturation to a pseudo-pressure, P_a, which is directly proportional to the mass or mole fraction of gas dissolved in brine:

$$P_a = x_g H,$$

where:

x_g = mole fraction of gas dissolved in brine,

H = Henry's law constant [Pa/mol fraction gas in solution].

When a gas phase is present, P_a is identical to P_g. When a single liquid phase is present, P_a is the gas pressure that would exist in equilibrium with the dissolved gas if a gas phase were present. In this manner, BRAGFLO

can still use the gas mass balance equation as one of the two equations being solved, but solves, in effect, for the nonzero dissolved gas mass fraction instead of the zero gas saturation. When LVARSWTCH = T, this switching of the dependent variables is done automatically and is transparent to the user, except that informational messages are printed to the screen and to the summary [.sum] file to indicate when the variables are switched and at which grid blocks. If LVARSWTCH = F when Henry's law is used to model gas dissolution, BRAGFLO will run smoothly only if a gas phase is always present. Unless this situation can be assured of holding true for the full duration of the run, LVARSWTCH = T should be used.

NOTE: Variable switching capability is not QA'd or used for WIPP Compliance Calculations.

Line 6.23. Descriptor. Upstream weighting frequencies; time step reduction factor; averaging methods for relative permeabilities and mass fractions.

One-line (up to 132 characters) descriptor for the following parameters:

Line 6.24. IUPRPFLAG, IUPMFFLAG, DELTFACTOR, ITRAVE, IMFRAVE.

IUPRPFLAG: Frequency of updating the inter-time step upstream weighting direction for relative permeabilities. The upstream weighting direction can be changed only when the Jacobian is reevaluated; thus, IUPRPFLAG is not simply the number of Newton-Raphson iterations between updating the upstream direction, but rather the number of Jacobian evaluations between updates. For example, if IJACINPUT (Line 6.22) = 3 (Jacobian reevaluated every third iteration) and IUPRPFLAG = 3, then the upstream direction for relative permeability is updated every 9 iterations. *This option has not been extensively tested,* but it appears that the upstream direction should not be changed every iteration, nor every other iteration (assuming IJACINPUT (Line 6.22) = 1), because this may cause the solution to oscillate and fail to converge. Recommended value: same as ITMAX (Line 6.22), which effectively turns this option off, anchoring the upstream direction at the first iteration. If convergence difficulties suggest that this option may improve convergence, a value of 3 should be tried first.

IUPMFFLAG: Frequency of updating the inter-time step upstream weighting direction for mass fractions. As with relative permeabilities, the upstream weighting direction can be changed only when the Jacobian is reevaluated. IUPMFFLAG the number of Jacobian evaluations between updates. This option will have an effect only if the dissolved gas option is activated (see Section 7.2.9); without dissolved gas, the mass fraction of gas dissolved in brine is always zero everywhere, and the mass fraction of brine component in the brine phase is always 1.0 everywhere, so the upstream direction is not only fixed, but has no impact on the solution. Recommended value: same as ITMAX (Line 6.22), which turns this option off, anchoring the

upstream direction at the first iteration. A value must be input even if the dissolved gas option is not activated.

NOTE: IUPMFFLAG capability is not QA'd or used for WIPP Compliance Calculations. Set IUPMFFLAG = ITMAX to disable.

DELTFACTOR: Time step reduction factor when non-convergence occurs. Recommended value: 0.5.

ITRAVE: Transmissivity averaging method at block interfaces. Recommended value: 1.

= 0: Use arithmetic average.

= 1: Use harmonic average.

NOTE: ITRAVE = 0 capability is not QA'd or used for WIPP Compliance Calculations.

IMFRAVE: Method for averaging mass fractions at block interfaces when dissolved gas option is activated. A value must be input even if the dissolved gas option is not activated. Recommended value: 0.

= 0: Use upstream value of mass fractions.

= 1: Use harmonic average.

Line 6.25. Descriptor. Jacobian reevaluation control parameters.

These parameters are invoked when difficulties arise that cause the time step to be cut back repeatedly, potentially causing the run to abort. The options permit the frequency of Jacobian reevaluation to be changed, convergence tolerances to be relaxed, and upstream directions to be updated at different frequencies. These changes remain in effect for a specified number of time steps before the original set of control parameter values is reinstated.

One-line (up to 132 characters) descriptor for the following parameters:

Line 6.26. IJACSWITCH, IJACMIN, IJACRESET, IUPRPLOOSE, IUPMFLOOSE.

IJACSWITCH: Number of time step reductions allowed before the new set of control parameters is temporarily invoked. This parameter controls when the Jacobian starts to be reevaluated every IJACMIN iterations instead of every IJACINPUT (Line 6.22) iterations, the looser convergence tolerances are invoked, and upstream direction update frequencies are changed. Recommended value: 10.

IJACMIN: Number of iterations allowed before the Jacobian is reevaluated after IJACSWITCH time step reductions have occurred; the Jacobian is now reevaluated every IJACMIN iterations. Reevaluating the Jacobian more frequently (if IJACINPUT > 1) can sometimes promote convergence when BRAGFLO is encountering difficulties. Although many iterations can be performed in much less computing time than is required for a single evaluation of the Jacobian, convergence is often achieved with a single

iteration after reevaluation. If IJACINPUT > 1, this parameter alone should be changed first, before tolerances are loosened or upstream direction frequencies are changed, because this parameter generally has the greatest impact on convergence. Recommended value: 1.

IJACRESET: Number of time steps during which IJACMIN, looser tolerances, and modified upstream direction update frequencies remain in effect following a time step in which IJACSWITCH time step reductions occurred. When BRAGFLO is having severe difficulties, reevaluating the Jacobian more frequently for a few time steps can help it through the difficult period. However, such trouble spots are usually of short duration, so more frequent reevaluations should not be continued indefinitely if not necessary. Looser convergence tolerances should also not be used any longer than necessary because, strictly speaking, the accuracy of the entire run is only as good as the looser tolerances, even though they were used only a few small time steps. Recommended value: 2.

IUPRPLOOSE: Frequency of updating the upstream direction for relative permeabilities. This is the "looser tolerances" value of IUPRPFLAG and is used for IJACRESET time steps.

NOTE: IUPRPLOOSE capability is not QA'd or used for WIPP Compliance Calculations. Set IUPRPLOOSE ≥ ITMAX to disable.

IUPMFLOOSE: Frequency of updating the upstream direction for mass fractions. This is the "looser tolerances" value of IUPMFFLAG and is used for IJACRESET time steps.

NOTE: IUPMFLOOSE capability is not QA'd or used for WIPP Compliance Calculations. Set IUPMFLOOSE ≥ ITMAX to disable.

Line 6.27. Descriptor. Relative changes for Jacobian elements.

One-line (up to 132 characters) descriptor for the following parameters:

Line 6.28. DH(1), DH(2).

DH(1): Relative change in gas saturation for Jacobian element derivative calculations. Because the equations being solved are so nonlinear, DH should be as small as possible without losing numerical precision. Recommended value: 1.0×10^{-8}.

DH(2): Relative change in brine pressure for Jacobian element derivative calculations. Recommended value: 1.0×10^{-8}.

Line 6.29. Descriptor. Minimum absolute change for Jacobian elements.

One-line (up to 132 characters) descriptor for the following parameters:

Line 6.30. HMIN(1), HMIN(2).

HMIN(1): Minimum absolute gas saturation change allowed for Jacobian element derivative calculations. This limit prevents the variable change calculated

using the *relative* change factor DH from becoming too small when the saturation is small. Recommended value: 1.0×10^{-10}.

HMIN(2): Minimum absolute brine pressure change allowed for Jacobian element derivative calculations [Pa or psi]. Recommended value: 0.01 Pa.

7.2.8 Material Maps and Material Properties

This section describes input that establishes material properties for each grid block. A material type grid map is input in which each grid block is assigned a material type index. This map applies during a specified time period. A series of material maps covers the duration of the run, allowing material properties in each grid block to change for discrete periods of time. Following the material maps, certain special materials are input; for these materials, specialized submodels apply, the most important example being Waste, in which chemical reactions occur that can occur in no other material. Material properties are input next. These include two-phase flow parameters, permeabilities, reference-condition porosities, and compressibilities. Finally, flags and parameters for submodels simulating fracturing and Klinkenberg effect are input.

Line 7.1. Descriptor. Number of material maps.

One-line (up to 132 characters) descriptor for the following parameters:

Line 7.2. NMATTIMES.

NMATTIMES: Number of times to specify a material map. NMATTIMES must be less than or equal to MAXMATTIMES, set in the PARAMETER statement. If NMATTIMES is less than one or greater than MAXMATTIMES, no error message will be printed, but BRAGFLO will abort at some time during the simulation.

Lines 7.3 - 7.6 are repeated NMATTIMES times.

Line 7.3. Descriptor. Start times.

One-line (up to 132 characters) descriptor for the following parameters:

Line 7.4. TIMEMAT.

TIMEMAT: Starting time at which the material map that follows is in effect [s or days]. If the first TIMEMAT is later than START, the starting time for the run, no error message is printed, but any results obtained before BRAGFLO aborts will be unpredictable and unreliable.

Line 7.5. Descriptor. Material map.

One-line (up to 132 characters) descriptor for the following parameters:

Line 7.6. (((IMAT(I,J,K), I=1, NX), J=1, NY), K=1, NZ).

IMAT(I,J,K): Material type number for grid block (I,J,K). This number is associated later with the material properties input. BRAGFLO finds the minimum and maximum material type numbers in all NMATTIMES maps and assumes that the total number of materials, NMAT, is equal to the maximum value found in the maps. If any IMAT(I,J,K) is less than 1 or

greater than MMAT (set in the PARAMETER statement), BRAGFLO will abort after printing the offending minimum or maximum value of IMAT, with the following message printed to the screen:

```
*** Aborted:  Input material type error in READMAT ***
```

One or more material type numbers between 0 and NMAT may, at the user's option, be omitted from the material maps without causing any problem. However, material properties (starting at Line 7.31 below) must be input for NMAT materials, regardless of how many material numbers are actually used in the maps. For example, if the maps have only two material types, numbered 2 and 8, properties for 8 materials must be input, even though the properties for only two of the eight materials will actually be used. Normally, NMAT materials would actually be used.

Line 7.7. Descriptor. Material numbers and names.

One-line (up to 132 characters) descriptor for the following parameters:

Line 7.8 is repeated NMATTIMES times.

Line 7.8. LABEL.

LABEL: Dummy CHARACTER*132 variable. Must be read in but is not used.

Must be read in, but the information on each line is not otherwise used in BRAGFLO. It is intended solely to provide space within the input file to help the user identify each material type.

7.2.8.1 Special Materials.

BRAGFLO has four special material types that have unique capabilities. These have evolved to handle situations encountered in modeling the WIPP, so they have names that apply to regions included in models of the WIPP, but actually have fairly generally applications. The materials are referred to as: Waste, DRZ (Disturbed Rock Zone), "Reset" materials, and Borehole.

Waste Material.

In Waste materials, and only in Waste, can chemical reactions take place. Specifically, corrosion of iron can occur, which consumes iron and water and produces hydrogen; microbial degradation of cellulosics can occur; this reaction consumes cellulosics and produces hydrogen, and, if indicated in the input (described later), can also consume or produce water. Hydration and carbonation of MgO can occur as described above in Section 4.13.5. Finally, radiolysis and decay can occur as described in Section 4.20.

Another special capability unique to Waste is simulation of creep closure, in which the porosity decreases over time, the rate depending on the rate of gas production and the pressure within the Waste. Porosity can change in any material as a result of pressure-dependent compressibility, but the change is generally quite small. In contrast, the porosity change resulting from creep closure of the Waste can be very large.

Only in Waste can there be an *initial* mass of radionuclides, the transport and decay of which can be modeled in any region as long as there was some amount initialized in the Waste. Finally, to be able to simulate an operational period in the WIPP, during which excavations are open to the

atmosphere and any brine seepage is removed by means of ventilation or pumping, the initial brine pressure and saturation in the Waste can be specified to be different from the initial conditions described in Section 7.2.6. Then, at some later time (TIMEICRESET), the conditions in the Waste can be reset to the initial conditions specified in Section 7.2.6.

There is one important constraint in how Waste regions are specified. If there are to be NWST regions that will contain waste (MAT_WASTEI), there must also be NWST Waste regions (MAT_WASTE) to "deposit" into these regions to be filled with Waste. Additionally, each NWST MAT_WASTE material index number must be unique even though the same Waste properties are desired to be placed in the NWST MAT_WASTEI regions. For example, assume NWST = 2 and the 2 MAT_WASTEI regions are empty excavations described by materials number 4 and 5 of the materials table defined in the section "Material Property Data" below (see lines 7.41 to 7.46). Also suppose that at some time during the simulation defined by TIMEICRESET in line 7.24 that Waste properties defined by material 6 are to replace the MAT_WASTEI materials 4 and 5. Since two MAT_WASTE material numbers are required and since these material identifiers must be unique, an additional material must be specified in the table (lines 7.41 to 7.46), say material 7, even though it has the same properties as material 6, the original Waste material. Therefore, in this example, NWST = 2, MAT_WASTEI(1) = 4, MAT_WASTEI(2) = 5, MAT_WASTE(1) = 6, and , MAT_WASTEI(2) = 7. An error check is performed in BRAGFLO to make sure NWST unique MAT_WASTE material identifiers are provided. If they are not BRAGFLO will abort with an error message printed to the screen and to the .sum file.

Line 7.9. Descriptor. Waste regions.

One-line (up to 132 characters) descriptor for the following parameters:

Line 7.10. NWST.

NWST: Number of Waste regions.

If NWST ≤ 0, the next two lines (7.11 and 7.12) are omitted. If NWST > MWST (set in the PARAMETER statement), the run will abort.

Line 7.11. Descriptor. Definition of Waste regions.

One-line (up to 132 characters) descriptor for the following parameters:

Line 7.12. (MAT_WASTEI(I), I=1, NWST), (MAT_WASTE(I), I=1, NWST).

MAT_WASTEI: Material type index of the material at time START that will *become* Waste at time TIMEICRESET. Prior to TIMEICRESET, materials designated as MAT_WASTEI have no special characteristics and receive no special treatment. It is necessary to know which regions are eventually going to become Waste regions, however, to calculate what will be the Waste region volume, because this information must be known before any initial conditions are printed or any other calculations are done.

MAT_WASTE: Material type index of Waste *after* TIMEICRESET. Porosity will be calculated using the creep closure sub-model only for this material type (provided that model is turned on; input controlling this sub-model will be discussed later, in Section 7.2.11). Corrosion and biodegradation reactions occur only in this material. There should be a one-to-one

correspondence between MAT_WASTEI(I) and MAT_WASTE(I); NWST values of each are read in.

Disturbed Rock Zone (DRZ) Material.

In this material, if the porosity increases at time TIMEICRESET, the brine volume is assumed to remain fixed over that change, and the brine saturation is adjusted to account for the increased pore volume. Gas is assumed to fill the additional pore space. The gas appears instantaneously; there is no source for this gas, *i.e.*, it does not flow from any other cell, is not introduced by well injection, and is not created by way of chemical reaction. It just appears suddenly to occupy newly created pore volume. The pressure in this material at TIMEICRESET is specified by input as PRESDRZ. This material arose as an option to simulate the disturbed rock zone surrounding excavations in halite. The time-dependent behavior of disturbed halite is not well understood, but it is considered likely that the porosity will be greater by the time the repository is filled and sealed. This behavior can be modeled very simply as an instantaneous increase in porosity at TIMEICRESET, with the additional pore space filled with gas that, in reality, would have migrated in from the adjacent excavated regions through cracks and borings. More than one DRZ material can be used, each with a different reset pressure (PRESDRZ). If used, it is recommended that pressure in the DRZ material is reset to PRESDRZ = 1 atm (101.325 kPa), the same as in the Waste at TIMEICRESET, so that the newly-introduced gas in the DRZ does not expand and unrealistically flow into the Waste.

Line 7.13. Descriptor. DRZ regions.

One-line (up to 132 characters) descriptor for the following parameters:

Line 7.14. NDRZ.

NDRZ: Number of DRZ material regions.

If NDRZ ≤ 0, the next two lines (7.15 and 7.16) are omitted. If NDRZ > MDRZ (set in the PARAMETER statement), the run will abort.

Line 7.15. Descriptor. DRZ materials.

One-line (up to 132 characters) descriptor for the following parameters:

Line 7.16. (MAT_DRZ(I), I=1, NDRZ), (MAT_DRZNEW(I), I=1, NDRZ).

MAT_DRZ: Original DRZ material type index number, from the first material map.

MAT_DRZNEW: The DRZ material type index number for the material map starting at time TIMEICRESET (Line 7.24); in this material type at time TIMEICRESET, saturations will be adjusted and pressures will be reset to PRESDRZ (Line 7.30).

"Reset" Material.

In this material, conditions will be reset to the initial conditions specified in Section 7.2.6. This differs from DRZ material in that both saturation and pressure are reset at time TIMEICRESET, and they are reset to the Section 7.2.6 conditions. In contrast, in DRZ material, the saturations are adjusted to maintain a fixed brine volume and the pressure is reset to PRESDRZ, rather than to the Section 7.2.6 initial pressure. This material arose as an option to model backfilled regions, which are initially excavations, but become backfill at TIMEICRESET. In this case, the

conditions calculated just prior to TIMEICRESET are inconsequential, and new specified conditions reflecting newly-emplaced backfill and seals are needed; because the backfilled and sealed regions may cover a large number of grid blocks, these new conditions are most conveniently provided in the original conditions in Section 7.2.6.

Line 7.17. Descriptor. "Reset" materials.

One-line (up to 132 characters) descriptor for the following parameters:

Line 7.18. NMATRESET.

NMATRESET: Number of material regions where initial conditions will be reset at time TIMEICRESET to the original initial conditions.

If NMATRESET ≤ 0, the next two lines (7.19 and 7.20) are omitted. If NMATRESET > NMAT, the run will abort.

Line 7.19. Descriptor. "Reset" materials.

One-line (up to 132 characters) descriptor for the following parameters:

Line 7.20. (MATRESET(I), I=1, NMATRESET).

MATRESET: Material type index numbers for materials in which the brine pressure, PO, and brine saturation, SO, will be reset to the original (Section 7.2.6) initial conditions, PINIT and SOINIT, respectively. Waste material index numbers should be included here if PO and SO are to be reset. The material index numbers used should be for the last material map *prior* to TIMEICRESET; this map may be (and generally is) the first map specified (at time START), but if more than one map is specified prior to TIMEICRESET, use the last map immediately before TIMEICRESET.

Borehole Material.

In this material, the solute concentration and solute mass are reset to zero when an intrusion borehole opens. This simulates the removal of radionuclides in both solid and dissolved phases when a drill cuts through the waste. It is a minor adjustment, but easily accomplished in BRAGFLO, so it is done just to make the results reflect reality slightly more accurately. It is used only when transport is activated. However, if transport is not being modeled, lines 7.21 and 7.22 must still be input, although MAT_BOREHOLE can be any number from 0 to NMAT and is not used.

Line 7.21. Descriptor. Borehole material.

One-line (up to 132 characters) descriptor for the following parameters:

Line 7.22. MAT_BOREHOLE.

MAT_BOREHOLE: Material type index number for borehole material, if transport is activated (see Section 7.2.12). If transport is not activated, MAT_BOREHOLE can be any number from 0 to NMAT, but a number must still be input.

Special Material Control and Reset Parameters.

Line 7.23. Descriptor. Reset control parameters.

One-line (up to 132 characters) descriptor for the following parameters:

Line 7.24. TIMEICRESET, ICWASTE.

TIMEICRESET: Time when initial conditions are reset [s or days]. Normally = 0. Used only when START is less than zero. Negative times (START<0) are used in WIPP PA simulations to cover the operational period of the WIPP, prior to the start of the regulatory compliance period, which begins at time zero. The primary objective of using these negative times is to enable realistic pressure distributions in the formations surrounding the WIPP repository to be calculated without doing this in a separate run. Designation of times as positive or negative is largely a question of semantics. All calculations could start at time zero, cover, say, a 20-year operational period and extend to 10,020 years total to cover the 10,000-year compliance period. However, then the plotting and other post-processing would need to deal with a time period of 20 to 10,020 years, instead of the more clearly understandable period of 0 to 10,000 years specified in regulations. Using negative times for the operational period, and omitting this period from plots and reports, makes discussions of the results simpler and more in line with compliance regulations.

No results are printed to the output files until TIMEICRESET. The initial conditions that are always printed to both the ASCII and binary output files are the conditions at TIMEICRESET, *after* all the special materials have been reset to their respective initial conditions.

If TIMEICRESET = START, the ICWASTE must be 0. Otherwise, BRAGFLO will abort with the message:

```
ICWASTE must be 0 when TIMEICRESET = START.
*** ICWASTE error in READMAT.
```

ICWASTE: Flag to indicate that waste initial conditions will differ from the initial conditions specified in Section 7.2.6. This flag overrides any implied reset control indicated by material type indexes in Lines 7.9 - 7.22, but these lines must still be input.

= 1: Initial conditions specified by POWASTEIC and SOWASTEIC (input next) will be used at time START instead of PINIT and SOINIT (from Section 7.2.5).

= 0: Initial conditions PINIT and SOINIT will be used at time START.

If ICWASTE is not 0 or 1, BRAGFLO will neither abort nor warn of an error, but results may be unpredictable.

Line 7.25. Descriptor. Pressure initial conditions.

One-line (up to 132 characters) descriptor for the following parameters:

Line 7.26. (POWASTEIC(I), I=1, NWST).

POWASTEIC(I): Brine pressure in Waste region I at time START, uniform throughout Waste region I [Pa or psi]. Used only when ICWASTE = 1, but NWST values must still be input even if ICWASTE = 0.

Line 7.27. Descriptor. Saturation initial conditions.

One-line (up to 132 characters) descriptor for the following parameters:

Line 7.28. (SOWASTEIC(I), I=1, NWST).

SOWASTEIC: Brine saturation in Waste region I at time START, uniform throughout Waste region I. Used only when ICWASTE = 1, but NWST values must still be input even if ICWASTE = 0.

Line 7.29. Descriptor. Reset DRZ pressure.

One-line (up to 132 characters) descriptor for the following parameters:

Line 7.30. (PRESDRZ(I), I=1, NDRZ).

PRESDRZ(I): Brine pressure to which DRZ region I will be reset at time TIMEICRESET [Pa or psi].

If NDRZ $\leq$ 0, then enter a blank line for Line 7.30.

Line 7.31. Descriptor. Number of times the borehole is to be reset

One-line (up to 132 characters) descriptor for the following parameters:

Line 7.32. NBORERESET

NBORERESET: Number of times at which a borehole (or other material) is to be reset to a new pressure and saturation. See Section 4.17.4 for a description of the subroutine RESETMID and how it is used. For example, if two separate materials were to be reset at two different material changes, then NBORERESET = 2.

If NBORERESET = 0, then Lines 7.33 through 7.40 are not entered

Line 7.33. Descriptor. NBORETIME(I), NMATBORE(I), MATBORE(I,NMATBORE), I = intrusion time index.

One-line (up to 132 characters) descriptor for the following parameters:

Line 7.34 is repeated NBORERESET times.

Line 7.34. NBORETIME(I), NMATBORE(I), MATBORE(I,NMATBORE).

NBORETIME: Index of the material change at which a borehole (or other material) is to be reset to a new pressure and saturation. 1 $\leq$ NBORETIME $\leq$ NMATTIMES.

NMATBORE: Number of materials to be changed at the intrusion time.

(MATBORE(I),I=1,NMATBORE): Material type numbers that are to be reset at NBORETIME.

Line 7.35. Descriptor. Borehole reset pressure.

One-line (up to 132 characters) descriptor for the following parameters:

Line 7.36 is repeated NBORERESET times.

Line 7.36. PORESET(I). I = intrusion index.

PORESET(I): Reset pressure [Pa or psi] for the materials identified in Line 7.34. All materials identified in MATBORE(I) are reset to PORESET(I) for a given intrusion index. Each material cannot be reset to a different pressure. If less than zero, the pressure will not be reset on the specified materials.

Line 7.37. Descriptor. Borehole reset saturation.

One-line (up to 132 characters) descriptor for the following parameters:

Line 7.38 is repeated NBORERESET times.

Line 7.38. SORESET(I). I = intrusion index.

SORESET(I): Reset saturation [dimensionless] for the materials identified in Line 7.34. All materials identified in MATBORE(I) are reset to SORESET(I) for a given intrusion index. Each material cannot be reset to a different saturation. If less than zero, the saturation will not be reset on the specified materials.

Line 7.39. Descriptor. ICHEM.

One-line (up to 132 characters) descriptor for the following parameters:

Line 7.40 is repeated NBORERESET times.

Line 7.40. ICHEM(I). I = intrusion index.

ICHEM: Flag which determines whether concentrations of Fe, cellulosics, and MgO are set to zero after an intrusion. If ICHEM = 1 then concentrations are set to zero, otherwise they are not.

7.2.8.2 Material Property Data.

In this section, material properties are input for each of the NMAT materials in the material map. Properties used include relative permeability and capillary pressure model parameters, intrinsic permeability values, porosities, and compressibilities.

Line 7.41. Descriptor. Relative permeability and capillary pressure model parameters.

If some material type numbers less than NMAT are not actually used in any material maps, NMAT property values must still be read in. If there are fewer than NMAT lines of property data, BRAGFLO will abort as a result of an input error while trying to read character data into INTEGER and REAL variables.

One-line (up to 132 characters) descriptor for the following parameters:

Line 7.42 is repeated NMAT times.

Line 7.42. I, XLAMDA(I), SBR(I), SGR(I).

I: Material type number.

XLAMDA(I): Pore-size distribution parameter, λ, for Brooks-Corey and van Genuchten-Parker relative permeability and capillary pressure models. The van Genuchten-Parker model uses a parameter, m, which is obtained from the Brooks-Corey parameter, λ:

$m = \lambda /(1+\lambda,)$.

SBR(I): Residual brine saturation, S_{br}.

SGR(I): Residual gas saturation, S_{gr}. The original Brooks-Corey and van Genuchten-Parker models do not use a residual gas saturation, but a value must still be input.

Line 7.43. Descriptor. More relative permeability and capillary pressure model parameters.

One-line (up to 132 characters) descriptor for the following parameters:

Line 7.44 is repeated NMAT times.

Line 7.44. I, SBMIN(I), POMIN(I), PCMAX(I), PCT_A(I), PCT_EXP(I), KRP(I), KPC(I), KPT(I).

I: Material type number.

SBMIN(I): Minimum brine saturation when using capillary pressure model number KPC(I) = 3. It is otherwise not used; however, a value must still be read in, and SBMIN(I) > SBR(I). If SBMIN(I) < SBR(I), BRAGFLO will abort, even if KPC(I) ≠ 3. Recommended value: 1.05 × SBR(I).

POMIN(I): Minimum brine pressure [Pa or psi]. Used to adjust capillary pressure when capillary pressure model KPC(I) = 3 is used. If KPC(I) ≠ 3, POMIN(I) is not used and any value can be input for POMIN(I); however, some value must be input regardless of the capillary pressure model used. If KPC(I) = 3, a value of POMIN(I) = 1.01325×10^5 Pa is recommended.

PCMAX(I): Maximum capillary pressure that can be used when capillary pressure model KPC(I) = 2 or 3 is used [Pa or psi]. A value of PCMAX(I) = 1.0×10^8 Pa is recommended. If KPC(I) = 1, 4, or 5, a value must still be read in, but PCMAX(I) is not used.

PCT_A(I): Constant, a, in function relating threshold capillary pressure, P_{ct}, to permeability, k:

$P_{ct} = a\, k^{\eta}$. Gives P_{ct} for the Brooks-Corey models. In the van Genuchten-Parker model, a capillary pressure constant, P_o, is used; it is calculated in BRAGFLO by equating the capillary pressure from each of the two models at an effective saturation, S_{e2}, of 0.5 and solving the expression for P_o.

PCT_EXP(I): Exponent, η, in function relating threshold capillary pressure, P_{ct}, to permeability [dimensionless].

KRP(I): Relative permeability model number:

= 1: Modified van Genuchten-Parker model; modified to use a nonzero residual gas saturation.

= 2: Original Brooks-Corey model, with zero residual gas saturation.

= 3: 1st Modified Brooks-Corey model; modified to use a residual gas saturation in calculating the effective saturation for both wetting and non-wetting phase relative permeabilities.

= 4: 2nd Modified Brooks-Corey model; modified to use a residual gas saturation in calculating the effective saturation for the non-wetting phase relative permeability only.

= 5: Linear relative permeabilities (model A): $k_{rb} = S_{eg}$; $k_{rg} = 1 - S_{eg}$, where:

$S_{eg} = (S_b - S_{br})/(1 - S_{gr} - S_{br})$ is the effective saturation using residual gas saturation.

= 6: Linear relative permeabilities (model B): $k_{rb} = S_e$; $k_{rg} = S_{eg}$, where S_{eg} is the same as given above for KRP(5), and $S_e = (S_b - S_{br})/(1 - S_{br})$ is the effective saturation without the gas saturation dependence.

= 7: Linear relative permeabilities (model D): $k_{rb} = k_{rg} = 1$.

= 8: Original van Genuchten-Parker model, with zero residual gas saturation.

= 11: Open Cavity modification for linear relative permeabilities between residual saturation and residual saturation plus a tolerance. The additional parameter TOL (*tol*) needed for this model is given below in Line 7.48.

= 12: Waste Area modification based on Brooks-Corey model, modified to use $S_{\min}$ (a cut off in saturation that is considered numerically dry) and $S_{eff\,\min}$ (a small tolerance which pushes the singularity in the capillary pressure equation to a saturation slightly below $S_{\min}$) instead of the residual brine saturation. The additional parameter SOCEFFMIN ($S_{eff\,\min}$) needed for this model is given below in Line 7.48. The additional parameter SMIN ($S_{\min}$) needed for this model is given below in Line 9.12.

Note that models 9, and 10 are specific to a regression test case and will not be discussed here.

KPC(I): Capillary pressure model number:

= 1: No special treatment. Numerical problems may occur as brine saturation approaches residual brine saturation and capillary pressure tends to infinity. Below residual brine saturation, the capillary pressure is zero.

= 2: Fixed maximum capillary pressure of PCMAX(I), thereby avoiding potential problems that might be encountered using KPC(I) = 1. BRAGFLO computes a minimum brine saturation at which the capillary pressure equals PCMAX; below this minimum brine saturation, the capillary pressure is PCMAX. This model is recommended.

= 3: Variable maximum capillary pressure. This model has not been fully tested, and its theoretical basis is uncertain. Use this model at your own risk.

= 4: Capillary pressure fixed at PTHRESH(I), which may be zero.

= 5: Linear capillary pressures.

KPT(I): Flag indicating whether threshold capillary pressure will be continuously updated as a function of dynamically varying permeability or fixed in time for a given material.:

= 0: Threshold capillary pressure is fixed in time for material I; computed in BRAGFLO using the function: $P_{ct} = a\, k^{\eta}$, as described above for PCT_A(I) and PCT_EXP(I). The intrinsic permeability in the *x*-direction, XKX(I) (input on Line 7.36), is used for *k*.

= 1: Threshold capillary pressure varies in time for material I; computed in BRAGFLO using the function: $P_{ct} = a\, k^{\eta}$, as described above for PCT_A(I) and PCT_EXP(I). Brine permeability in the *x*-direction is used for *k*; it varies as a function of time-dependent porosity in materials that undergo fracturing or creep closure. Fracturing is described below starting at Line 7.37. Creep closure is discussed in Section 7.2.11.

Line 7.45. Descriptor. Intrinsic properties.

One-line (up to 132 characters) descriptor for the following parameters:

Line 7.46 is repeated NMAT times.

Line 7.46. I, XKX(I), YKY(I), ZKZ(I), PORREFROCK(I), CROCK(I)

I: Material type number.

XKX(I): Intrinsic permeability of material I in the *x*-direction [m^2 or darcy].

YKY(I): Intrinsic permeability of material I in the *y*-direction [m^2 or darcy].

ZKZ(I): Intrinsic permeability of material I in the *z*-direction [m^2 or darcy].

PORREFROCK(I): Porosity of material I at a reference pressure equal to the initial pressure, PINIT, which may be different in each grid block [fraction]. If material I is to undergo creep closure (see Section 7.2.11.), PORREFROCK(I) is not used unless material I is used before TIMEICRESET, when creep closure is not yet activated. If a material that will undergo creep closure is used before TIMEICRESET, an appropriate value of PORREFROCK(I) must be input. If such a material is not used

until after TIMEICRESET (this is normally the case in WIPP PA), then the input value of PORREFROCK(I) is not used, and any value can be input. If creep closure is later turned off in this material because pressure or time limitations are exceeded, BRAGFLO resets PORREFROCK(I) at the value of porosity that exists at the time when closure is turned off; the reference pressure is reset at the same time and is equal to the current brine pressure in the material or grid block.

CROCK(I): Pore compressibility of material I (i.e., bulk rock compressibility / porosity) at a reference pressure equal to the initial pressure, PINIT [Pa^{-1} or psi^{-1}].

Various checks are done on the material properties input. Errors or inconsistencies may cause BRAGFLO to abort with error messages printed to the screen and to the .sum file.

Line 7.47. Descriptor. Tol and SOCEFFMIN for permeability models 11 and 12.

One-line (up to 132 characters) descriptor for the following parameters:

Line 7.48. TOL, SOCEFFMIN.

TOL: Tolerance over which the relative permeability changes from zero to 1 for KRP = 11.

SOCEFFMIN: Small tolerance which pushes the singularity in the capillary pressure equation to a saturation slightly below S_{min} for KRP = 12.

Line 7.49. Descriptor. Number of materials to use the smooth permeability transition model.

See Section 4.18 for a complete description of this module.

One-line (up to 132 characters) descriptor for the following parameters:

Line 7.50. NMATSP

NMATSP: Number of materials which will use the smooth permeability transition model. See Section 4.18 for a complete description of this module.

Line 7.51. Descriptor. MATSP, MATSPF, TEND, TCHANGE.

One-line (up to 132 characters) descriptor for the following parameters:

Line 7.52 is repeated NMATSP times.

Line 7.52. MATSP(I), MATSPF(I), TEND(I), TCHANGE(I).

MATSP(I): Starting material type number for the material in which to use the smooth permeability model. See Section 4.18 for a complete description of this module.

MATSPF(I): Final material type number that material MAPSP(I) will become at the end of the smoothed permeability change. See Section 4.18 for a complete description of this module.

TEND(I): Time at which material MATSP(I) will have completed its smooth change to material MATSPF(I). See Section 4.18 for a complete description of this module.

TCHANGE(I): Time over which the material change will occur. From TCHANGE(I) and TEND(I), the time at which the material change begins TINIT(I) = TEND(I) – TCHANGE(I). See Section 4.18 for a complete description of this module.

Line 7.53. Descriptor. NSMPRMC, SMPRMC.

One-line (up to 132 characters) descriptor for the following parameters:

Line 7.54 is repeated NMATSP times.

Line 7.54. NSMPRMC(I), SMPRMC(I).

NSMPRMC(I): Number of coefficients, i.e. order of the polynomial + 1, to be used in the smooth permeability model. See Section 4.18 for a complete description of this module.

(SMPRMC(I,J),J=1,NSMPRMC(I)): Coefficients a_j of the polynomial that smoothly changes permeability from that of the material MATSP(I) to that of MATSPF(I). See equation (200) and the supporting text of Section 4.18 for a complete description.

7.2.8.3 Fracture Model.

The rock fracture model in BRAGFLO allows the porosity and permeability to increase in a fractured network as pore pressure increases above a threshold value. The implementation uses a pressure-dependent pore compressibility (*i.e.*, bulk rock compressibility / porosity) to determine fracture porosity. Permeability in the fractured layer is varied with porosity according to a power law function:

$$k = k_o \left[\frac{\phi_f}{\phi_o} \right]^n ,$$

where k = fractured permeability [m^2];

k_o = intact permeability [m^2];

ϕ_f = fractured porosity [m^3 void/m^3 rock];

ϕ_o = intact porosity [m^3 void/m^3 rock];

n = exponent [dimensionless].

Line 7.55. Descriptor. Fracture model control.

One-line (up to 132 characters) descriptor for the following parameters:

Line 7.56. KFRACTURE.

KFRACTURE: Logical flag indicating whether the fracture model will be used and whether the fracture model parameters will be read in.

= .TRUE.: Use the fracture model in BRAGFLO and read in parameters.

= .FALSE.: Do not use the fracture model, and do not read in fracture model parameters.

Lines 7.57 -7.60 are input *only* if KFRACTURE = .TRUE.

Line 7.57. Descriptor. Number of materials in which the fracture model can be applied.

One-line (up to 132 characters) descriptor for the following parameters:

Line 7.58. NFRAC.

NFRAC: Number of materials in which the fracture model can be applied.

Line 7.59 and 7.60 are repeated NFRAC times.

Line 7.59. Descriptor. Fracture model parameters.

One-line (up to 132 characters) descriptor for the following parameters:

Line 7.60. I, FRPI(I), FRPF(I), FRPHIMAX(I), FRPRMEXP(I), IFRX(I), IFRY(I), IFRZ(I), LFPC(I).

I: Material type number for the material in which fracturing can occur.

FRPI(I): Pressure increment above the initial pressure, PINIT, at which fracturing will initially occur. [Pa or psi]. Typical value: 1.39×10^6 Pa.

FRPF(I): Pressure increment above the fracture initiation pressure (*i.e.*, increment above PINIT + FRPI), at which the fracture is fully-developed, *i.e.*, the porosity of the fractured material is at its maximum [Pa or psi]. Typical value: 2.5×10^6 Pa.

FRPHIMAX(I): [m^3 void/m^3 rock] Maximum allowable fracture porosity. The pressure-dependent porosity will be limited to this value. Typical value: 0.10.

FRPRMEXP(I): Exponent, *n*, in the permeability-porosity power law relationship [dimensionless]. Typical value: 9.5.

IFRX(I): Flag to indicate whether *x*-direction permeability will be calculated for fractured material. Recommended value: 1.

= 1: Do calculate permeability for fractured material.

= 0: Permeability will remain the same as the intact permeability for material I.

IFRY(I): Flag to indicate whether *y*-direction permeability will be calculated for fractured material. Recommended value: 0.

= 1: Do calculate permeability for fractured material.

= 0: Permeability will remain the same as the intact permeability for material I.

IFRZ(I): Flag to indicate whether *z*-direction permeability will be calculated for fractured material. Recommended value: 0.

= 1: Do calculate permeability for fractured material.

= 0: Permeability will remain the same as the intact permeability for material I.

LFPC(I): Flag to indicate whether to use constant pressure during fracturing model. Recommended value: F.

= T: Use constant pressure during fracturing model.

= F: Use original fracture model.

7.2.8.4 Klinkenberg Effect.

At low pressures and in low-permeability materials, the gas phase intrinsic permeability can be significantly higher than the liquid phase intrinsic permeability. This is the Klinkenberg effect. The gas or non-wetting phase permeability, k_{nw}, can be correlated to the brine or wetting phase permeability, k_w, by the Klinkenberg equation:

$$k_{nw} = k_w \left(1 + b / P \right)$$

where

k_w = brine phase intrinsic permeability [m^2],

P = brine pressure [Pa],

b = Klinkenberg coefficient [Pa]

$$= \text{BKLINK} \bullet \left(k_w \right)^{\text{EXPLINK}},$$

BKLINK = linear parameter in Klinkenberg equation [Pa],

EXPKLINK = exponent in Klinkenberg equation [dimensionless].

It is assumed in BRAGFLO that input values of intrinsic permeability (Line 7.46) are brine phase intrinsic permeabilities. If the Klinkenberg effect is modeled, gas phase intrinsic permeabilities are obtained from the Klinkenberg equation from the input values of brine phase intrinsic permeability. If the fracture model is also activated (Line 7.38; KFRACTURE = .TRUE.), brine phase intrinsic permeabilities are calculated first, using the fracture model parameters, and then gas phase intrinsic permeabilities are calculated using the Klinkenberg equation.

Line 7.61. Descriptor. Klinkenberg effect control parameter.

One-line (up to 132 characters) descriptor for the following parameters:

Line 7.62. KLINK.

KLINK: Logical flag controlling use of Klinkenberg effect:

= .TRUE.: Do include Klinkenberg effect and read in the two parameters.

= .FALSE.: Do not include Klinkenberg effect and do not read in the two parameters.

Lines 7.45 and 7.46 are read in only if KLINK = .TRUE.

Line 7.63. Descriptor. Klinkenberg parameters.

One-line (up to 132 characters) descriptor for the following parameters:

Line 7.64. BKLINK, EXPKLINK.

BKLINK: Linear parameter in Klinkenberg equation [Pa]. Recommended value: 0.336 Pa.

EXPKLINK: Exponent in Klinkenberg equation [dimensionless]. Recommended value: -0.336.

7.2.9 Fluid Properties.

This section discusses input for fluid properties and parameters that control their use. BRAGFLO has two fluids: brine and gas. Brine is composed of water and an unspecified solute, the composition of which is of no consequence in BRAGFLO. The gas is a mixture of any of six gases: hydrogen (H_2), carbon dioxide (CO_2), methane (CH_4), nitrogen (N_2), oxygen (O_2), and hydrogen sulfide (H_2S). Brine is treated as an ideal fluid. Gases can be treated either as ideal gases or as real gases using the Redlich-Kwong-Soave equation of state. As an option, gas can dissolve in brine; using either a Henry's law treatment or an unreliable, untested bubble point calculation. Gas dissolution will not be included in the WIPP certification compliance calculations. Additionally, as mentioned in Section 4.20, the gas phase is assumed to be all H_2.

Line 8.0. Descriptor. Gravity Constant, GSTD, and Gas Constant, R.

One-line (up to 132 characters) descriptor for the following parameters:

Line 8.1. GSTD, R.

GSTD: Gravity Acceleration Constant at WIPP [m/s^2 or ft/day^2]

R: Gas Constant [J/(gm-mol*K) or Btu/(lbmol*R)]

Line 8.2. Descriptor. Reference conditions.

One-line (up to 132 characters) descriptor for the following parameters:

Line 8.3. TREF, PREF.

TREF: Reference temperature for standard densities [K or °R].

PREF: Reference pressure for standard densities [Pa or psi].

Line 8.4. Descriptor. Brine property parameters.

One-line (up to 132 characters) descriptor for the following parameters:

Line 8.5. SALT, DENOSC, KGSAT, IDGAS, BRCOMP, WMSALT, WMH2O.

SALT: Brine salinity [wt % solute].

DENOSC: Density of brine at reference conditions [kg/m^3 or lb/ft^3].

KGSAT: Flag to indicate initial gas content of brine:

= 0: Brine is initially gas-free.

= 1: Brine is initially saturated with gas. This is the recommended input value.

IDGAS: Flag to indicate treatment of dissolved gas in brine:

= 0: Gas does not dissolve in brine.

= 1: Gas does dissolve in brine, using bubble point tracking.

= 2: Gas does dissolve in brine, using Henry's law treatment.

BRCOMP: Brine compressibility, β [Pa^{-1} or psi^{-1}]. The compressibility of WIPP brine is 2.5×10^{-10} Pa^{-1}. The equation BRAGFLO uses to evaluate brine density is:

$$\rho = \rho_o \exp[\beta(p - p_o)]$$

where:

p = brine pressure [Pa],

p_o = reference pressure, PREF (Line 8.3) [Pa],

ρ_o = brine density, DENOSC, at reference pressure [kg/m^3].

WMSALT: Molecular weight of salt component of the brine [kg/gm-mol or lb/lbmol]. Assumed to have the molecular weight of NaCl.

WMH2O: Molecular weight of water component of the brine [kg/gm-mol or lb/lbmol].

NOTE: If IDGAS = 0 (Line 8.5), then no additional gas dissolution parameters are read in (i.e., Do not enter lines 8.5.1-8.5.4). IDGAS = 0 capability is QA'd for use in WIPP Compliance Calculations.

NOTE: If IDGAS = 1 (Line 8.5), then input Lines 8.5.1- 8.5.4. IDGAS = 1 capability is not QA'd or used for WIPP Compliance Calculations.

NOTE: If IDGAS = 2 (Line 8.5), then input Lines 8.5.1- 8.5.2. Also, LVARSWTCH = T should be used; see Line 6.22. IDGAS = 2 capability is not QA'd or used for WIPP Compliance Calculations.

Line 8.5.1. Descriptor. Gas solubility parameters.

The input parameters are coefficients in the empirical correlation relating gas solubility to gas partial pressure. This correlation is commonly used, but it is used in BRAGFLO specifically to account for the solubility of hydrogen in WIPP brine.

$$\ln x_g = D_0 + D_1 \ln P$$

where

x_g = mole fraction of gas in solution in brine.

D_0 = adjustable fitting coefficient. For hydrogen dissolved in 5 N NaCl brine, $D_0 = 10.0789$.

D_1 = adjustable fitting coefficient. For hydrogen dissolved in 5 N NaCl brine, $D_1 = 0.8205$.

P = partial pressure of the gas of interest in the gas phase [MPa].

The bubble point tracking treatment used in BRAGFLO is believed to be flawed, and its use is not recommended. If a user wishes to investigate this feature, the logic can be retained while the bubble point tracking is effectively turned off by using input values for RSOD0 of -100. and RSOD1 of 5.

One-line (up to 132 characters) descriptor for the following parameters:

Line 8.5.2. SGBUBMIN, RSOD0, RSOD1.

SGBUBMIN: Minimum gas saturation required for calculating new bubble point. Recommended value: -1.0.

RSOD0: Gas solubility correlation coefficient, D_0.

RSOD1: Gas solubility correlation coefficient, D_1.

Line 8.5.3. Descriptor. Slopes of parameters at pressures greater than the bubble pressure.

One-line (up to 132 characters) descriptor for the following parameters:

Line 8.5.4. BSLOPE, RSLOPE, VSLOPE.

BSLOPE: Slope of the brine formation volume factor versus pressure curve for undersaturated brine (pressure above initial brine bubble point pressure): d (formation volume factor) / dP [Pa^{-1} or psi^{-1}]. Recommended value: 0.

RSLOPE: Slope of the solution gas-brine ratio versus pressure curve for undersaturated brine (pressure above initial brine bubble point pressure): d (R_{so}) / dP [Pa^{-1} or ft^3/(bbl psi)]. Recommended value: 0.

VSLOPE: Slope of the brine viscosity versus pressure curve for undersaturated brine (pressure above initial brine bubble point pressure): d (brine viscosity) / dP [s or cP/psi]. Recommended value: 0.

Line 8.5.1. Descriptor. Henry's law constant.

One-line (up to 132 characters) descriptor for the following parameters:

Line 8.5.2. HENRYC.

HENRYC: Henry's law constant [Pa/mol fraction gas dissolved in brine]. If selected, i.e. when IDGAS = 2, a single value is used for all gases, independent of the actual composition, at a fixed temperature. WIPP PA uses 4.0×10^{10} Pa/mol fraction gas. BRAGFLO assumes that the dissolved gas is N_2, regardless of the actual composition of the gas phase, which WIPP PA generally assumes to be pure H_2. These conflicting assumptions are used because the gas found dissolved in native WIPP brines is mostly N_2, whereas the gas generated in the waste, especially by anoxic corrosion of

ferrous metals, is mostly H_2. To deal with this situation correctly would require tracking multiple gas components in both the gas phase and in the brine phase. Although BRAGFLO is capable of tracking multiple components in the gas phase, it cannot currently do this in the brine phase, and the computational effort to do so cannot be justified to correct the small errors resulting from these assumptions.

Line 8.6. Descriptor. Fluid viscosities.

BRAGFLO does not account for the effects of pressure and composition on viscosity. A single constant value each for brine viscosity and gas viscosity at a temperature, TREF, is read in.

One-line (up to 132 characters) descriptor for the following parameters:

Line 8.7. VISO, VISG.

VISO: Brine viscosity [Pa s or cP].

VISG: Gas viscosity [Pa s or cP].

Line 8.8. Descriptor. Gas density flag.

One-line (up to 132 characters) descriptor for the following parameters:

Line 8.9. INTERPDENG.

INTERPDENG: Flag indicating how gas density will be calculated:

= 1: Interpolate from table set up by BRAGFLO using the Redlich-Kwong-Soave equation of state. This is a very fast and efficient means for calculating gas density accurately, but it can be used only when a single pure gas is used.

= 0: Calculate gas density using the Redlich-Kwong-Soave equation of state. This option provides the greatest accuracy and can be used with any combination of the six gases that can be modeled in BRAGFLO: H_2, CO_2, CH_4, N_2, O_2, and H_2S. However, it is by far the slowest method for calculating gas density. The gases that are available is severely limited because of the lack of binary interaction coefficients for other gases.

= -1: Interpolate from table set up by BRAGFLO using the ideal gas law. This option is made available as a counterpart to INTERPDENG = 1, but because the ideal gas law is so simple and fast, setting up an interpolation table is generally not recommended.

= -2: Use ideal gas law. This option is the fastest method for calculating gas density but is not as accurate as the Redlich-Kwong-Soave equation of state. Other gases, in addition to the six currently available, could easily be added because the only data required is molecular weight. When using the multi-component gas transport option (Section 7.2.12), the ideal gas law should always be used

because the transport model introduces enough inaccuracies that the substantial additional computing time required to use INTERPDENG = 0 is not justified.

If a single pure gas such as hydrogen is used, it is best to interpolate from a table, because it is much faster computationally. In this case, BRAGFLO sets up a table of calculated gas densities using the Redlich-Kwong-Soave equation of state at fixed pressure intervals of 10,000 Pa. The number of table entries is specified in the PARAMETER statement by the constant, NPINT. Intervals of 10,000 Pa provides a sufficiently smooth density curve versus pressure. If much larger intervals are used, results can be noticeably affected; pressure vs. time plots, for example, will acquire a staircase appearance and the results may be seriously in error. To ensure that table values cover the full range of expected pressures, NPINT must be large. It is currently set at NPINT = 10,000, giving a maximum table entry of 100 MPa. If memory is limited, this can be safely reduced to a more practical limit of, say, 20 MPa, or NPINT = 2,000. If pressures higher than the maximum table entry are encountered, BRAGFLO will extrapolate from the two highest entries. If the pressure, P_g, is between 0 and 10,000 Pa, the density is calculated as (P_g/10000) times the density at 10,000 Pa. If the pressure is less than zero, the density is set to 1/10 of the density at 10,000 Pa.

If more than one gas is used, interpolation is not possible, and the full Redlich-Kwong-Soave (RKS) equation of state (EOS) (INTERPDENG = 0) must be solved each time a new density is needed.

If INTERPDENG $\geq$ 0 then the RKS EOS has been selected. The required RKS parameters are specified on Lines 8.16-8.26.

Line 8.10. Descriptor. Gas composition.

One-line (up to 132 characters) descriptor for the following parameters:

Line 8.11. (YGAS(I), I=1, MGAS).

YGAS: Initial mole fraction of each of the MGAS gases currently available in BRAGFLO (MGAS = 6); set in the PARAMETER statement. If the gas transport option is used, this composition can change during the run. If gas transport is not used, this initial gas composition will remain fixed for all time. All MGAS entries are required.

YGAS(1) = mole fraction of H_2 [dimensionless].

YGAS(2) = mole fraction of CO_2 [dimensionless].

YGAS(3) = mole fraction of CH_4 [dimensionless].

YGAS(4) = mole fraction of N_2 [dimensionless].

YGAS(5) = mole fraction of H_2S [dimensionless].

YGAS(6) = mole fraction of O_2 [dimensionless].

Line 8.12. Descriptor. Gas component molecular weights.

One-line (up to 132 characters) descriptor for the following parameters:

Line 8.13. (MWGAS(I), I=1, MGAS)

WMGAS: Molecular weights of the 6 possible gas phase components allowed by BRAGFLO. All MGAS entries are required.

MWGAS(1) = Molecular Weight of H_2 [kg/gm-mol or lb/lbmol].

MWGAS(2) = Molecular Weight of CO_2 [kg/gm-mol or lb/lbmol].

MWGAS(3) = Molecular Weight of CH_4 [kg/gm-mol or lb/lbmol].

MWGAS(4) = Molecular Weight of N_2 [kg/gm-mol or lb/lbmol].

MWGAS(5) = Molecular Weight of H_2S [kg/gm-mol or lb/lbmol].

MWGAS(6) = Molecular Weight of O_2 [kg/gm-mol or lb/lbmol].

Line 8.14. Descriptor. Number of gas components used and index number.

One-line (up to 132 characters) descriptor for the following parameters:

Line 8.15. NGAS, N1GAS.

NGAS: Number of gases actually being used in the problem.

N1GAS: Gas number from the current list: 1 = H_2, 2 = CO_2, 3 = CH_4, 4 = N_2, 5 = H_2S , 6 = O_2,. This is used only if NGAS = 1; otherwise, it can be any number. This parameter is used to simplify the gas density calculation when only one gas is present.

Line 8.16. Descriptor. RKS specified- TC: for H_2, CO_2, CH_4, N_2, H_2S, O_2.

One-line (up to 132 characters) descriptor for the following parameters:

Line 8.17. (TC(I), I=1, MGAS).

TC: Critical temperatures of the 6 possible gas phase components allowed by BRAGFLO. All MGAS entries are required.

TC(1) = Critical Temperature of H_2 [K or R].

TC(2) = Critical Temperature of CO_2 [K or R].

TC(3) = Critical Temperature of CH_4 [K or R].

TC(4) = Critical Temperature of N_2 [K or R].

TC(5) = Critical Temperature of H_2S [K or R].

TC(6) = Critical Temperature of O_2 [K or R].

Line 8.18. Descriptor. RKS specified- PC for H_2, CO_2, CH_4, N_2, H_2S, O_2.

One-line (up to 132 characters) descriptor for the following parameters:

Line 8.19. (PC(I), I=1, MGAS).

PC: Critical pressure of the 6 possible gas phase components allowed by BRAGFLO. All MGAS entries are required.

PC(1) = Critical Pressure of H_2 [Pa or psi].

PC(2) = Critical Pressure of CO_2 [Pa or psi].

PC(3) = Critical Pressure of CH_4 [Pa or psi].

PC(4) = Critical Pressure of N_2 [Pa or psi].

PC(5) = Critical Pressure of H_2S [Pa or psi].

PC(6) = Critical Pressure of O_2 [Pa or psi].

Line 8.20. Descriptor. RKS specified- ACEN for H_2, CO_2, CH_4, N_2, H_2S, O_2.

One-line (up to 132 characters) descriptor for the following parameters:

Line 8.21. (ACEN(I), I=1, MGAS).

ACEN: Acentric Factors for the 6 possible gas phase components allowed by BRAGFLO. All MGAS entries are required.

ACEN(1) = Acentric factor for H_2 [dimensionless].

ACEN(2) = Acentric factor for CO_2 [dimensionless].

ACEN(3) = Acentric factor for CH_4 [dimensionless].

ACEN(4) = Acentric factor for N_2 [dimensionless].

ACEN(5) = Acentric factor for H_2S [dimensionless].

ACEN(6) = Acentric factor for O_2 [dimensionless].

Line 8.22. Descriptor. RKS specified- Special properties for H_2.

One-line (up to 132 characters) descriptor for the following parameters:

Line 8.23. TCH2, PCH2, WMH2.

TCH2: Special critical temperature for H_2 [K or R].

PCH2: Special critical pressure for H_2 [Pa or psi].

WMH2: Special molecular weight for H_2 [kg/gm-mol or lb/lbmol].

Line 8.24. Descriptor. RKS specified- OMEGAA and OMEGAB constants.

One-line (up to 132 characters) descriptor for the following parameters:

Line 8.25. OMEGAA OMEGAB.

OMEGAA: RKS constant [dimensionless].

OMEGAB: RKS constant [dimensionless].

Line 8.26. Descriptor. RKS specified- Binary Interaction Parameters.

One-line (up to 132 characters) descriptor for the following parameters:

Line 8.26.1. Descriptor. RKS specified- Binary Interaction Parameters for H_2.

One-line (up to 132 characters) descriptor for the following parameters:

Line 8.26.2. AKIJ(1,1:MGAS) = Binary Interaction Parameter for H_2 [dimensionless].

H_2 interaction with H_2, CO_2, CH_4, N_2, H_2S, O_2, respectively.

Line 8.26.3. Descriptor. RKS specified- Binary Interaction Parameters for CO_2.

One-line (up to 132 characters) descriptor for the following parameters:

Line 8.26.4. AKIJ(2,1:MGAS) = Binary Interaction Parameter for CO_2 [dimensionless].

CO_2 interaction with H_2, CO_2, CH_4, N_2, H_2S, O_2, respectively.

Line 8.26.5. Descriptor. RKS specified- Binary Interaction Parameters for CH_4.

One-line (up to 132 characters) descriptor for the following parameters:

Line 8.26.6 AKIJ(3,1:MGAS) = Binary Interaction Parameter for CH_4 [dimensionless].

CH_4 interaction with H_2, CO_2, CH_4, N_2, H_2S, O_2, respectively.

Line 8.26.7. Descriptor. RKS specified- Binary Interaction Parameters for N_2.

One-line (up to 132 characters) descriptor for the following parameters:

Line 8.26.8. AKIJ(4,1:MGAS) = Binary Interaction Parameter for N_2 [dimensionless].

N_2 interaction with H_2, CO_2, CH_4, N_2, H_2S, O_2, respectively.

Line 8.26.9. Descriptor. RKS specified- Binary Interaction Parameters for H_2S.

One-line (up to 132 characters) descriptor for the following parameters:

Line 8.26.10. AKIJ(5,1:MGAS) = Binary Interaction Parameter for H_2S [dimensionless].

H_2S interaction with H_2, CO_2, CH_4, N_2, H_2S, O_2, respectively.

Line 8.26.11. Descriptor. RKS specified- Binary Interaction Parameters for O_2.

One-line (up to 132 characters) descriptor for the following parameters:

Line 8.26.12. AKIJ(6,1:MGAS) = Binary Interaction Parameter for O_2 [dimensionless].

O_2 interaction with H_2, CO_2, CH_4, N_2, H_2S, O_2, respectively.

7.2.10 Chemical Reaction Parameters

These parameters govern the chemical reactions that are modeled in BRAGFLO. THE AVERAGE STOICHIOMETRY MODEL IS THE QUAIFIED GAS GENERATION MODEL TO BE USED FOR WIPP COMPLIANCE CALCULATIONS. This is explained fully in Section 4.13. These reactions take place only in the Waste Areas. Cellulose is approximated by the pseudo- molecule,, $[C_6H_{10}O_5/6]$, having a molecular weight of 27.023 x 10^{-3} [kg/gm-mol]. The gas produced or consumed in these reactions is assumed to have the physical properties of hydrogen.

Line 9.1. Descriptor. Chemical Reaction Parameters.

One-line (up to 132 characters) descriptor for the following parameters:

Line 9.2. IGASVAR.

IGASVAR: Gas generation reaction flag:

= 0: No Fe or $[C_6H_{10}O_5]/6$ consumption and no gas generation.

= 1: Fe and $[C_6H_{10}O_5]/6$ consumption with gas generation (Average Stoichiometry Model. This is the qualified option for WIPP compliance calculations.).

= 2: Reaction path gas generation model. (Not yet available).

NOTE: If IGASVAR = 0 (Line 9.2), then no more chemical reaction parameters are input; go to Section 7.2.11. Lines 9.19-9.22 must be entered even if IGASVAR = 0.

NOTE: If IGASVAR = 1 (Line 9.2), then input Lines 9.3-9.12. IGASVAR = 1 capability is QA'd and used for WIPP Compliance Calculations.

NOTE: If IGASVAR = 2 (Line 9.2), then skip to Line 9.13. IGASVAR = 2 capability is not available.

Line 9.3. Descriptor. Reaction rate constants for brine-inundated conditions.

One-line (up to 132 characters) descriptor for the following parameters:

Line 9.4. RK(1), RK(2), LINTRIN.

RK(1): Corrosion reaction rate constant under brine-inundated conditions [gm-mol Fe/(s m^3) or lbmol Fe/(day ft^3)], unless LINTRIN = .TRUE. (see below) and then the units should be [gm-mol Fe/(s kg)].

RK(2): Biodegradation reaction rate constant under brine-inundated conditions [gm-mol $[C_6H_{10}O_5]/6$ /(s m^3) or lbmol $[C_6H_{10}O_5]/6$ /(day ft^3)], unless LINTRIN = .TRUE. (see below) and then the units should be [gm-mol $[C_6H_{10}O_5]/6$ /(s kg)].

LINTRIN: Parameter to decide whether to use intrinsic or extrinsic rates.

= .TRUE.: Then the chemical rates are multiplied by the initial concentration of the consumed material, on an element by element basis. For example in CORSAT and CORHUM, RK(1) would be multiplied by the initial concentration of Fe in the element in which the rate is being calculated. In this case the units of RK(1) in the input file should be [gm-mol Fe/(s kg)] and not [gm-mol Fe/(s m^3)]. This option is for iron corrosion, biodegradation, and MgO hydration and carbonation. The purpose of this option is to allow for different initial concentrations in each element of the BRAGFLO grid.

= .FALSE.: Then the rates are used as is and should be entered in the input file in units of [gm-mol/(s m^3)].

Line 9.5. Descriptor. Humid rate factors.

One-line (up to 132 characters) descriptor for the following parameters:

Line 9.6. HF(1), HF(2).

HF(1): Factor multiplying RK(1) to get the corrosion reaction rate constant under humid conditions [dimensionless].

HF(2): Factor multiplying RK(2) to get the biodegradation reaction rate constant under humid conditions [dimensionless].

Line 9.7. Descriptor. Inundated and humid MgO hydration rates and hydromagnesite conversion rate.

One-line (up to 132 characters) descriptor for the following parameters:

Line 9.8. BRUCITEI, BRUCITEH, HYMAGCON.

BRUCITEI: Inundated MgO hydration rate in units of [gm-mol MgO/(s m^3)] or [lbmol Fe/(day ft^3)], unless LINTRIN = .TRUE., in which case the units should be [gm-mol MgO/(s kg)] or [lbmol Fe/(day lb)].

BRUCITEH: Humid MgO hydration rate in units of [gm-mol MgO/(s m^3)] or [lbmol Fe/(day ft^3)], unless LINTRIN = .TRUE., in which case the units should be [gm-mol MgO/(s kg)] or [lbmol Fe/(day lb)].

HYMAGCON: Hydromagnesite conversion rate in units of [gm-mol MgO/(s kg)] or [lbmol Fe/(day lb)].

Line 9.9. Descriptor. RXH2S and RXCO2.

One-line (up to 132 characters) descriptor for the following parameters:

The next line is repeated NWST times

Line 9.10. RXH2S(I), RXCO2(I).

RXH2S(I): Moles of iron sulfidized per mole of organic carbon consumed. See Section 4.13.3.

RXCO2(I): Moles of magnesium needed to carbonate one mole of CO_2. See Section 4.13.5.

Line 9.11. Descriptor. SMIN.

One-line (up to 132 characters) descriptor for the following parameters:

Line 9.12. SMIN.

SMIN: Minimum brine saturation below which all chemistry ceases. This is discussed in Section 4.13.1. Recommend SMIN = 0.015.

Line 9.13. Descriptor. Reactant/product molecular weights, WM(1:4).

One-line (up to 132 characters) descriptor for the following parameters:

Line 9.14. (WM(I),I=1,4).

WM : Molecular weights for the reactants and products in the Average Stoichiometry Model.

WM(1): Molecular weight for H_2 [kg/gm-mol or lb/lbmol].

WM(2): Molecular weight for H_2O [kg/gm-mol or lb/lbmol].

WM(3): Molecular weight for FE [kg/gm-mol or lb/lbmol].

WM(4): Molecular weight for $[C_6H_{10}O_5]/6$ [kg/gm-mol or lb/lbmol].

Line 9.15. Descriptor. Reactant/product molecular weights, WM(5:10).

One-line (up to 132 characters) descriptor for the following parameters:

Line 9.16. (WM(I),I=5,10).

WM(5): Molecular weight for $Fe(OH)_2$ [kg/gm-mol or lb/lbmol].

WM(6): Molecular weight for FeS [kg/gm-mol or lb/lbmol].

WM(7): Molecular weight for MgO [kg/gm-mol or lb/lbmol].

WM(8): Molecular weight for $Mg(OH)_2$ [kg/gm-mol or lb/lbmol].

WM(9): Molecular weight for Hydromagnesite [kg/gm-mol or lb/lbmol].

WM(10): Molecular weight for $MgCO_3$ [kg/gm-mol or lb/lbmol].

Line 9.17. Descriptor. Stoichiometry Matrix.

One-line (up to 132 characters) descriptor for the following parameters:

Line 9.18. S(I,J)

S(I,J): Stoichiometry coefficient matrix for the eight reactions currently considered in the average stoichiometry model [dimensionless]. The matrix is entered in rows and columns with I being the row and J being the column. The identity of each entry is described in Section 4.13.2, with the meaning of each row given in Table 1, and the meaning of each column given in Table 2. Guidance for the values of these coefficients is given in Subsections 4.13.3-4.13.5.

NOTE: Lines 9.19-9.22 must be entered even if IGASVAR = 0.

Line 9.19. Descriptor. Reactant/Product Densities DEN(1:4).

One-line (up to 132 characters) descriptor for the following parameters:

Line 9.20. (DEN(I),I=1,4).

DEN(I): Densities listed in Table 3 for I = 1,4 in units of [kg/m^3] or [lb/ft^3]. The index and corresponding identity are given in Table 3, and will not be repeated here.

Line 9.21. Descriptor. Reactant/Product Densities DEN(5:9).

One-line (up to 132 characters) descriptor for the following parameters:

Line 9.22. (DEN(I),I=5,9).

DEN(I): Densities listed in Table 3 for I = 5,9 in units of [kg/m^3] or [lb/ft^3]. The index and corresponding identity are given in Table 3, and will not be repeated here.

Line 9.23. Descriptor. Additional reaction parameters.

One-line (up to 132 characters) descriptor for the following parameters:

Line 9.24. SATWICK, LARXN, LARXN2, ALPHARXN.

SATWICK: Term modifying the brine saturation to simulate the effect of wicking on the net reaction rate by increasing the inundated rate and decreasing the humid rate [dimensionless]. Valid range: 0.0-1.0. A value of 0.0 will turn this feature off. Instead of using the actual brine saturation, S_b, to calculate reaction rates, the effective saturation S_{eff} is used as described in Section 4.13.1.

LARXN: Logical flag indicating whether to smooth humid reaction rates (.TRUE.) using the factor ALPHARXN, or use unmodified, discontinuous humid rates (.FALSE.). Recommended value: T.

LARXN2: Logical flag indicating whether to use concentration smoothing (.TRUE.) using the factor ALPHARXN or use discontinuous rates (.FALSE) when reactants run out. See Section 4.13.6 for a discussion of this feature.

ALPHARXN: Term used in smoothing functions to eliminate a discontinuity at brine saturation, $S_b = 0$, as described in Section 4.13.1. Always used in expression to obtain S_{eff} when wicking is modeled (*i.e.*, when SATWICK > 0.). When LARXN = T, ALPHARXN (or α) is used in the smoothing function for all humid rates:

$$r_{h,eff} = r_h\left(1 - e^{\alpha S_{eff}}\right)$$

where:

r_h = humid rate
= HF(1) × RK(1), or HF(2) × RK(2);
$r_{h,eff}$ = effective (smoothed) humid rate.

If LARXN = F, then ALPHARXN is not used for the humid corrosion and biodegradation rates, and $r_{h,eff} = r_h$. The full rate is given by [where r_i is the inundated rate]:

$$r = S_{eff} r_i + \left(1 - S_{eff}\right) r_{h,eff}, \quad S_{eff} > 0$$
$$= 0, \qquad S_{eff} = 0$$

so, unless $r_{h,eff} = 0$, r will be discontinuous at $S_{eff} = 0$. This discontinuity tends to cause numerical problems. Generally, BRAGFLO will run better when LARXN = T, although exceptions to this rule have been encountered. ALPHARXN must be a negative value; if a positive value is input, BRAGFLO will convert the input value to a negative value before using it. Recommended value: -1000. A large negative value for ALPHARXN will approximate more closely the discontinuous function originally intended for r while remaining smooth enough to ease the numerical difficulties. Small negative values of ALPHARXN will result

in values of $r_{h,eff}$ that are significantly different from r_h, and a value of zero will cause $r_{h,eff}$ to be zero.

NOTE: If IGASVAR ≠ 2 (Line 9.2), then skip to Section 7.2.11.

Line 9.25. Descriptor. Reactant/product molecular weights, WMRXN(1:MSPEC).

One-line (up to 132 characters) descriptor for the following parameters:

Line 9.26. (WMRXN(I),I=1,MSPEC).

WMRXN : Molecular weights for the reactants and products in the Reaction Path Model. MSPEC values are required. MSPEC is defined in the BRAGFLO PARAMETER INCLUDE STATEMENT and is assigned a value of 23.

WMRXN(1): Molecular weight for H_2 [kg/gm-mol or lb/lbmol].

WMRXN(2): Molecular weight for CO_2 [kg/gm-mol or lb/lbmol].

WMRXN(3): Molecular weight for CH_4 [kg/gm-mol or lb/lbmol].

WMRXN(4): Molecular weight for N_2 [kg/gm-mol or lb/lbmol].

WMRXN(5): Molecular weight for H_2S [kg/gm-mol or lb/lbmol].

WMRXN(6): Molecular weight for O_2 [kg/gm-mol or lb/lbmol].

WMRXN(7): Molecular weight for H_2O [kg/gm-mol or lb/lbmol].

WMRXN(8): Molecular weight for H_2SO_4 [kg/gm-mol or lb/lbmol].

WMRXN(9): Molecular weight for HNO_3 [kg/gm-mol or lb/lbmol].

WMRXN(10): Molecular weight for $[C_6H_{10}O_5]/6$ [kg/gm-mol or lb/lbmol].

WMRXN(11): Molecular weight for FE [kg/gm-mol or lb/lbmol].

WMRXN(12): Molecular weight for FES_2-F [kg/gm-mol or lb/lbmol].

WMRXN(13): Molecular weight for FES_2-O [kg/gm-mol or lb/lbmol].

WMRXN(14): Molecular weight for $FECO_3$ [kg/gm-mol or lb/lbmol].

WMRXN(15): Molecular weight for $FECO_3$-O [kg/gm-mol or lb/lbmol].

WMRXN(16): Molecular weight for $FE(OH)_2$ [kg/gm-mol or lb/lbmol].

WMRXN(17): Molecular weight for FEO(OH) [kg/gm-mol or lb/lbmol].

WMRXN(18): Molecular weight for FE_3O_4 [kg/gm-mol or lb/lbmol].

WMRXN(19): Molecular weight for FES [kg/gm-mol or lb/lbmol].

WMRXN(20): Molecular weight for CAO [kg/gm-mol or lb/lbmol].

WMRXN(21): Molecular weight for $CA(OH)_2$ [kg/gm-mol or lb/lbmol].

WMRXN(22): Molecular weight for $CACO_3$ [kg/gm-mol or lb/lbmol].

WMRXN(23): Molecular weight for H_2_RAD [kg/gm-mol or lb/lbmol].

7.2.11 Creep Closure Parameters

These parameters activate the creep closure sub-model. Using this model, the porosity of the Waste is calculated to simulate salt creep that, over time, closes in on the waste, compressing it. Four closure models, or "surfaces," are available, three that apply to waste and one for non-back-filled drifts. Two options are available for interpolating over the closure models. The porosity can be based on the quantity of gas present in the waste or on the pressure in the waste. The latter option is more current and conforms more closely to the theoretical basis on which creep closure is modeled.

Line 10.1. Descriptor. Creep closure control flag.

One-line (up to 132 characters) descriptor for the following parameters:

Line 10.2. CLOSURE.

CLOSURE: LOGICAL flag.

= .TRUE., the porosity of the waste will be calculated using the creep closure model.

= .FALSE., the porosity of the waste will instead be calculated based simply on the compressibility of the waste, in the same manner as for all other materials.

NOTE: If CLOSURE = .TRUE., then Lines 10.3-10.10 must be entered. Additionally, an external file containing the closure look-up table data is also required. The description and format of this data is defined in Section 7.4.

NOTE: If CLOSURE = .FALSE., then no more closure parameters are input; go to Section 7.2.12.

Even if CLOSURE = .TRUE., the creep closure model is not used at any time prior to TIMEICRESET. The creep closure model is used only up to the maximum data time for each closure model, TIMEDATA_MAX (3.78716×10^{11} s, or 12,000 yr, in the current version of BRAGFLO. An upper limit of 12,000 yr, instead of 10,000 yr, is used to ensure that interpolation is done properly if a WIPP run goes slightly past 10,000 yr; for example, the completion time [FINISH] for a run is typically set at 3.1557×10^{11} s, which is 10,000.02 yr.); after that time, the porosity of the waste is computed from the compressibility. In order to preserve the waste porosity as a continuous function of time after TIMEDATA_MAX, BRAGFLO sets the reference pressure for porosity calculation, PREFROCK, equal to the current waste pressure, which is uniform throughout the waste in the creep closure model. In addition, the reference porosity, PORREFROCK, is set equal to the current waste porosity, which is also uniform throughout the waste.

Line 10.3. Descriptor. Creep closure parameters.

One-line (up to 132 characters) descriptor for the following parameters:

Line 10.4. NKLOS, KLOSINT, KLOSAVE.

NKLOS: Number of closure models to be used in this run. BRAGFLO currently has three closure surfaces from which to choose. NKLOS must be > 0 and ≤ MKLOS, set in the PARAMETER statement; currently, MKLOS = 4.

KLOSINT: Flag indicating the basis on which interpolation on the creep closure data will be done. Recommended value: 1. KLOSINT = 0 was used exclusively in early versions of BRAGFLO that had closure surface capabilities, but is no longer considered reliable, especially with closure surfaces 1, 2, and 4 (surface 3 is the original closure surface). If KLOSAVE = 2 is used, KLOSINT = 0 may *not* be used.

= 0: Interpolation based on gas generation rate and quantity of gas present.

= 1: Interpolation based on average waste pore pressure.

KLOSAVE: Flag indicating the scale over which properties are averaged for application of a closure model. Recommended value: 2.

= 1: Average brine pressures in all grid blocks using a given closure model to determine the porosity, which will be identical in all those grid blocks. This is done only when evaluating residuals; creep closure is not modeled when calculating the Jacobian. This averaging method was used exclusively in earlier versions of BRAGFLO. However, because creep closure effects cannot be accounted for in evaluating the Jacobian, convergence problems often arise. In general, this method should not be used except to replicate earlier results. On the other hand, in some instances solutions have been obtained using KLOSAVE = 1 where using KLOSAVE = 2 causes the run to fail.

= 2: Do no averaging; use only the brine pressure in individual grid blocks to obtain porosity from a closure surface, both for evaluating residuals and for evaluating the Jacobian. Because creep closure effects are properly accounted for in the Jacobian, convergence behavior should be superior to using KLOSAVE = 1. If KLOSINT = 0, BRAGFLO will abort with a message warning that KLOSINT must be 1 when KLOSAVE = 2.

Line 10.5. Descriptor. Creep closure parameters.

One-line (up to 132 characters) descriptor for the following parameters:

Line 10.6 is repeated NKLOS times:

Line 10.6. I, PLITHO(I), TIME_CLOSOFF(I), MODPERM(I), INCR_PORO(I), LSOLPROD(I).

I: Closure surface or model number (1, 2, 3, or 4).

PLITHO(I): Maximum pressure allowed for closure to continue. If waste brine pressure exceeds PLITHO(I), closure is tuned off permanently. The user

is informed if and when this happens by a warning printed to the screen and to the .sum file if it is used. If closure is turned off, the porosity of the waste may continue to vary with pressure depending on the value of compressibility of the waste, as specified in Line 7.45. For this purpose, the reference porosity and reference pressure are the values that exist in the closure region (if KLOSAVE = 1) or in the grid block undergoing closure (if KLOSAVE = 2) at the time when closure is turned off.

TIME_CLOSOFF(I): Time limit for creep closure to be active [s]. As an example, creep closure modeling may be turned off when a human intrusion occurs, since the closure surface is no longer valid under those circumstances. If there is no time limit on creep closure, a value equal to or greater than TIMEDATA_MAX(I) or FINISH (Line 1.7, end time for the run) can be input.

MODPERM(I): Model to use for determining changes in permeability with changes in porosity for regions that experience closure.

= 1: Use model of the form $k = a\phi^{\eta}$, where a and η are constants set by CLOSPERMFACT(I) and CLOSPERMEXP(I) described below in Line 10.8, k is the intrinsic permeability [m^2], and ϕ is the porosity in each region undergoing dynamic creep closure [m^2].

= 2: Use a Koseny-Carman like model

$$k = k_{inp} \quad for\ \phi \geq \phi_{HIGH} \tag{207}$$

$$k = a\frac{\phi^3}{(1-\phi)^2} \quad for\ \phi_{LOW} \leq \phi < \phi_{HIGH} \tag{208}$$

$$k = a\frac{\phi_{LOW}^{\ 3}}{(1-\phi_{LOW})^2} \quad for\ \phi \leq \phi_{LOW} \tag{209}$$

where k_{inp} is the initial intrinsic permeability for the waste area given in Line 7.46, and the constant a is set in BRAGFLO by matching the intrinsic permeability for the waste area at some porosity ϕ_{HIGH} (set by PHIUPPER given in Line 10.8 below) chosen by the user. These models are in the subroutine CONSOL1.

INCR_PORO(I): Flag to decide whether or not to allow the porosity to increase with time.

= .TRUE.: Only allow porosity to decrease with time.

= .FALSE.: Porosity can increase or decrease with time.

LSOLPROD(I): Flag to decide whether or not to use a model (i.e., 1 or 2) for changes in permeability due to changes in porosity in regions that experience closure.

= .TRUE.: Use model given by MODPERM(I) to determine permeability in the waste area.

= .FALSE.: Ignore effect of changes of porosity on permeability.

NOTE: Note that Lines 10.7 and 10.8 must be entered regardless of LSOLPROD(I).

Line 10.7. Descriptor. Parameters for the permeability versus porosity models.

One-line (up to 132 characters) descriptor for the following parameters:

Line 10.8 is repeated NKLOS times:

Line 10.8. CLOSPERMFACT(I), CLOSPERMEXP(I).

If MODPERM(I) *(Line 10.6) = 1:*

CLOSPERMFACT(I): Constant factor, a, in expression relating permeability, k, to porosity, ϕ, in each region undergoing dynamic creep closure [m^2]. If the permeability of any region (KLOSAVE = 1) or grid block (KLOSAVE = 2) undergoing creep closure is to be constant, set CLOSPERMFACT(I) to the initial permeability for that material, XKX (Line 7.46). If KLOSAVE = 1, all grid blocks using the same closure surface will have the same porosity and, consequently, the same permeability.

CLOSPERMEXP(I): Exponent, η, in expression relating permeability, k, to porosity, ϕ, in each region undergoing dynamic creep closure [dimensionless]. If the permeability of any region or grid block is to be constant, set CLOSPERMEXP(I) to zero. Recommended value: 4.6.

Line 10.8. PHIUPPER(I), PHILOWER(I).

If MODPERM(I) *(Line 10.6) = 2:*

PHIUPPER(I) = ϕ_{HIGH} described above in Line 10.6. This value represents the upper porosity at which changes in permeability with porosity are no longer significant. It is also the value of porosity at which the model sets the permeability equal to the initial intrinsic permeability of the material experiencing closure.

PHILOWER(I) = ϕ_{LOW} described above in Line 10.6. This value represents the lower porosity below which changes in permeability are not significant.

Line 10.9. Descriptor. Creep closure material control parameter.

One-line (up to 132 characters) descriptor for the following parameters:

Line 10.10. NMATCLOS.

NMATCLOS: Number of materials in which closure will take place. Each material that undergoes creep closure is referred to as a closure region. The number of closure regions cannot be greater than the number of materials. Thus,

NMATCLOS must be ≤ MMAT (set in the PARAMETER statement) and must be ≥ 0.

NOTE: If NMATCLOS = 0, no more closure data are input; go to Section 7.2.12.

Line 10.11. Descriptor. Creep closure parameters associating a material number with a creep closure model number.

One-line (up to 132 characters) descriptor for the following parameters:

Line 10.12 is repeated NMATCLOS times:

Line 10.12. I, MATCLOS(I), MODELCLOS(I).

I: Closure region number.

I must be > 0 and ≤ MMAT (set in the PARAMETER statement).

MATCLOS(I): Material type number from the material map that will be a closure region.

MATCLOS(I) must be > 0 and ≤ MMAT (set in the PARAMETER statement). It is permissible for a material number not to be used in any material map, but there is no check to be sure that material MATCLOS(I) is used in any map. For example, if an input file has one material map with two materials, numbered, say, 1 and 14 (and 14 sets of material properties are input in Section 7.2.8), one may input a value of, say, MATCLOS(I) = 5 here, which does not refer to any material actually used in the run. Creep closure will be calculated for material 5 even though it does not exist. This may have no effect on the run, but it may cause the run to abort (after it has reached TIMEICRESET) when the creep closure model tries to interpolate on the closure surface using brine pressures of 0.0, which is the default value when a material has not been defined. Thus, it is up to the user to ensure that valid material numbers are used as closure regions.

MODELCLOS(I): Creep closure surface or model number used by closure region MATCLOS(I).

MODELCLOS(I) must be >0 and ≤ MKLOS (set in PARAMETER statement; currently, MKLOS = 4). The available options are:

= 1: Waste without backfill. Used during 1995, this model is no longer considered the best available for application to waste but is retained in BRAGFLO to enable earlier calculations to be reproduced.

= 2: Drift without backfill. This model was applied to access drifts ("North End") and the Experimental Region excavations during 1995. It is no longer required for application to WIPP but is retained in BRAGFLO for future use and to enable earlier calculations to be reproduced.

= 3: Waste with backfill. This model was used in the 1992 Preliminary Performance Assessment and in subsequent calculations, until early 1995. Although the waste configuration is no longer considered likely, this model is retained in BRAGFLO to enable earlier calculations to be reproduced.

= 4: Waste without backfill. This model is used in the 1996 Compliance Certification Application (CCA) calculations (Stone, 1995).

7.2.12 Radiolysis and Radionuclide Decay Parameters

The "transport" model that was deprecated in BRAGFLO 7.00 was a simple particle-tracking model. Radionuclides originating in waste blocks were carried to other grid blocks by simple advection. BRAGFLO 7.00, to facilitate the qualification of radiolysis and radionuclide decay with minimal impact, retains the previous transport-based input deck line format. However, transport mode is inoperable such that LTRANS should always be set to .FALSE.

Line 11.1. Descriptor. On/off flag for radionuclide decay.

One-line (up to 132 characters) descriptor for the following parameters:

Line 11.2. LRADDK.

LRADDK: Logical flag indicating whether radionuclide decay will be calculated.

= .TRUE., decay will be calculated

= .FALSE., decay will not be calculated

Line 11.3. Descriptor. On/off flag for transport.

One-line (up to 132 characters) descriptor for the following parameters:

Line 11.4. LTRANS.

LTRANS: Logical flag indicating whether transport will be calculated.

= .TRUE., deprecated feature will be automatically set to .FALSE. and transport will not be calculated

= .FALSE., transport will not be calculated

NOTE: LTRANS capability is not activated, QA'd, nor used for WIPP Compliance Calculations. Set LTRANS = .FALSE. to disable.

Line 11.5. Descriptor. On/off flag for radiolysis.

One-line (up to 132 characters) descriptor for the following parameters:

Line 11.6. LRADLSIS.

LRADLSIS: Logical flag indicating whether radiolysis will be calculated.

= .TRUE., radiolysis will be calculated

= .FALSE., radiolysis will not be calculated

NOTE: If LRADLSIS = .FALSE. and LTRANS = .FALSE., then BRAGFLO sets LRADDK to .FALSE. even if it was input as .TRUE., and no additional radionuclide decay parameters are input; go to Section 7.2.13..

Line 11.7. Descriptor. Number of radionuclides.

One-line (up to 132 characters) descriptor for the following parameters:

Line 11.8. NRAD.

NRAD: Number of radionuclide species to be tracked in the transport and decay models.

NRAD must be greater than zero and less than or equal to MRAD, which is set in the PARAMETER statement. Otherwise, BRAGFLO will abort with the message:

```
*** Aborted in READRAD:  Invalid NRAD value input.
```

The following two lines (11.9 and 11.10) are read in only if LRADDK = .TRUE.:

Line 11.9. Descriptor. Radiolysis and decay control parameters.

One-line (up to 132 characters) descriptor for the following parameters:

Line 11.10. XLIM, HALFMAX, T_SCALE, SRADO2, GH2AVG, GDEPFAC.

XLIM: Minimum decay factor; decay factor is set to zero when it is below XLIM [dimensionless]. Recommended value: 1.0×10^{-7}.

HALFMAX: Maximum number of half-lives during which decay will be calculated. Recommended value: 50.

T_SCALE: Time above which half-life is too large to bother calculating decay; used to shorten the decay chain [s]. Recommended value: 3.1557×10^{7} s (1.0 yr).

SRADO2: Stoichiometric coefficient for O_2 from radiolysis [gm-mol O_2/gm-mol H_2]:

$$H_2O \rightarrow H_2 + (\text{SRADO2})\ O_2.$$

The value of SRADO2 should be between 0.0 and 0.5:

= 0.0 if O_2 is assumed to react immediately with other materials;

= 0.5 if O_2 is assumed to be inert.

Note that BRAGFLO, as used in WIPP PA calculations, assumes all gas to be H_2. The mass of gas produced by radiolysis as O_2 is:

$$M_{w,O_2} \cdot \text{SRADO2} = 31.988 \times 10^{-3}\ \text{SRADO2}\ [\text{kg } O_2 / \text{gm-mol } H_2],$$

where:

M_{w,O_2} = molecular weight of O_2 [kg O_2 / gm-mol O_2],

M_{w,H_2} = molecular weight of H_2 [kg H_2 / gm-mol H_2],

When this mass is treated as an equal mass of H_2, it is equivalent to:

$$\frac{M_{w,O_2}\cdot \text{SRADO2}}{M_{w,H_2}} = \frac{31.9988\times10^{-3}\text{SRADO2}\left[\frac{\text{kgH}_2(=\text{kgO}_2)}{\text{gm-molH}_2}\right]}{2.01588\times10^{-3}\left[\frac{\text{kgH}_2}{\text{gm-molH}_2}\right]}$$

$$= 15.8734 \cdot \text{SRADO2}\ [\text{gm-mol H}_2 / \text{gm-mol H}_2]$$

$$= 7.93668\ [\text{gm-mol H}_2/\text{gm-mol H}_2]$$

When SRADO2 = 0.5, this results in a far greater volume of gas (as H_2) than is realistically produced. It may be more realistic in BRAGFLO to consider radiolysis as producing 1/2 *moles* of H_2 (assuming the gas to be inert) (*i.e.*, $H_2O \rightarrow H_2 + 1/2H_2$), rather than $M_{w,O_2} \cdot \text{SRADO2}$ kg of H_2. Then the value SRADO2 should have in order to produce 0.5 gm-mol H_2 can be calculated from:

$$\frac{1}{2}\left[\text{mol H}_2 / \text{mol H}_2\right] = \frac{M_{w,O_2}\cdot \text{SRADO2}}{M_{w,H_2}},$$

or,

$$\text{SRADO2} = \frac{\frac{1}{2}M_{w,H_2}}{M_{w,O_2}}$$

$$= \frac{\left(\frac{1}{2}\right)2.01588\times10^{-3}}{31.9988\times10^{-3}}$$

$$= 0.314993.$$

GH2AVG: Average "G" value for H_2 [molecule/eV].

GDEPFAC: The energy deposition probability for wetted solids [dimensionless].

The value of GDEPFAC should be between 0.0 and 1.0:

= 0.0, if brine radiolysis is only occurring due radionuclides in solution

≥ 0.0, if brine radiolysis is both occurring due to radionuclides in solution and radionuclides that are in contact with brine (wetted) in solid form (precipitated); set equal to the fraction of the total disintegration energy from the wetted solid radionuclides that is contributing to brine radiolysis

Line 11.11. Descriptor. Isotope names.

One-line (up to 132 characters) descriptor for the following parameters:

Line 11.12. (IDION(I),I=1,NRAD).

IDION: Name of parent isotope. This is a CHARACTER*8 variable, read in free format, so it must be enclosed in tick marks. The name should be the element symbol followed by the atomic number (*e. g.*, 'Pu238') with no spaces or other punctuation between the element symbol and the atomic number. The element symbol can be either all upper case or upper and lower case. Trailing blanks are optional.

Line 11.13. Descriptor. Daughter names.

One-line (up to 132 characters) descriptor for the following parameters:

Line 11.14. (IDAUG(I),I=1,NRAD).

IDAUG: Name of immediate daughter isotope from the decay of isotope IDION(I). Same input rules as for the parent isotopes. If there is no daughter, use a blank: one to eight spaces between tick marks.

Line 11.15. Descriptor. Element indexes.

One-line (up to 132 characters) descriptor for the following parameters:

Line 11.16. (IELE(I),I=1,NRAD).

IELE: Element index for each isotope; must range from 1 to a maximum of NRAD, depending on how many elements there are. Applies to IDION only. Thus, all IDION isotopes of Pu, for example, will have the same IELE index, and all isotopes of Th will have another IELE index, all the same, but different from the index used for Pu. These are used to calculate the solubility when more than one isotope of an element is present, since the input solubility is of an element, not an isotope.

Line 11.17. Descriptor. Half lives.

One-line (up to 132 characters) descriptor for the following parameters:

Line 11.18. (THALF(I),I=1,NRAD).

THALF: Half-life of isotope IDION [s or yr].

Line 11.19. Descriptor. Atomic weights.

One-line (up to 132 characters) descriptor for the following parameters:

Line 11.20. (AWT(I),I=1,NRAD).

AWT: Atomic weight of isotope IDION [kg/gm-mol or lb/lbmol].

Line 11.21. Descriptor. Solubilities.

One-line (up to 132 characters) descriptor for the following parameters:

Line 11.22. (SOLB_LIM(I),I=1,NRAD).

SOLB_LIM: Solubility limit (total mobilization potential) of element in brine [gm-mol/m^3 or lbmol/ft^3]. Same value should be input for each isotope IDION of the element; *i.e.*, all IDION with the same IELE should have the same SOLB_LIM.

Line 11.23. Descriptor. Disintegration energy.

One-line (up to 132 characters) descriptor for the following parameters:

Line 11.24. (EVDP(I),I=1,NRAD).

EVDP: Disintegration energy if isotope IDION [MeV/disintegration]. Note that input units are MeV/dis; BRAGFLO converts to eV/dis.

Lines 11.25 and 11.26 are repeated NRAD times, once for each radionuclide.

Line 11.25. Descriptor. Initial inventory.

One-line (up to 132 characters) descriptor for the following parameters:

Line 11.26. RADINIT(I).

RADINIT(I): Initial total quantity of radionuclide IDION(I) in waste [gm-mol]. Assumed to exist initially in solid phase only; BRAGFLO will then calculate how much is dissolved in brine, based on input solubilities. This initial inventory is distributed to all grid blocks having initial material type index MAT_WASTEI (Line 7.12) in proportion to the volume of each grid block relative to the total waste volume.

NOTE: Lines 11.27 and 11.28 are input only if LTRANS = .TRUE. Again, note that LTRANS is deprecated and set to .FALSE., so the following lines are retained only for future use.

Line 11.27. Descriptor. Transport control parameters.

One-line (up to 132 characters) descriptor for the following parameters:

Line 11.28. SOLB_MULT, Q_BVOL_RATIO, TSUB_MAX.

SOLB_MULT: Multiplier on SOLB_LIM (solubility limit of radionuclide species in brine, Line 11.22) to avoid unrealistic precipitation of radionuclide outside of the waste regions [dimensionless]. Recommended value: 1.0×10^5.

Q_BVOL_RATIO: Maximum inter-block flow allowed during transport calculation [fraction of grid block volume]. Recommended value: 0.10.

TSUB_MAX: Maximum number of times that BRAGFLO time step DELT is sub-divided to keep the transport solution stable. Larger values may actually be needed, but the calculation may then require excessive computing time, so it is best to set some reasonable limit and hope it remains stable. Recommended value: 100 - 200. If the solution becomes unstable, TSUB_MAX should be increased. Q_BVOL_RATIO can be increased but should remain below 1.0. Increasing either of these will increase the computational effort.

7.2.13 Multi-Component Gas Transport Parameters

BRAGFLO has the capability to track multiple components of the gas phase as they are produced, consumed, and transported. This transport model accounts only for advective flow; diffusion and retardation are not considered. This feature is intended to supplement the reaction path gas generation model and gas dissolution model. Because the reaction path model has not yet been implemented, the gas transport model has not yet been tested or even debugged, so it should not be used except for testing purposes.

NOTE: Multi-component gas transport capability is not QA'd or used for WIPP Compliance Calculations.

Line 12.1. Descriptor. Gas transport control flag.

One-line (up to 132 characters) descriptor for the following parameters:

Line 12.2. LRXGAST.

LRXGAST: Logical flag (.TRUE. or .FALSE.) indicating whether gas component transport will be used.

= .TRUE., gas component transport will be calculated

= .FALSE., gas component transport will not be calculated

If LRXGAST = .FALSE., this is the end of the BRAGFLO input.

The next two lines are repeated MGAS times, where MGAS is the number of gas components, set in the PARAMETER statement.

Lines 12.3 and 12.4 are input MGAS times (where MGAS is the number of gas components, set in the PARAMETER statement) only if LRXGAST = .TRUE. Otherwise, this is the end of the BRAGFLO input.

Line 12.3. Descriptor. Initial gas component concentration.

One-line (up to 132 characters) descriptor for the following parameters:

Line 12.4. (((AFTER(I,J,K), I=1, NX), J=1, NY), K=1, NZ).

AFTER: Initial mole fraction of each gas component [mol fraction].

7.3 Restart Capability

NOTE: Restart capability is not QA'd or used for WIPP Compliance Calculations.

The restart capability in BRAGFLO enables runs to be restarted from any point specified in the input file and from the end of a run. The restarted run will continue exactly as it would have if the run had been done from the beginning without interruption. This capability is most useful for debugging, but also allows troublesome runs to be stopped and analyzed before wasting computing time. Occasionally, control parameters can be changed part way through a run, enabling a run to finish when it would otherwise remain stuck.

Some basic information on how to use the restart capability was presented earlier under "Files used by BRAGFLO." Initially, the input file must specify that a restart output file is to be

written. This is indicated by setting the logical flag, LWRST, on Line 1.3 to T (.TRUE.). If LWRST is .FALSE., no restart output will be written, and the run cannot be restarted. If LWRST is .TRUE., a restart record will be written as specified in Section 7.2. Restart records, like ASCII and binary output, can be written at specified times, at specified time intervals, or at a specified time step frequency. If LWRST is .TRUE., a restart record will automatically be written at the end of a run, regardless of how they are specified to be written during a run. The restart record contains all the information needed to resume from the last converged time step before the restart record is written. Although there is no limit to the number of restart records that can be written during a run, the number of restart records needed is generally very small, at most a couple, or perhaps every 500 years in a 10,000-year run. The user has to know when the restart records are written in order to do a restart. This information is written to the screen or log file, to the ASCII output file [if one is being written (LWASC is .TRUE. on Line 1.3)], and to the .sum file [if one is being written (LWSUM is .TRUE. on Line 1.3)] each time a restart record is written.

The procedure for restarting a BRAGFLO run is as follows:

1. Copy the restart output file [.xrot] into a restart input file [.xrin]. The name of the restart input file does not have to be the same as the restart output file, but it does have to be the same (except for the .xrin extension) as the ASCII input file that will be used for the restart.
2. Edit the ASCII input [.inp] file used in the initial run. If the flag LRRST in Line 1.3 is F, it must be changed to T, indicating that a restart input file will be read. The flag LWRST in Line 1.3 had to have been T in the initial run; it can (and probably should) be left as T, or can be changed to F for the restart, depending on whether the user wished to write any more restart output records during the restart run. If the initial run completed the maximum number of time steps allowed, then MAXITF (Line 1.7) must be increased, or the restart run will stop immediately, having already completed MAXITF steps. If the run is being restarted simply because MAXITF was too small in the initial run, or if the restart is a debugging run, these are the only changes needed. Almost anything in the ASCII input file can be changed for the restart run, with the exception of the dimensions of the problem (NX, NY, NZ, Line 1.5). If these are changed, the restart run will abort. Any parameter specifying the number of something, such as the number of wells, the number of material types, or the number of history variables, can be changed, but should not be changed because it will likely confuse both the user and BRAGFLO and probably eventually abort. Print flags should not be changed because post-processing will be messed up. Grid block sizes and initial conditions should not be changed. Logically, the only changes that should be considered, other than file specifications, time or time step limits, and output times or frequencies, are numerical control parameters. In rare instances, one might want to modify material properties. Keep in mind that any changes to the input file that are in effect only at times earlier than the time of the restart, and are no longer in effect at the restart time, will not have any effect on the restart run. For example, if the restart is at 1000 years, and the input file is changed to request additional ASCII output at 500 years, the output at 500 years will not be written. The .inp file name can be changed from the initial run, but the name has to be the same as the restart input file name, except for the .inp extension.

3. Run BRAGFLO. As usual, BRAGFLO prompts for the name of the .inp file. Then it requests the number of the restart record from the restart input .rin file. If the user wished to start the run from the beginning again (having made changes to the input file), a zero can be entered here. If a number greater than the number of restart records in the .rin file is entered, the run will abort trying to read past the end of the .rin file.
4. Post-processing. The binary file from the restart run will have the same structure as the initial run but start from the restart time. Before post-processing in the CAMCON system using POSTBRAG, it is necessary first to run a utility which merges the two binary files into a single binary file.

7.4 External Input File Containing Closure Look-up Table Data

This data is only required if creep closure has been selected, i.e. CLOSURE=.TRUE.. For each included Look-up Table, the data consists of two dependent variables, porosity and pressure as a function of two independent variables, an F Factor (related to gas generation rate), and time. This data has been generated external to BRAGFLO by a rock mechanics code. Since the rock mechanics codes uses a different definition or basis for determining porosity than does BRAGFLO, the rock-mechanics code porosity values were converted to those consistent with BRAGFLO's usage.

The dimensions of the data are defined on BRAGFLO's PARAMETER INCLUDE file. The defining dimensions are

1) MKLOS, the number of Look-up" Tables included on the file. Currently 4.
    1: Porosity Surface #1, for Waste w/o Backfill. First used in SPM2 in January 1995. Raw data were SANCHO porosities, based on current time-dependent room volume; these were converted to initial room volume basis before inserting into BRAGFLO.
    2: Porosity Surface #2, for North End w/o Backfill. First used in SPM2 in January 1995. Raw data were SANCHO current time-dependent room volumes (SANCHO porosities are always 1.0); these were converted to porosities based on initial room volume before inserting in BRAGFLO.
    3: Porosity Surface #3, the Original porosity surface used before SPM2 in January 1995. Raw data were SANCHO porosities, based on current time-dependent room volume; these were converted to initial room volume basis before inserting into BRAGFLO.
    4: Porosity Surface #4, for Waste w/o Backfill, an improved version of Surface #1, installed 01/21/96. This is surface that was used in the 1996 CCA, 1997 PAVT PA, and the CRA-2004 and CRA-2004 PABC.
2) NSDATA, then number of F Factors considered in the table.
3) NTDATA, the number of times at which data is defined in the table.

The data arrays are sized according to the largest set of data. MKLOS =4, NSDATA =13, NTDATA = 214. For each of the MKLOS data sets there must be entries for each of the

NSDAT x NTDATA points. Since the dependent variable arrays are sized according to the largest set of data, a given table may not have sufficient calculated entries. In these cases, the remaining portion of the table is zero filed. Similarly, the independent variable arrays are sized according to the largest set of data, in the event that there are not NSDATA F Factors defining the table, the remaining portion of the F Factor array is zero filled. In the event that there are not NTDATA times corresponding to data in the table, the remaining portion of the time array is zero filled. This will become clearer below. Because of the large amount of data on the closure data input file, a generous number of "descriptor lines" are include and required to help the user clearly delineate the data being entered.

Line 1.0 Descriptor. Minimum porosity value for each look-up table (surface)

Line 2.0 (PHIMIN_BRAG(I),I=1,MKLOS)

Line 3.0 Descriptor. Maximum porosity value for each look-up table (surface)

Line 4.0 (PHIMAX_BRAG(I),I=1,MKLOS)

Line 5.0 Descriptor. Maximum time of data for each look-up table (surface)

Line 6.0 (TIME_DATA_MAX (I),I=1,MKLOS)

Line 7.0 Descriptor. F Factor Data

Repeat Line 8.0 and 9.0 MKLOS times

Line 8.0 Descriptor. F Factor Data for Look-up Table J, J=1 to MKLOS.

Line 9.0 (FDATA(I,J),I=1,NSDATA)

FDATA: Fraction of base gas generation rate [dimensionless]. MKLOS values are required. If there are not MKLOS values then fill the remaining entries with 0.

Line 10.0 Descriptor. Time data.

Line 11.0 Descriptor. TDATA(1:NTDATA)

Line 12.0 (TDATA(I,),I=1,NTDATA)

TDATA: Time corresponding to data entry [sec or day]. NTDATA values are required. All the look-up tables in use have the same number and times at which data is entered. Therefore, TDATA is only a one-dimensional array.

Repeat Line 13.0 to 21.0, K=1 to MKLOS times

Line 13.0 Descriptor. Description of Look-up Table K, K=1 to MKLOS.

Line 14.0 Descriptor. PDATA and SDATA.

Line 15.0 Descriptor. For Look-up Table K data for xxx F Factors are used.

Repeat Line 16.0 to 21.0 J=1 to NSDATA times

Line 16.0 Descriptor. PDATA For Look-Up Table K, and F Factor (J).

Line 17.0 Descriptor. (PDATA(J,I,K) ,I=1,NTDATA)

Line 18.0 (PDATA(J,I,K) ,I=1,NTDATA)

PDATA(J,I,K): Time varying pressure data for Kth look-up table and Jth F Factor [Pa or psi]. NTDATA values are required. If there are not NTDATA values, the remaining entries should be zero filled.

Line 19.0 Descriptor. SDATA For Look-Up Table K, and F Factor (J).

Line 20.0 Descriptor. (SDATA(J,I,K) ,I=1,NTDATA)

Line 21.0 (SDATA(J,I,K) ,I=1,NTDATA)

SDATA(J,I,K): Time varying porosity data for Kth look-up table and Jth F factor [Pa or psi]. NTDATA values are required. If there are not NTDATA values, the remaining entries should be zero filled.

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8.0 ERROR MESSAGES

BRAGFLO outputs a number of error messages and aborts execution when it detects invalid input parameters. The following list of error messages are common and discussed in Section 6.0. However, nearly every line in the input file has a corresponding error message if it detects something wrong or inconsistent. We refer the user to the source code in the event that such an error message appears.

Section 7.2.2, Line 1.5

```
*** MODTYPE Error in READSTARTUP ***
```

The ASCII output file provides additional information:

```
**FATAL ERROR in Input:  MODTYPE = <input value>
**MODTYPE must be 1, 2, or 3.
```

Section 7.2.2, Line 1.5

```
*** Size error in READSTARTUP; invalid NX, NY, or NZ
```

The ASCII output file provides additional information:

```
** FATAL ERROR in Input:         NX,NY,NZ = <input values>
** Maximum values dimensioned:  MX,MY,MZ = <values set in PARAMETER
statement>
** Minimum values allowed:     MX,MY,MZ =     1     1     1
```

Section 7.2.2, Line 1.11

```
*** ERROR in READSTARTUP:  NDTFIXMAX needs to be larger;
     NDTFIX = <input value>
*** NDTFIX error in READSTARTUP ***
```

Section 7.2.3, Line 2.20

```
*** ERROR:  Too many Monitor Blocks in Input:
    Specified: NMON = <NMON input value>
    Maximum:   MMON = <MMON value set in PARAMETER statement>
*** Monitor error in READPRTYPE ***
```

Section 7.2.4, Line 3.2

```
Number of FATAL errors in READMESH = <number of errors>
*** FATAL geometry input errors in READMESH ***
```

Section 7.2.5, Line 4.2

```
In READWELL, NWTIME needs to be larger. NWELLTIMES = <NWELLTIMES input
value>
*** Well time errors in READWELL ***
```

Section 7.2.8, Line 7.24

```
ICWASTE must be 0 when TIMEICRESET = START.
```

```
*** ICWASTE error in READMAT.
```

9.0 DESCRIPTION OF OUTPUT FILES

There can be up to 4 output files created by BRAGFLO. They are as follows:

1. The BRAGFLO binary output (.xbin). This file is the primary results file that is converted by POSTBRAG into CAMDAT Database (.cdb) format.
2. The BRAGFLO ASCII output (.xout). This file echoes input and provides user-readable output and QA information.
3. The BRAGFLO summary (.sum). This file contains a limited amount of summary information on results at each time step for monitoring progress of the solution over time.
4. The BRAGFLO restart output (.xrot). Enough information is stored in this binary file to permit restarting BRAGFLO if execution is halted.

9.1 Binary Output (.xbin) File

This file is the primary results file that is converted by POSTBRAG into standard .cdb format. This file contains output in a more compact form than is possible in an ASCII output file. Most results of interest printed typically every 5 or so time steps and a more limited amount of information printed every time step. The beginning of the file contains QA information, as in the ASCII file (Section 9.2). It also contains an output variable glossary. Enough information is stored to enable a postprocessor, POSTBRAG to read the file and place the results into a CAMDAT data base for additional post-processing and analysis by the downstream codes. The structure of this file is described below. Although it does not contain all the information used in a BRAGFLO run (for example, material properties are absent), it can contain all the results needed for a complete analysis of the results, so it should not be necessary to modify the code or to write additional output files for further post-processing.

A FORTRAN program that will read the binary output file is listed on the following page to illustrate the structure of the file. In this program, the header information is read and saved as variables whose values are not changed later. The information at each time step is read and stored in local variables that are over-written at the next time step, so this information must be written to the output file at each time step as needed for subsequent analysis and post-processing. Although the code BINREAD dates from 1996, the source code has been visually checked to ensure that it accurately represents the .xbin output format for BRAGFLO Version 7.00. Additional comments have been added for clarity. The grid dimensions in the parameter statement in the program BINREAD do not reflect the current WIPP PA grid for BRAGFLO.

```
PROGRAM BINREAD
C
C     Translates BRAGFLO binary file into ASCII file.
C     J. Schreiber, SAIC, 03/08/96
C       Additional comments added by M. Nemer 3/4/07
C     Nemer: Ignore the fact that the dimensions below do not reflect current
C     WIPP PA grid.  Not relevant for understanding BRAGFLO BIN output format
C
      PARAMETER (MX=50,MY=40,MZ=10,NVPR=107,MXHIV=15000,
     1   MVHIV=MX*MY*MZ,MGVAR=10)
C
      CHARACTER*8   RTIME(2),PNAME(2),VRSION(2),UNITS,REVDATE(2)
      CHARACTER*8   NAMVAREL(NVPR),NAMVARHI(MXHIV),NAMVARGL(MGVAR)
      CHARACTER*50  LABELEL(NVPR),LABELHI(MXHIV),LABELGL(MGVAR)
      CHARACTER*20  LABUNTEL(NVPR),LABUNTHI(MXHIV),LABUNTGL(MGVAR)
      CHARACTER*9   DATE(2)
      CHARACTER*32  CPUNAME
      CHARACTER*1   FILTYP
      CHARACTER*80  FILNAM(6),BRAGNAM
      CHARACTER*132 TITLE
      DIMENSION IIHIV(MVHIV,NVPR),JJHIV(MVHIV,NVPR),KKHIV(MVHIV,NVPR)
      DIMENSION UNTCNVEL(NVPR),UNTCNVHI(MXHIV),UNTCNVGL(MGVAR)
      DIMENSION DXGRID(MX,MY,MZ),DYGRID(MX,MY,MZ),DZGRID(MX,MY,MZ)
      DIMENSION GRIDVOL(MX,MY,MZ),LHI(NVPR),LE(NVPR),LH(MXHIV),LG(MGVAR)
      DIMENSION HVAR(MXHIV),YY(MX,MY,MZ),NGBHIV(NVPR)
      REAL IBBALMX,JBBALMX,KBBALMX,IGBALMX,JGBALMX,KGBALMX
C
C
      WRITE (*,*) 'Enter name of BRAGFLO binary file.'
      READ  (*,'(A)') BRAGNAM
C
      OPEN (8,FILE=BRAGNAM,STATUS='OLD',FORM='UNFORMATTED')
      OPEN (9,FILE='ASCII.OUT',STATUS='NEW')
C
C     Read header section with QA info, vbl glossary, grid dimensions:
C       Note:  If first record is 'PREBRAG', then the file starts with
C              PREBRAG QA info; otherwise, there is no PREBRAG info, and
C              the file starts with BRAGFLO QA info.
C       PNAME(1)   = Preprocessor name (PREBRAG).
C       VRSION(1)  = PREBRAG version number.
C       REVDATE(1) = PREBRAG revision date.
C       DATE(1)    = PREBRAG run date.
C       RTIME(1)   = PREBRAG run time.
C       DATE(2)    = BRAGFLO run date.
C       RTIME(2)   = BRAGFLO run time.
C       PNAME(2)   = Program name (BRAGFLO).
C       VRSION(2)  = BRAGFLO version number.
```

```
C       REVDATE(2) = BRAGFLO revision date.
C       CPUNAME    = Name of machine on which BRAGFLO was run.
C       FILTYPE    = Type of file ('B'=binary).
C       NUMFIL     = Number of files used in the BRAGFLO run.
C       FILNAM     = Names of NUMFIL files used by BRAGFLO.
C       TITLE      = Title of run.
C       NX,NY,NZ   = Dimensions of problem run.
C       UNITSO     = Units system used for ouput ('SI' or 'ENGLISH').
C       NVAREL     = Number of element variables.
C       MHIVM      = Number of time- & performance-related history vbls.
C       MHIV       = Total no. of element vbl-based history vbls printed
C                    at each time step.
C       NHIV       = No. of element vbls that are printed as history vbls.
C       NGVAR      = Number of global variables.
C
      READ (8) PNAME(1)
      IF (PNAME(1)(1:7) .EQ. 'PREBRAG') THEN
         READ (8) VRSION(1)
         READ (8) REVDATE(1)
         READ (8) DATE(1)
         READ (8) RTIME(1)
         READ (8) DATE(2)
      ELSE
         DATE(2) = PNAME(1)
      END IF
C
      READ (8) RTIME(2)
      READ (8) PNAME(2)
      READ (8) VRSION(2)
      READ (8) REVDATE(2)
      READ (8) CPUNAME
      READ (8) FILTYP
      READ (8) NUMFIL
      DO 10 I=1,NUMFIL
         READ (8) FILNAM(I)
   10 CONTINUE
      READ (8) TITLE
      READ (8) NX,NY,NZ
      READ (8) UNITS
      READ (8) NVAREL,MHIVM,MHIV,NHIV,NGVAR
      MHIVT = MHIVM + MHIV
C
C     Read glossary of variables:
C       LHI      = Element vbl no. from User Manual Table 7 for this
C                  history vbl.
C       NGBHIV   = No. of grid blocks to be printed as history vbl for
C                  variable LHI.
C       IIHIV    = I-index of grid block for this history variable.
C       JJHIV    = J-index of grid block for this history variable.
```

```
C       KKHIV    = K-index of grid block for this history variable.
C       LE       = Number of the element variable.
C       NAMVAREL = Variable name to be used in POSTBRAG.
C       LABELEL  = Description of this variable.
C       LABUNTEL = Units label for this variable (e.g., Pa).
C       UNTCNVEL = Factor to convert from UNITSO to SI units.
C       LH       = Number of the history variable.
C       NAMVARHI = Variable name to be used in POSTBRAG.
C       LABELHI  = Description of this variable.
C       LABUNTHI = Units label for this variable (e.g., Pa).
C       UNTCNVHI = Factor to convert from UNITSO to SI units.
C       LG       = Number of the global variable.
C       NAMVARGL = Variable name to be used in POSTBRAG.
C       LABELGL  = Description of this variable.
C       LABUNTGL = Units label for this variable (e.g., kg).
C       UNTCNVGL = Factor to convert from UNITSO to SI units.
C
      DO 20 I=1,NHIV
         READ (8) LHI(I),NGBHIV(I),(IIHIV(J,I),JJHIV(J,I),KKHIV(J,I),
     1       J=1,NGBHIV(I))
   20 CONTINUE
      DO 30 I=1,NVAREL
         READ (8) LE(I),NAMVAREL(I),LABELEL(I),LABUNTEL(I),UNTCNVEL(I)
   30 CONTINUE
      DO 40 I=1,MHIVT
         READ (8) LH(I),NAMVARHI(I),LABELHI(I),LABUNTHI(I),UNTCNVHI(I)
   40 CONTINUE
      DO 50 I=1,NGVAR
         READ (8) LG(I),NAMVARGL(I),LABELGL(I),LABUNTGL(I),UNTCNVGL(I)
   50 CONTINUE
C
C     Mesh dimensions and grid block volumes.
C
      READ (8) (((DXGRID(I,J,K),I=1,NX),J=1,NY),K=1,NZ)
      READ (8) (((DYGRID(I,J,K),I=1,NX),J=1,NY),K=1,NZ)
      READ (8) (((DZGRID(I,J,K),I=1,NX),J=1,NY),K=1,NZ)
      READ (8) (((GRIDVOL(I,J,K),I=1,NX),J=1,NY),K=1,NZ)
C
C     *** End of header section (READ) ***
C
C
      IF (PNAME(1)(1:7) .EQ. 'PREBRAG') THEN
         WRITE (9,*) '** PREBRAG Program Name **'
         WRITE (9,*) PNAME(1)
         WRITE (9,*) '** PREBRAG Version Number **'
         WRITE (9,*) VRSION(1)
         WRITE (9,*) '** PREBRAG Revision Date **'
         WRITE (9,*) REVDATE(1)
         WRITE (9,*) '** PREBRAG Run Date **'
         WRITE (9,*) DATE(1)
         WRITE (9,*) '** PREBRAG Run Time **'
         WRITE (9,*) RTIME(1)
      END IF
C
```

```
      WRITE (9,*) '** BRAGFLO Run Date **'
      WRITE (9,*) DATE(2)
      WRITE (9,*) '** BRAGFLO Run Time **'
      WRITE (9,*) RTIME(2)
      WRITE (9,*) '** BRAGFLO Program Name **'
      WRITE (9,*) PNAME(2)
      WRITE (9,*) '** BRAGFLO Version Number **'
      WRITE (9,*) VRSION(2)
      WRITE (9,*) '** BRAGFLO Revision Date **'
      WRITE (9,*) REVDATE(2)
C
      WRITE (9,*) '** Computer Name **'
      WRITE (9,*) CPUNAME
      WRITE (9,*) '** Output File Type **'
      WRITE (9,*) FILTYP
      WRITE (9,*) '** Number of Files Used **'
      WRITE (9,*) NUMFIL
      WRITE (9,*) '** Names of Files Used **'
      DO 60 I=1,NUMFIL
         WRITE (9,*) FILNAM(I)
   60 CONTINUE
C
      WRITE (9,*) '** Title of Run **'
      WRITE (9,'(A)') TITLE
      WRITE (9,*) '** NX, NY, NZ **'
      WRITE (9,*) NX,NY,NZ
      WRITE (9,*) '** Output Units **'
      WRITE (9,*) UNITS
C
      WRITE (9,*) '** NVAREL, MHIVM, MHIV, NHIV, MGVAR **'
      WRITE (9,*) NVAREL,MHIVM,MHIV,NHIV,NGVAR
      WRITE (9,*)
      WRITE (9,*) '** History Vbl Locations **'
      DO 70 I=1,NHIV
         WRITE (9,'(2I5,10(3X,3I3))') LHI(I),NGBHIV(I),
     1       (IIHIV(J,I),JJHIV(J,I),KKHIV(J,I),J=1,NGBHIV(I))
   70 CONTINUE
      WRITE (9,*)
      WRITE (9,*) '** Element Vbl Labels **'
      DO 80 I=1,NVAREL
         WRITE (9,'(I4,2X,A,2X,A,2X,A,1PE16.6)') LE(I),NAMVAREL(I),
     1       LABELEL(I),LABUNTEL(I),UNTCNVEL(I)
   80 CONTINUE
      WRITE (9,*)
      WRITE (9,*) '** History Vbl Labels **'
      DO 90 I=1,MHIVT
         WRITE (9,'(I4,2X,A,2X,A,2X,A,1PE16.6)') LH(I),NAMVARHI(I),
     1       LABELHI(I),LABUNTHI(I),UNTCNVHI(I)
   90 CONTINUE
      WRITE (9,*)
      WRITE (9,*) '** Global Vbl Labels  **'
      DO 100 I=1,NGVAR
         WRITE (9,'(I4,2X,A,2X,A,2X,A,1PE16.6)') LG(I),NAMVARGL(I),
     1       LABELGL(I),LABUNTGL(I),UNTCNVGL(I)
  100 CONTINUE
C
      WRITE (9,*)
      WRITE (9,*) '** Mesh Sizes:  DXGRID **'
      WRITE (9,*) (((DXGRID(I,J,K),I=1,NX),J=1,NY),K=1,NZ)
      WRITE (9,*)
      WRITE (9,*) '** Mesh Sizes:  DYGRID **'
      WRITE (9,*) (((DYGRID(I,J,K),I=1,NX),J=1,NY),K=1,NZ)
      WRITE (9,*)
```

```
      WRITE (9,*) '** Mesh Sizes:  DZGRID **'
      WRITE (9,*) (((DZGRID(I,J,K),I=1,NX),J=1,NY),K=1,NZ)
      WRITE (9,*)
      WRITE (9,*) '** Mesh Sizes:  GRIDVOL **'
      WRITE (9,*) (((GRIDVOL(I,J,K),I=1,NX),J=1,NY),K=1,NZ)
C
C     *** End of header section (WRITE) ***
C
C
C     *** Cycle through time steps ***
C
C     First read time, time step, CPU time, performance measures:
C       TIME     = Elapsed simulation time [s].
C       TIMED    = Elapsed simulation time [days].
C       TIMEYR   = Elapsed simulation time [yr].
C       DELT     = Time step [s].
C       DELTD    = Time step [days].
C       DELTYR   = Time step [yr].
C       AVGITER  = Average Newton-Raphson iterations per time step.
C       CPUS     = CPU time used for this time step [s].
C       CPUHR    = Total CPU time used so far in the run [hr].
C       RNSTEP   = Time step number (REAL).
C       RITERTOT = Total Newton-Raphson iterations so far (REAL).
C       KBIN     = Flag indicating:
C                    =0: only history vbl output will follow.
C                    =1: history vbls and global and element vbls output
C                        will follow at this time step.
C
      NPO = 0
  110 READ (8,END=130) TIME,TIMED,TIMEYR,DELT,DELTD,DELTYR,AVGITER,
     1   CPUS,CPUHR,RNSTEP,RITERTOT,KBIN

C  Read history variables, if there are any.

      IF (MHIV .GT. 0) READ (8,END=130) (HVAR(I),I=1,MHIV)
C
      WRITE (9,*)
      WRITE (9,*)
      WRITE (9,*) '** TIME (s,d,y), DELT (s,d,y), IterAvg, CPU (s,hr),'
     1   //' Step No., IterTot, KBIN'
      WRITE (9,*) TIME,TIMED,TIMEYR,DELT,DELTD,DELTYR,AVGITER,
     1   CPUS,CPUHR,RNSTEP,RITERTOT,KBIN
      WRITE (9,*)
      WRITE (9,*) '** History Vbls at Time Step',RNSTEP
      IF (MHIV .LE. 0) THEN
         WRITE (9,*) '   (no element-variable-based history variables)'
      ELSE
         WRITE (9,*) (HVAR(I),I=1,MHIV)
      END IF
C
C     (History vbls only, if KBIN=0)
C
      IF (KBIN .EQ. 1) THEN
C
C        Global vbls (mass balance info at current step) are read next:
C          BBALC   = Brine mass balance error over entire mesh [kg].
C          GBALC   = Gas mass balance error over entire mesh [kg].
C          BBALMX  = Max relative brine mass bal error in any grid block.
C          GBALMX  = Max relative gas mass bal error in any grid block.
C          IBBALMX = I-index of grid block with BBALMX \
C          JBBALMX = J-index of grid block with BBALMX  |  These are
C          KBBALMX = K-index of grid block with BBALMX  |_ saved as
C          IGBALMX = I-index of grid block with GBALMX  |  REAL vbls
```

```
C          JGBALMX = J-index of grid block with GBALMX  |
C          KGBALMX = K-index of grid block with GBALMX /
C
          READ (8,END=130) BBALC,GBALC,BBALMX,GBALMX,
     1       IBBALMX,JBBALMX,KBBALMX,IGBALMX,JGBALMX,KGBALMX
C
          NPO = NPO + 1
          WRITE (9,*)
          WRITE (9,*) '** Mass Balances (Global Vbls) Printout No.',NPO
          WRITE (9,*) BBALC,GBALC,BBALMX,GBALMX
          WRITE (9,*) IBBALMX,JBBALMX,KBBALMX,IGBALMX,JGBALMX,KGBALMX
C
C
C         The Element vbl distributions are read next.
C
          DO 120 L=1,NVAREL
             READ  (8,END=130) (((YY(I,J,K),I=1,NX),J=1,NY),K=1,NZ)
             WRITE (9,*)
             WRITE (9,'(A,I3,3X,A,F10.1)') ' ** Element Vbl: (No., Name,'
     1          //'Time Step No.) =',L,NAMVAREL(L),RNSTEP
             WRITE (9,*) (((YY(I,J,K),I=1,NX),J=1,NY),K=1,NZ)
  120     CONTINUE
       END IF
C
C      Continue to next time step.
C
       GO TO 110
C
  130  CLOSE (8)
       CLOSE (9)
       STOP '** Normal Completion **'
C
       END
```

9.2 ASCII Output (.xout) File

This file echoes input and provides user-readable output and QA information. It has a "standard" text file format. It starts with QA information, including a time-and-date-of-run stamp, BRAGFLO version number, and revision date. It then echoes the input, but with more information and annotation than found (or allowed) in the input file. Therefore, when problems are encountered with the input, this file should be checked first to be sure that the input was read as intended. Some processed input is then printed out, including information on grid sizes and volumes of each grid block, since this is not necessarily input directly. Then initial conditions are printed, with the amount of information specified by the user. Results specified by the user are printed periodically, at times or frequencies specified by the user. Results at the end of the run are also printed, the amount of information printed being specified by the user. Finally, an ending time-and-date stamp is printed. Use of this file is optional when BRAGFLO is run but is strongly recommended because it always contains an echo of the input, the initial conditions, and results at the end of the run, which makes it useful for debugging input. Additional results are at the discretion of the user and depend on user input. A sample output file is provided in Section 11.3 (Appendix C).

9.3 Summary (.sum) File

A limited amount of summary information is written at each time step to the screen (when BRAGFLO is run interactively) or to a log file (when run in background). The same information is written to this summary file so that a detailed time step summary is available later if BRAGFLO is run interactively. This information is often useful for diagnostic purposes when problems occur.

A typical summary output at one time step appears as follows:

```
                 3.376E-03  8.043E-08   8.951E-01  6.868E-02
                  15 12  1    2 20  1    11 27  1    1 20  1
 1146  1.226E+03  1.101E+03  3    3.31   9.96E-03 10 14  1  3.50E+04 19  8  1
      -8.44E-05 15 12  1  3.16E-08 11  9  1   8.48E-14  3.21E-18 LU
** Monitor Block Arrays:  PO,       PG,       SO,       SOEFC
                         PERMGX,   QR(1),    PHI,      PORSOLID
                         QOBLOCKI, QOBLOCKJ, QGBLOCKI, QGBLOCKJ
                         CONCFE,   CONCBIO,  CONCMGO,  CONCHYDRO
   Monitor Block # 1: ( 26, 12,  1)
   3.9152210460E+06   3.9152210460E+06   1.5000093210E-02   9.3769648059E-08
   2.4032401063E-13   4.3464428375E-17   7.0246988282E-02   1.8071445869E-02
   0.0000000000E+00   0.0000000000E+00   8.4023003688E-07  -1.4217272580E-11
   1.1738049324E+02   1.8251680998E+01   6.7933538603E+01   2.0502677594E-02
   Monitor Block # 2: ( 32, 12,  1)
   2.6628900596E+06   2.6628900596E+06   1.5000107635E-02   1.0838170744E-07
   2.4048109254E-13   5.0244935991E-17   5.5314077124E-02   1.7453495760E-02
   2.0895341248E-12   0.0000000000E+00   1.2491024208E-07  -9.9230520030E-07
   1.1738069953E+02   1.8251873662E+01   6.9367286781E+01   2.0008960985E-02
   Monitor Block # 3: ( 36, 12,  1)
   1.7762631345E+06   1.7762631345E+06   1.5000196086E-02   1.9856475257E-07
   2.4072622281E-13   9.2045625566E-17   4.8978107400E-02   1.7674502997E-02
   1.5659264471E-11   0.0000000000E+00   0.0000000000E+00  -5.5313414058E-07
   1.1738062711E+02   1.8251804889E+01   6.8854557479E+01   2.0282501408E-02
```

Lines 1-2 contain information on how well the variable change or mass balance meets or does not meet the convergence criteria specified in the input. The variables that are written are as follows:

Line 1: EPSMAX(1), EPSMAX(2), FTOLMAX(1), FTOLMAX(2)

Line 2: IEPS(1), JEPS(1), KEPS(1), IEPS(2), JEPS(2), KEPS(2),IFTOL(1), JFTOL(1), KFTOL(1) ,IFTOL(2), JFTOL(2), KFTOL(2)

where

$$\text{EPSMAX(1)}=\max\left(\Delta S_g \times 10^{\varepsilon_1}\right),$$

$$\text{EPSMAX(2)}=\max\left(\frac{\Delta P_b}{P_b \varepsilon_2}\right).$$

ΔS_g = change in gas saturation in a grid block since last iteration,

ΔP_b = change in brine pressure in a grid block since last iteration,

P_b = brine pressure at end of current iteration.

$$\text{FTOLMAX(1)} = \begin{cases} \max\left(\dfrac{F_1 / T_{3g}}{f_1}\right), & T_{3g} \geq T_{3o} \text{ and } F_1 > f_1, \\ \max\left(\dfrac{F_1}{f_1}\right), & T_{3g} \geq T_{3o} \text{ and } F_1 \leq f_1, \\ 0., & T_{3g} < T_{3o} \end{cases}$$

$$\text{FTOLMAX(2)} = \begin{cases} \max\left(\dfrac{F_2 / T_{3b}}{f_2}\right), & T_{3b} \geq T_{3o} \text{ and } F_2 > f_2, \\ \max\left(\dfrac{F_2}{f_2}\right), & T_{3g} \geq T_{3o} \text{ and } F_2 \leq f_2, \\ 0., & T_{3g} < T_{3o} \end{cases}$$

F_1 = discretized gas mass balance equation (see equation (92)),

F_2 = discretized brine mass balance equation,

and the grid block locations where these occur are, respectively:

[IEPS(1),JEPS(1),KEPS(1)],

[IEPS(2),JEPS(2),KEPS(2)],

[IFTOL(1),JFTOL(1),KFTOL(1)],

[IFTOL(2),JFTOL(2),KFTOL(2)].

T_{3g} and T_{3b} are, respectively, the mass of gas and mass of brine in a grid block in [(kg phase)/(m^3 grid block)]. T_{3o} is a small number, set at 1.0×10^{-15} kg/m^3, intended to prevent division by zero and to de-emphasize minute amounts of phase that may be nothing more than round-off.

The maxima are taken over the entire grid for the Newton-Raphson iteration just completed.

The convergence limits are specified in the input [Lines 6.10 and 6.14 in Section 7.2.7]:

ε_1 = EPSNORM(1) = required number of digits of accuracy to the right of the decimal in the change in gas saturation from the last time step.

ε_2 = EPSNORM(2) = maximum relative change allowed in brine pressure over a time step.

f_1 = FTOLNORM(1) = maximum allowable residual for the gas mass balance, normalized by the amount of gas present in the grid block.

f_2 = FTOLNORM(2) = maximum allowable residual for the brine mass balance, normalized by the amount of brine present in the grid block.

Thus, EPSMAX(1) is the maximum fraction of the total allowable change in the gas saturation. It should have a value less than 1.0 when the solution has converged at each time step if ICONVTEST [Line 6.8 in Section 7.2.7] has a value of 1. If ICONVTEST = 0, EPSMAX(1)may be greater than 1.0 when the solution has converged. (In this case, at least two of the values on Line 1 above must be less than or equal to 1.0.)

EPSMAX(2) is the maximum fraction of the allowable change in the brine pressure over an iteration that was obtained in the time step just completed. It should have a value less than 1.0 if ICONVTEST =1. If ICONVTEST = 0, EPSMAX(2) may be greater than 1.0 when the solution has converged (but at least two other values on Line 1 will be less than 1.0).

FTOLMAX(1) is the maximum fraction of the allowable normalized residual in the gas mass balance that was obtained in the time step just completed. It should have a value less than 1.0 if ICONVTEST = 1 but may be greater than 1.0 if ICONVTEST = 0.

FTOLMAX(2) is the maximum fraction of the allowable normalized residual in the brine mass balance that was obtained in the time step just completed. It should have a value less than 1.0 if ICONVTEST = 1 but may be greater than 1.0 if ICONVTEST = 0.

Occasionally, BRAGFLO encounters difficulty in converging to a solution. If a solution has not been obtained at a particular time step after numerous (30-50) time step reductions, it is quite likely that further time step reductions will not improve the solution sufficiently to satisfy the normal convergence criteria, EPSNORM(1) and EPSNORM(2) and FTOLNORM(1) and FTOLNORM(2). One option at this point is for BRAGFLO to abort. The user would then rerun the problem after adjusting one or more of the control parameters and hope for better results. However, it is often the case that BRAGFLO's difficulties are temporary, and that if it can get past the trouble spot, it will complete the run without further major difficulties. Thus, a second option has been built into BRAGFLO to handle those occasions when repeated time step reductions fail to provide convergence: The convergence criteria are temporarily relaxed. These relaxed criteria are applied after user-specified IJACSWITCH time step reductions have occurred, and they continue to be applied only until convergence is obtained at that time step. After IJACRESET time steps, and at all subsequent time steps, the normal convergence criteria are used. This capability makes BRAGFLO a little more robust, enabling it to complete runs that would otherwise abort and require input modifications before rerunning, at only a minor cost in overall accuracy. This feature becomes important when carrying out

large number of runs in automated batch systems. It can be turned off by setting all input values of the loosened criteria equal to the normal criteria. Caution is advised when using this feature because large mass balance errors can be introduced which may not be apparent in a cursory examination of the results. The following BRAGFLO Input control file parameters define the looser convergence criteria:

EPSLOOSE(1): Same meaning as EPSNORM(1); used after IJACSWITCH time step reductions have occurred. Recommended value range: 1 to 4 with a best estimate of 2.

EPSLOOSE(2): Same meaning as EPSNORM(2); used after IJACSWITCH time step reductions have occurred. Recommended value range: 1.0×10^{-1} to 1.0×10^{-4} with a best estimate of 1.0×10^{-2}.

FTOLLOOSE(1): Relaxed value of normalized residual for gas saturation below which convergence is accepted regardless of EPSLOOSE(1); used after IJACSWITCH time step reductions have occurred [kg gas in residual/kg gas in grid block]. Recommended value range: 1.0×10^{-1} to 1.0×10^{-5} with a best estimate of 1.0×10^{-1}.

FTOLLOOSE(2): Relaxed value of normalized residual for brine pressure below which convergence is accepted regardless of EPSLOOSE(2); used after IJACSWITCH time step reductions have occurred [kg brine in residual/kg brine in grid block]. Recommended value range: 1.0×10^{-1} to 1.0×10^{-5} with a best estimate of 1.0×10^{-1}.

When convergence is *not* obtained within ITMAX [Line 6.22 in Section 7.2.7] iterations, lines 1 and 2 are still printed out, providing valuable information as to the magnitude of the convergence problems and where those problems are occurring.

Lines 3 and 4 include time information and global mass balance results, along with grid block locations where maximum mass balance errors occur:

Line 3: IPRINT, TIME*SECYR, DELT/DAYSEC, ITER, CPU, DELTASATMAX, IDEPMAX(1), JDEPMAX(1), KDEPMAX(1), DELTAPRESMAX, IDEPMAX(2), JDEPMAX(2), KDEPMAX(2),

Line 4: GASBALMAX, IGBALMX, JGBALMX, KGBALMX, BRNBALMAX, IBBALMX, JBBALMX, KBBALMX, GASBALCUM, BRNBALCUM, CHSOLVER.

where:

IPRINT	=	time step number;
TIME*SECYR	=	elapsed simulation time since start of run [yr];
DELT/DAYSEC	=	time step size [days];
ITER	=	number of Newton-Raphson iterations to reach convergence;
CPU	=	CPU time to complete this time step [s];
DELTASATMAX	=	maximum saturation change since last time step anywhere in the grid;

IDEPMAX(1)	=	I-index of grid block where DELTASATMAX occurred;
JDEPMAX(1)	=	J-index of grid block where DELTASATMAX occurred;
KDEPMAX(1)	=	K-index of grid block where DELTASATMAX occurred;
DELTAPRESMAX	=	maximum brine pressure change since last time step anywhere in the grid [Pa];
IDEPMAX(2)	=	I-index of grid block where DELTAPRESMAX occurred;
JDEPMAX(2)	=	J-index of grid block where DELTAPRESMAX occurred;
KDEPMAX(2)	=	K-index of grid block where DELTAPRESMAX occurred;
GASBALMAX	=	maximum gas mass balance error relative to mass of gas present in a grid block [kg gas (error)/kg gas in grid block];
IGBALMX	=	I-index of grid block where GASBALMAX occurred;
JGBALMX	=	J-index of grid block where GASBALMAX occurred;
KGBALMX	=	K-index of grid block where GASBALMAX occurred;
BRNBALMAX	=	maximum brine mass balance error relative to mass of brine present in a grid block [kg brine (error)/kg brine in grid block];
IBBALMX	=	I-index of grid block where BRNBALMAX occurred;
JBBALMX	=	J-index of grid block where BRNBALMAX occurred;
KBBALMX	=	K-index of grid block where BRNBALMAX occurred;
GASBALCUM	=	sum of gas mass balance errors over all grid blocks for this time step normalized by the mass of gas in the entire mesh [kg gas(error)/kg gas total grid].
BRNBALCUM	=	sum of brine mass balance errors over all grid blocks for this time step, normalized by the mass of brine in the entire mesh [kg brine (error)/kg brine total grid].
CHSOLVER	=	linear equation solver being used [input on Line 6.20 in Section 7.2.7].

GASBALMAX and BRNBALMAX are computed as follows:

GASBALMAX	=	$\max(F_1)$.
BRNBALMAX	=	$\max(F_2)$.

These mass balance measures are closely related to FTOLMAX(1) and FTOLMAX(2), respectively, the latter being normalized by $T_{3_g} f_1$ or $T_{3_b} f_2$ in the denominator.

Lines 5 through 8 indicate which arrays are being monitored (see discussion of Monitor Blocks, Lines 2.17 - 2.22, in Section 7.2.3). In this example, three grid blocks are being monitored; the grid block locations are indicated on lines 9, 14, and 19. For each monitored grid block, the 16 array values being monitored are listed on the four lines that follow the grid block location.

In BRAGFLO, the following sixteen variables are printed at the monitor grid blocks: PO (brine pressure, Pa), PG (gas pressure, Pa), SO (brine saturation), SOEFC (effective brine saturation), PERMGX (permeability to gas in the x-direction, m^2), QR(1) [H_2 generation rate, kg/(s m^3)], PHI (porosity), PORSOLID (volume change due to chemistry m^3/m^3), QOBLOCKI (inter-block brine flow in x-direction, m^3/s at reference conditions), QOBLOCKJ (inter-block brine flow in y-direction, m^3/s at reference conditions), QGBLOCKI (inter-block gas flow in x-direction, m^3/s at reference conditions), QGBLOCKJ (inter-block gas flow in y-direction, m^3/s at reference conditions), CONCFE (iron concentration, kg/m^3), CONCBIO (cellulosics concentration, kg/m^3), CONCMGO (MgO concentration, kg/m^3), CONCHYDRO (hydromagnesite concentration, kg/m^3).

9.4 Restart Output (.xrot) File

This binary file is written, if requested in the input, at specified times during a run. It is always written at the end of a run if the restart write flag has been set in the input. Enough information is saved to enable BRAGFLO to pick up from where it left off. Each batch of information written is referred to as a restart record. It is up to the user to keep track of when each restart record is written so that if a restart run is needed, the point where BRAGFLO is to resume can be indicated by the number of the restart record. Periodic writing of restart records is strongly recommended in calculations that are anticipated to be lengthy as a precaution against computer or power failures or unforeseen input errors that do not go into effect until late in the calculation. A message is written to the screen and to the summary file (if one is being written) when a restart record is written to assist the user in keeping track of when and how many restart records were written.

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11.0 APPENDICES

11.1 Appendix A: Sample BRAGFLO Input Control File

Below is a sample BRAGFLO input control file. This file is given for illustrative purposes only. Its contents are not necessarily those that would be run for a WIPP compliance PA.

```
**QA**        = PREBRAG QA RECORDS                                                                                    (Line 0.1)
PREBRAG       = PROGRAM NAME                                                                                          (Line 0.2)
9.00          = PROGRAM VERSION                                                                                       (Line 0.3)
08/16/18      = PROGRAM REVISION DATE                                                                                 (Line 0.4)
10/02/18      = PROGRAM RUN DATE                                                                                      (Line 0.5)
10:52:56      = PROGRAM RUN TIME                                                                                      (Line 0.6)
BRAGFLO S2-BF FOR EXAMPLE IO                                                                                          (Line 1.1)
FILE FLAGS...ASCII, BINARY, SUMMARY, RESTART OUT, RESTART INPUT                                                       (Line 1.2)
T T T T F                                                                                                             (Line 1.3)
MODEL TYPE AND NUMBER OF GRID BLOCKS IN X, Y, AND Z                                                                   (Line 1.4)
   2   68   33    1                                                                                                   (Line 1.5)
TSTART,    TMAX,       MAXSTEPS,        YRSEC,    SECYR                                                           (Line 1.6)
 -1.5778E+08   3.1557E+11  30000   3.15569300000000E+07   3.16887700000000E-08                                      (Line 1.7)
DT_INIT,  DT_MIN,    DT_MAX,    DT_INCR, IAUTODT, TSWITCH                                                         (Line 1.8)
  8.6400E+00   8.6400E-04   3.1557E+08   1.2500E+00  1     1.0000E+00                                              (Line 1.9)
TIME-STEP CHANGES: NUMBER OF CHANGES, TIME OF CHANGE, DELT USED                                                     (Line 1.10)
   6                                                                                                                (Line 1.11)
  0.0000E+00   8.6400E+02                                                                                         (Line 1.12)
  3.1557E+09   8.6400E+02
  6.3114E+09   8.6400E+02
  1.1045E+10   8.6400E+02
  1.7356E+10   8.6400E+02
  4.8913E+10   8.6400E+02                                                                                         (Line 1.12)
IPRTYPEASC IPRTYPEBIN IPRTYPERST UNITSI UNITSO                                                                        (Line 2.1)
   2    0    2     'SI'     'SI'                                                                                    (Line 2.2)
ASCII PRINTOUT CONTROLLED BY USER SPECIFIED TIMES                                                                     (Line 2.3)
   9                                                                                                                (Line 2.4)
USER REQUESTED PRINTOUT TIMES                                                                                       (Line 2.4.1)
 0.0000E+00   3.1557E+09   1.1045E+10   3.1557E+10   9.4671E+10   1.5778E+11                                      (Line 2.4.2)
 2.2090E+11   2.8401E+11   3.1557E+11
BINARY PRINTOUT CONTROLLED BY STEP INTERVAL, IPRNTBIN                                                                 (Line 2.5)
   5                                                                                                                (Line 2.6)
RESTART PRINTOUT CONTROLLED BY USER SPECIFIED TIMES                                                                   (Line 2.7)
   1                                                                                                                (Line 2.8)
USER REQUESTED RESTART TIMES                                                                                        (Line 2.8.1)
 3.1557E+11                                                                                                         (Line 2.8.2)
ASCII PRINT FLAGS                                                                                                     (Line 2.9)
 1 1 0 0 0  1 0 0 0 0  0 0 0 0 0  0 0 1 0 0  0 0 0 0 0                                                             (Line 2.10)
```

```
 0 0 0 0 0  0 0 0 0 0  0 0 0 0 0  0 0 0 0 0  0 0 0 1 0
 0 0 0 0 0  0 0 0 1 1  0 0 1 0 0  0 0 0 0 0  0 0 0 0 0
 0 0 0 0 0  0 0 0 0 0  0 0 0 0 0  1 0 0 0 0  0 0 0 0 0
 0 0 0 0 0  0 0 0 0 0  0 0 0 0 0
 1 1 1 1 1  1 1 1 1 1                                                    (Line 2.10)
BINARY PRINT FLAGS                                                       (Line 2.11)
 1 1 0 0 0  1 0 0 0 1  1 0 0 1 0  0 0 1 0 0  0 0 0 0 0                   (Line 2.12)
 0 0 0 0 0  1 1 0 1 1  0 0 0 0 0  0 0 0 0 0  0 0 0 1 1
 0 0 0 0 0  0 0 0 1 1  0 0 1 0 0  0 0 0 0 0  0 0 0 0 0
 0 0 0 0 0  0 0 0 0 0  0 0 0 0 0  1 0 0 0 0  0 0 0 0 0
 0 0 0 0 0  0 0 0 0 0  0 0 0 0 0
 1 1 1 1 1  1 1 1 1 1                                                    (Line 2.12)
HISTORY VARIABLE OUTPUT                                                  (Line 2.13)
   0                                                                     (Line 2.14)
MONITOR PARAMETER VALUES AT GRIDBLOCK(S)                                 (Line 2.17)
T                                                                        (Line 2.18)
NUMBER OF MONITOR BLOCKS                                                 (Line 2.19)
   3                                                                     (Line 2.20)
MONITOR BLOCKS (I,J,K)                                                   (Line 2.21)
  26   12    1                                                          (Line 2.22)
  32   12    1
  36   12    1                                                          (Line 2.22)
GRID DATA FLAGS: IDXFLAG, IDYFLAG, IDZFLAG, IDEPTHFLAG                   (Line 3.1)
   1    2    1    7                                                     (Line 3.2)
GRID DATA CARDS: GRID BLOCK DX'S                                         (Line 3.3)
1.220383E+04  3.126850E+03  2.156450E+03  1.487210E+03  1.025660E+03  7.073500E+02   (Line 3.4)
5.266800E+02  3.632300E+02  2.505000E+02  1.727600E+02  1.191500E+02  8.217000E+01
5.667000E+01  3.908000E+01  2.695000E+01  1.859000E+01  1.282000E+01  8.840000E+00
6.100000E+00  4.200000E+00  2.900000E+00  2.000000E+00  4.380000E+01  1.000000E+01
2.000000E+00  2.757500E-01  2.000000E+00  1.000000E+01  4.380000E+01  1.524000E+01
1.524000E+01  1.402000E+02  1.402000E+02  1.524000E+01  1.524000E+01  1.402000E+02
1.402000E+02  3.048000E+01  3.048000E+01  9.870000E+01  9.870000E+01  9.870000E+01
1.000000E+01  3.616500E+02  3.616500E+02  2.000000E+00  2.900000E+00  4.200000E+00
6.100000E+00  8.840000E+00  1.282000E+01  1.859000E+01  2.695000E+01  3.908000E+01
5.667000E+01  8.217000E+01  1.191500E+02  1.727600E+02  2.505000E+02  3.632300E+02
5.266800E+02  7.073500E+02  1.025660E+03  1.487210E+03  2.156450E+03  3.126850E+03
4.533940E+03  7.669890E+03                                               (Line 3.4)
GRID DATA CARDS: GRID BLOCK DY'S                                         (Line 3.5)
1.258300E+02  5.227000E+01  6.672000E+01  6.672000E+01  6.572000E+01  1.000000E+00   (Line 3.6)
8.500000E-01  6.900000E-01  6.900000E-01  1.320000E+00  1.320000E+00  1.320000E+00
2.620000E+00  2.700000E-01  4.530000E+00  4.530000E+00  1.800000E-01  5.473000E+01
5.473000E+01  5.473000E+01  5.473000E+01  5.473000E+01  5.473000E+01  5.473000E+01
3.600000E+01  7.700000E+00  2.480000E+01  8.500000E+00  1.730000E+01  1.060000E+02
4.330000E+01  1.566000E+01  1.000000E-01                                   (Line 3.6)
GRID DATA CARDS: GRID BLOCK DZ'S                                         (Line 3.7)
6.617707E+04  3.551571E+04  2.494910E+04  1.766178E+04  1.263605E+04  9.170020E+03   (Line 3.8)
6.701950E+03  4.922120E+03  3.694660E+03  2.848130E+03  2.264310E+03  1.861680E+03
1.584010E+03  1.392510E+03  1.260440E+03  1.169360E+03  1.106540E+03  1.063220E+03
1.033340E+03  1.012740E+03  9.985300E+02  9.887300E+02  1.262000E+02  2.880000E+01
4.800000E+00  2.757500E-01  4.800000E+00  2.880000E+01  1.262000E+02  2.000000E+01
2.000000E+01  1.569040E+02  1.569040E+02  4.000000E+01  4.000000E+01  1.961300E+02
```

```
 1.961300E+02  4.000000E+01  4.000000E+01  3.218000E+01  3.218000E+01  3.218000E+01
 9.500000E+00  5.167000E+01  5.168000E+01  2.839580E+03  2.849380E+03  2.863590E+03
 2.884190E+03  2.914070E+03  2.957390E+03  3.020200E+03  3.111290E+03  3.243360E+03
 3.434860E+03  3.712530E+03  4.115160E+03  4.698980E+03  5.545500E+03  6.772970E+03
 8.552800E+03  1.102087E+04  1.448690E+04  1.951263E+04  2.679995E+04  3.736656E+04
 5.268814E+04  7.709580E+04                                                    (Line 3.8)
GRID BLOCK ELEVATIONS                                                         (Line 3.9)
 68*+6.291500E+01                                                             (Line 3.10)
 68*+1.519650E+02
  1*-9.207772E+01    1*+4.170092E+01    1*+8.780408E+01    1*+1.195994E+02
  1*+1.415272E+02    1*+1.566498E+02    1*+1.674182E+02    1*+1.751837E+02
  1*+1.805393E+02    1*+1.842327E+02    1*+1.867800E+02    1*+1.885368E+02
  1*+1.897483E+02    1*+1.905838E+02    1*+1.911600E+02    1*+1.915574E+02
  1*+1.918315E+02    1*+1.920205E+02    1*+1.921509E+02    1*+1.922408E+02
  1*+1.923027E+02    1*+1.923455E+02    1*+1.927451E+02    1*+1.932146E+02
  1*+1.933193E+02    1*+1.933392E+02    1*+1.933590E+02    1*+1.934638E+02
  1*+1.939332E+02    1*+1.944484E+02    1*+1.947144E+02    1*+1.960708E+02
  1*+1.985176E+02    1*+1.998740E+02    1*+2.001400E+02    1*+2.014964E+02
  1*+2.039432E+02    1*+2.054326E+02    1*+2.059646E+02    1*+2.070918E+02
  1*+2.088144E+02    1*+2.105369E+02    1*+2.114855E+02    1*+2.147286E+02
  1*+2.210402E+02    1*+2.242135E+02    1*+2.242563E+02    1*+2.243182E+02
  1*+2.244081E+02    1*+2.245385E+02    1*+2.247275E+02    1*+2.250016E+02
  1*+2.253990E+02    1*+2.259752E+02    1*+2.268107E+02    1*+2.280222E+02
  1*+2.297790E+02    1*+2.323263E+02    1*+2.360197E+02    1*+2.413752E+02
  1*+2.491408E+02    1*+2.599092E+02    1*+2.750318E+02    1*+2.969596E+02
  1*+3.287549E+02    1*+3.748581E+02    1*+4.417077E+02    1*+5.482008E+02
  1*-2.536788E+01    1*+1.084108E+02    1*+1.545139E+02    1*+1.863092E+02
  1*+2.082371E+02    1*+2.233597E+02    1*+2.341281E+02    1*+2.418936E+02
  1*+2.472491E+02    1*+2.509426E+02    1*+2.534898E+02    1*+2.552466E+02
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1*+8.604015E+01    1*+2.198188E+02    1*+2.659219E+02    1*+2.977173E+02
1*+3.196451E+02    1*+3.347677E+02    1*+3.455361E+02    1*+3.533016E+02
1*+3.586571E+02    1*+3.623506E+02    1*+3.648979E+02    1*+3.666546E+02
1*+3.678662E+02    1*+3.687017E+02    1*+3.692779E+02    1*+3.696753E+02
1*+3.699494E+02    1*+3.701384E+02    1*+3.702688E+02    1*+3.703586E+02
1*+3.704206E+02    1*+3.704634E+02    1*+3.708630E+02    1*+3.713325E+02
1*+3.714372E+02    1*+3.714571E+02    1*+3.714769E+02    1*+3.715816E+02
1*+3.720511E+02    1*+3.725663E+02    1*+3.728323E+02    1*+3.741887E+02
1*+3.766355E+02    1*+3.779919E+02    1*+3.782579E+02    1*+3.796143E+02
1*+3.820611E+02    1*+3.835505E+02    1*+3.840824E+02    1*+3.852097E+02
1*+3.869322E+02    1*+3.886548E+02    1*+3.896033E+02    1*+3.928464E+02
1*+3.991581E+02    1*+4.023314E+02    1*+4.023741E+02    1*+4.024361E+02
1*+4.025260E+02    1*+4.026563E+02    1*+4.028454E+02    1*+4.031194E+02
1*+4.035168E+02    1*+4.040930E+02    1*+4.049286E+02    1*+4.061401E+02
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1*+4.272587E+02    1*+4.380271E+02    1*+4.531496E+02    1*+4.750775E+02
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1*+3.241744E+02    1*+3.392970E+02    1*+3.500654E+02    1*+3.578309E+02
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1*+3.789351E+02    1*+3.794502E+02    1*+3.797162E+02    1*+3.810726E+02
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   1*+8.148159E+02    1*+8.609190E+02    1*+9.277687E+02    1*+1.034262E+03
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  42*+8.653400E+02    1*+8.652659E+02   25*+8.653400E+02
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  42*+1.031120E+03    1*+1.031021E+03   25*+1.031120E+03
  42*+1.039000E+03    1*+1.038899E+03   25*+1.039000E+03                    (Line 3.10)
WELL DATA                                                                  (Line 4.1)
 0                                                                         (Line 4.2)
DIRICHLET CONDITIONS                                                       (Line 4.7)
T     72                                                                   (Line 4.8)
   1  26   1   T   F   9.333000E+05   0.000000E+00                         (Line 4.9)
  68  26   1   T   F   9.333000E+05   0.000000E+00
   1  28   1   T   F   9.631000E+05   0.000000E+00
  68  28   1   T   F   9.631000E+05   0.000000E+00
   1  33   1   T   T   1.013250E+05   8.363000E-02
   2  33   1   T   T   1.013250E+05   8.363000E-02
   3  33   1   T   T   1.013250E+05   8.363000E-02
   4  33   1   T   T   1.013250E+05   8.363000E-02
   5  33   1   T   T   1.013250E+05   8.363000E-02
   6  33   1   T   T   1.013250E+05   8.363000E-02
   7  33   1   T   T   1.013250E+05   8.363000E-02
   8  33   1   T   T   1.013250E+05   8.363000E-02
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9	33	1	T	T	1.013250E+05	8.363000E-02
10	33	1	T	T	1.013250E+05	8.363000E-02
11	33	1	T	T	1.013250E+05	8.363000E-02
12	33	1	T	T	1.013250E+05	8.363000E-02
13	33	1	T	T	1.013250E+05	8.363000E-02
14	33	1	T	T	1.013250E+05	8.363000E-02
15	33	1	T	T	1.013250E+05	8.363000E-02
16	33	1	T	T	1.013250E+05	8.363000E-02
17	33	1	T	T	1.013250E+05	8.363000E-02
18	33	1	T	T	1.013250E+05	8.363000E-02
19	33	1	T	T	1.013250E+05	8.363000E-02
20	33	1	T	T	1.013250E+05	8.363000E-02
21	33	1	T	T	1.013250E+05	8.363000E-02
22	33	1	T	T	1.013250E+05	8.363000E-02
23	33	1	T	T	1.013250E+05	8.363000E-02
24	33	1	T	T	1.013250E+05	8.363000E-02
25	33	1	T	T	1.013250E+05	8.363000E-02
26	33	1	T	T	1.013250E+05	8.363000E-02
27	33	1	T	T	1.013250E+05	8.363000E-02
28	33	1	T	T	1.013250E+05	8.363000E-02
29	33	1	T	T	1.013250E+05	8.363000E-02
30	33	1	T	T	1.013250E+05	8.363000E-02
31	33	1	T	T	1.013250E+05	8.363000E-02
32	33	1	T	T	1.013250E+05	8.363000E-02
33	33	1	T	T	1.013250E+05	8.363000E-02
34	33	1	T	T	1.013250E+05	8.363000E-02
35	33	1	T	T	1.013250E+05	8.363000E-02
36	33	1	T	T	1.013250E+05	8.363000E-02
37	33	1	T	T	1.013250E+05	8.363000E-02
38	33	1	T	T	1.013250E+05	8.363000E-02
39	33	1	T	T	1.013250E+05	8.363000E-02
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41	33	1	T	T	1.013250E+05	8.363000E-02
42	33	1	T	T	1.013250E+05	8.363000E-02
43	33	1	T	F	1.013250E+05	0.000000E+00
44	33	1	T	T	1.013250E+05	8.363000E-02
45	33	1	T	T	1.013250E+05	8.363000E-02
46	33	1	T	T	1.013250E+05	8.363000E-02
47	33	1	T	T	1.013250E+05	8.363000E-02
48	33	1	T	T	1.013250E+05	8.363000E-02
49	33	1	T	T	1.013250E+05	8.363000E-02
50	33	1	T	T	1.013250E+05	8.363000E-02
51	33	1	T	T	1.013250E+05	8.363000E-02
52	33	1	T	T	1.013250E+05	8.363000E-02
53	33	1	T	T	1.013250E+05	8.363000E-02
54	33	1	T	T	1.013250E+05	8.363000E-02
55	33	1	T	T	1.013250E+05	8.363000E-02
56	33	1	T	T	1.013250E+05	8.363000E-02
57	33	1	T	T	1.013250E+05	8.363000E-02
58	33	1	T	T	1.013250E+05	8.363000E-02
59	33	1	T	T	1.013250E+05	8.363000E-02

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  62  33   1   T   T   1.013250E+05   8.363000E-02
  63  33   1   T   T   1.013250E+05   8.363000E-02
  64  33   1   T   T   1.013250E+05   8.363000E-02
  65  33   1   T   T   1.013250E+05   8.363000E-02
  66  33   1   T   T   1.013250E+05   8.363000E-02
  67  33   1   T   T   1.013250E+05   8.363000E-02
  68  33   1   T   T   1.013250E+05   8.363000E-02                                    (Line 4.9)
GRID BLOCK BRINE PRESSURE INITIAL CONDITIONS                                       (Line 5.1)
 22*+1.599190E+07   23*+1.331219E+07   23*+1.599190E+07                             (Line 5.2)
 68*+1.492134E+07
  1*+1.785614E+07    1*+1.624692E+07    1*+1.569261E+07    1*+1.531038E+07
  1*+1.504681E+07    1*+1.486504E+07    1*+1.473562E+07    1*+1.464229E+07
  1*+1.457793E+07    1*+1.453354E+07    1*+1.450293E+07    1*+1.448181E+07
  1*+1.446725E+07    1*+1.445721E+07    1*+1.445029E+07    1*+1.444551E+07
  1*+1.444222E+07    1*+1.443995E+07    1*+1.443838E+07    1*+1.443730E+07
  1*+1.443656E+07    1*+1.443604E+07    1*+1.443124E+07    1*+1.442560E+07
  1*+1.442434E+07    1*+1.442410E+07    1*+1.442386E+07    1*+1.442260E+07
  1*+1.441696E+07    1*+1.441077E+07    1*+1.440757E+07    1*+1.439127E+07
  1*+1.436187E+07    1*+1.434557E+07    1*+1.434237E+07    1*+1.432607E+07
  1*+1.429667E+07    1*+1.427877E+07    1*+1.427238E+07    1*+1.425884E+07
  1*+1.423814E+07    1*+1.421744E+07    1*+1.420604E+07    1*+1.416707E+07
  1*+1.409123E+07    1*+1.405309E+07    1*+1.405258E+07    1*+1.405184E+07
  1*+1.405076E+07    1*+1.404919E+07    1*+1.404692E+07    1*+1.404363E+07
  1*+1.403885E+07    1*+1.403193E+07    1*+1.402189E+07    1*+1.400733E+07
  1*+1.398622E+07    1*+1.395561E+07    1*+1.391124E+07    1*+1.384689E+07
  1*+1.375358E+07    1*+1.362421E+07    1*+1.344252E+07    1*+1.317910E+07
  1*+1.279718E+07    1*+1.224348E+07    1*+1.144078E+07    1*+1.016252E+07
  1*+1.705371E+07    1*+1.544489E+07    1*+1.489072E+07    1*+1.450859E+07
  1*+1.424508E+07    1*+1.406336E+07    1*+1.393396E+07    1*+1.384066E+07
  1*+1.377631E+07    1*+1.373194E+07    1*+1.370133E+07    1*+1.368022E+07
  1*+1.366567E+07    1*+1.365563E+07    1*+1.364871E+07    1*+1.364393E+07
  1*+1.364064E+07    1*+1.363837E+07    1*+1.363680E+07    1*+1.363572E+07
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1*+8.631285E+06    1*+8.621262E+06    1*+8.614350E+06    1*+8.609583E+06
1*+8.606295E+06    1*+8.604028E+06    1*+8.602464E+06    1*+8.601386E+06
1*+8.600642E+06    1*+8.600129E+06    1*+8.595335E+06    1*+8.589704E+06
1*+8.588448E+06    1*+8.588209E+06    1*+8.587971E+06    1*+8.586715E+06
1*+8.581083E+06    1*+8.574903E+06    1*+8.571713E+06    1*+8.555442E+06
1*+8.526091E+06    1*+8.509821E+06    1*+8.506630E+06    1*+8.490360E+06
1*+8.461010E+06    1*+8.443144E+06    1*+8.436763E+06    1*+8.423242E+06
1*+8.402580E+06    1*+8.381918E+06    1*+1.013250E+05    1*+8.331641E+06
1*+8.255935E+06    1*+8.217874E+06    1*+8.217361E+06    1*+8.216618E+06
1*+8.215540E+06    1*+8.213976E+06    1*+8.211709E+06    1*+8.208421E+06
1*+8.203655E+06    1*+8.196744E+06    1*+8.186723E+06    1*+8.172191E+06
1*+8.151120E+06    1*+8.120569E+06    1*+8.076270E+06    1*+8.012038E+06
1*+7.918904E+06    1*+7.789760E+06    1*+7.608406E+06    1*+7.345460E+06
1*+6.964229E+06    1*+6.411527E+06    1*+5.610282E+06    1*+4.334326E+06
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   1*+1.135699E+07     1*+9.751011E+06     1*+9.197814E+06     1*+8.816356E+06
   1*+8.553308E+06     1*+8.371909E+06     1*+8.242746E+06     1*+8.149604E+06
   1*+8.085371E+06     1*+8.041073E+06     1*+8.010522E+06     1*+7.989452E+06
   1*+7.974922E+06     1*+7.964901E+06     1*+7.957990E+06     1*+7.953224E+06
   1*+7.949937E+06     1*+7.947670E+06     1*+7.946107E+06     1*+7.945029E+06
   1*+7.944286E+06     1*+7.943773E+06     1*+7.938980E+06     1*+7.933349E+06
   1*+7.932093E+06     1*+7.931855E+06     1*+7.931617E+06     1*+7.930361E+06
   1*+7.924731E+06     1*+7.918552E+06     1*+7.915362E+06     1*+7.899095E+06
   1*+7.869750E+06     1*+7.853483E+06     1*+7.850293E+06     1*+7.834026E+06
   1*+7.804681E+06     1*+7.786820E+06     1*+7.780440E+06     1*+7.766921E+06
   1*+7.746264E+06     1*+7.725606E+06     1*+1.013250E+05     1*+7.675339E+06
   1*+7.599649E+06     1*+7.561595E+06     1*+7.561082E+06     1*+7.560339E+06
   1*+7.559261E+06     1*+7.557698E+06     1*+7.555431E+06     1*+7.552145E+06
   1*+7.547379E+06     1*+7.540470E+06     1*+7.530450E+06     1*+7.515922E+06
   1*+7.494855E+06     1*+7.464310E+06     1*+7.420020E+06     1*+7.355801E+06
   1*+7.262686E+06     1*+7.133568E+06     1*+6.952251E+06     1*+6.689359E+06
   1*+6.308205E+06     1*+5.755615E+06     1*+4.954534E+06     1*+3.678837E+06
  42*+2.283128E+06     1*+1.013250E+05    25*+2.283128E+06
  42*+9.333000E+05     1*+1.013250E+05    25*+9.333000E+05
  42*+1.827015E+06     1*+1.013250E+05    25*+1.827015E+06
  42*+9.631000E+05     1*+1.013250E+05    25*+9.631000E+05
  42*+1.473304E+06     1*+1.013250E+05    25*+1.473304E+06
  42*+7.355477E+05     1*+1.013250E+05    25*+7.355477E+05
  68*+1.013250E+05
  68*+1.013250E+05
  68*+1.013250E+05                                                                (Line 5.2)
 GRID BLOCK BRINE SATURATION INITIAL CONDITIONS                                   (Line 5.3)
  68*+1.000000E+00                                                                (Line 5.4)
  68*+1.000000E+00
  68*+1.000000E+00
  68*+1.000000E+00
  68*+1.000000E+00
  68*+1.000000E+00
  68*+1.000000E+00
  42*+1.000000E+00     1*+9.999999E-01    25*+1.000000E+00
  42*+1.000000E+00     1*+9.999999E-01    25*+1.000000E+00
  22*+1.000000E+00     7*+1.500000E-02     2*+0.000000E+00     2*+1.500000E-02
   2*+5.664186E-01     2*+1.500000E-02     2*+5.664186E-01     3*+0.000000E+00
   1*+9.999999E-01     2*+0.000000E+00    23*+1.000000E+00
  22*+1.000000E+00     7*+1.500000E-02     2*+0.000000E+00     2*+1.500000E-02
   2*+5.664186E-01     2*+1.500000E-02     2*+5.664186E-01     3*+0.000000E+00
   1*+9.999999E-01     2*+0.000000E+00    23*+1.000000E+00
  22*+1.000000E+00     7*+1.500000E-02     2*+0.000000E+00     2*+1.500000E-02
   2*+5.664186E-01     2*+1.500000E-02     2*+5.664186E-01     3*+0.000000E+00
   1*+9.999999E-01     2*+0.000000E+00    23*+1.000000E+00
  42*+1.000000E+00     1*+9.999999E-01    25*+1.000000E+00
  68*+1.000000E+00
  42*+1.000000E+00     1*+9.999999E-01    25*+1.000000E+00
  42*+1.000000E+00     1*+9.999999E-01    25*+1.000000E+00
  68*+1.000000E+00
  42*+1.000000E+00     1*+9.999999E-01    25*+1.000000E+00
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  42*+1.000000E+00    1*+9.999999E-01   25*+1.000000E+00
  42*+1.000000E+00    1*+9.999999E-01   25*+1.000000E+00
  42*+1.000000E+00    1*+9.999999E-01   25*+1.000000E+00
  42*+1.000000E+00    1*+9.999999E-01   25*+1.000000E+00
  42*+1.000000E+00    1*+9.999999E-01   25*+1.000000E+00
  42*+1.000000E+00    1*+9.999999E-01   25*+1.000000E+00
  42*+1.000000E+00    1*+9.999999E-01   25*+1.000000E+00
  42*+1.000000E+00    1*+9.999999E-01   25*+1.000000E+00
  42*+1.000000E+00    1*+9.999999E-01   25*+1.000000E+00
  42*+1.000000E+00    1*+9.999999E-01   25*+1.000000E+00
  42*+1.000000E+00    1*+9.999999E-01   25*+1.000000E+00
  42*+1.000000E+00    1*+9.999999E-01   25*+1.000000E+00
  42*+8.360000E-02    1*+9.999999E-01   25*+8.360000E-02
  42*+8.363000E-02    1*+9.999999E-01   25*+8.363000E-02
  42*+8.363000E-02    1*+9.999999E-01   25*+8.363000E-02                                                                     (Line 5.4)
 GRID BLOCK FE CONCENTRATION INITIAL CONDITIONS                                                                              (Line 5.5)
  68*+0.000000E+00                                                                                                           (Line 5.6)
  68*+0.000000E+00
  68*+0.000000E+00
  68*+0.000000E+00
  68*+0.000000E+00
  68*+0.000000E+00
  68*+0.000000E+00
  68*+0.000000E+00
  68*+0.000000E+00
  22*+0.000000E+00    7*+1.341199E+02    2*+0.000000E+00    2*+1.341199E+02
   2*+0.000000E+00    2*+1.341199E+02   31*+0.000000E+00
  22*+0.000000E+00    7*+1.341199E+02    2*+0.000000E+00    2*+1.341199E+02
   2*+0.000000E+00    2*+1.341199E+02   31*+0.000000E+00
  22*+0.000000E+00    7*+1.341199E+02    2*+0.000000E+00    2*+1.341199E+02
   2*+0.000000E+00    2*+1.341199E+02   31*+0.000000E+00
  68*+0.000000E+00
  68*+0.000000E+00
  68*+0.000000E+00
  68*+0.000000E+00
  68*+0.000000E+00
  68*+0.000000E+00
  68*+0.000000E+00
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  68*+0.000000E+00
  68*+0.000000E+00
  68*+0.000000E+00
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  68*+0.000000E+00                                                                                    (Line 5.6)
 GRID BLOCK CH2O CONCENTRATION INITIAL CONDITIONS                                                      (Line 5.7)
  68*+0.000000E+00                                                                                    (Line 5.8)
  68*+0.000000E+00
  68*+0.000000E+00
  68*+0.000000E+00
  68*+0.000000E+00
  68*+0.000000E+00
  68*+0.000000E+00
  68*+0.000000E+00
  68*+0.000000E+00
  22*+0.000000E+00    7*+1.973741E+01    2*+0.000000E+00    2*+1.973741E+01
   2*+0.000000E+00    2*+1.973741E+01   31*+0.000000E+00
  22*+0.000000E+00    7*+1.973741E+01    2*+0.000000E+00    2*+1.973741E+01
   2*+0.000000E+00    2*+1.973741E+01   31*+0.000000E+00
  22*+0.000000E+00    7*+1.973741E+01    2*+0.000000E+00    2*+1.973741E+01
   2*+0.000000E+00    2*+1.973741E+01   31*+0.000000E+00
  68*+0.000000E+00
  68*+0.000000E+00
  68*+0.000000E+00
  68*+0.000000E+00
  68*+0.000000E+00
  68*+0.000000E+00
  68*+0.000000E+00
  68*+0.000000E+00
  68*+0.000000E+00
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  68*+0.000000E+00
  68*+0.000000E+00
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  68*+0.000000E+00
  68*+0.000000E+00
  68*+0.000000E+00
  68*+0.000000E+00
  68*+0.000000E+00                                                                                    (Line 5.8)
 GRID BLOCK MGO CONCENTRATION INITIAL CONDITIONS                                                       (Line 5.9)
  68*+0.000000E+00                                                                                   (Line 5.10)
  68*+0.000000E+00
  68*+0.000000E+00
  68*+0.000000E+00
  68*+0.000000E+00
  68*+0.000000E+00
  68*+0.000000E+00
  68*+0.000000E+00
  68*+0.000000E+00
  68*+0.000000E+00
  22*+0.000000E+00    7*+1.093308E+02    2*+0.000000E+00    2*+1.093308E+02
   2*+0.000000E+00    2*+1.093308E+02   31*+0.000000E+00
  22*+0.000000E+00    7*+1.093308E+02    2*+0.000000E+00    2*+1.093308E+02
```

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  2*+0.000000E+00    2*+1.093308E+02   31*+0.000000E+00
 22*+0.000000E+00    7*+1.093308E+02    2*+0.000000E+00    2*+1.093308E+02
  2*+0.000000E+00    2*+1.093308E+02   31*+0.000000E+00
 68*+0.000000E+00
 68*+0.000000E+00
 68*+0.000000E+00
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 68*+0.000000E+00
 68*+0.000000E+00
 68*+0.000000E+00
 68*+0.000000E+00                                                    (Line 5.10)
DSATLIM, DPRESLIM, SATLIMIT                                          (Line 6.1)
  2.0000E-01  -1.0000E+08   1.0000E-03                               (Line 6.2)
SATNORM, PRESNORM: NOMINAL CHANGE DEPENDENT VARIABLE                 (Line 6.3)
  3.0000E-01   5.0000E+05                                            (Line 6.4)
MAXIMUM ALLOWABLE VARIABLE CHANGES: DSAT_MAX  DPRES_MAX              (Line 6.5)
  1.0000E+00   1.0000E+07                                            (Line 6.6)
CONVERGENGE TEST FLAG: 0=OR/1=AND                                    (Line 6.7)
   1                                                                 (Line 6.8)
EPS_SAT, EPS_PRES:  NORMAL CONVERGENCE CRITERIA                      (Line 6.9)
  3.0000E+00   1.0000E-02                                           (Line 6.10)
EPS_SAT, EPS_PRES:  RELAXED CONVERGENCE CRITERIA                     (Line 6.11)
  3.0000E+00   1.0000E-02                                           (Line 6.12)
FTOL_SAT   FTOL_PRES:  NORMAL RESIDUAL TOLERANCE                     (Line 6.13)
  1.0000E-02   1.0000E-02                                           (Line 6.14)
FTOL_SAT   FTOL_PRES:  RELAXED RESIDUAL TOLERANCE                    (Line 6.15)
  1.0000E-02   1.0000E-02                                           (Line 6.16)
GAS TRANSPORT TOLERANCES                                             (Line 6.17)
  1.0000E-05   1.0000E-05   1.0000E-05   1.0000E-05                  (Line 6.18)
LINEAR EQUATION SOLVER TYPE                                          (Line 6.19)
LU                                                                   (Line 6.20)
ITMAX, IRESETMAX, IJACINT, LSCALE, P_SCALE, LVARSWITCH               (Line 6.21)
   8   40    1   T     1.0000E+07 F                                  (Line 6.22)
IUPRPFLAG, IUPMFLAG, DT_REDU, ITRAVE, IMFRAVE                        (Line 6.23)
   9    9   5.0000E-01    1    0                                     (Line 6.24)
IJACSWITCH, IJACMIN, IJACRESET, IUPRPLOOSE, IUPMFLOOSE               (Line 6.25)
  41    1    5    9    9                                            (Line 6.26)
DHSAT_REL, DHPRES_REL: REL. CHANGE FOR JACOBIAN ELEMENT CALCS        (Line 6.27)
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   1.0000E-08   1.0000E-08                                                    (Line 6.28)
 DHSAT_MIN, DHPRES_MIN: MIN. CHANGE ALLOWED FOR JACOBIAN CALCS               (Line 6.29)
   1.0000E-10   1.0000E-02                                                   (Line 6.30)
 NUMBER OF TIMES FOR SPECIFYING MATERIAL MAP                                 (Line 7.1)
 7                                                                           (Line 7.2)
 START TIME FOR MAP 1                                                        (Line 7.3)
-1.5778E+08                                                                  (Line 7.4)
 MATERIAL TYPE GRID MAP                                                      (Line 7.5)
  22*10    23*11    23*10                                                   (Line 7.6)
  68*10
  68*1
  68*1
  68*1
  68*1
  22*3      7*2      2*3      2*2      2*3      2*2      2*3      3*12     1*3      2*12     23*3
  22*1      7*2      2*13     2*2      2*13     2*2      2*13     3*12     1*9      2*12     23*1
  22*1      7*2      2*13     2*2      2*13     2*2      2*13     3*12     1*9      2*12     23*1
  22*1      7*6      2*14     2*7      2*14     2*7      2*14     3*8      1*9      2*8      23*1
  22*1      7*6      2*14     2*7      2*14     2*7      2*14     3*8      1*9      2*8      23*1
  22*1      7*6      2*14     2*7      2*14     2*7      2*14     3*8      1*9      2*8      23*1
  22*1      7*2      2*13     2*2      2*13     2*2      2*13     3*12     1*9      2*12     23*1
  22*4      7*2      2*4      2*2      2*4      2*2      2*4      3*12     1*4      2*12     23*4
  22*1      7*2      2*13     2*2      2*13     2*2      2*13     3*12     1*9      2*12     23*1
  22*1      7*2      2*13     2*2      2*13     2*2      2*13     3*12     1*9      2*12     23*1
  68*5
  42*1      1*9     25*1
  42*1      1*9     25*1
  42*1      1*9     25*1
  42*1      1*9     25*1
  42*1      1*9     25*1
  42*1      1*9     25*1
  42*1      1*9     25*1
  42*10     1*9     25*10
  42*10     1*9     25*10
  42*10     1*9     25*10
  42*10     1*9     25*10
  42*10     1*9     25*10
  42*10     1*9     25*10
  42*10     1*9     25*10
  42*10     1*9     25*10
  42*10     1*9     25*10                                                   (Line 7.6)
 START TIME FOR MAP 2                                                        (Line 7.3)
 0.0000E+00                                                                  (Line 7.4)
 MATERIAL TYPE GRID MAP                                                      (Line 7.5)
  22*10    23*11    23*10                                                   (Line 7.6)
  68*10
  68*1
  68*1
  68*1
  68*1
  22*3     11*22     2*3      2*22     2*3      3*37     1*3      2*37     23*3
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 22*1     11*22     2*23     2*22     2*23     3*37     1*33     2*37    23*1
 22*1     11*22     2*23     2*22     2*23     3*37     1*33     2*37    23*1
 22*1      7*21     2*41     2*32     2*24     2*32     2*24     3*15     1*33     2*16    23*1
 22*1      7*21     2*41     2*32     2*24     2*32     2*24     3*15     1*33     2*16    23*1
 22*1      7*21     2*41     2*32     2*24     2*32     2*24     3*15     1*33     2*16    23*1
 22*1     11*22     2*23     2*22     2*23     3*37     1*33     2*37    23*1
 22*4     11*22     2*4      2*22     2*4      3*37     1*4      2*37    23*4
 22*1     11*22     2*23     2*22     2*23     3*37     1*35     2*37    23*1
 22*1     11*22     2*23     2*22     2*23     3*37     1*35     2*37    23*1
 68*5
 42*1      1*35    25*1
 42*1      1*35    25*1
 42*1      1*35    25*1
 42*1      1*35    25*1
 42*1      1*35    25*1
 42*1      1*35    25*1
 42*1      1*35    25*1
 42*29     1*34    25*29
 42*17     1*34    25*17
 42*30     1*34    25*30
 42*18     1*34    25*18
 42*31     1*34    25*31
 42*19     1*34    25*19
 42*19     1*34    25*19
 42*20     1*34    25*20
 42*20     1*34    25*20                                                              (Line 7.6)
START TIME FOR MAP 3                                                                (Line 7.3)
3.1557E+09                                                                          (Line 7.4)
MATERIAL TYPE GRID MAP                                                              (Line 7.5)
 22*10    23*11    23*10                                                           (Line 7.6)
 68*10
 68*1
 68*1
 68*1
 68*1
 22*3     11*22     2*3      2*22     2*3      3*37     1*3      2*37    23*3
 22*1     11*22     2*23     2*22     2*23     3*37     1*33     2*37    23*1
 22*1     11*22     2*23     2*22     2*23     3*37     1*33     2*37    23*1
 22*1      7*21     2*41     2*32     2*38     2*32     2*38     3*15     1*33     2*16    23*1
 22*1      7*21     2*41     2*32     2*38     2*32     2*38     3*15     1*33     2*16    23*1
 22*1      7*21     2*41     2*32     2*38     2*32     2*38     3*15     1*33     2*16    23*1
 22*1     11*22     2*23     2*22     2*23     3*37     1*33     2*37    23*1
 22*4     11*22     2*4      2*22     2*4      3*37     1*4      2*37    23*4
 22*1     11*22     2*23     2*22     2*23     3*37     1*35     2*37    23*1
 22*1     11*22     2*23     2*22     2*23     3*37     1*35     2*37    23*1
 68*5
 42*1      1*35    25*1
 42*1      1*35    25*1
 42*1      1*35    25*1
 42*1      1*35    25*1
 42*1      1*35    25*1
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  42*1       1*35     25*1
  42*1       1*35     25*1
  42*29      1*34     25*29
  42*17      1*34     25*17
  42*30      1*34     25*30
  42*18      1*34     25*18
  42*31      1*34     25*31
  42*19      1*34     25*19
  42*19      1*34     25*19
  42*20      1*34     25*20
  42*20      1*34     25*20                                                                    (Line 7.6)
START TIME FOR MAP 4                                                                          (Line 7.3)
6.3114E+09                                                                                    (Line 7.4)
MATERIAL TYPE GRID MAP                                                                        (Line 7.5)
 22*10     23*11     23*10                                                                    (Line 7.6)
 68*10
 68*1
 68*1
 68*1
 68*1
 22*3      11*22      2*3       2*22      2*3       3*37      1*3       2*37     23*3
 22*1      11*22      2*40      2*22      2*40      3*37      1*33      2*37     23*1
 22*1      11*22      2*40      2*22      2*40      3*37      1*33      2*37     23*1
 22*1       7*21      2*41      2*32      2*39      2*32      2*39      3*15      1*33      2*16     23*1
 22*1       7*21      2*41      2*32      2*39      2*32      2*39      3*15      1*33      2*16     23*1
 22*1       7*21      2*41      2*32      2*39      2*32      2*39      3*15      1*33      2*16     23*1
 22*1      11*22      2*40      2*22      2*40      3*37      1*33      2*37     23*1
 22*4      11*22      2*4       2*22      2*4       3*37      1*4       2*37     23*4
 22*1      11*22      2*40      2*22      2*40      3*37      1*36      2*37     23*1
 22*1      11*22      2*40      2*22      2*40      3*37      1*36      2*37     23*1
 68*5
 42*1       1*36     25*1
 42*1       1*36     25*1
 42*1       1*36     25*1
 42*1       1*36     25*1
 42*1       1*36     25*1
 42*1       1*36     25*1
 42*1       1*36     25*1
 42*29      1*34     25*29
 42*17      1*34     25*17
 42*30      1*34     25*30
 42*18      1*34     25*18
 42*31      1*34     25*31
 42*19      1*34     25*19
 42*19      1*34     25*19
 42*20      1*34     25*20
 42*20      1*34     25*20                                                                    (Line 7.6)
START TIME FOR MAP 5                                                                          (Line 7.3)
1.1045E+10                                                                                    (Line 7.4)
MATERIAL TYPE GRID MAP                                                                        (Line 7.5)
 22*10      3*11      1*26     19*11     23*10                                               (Line 7.6)
```

```
 25*10     1*26    42*10
 25*1      1*26    42*1
 25*1      1*26    42*1
 25*1      1*26    42*1
 25*1      1*26    42*1
 22*3      3*22     1*26     7*22     2*3      2*22     2*3      3*37     1*3      2*37     23*3
 22*1      3*22     1*26     7*22     2*40     2*22     2*40     3*37     1*33     2*37     23*1
 22*1      3*22     1*26     7*22     2*40     2*22     2*40     3*37     1*33     2*37     23*1
 22*1      3*21     1*26     3*21     2*41     2*32     2*39     2*32     2*39     3*15      1*33     2*16     23*1
 22*1      3*21     1*26     3*21     2*41     2*32     2*39     2*32     2*39     3*15      1*33     2*16     23*1
 22*1      3*21     1*26     3*21     2*41     2*32     2*39     2*32     2*39     3*15      1*33     2*16     23*1
 22*1      3*22     1*26     7*22     2*40     2*22     2*40     3*37     1*33     2*37     23*1
 22*4      3*22     1*26     7*22     2*4      2*22     2*4      3*37     1*4      2*37     23*4
 22*1      3*22     1*26     7*22     2*40     2*22     2*40     3*37     1*36     2*37     23*1
 22*1      3*22     1*26     7*22     2*40     2*22     2*40     3*37     1*36     2*37     23*1
 25*5      1*26    42*5
 25*1      1*26    16*1      1*36     25*1
 25*1      1*26    16*1      1*36     25*1
 25*1      1*26    16*1      1*36     25*1
 25*1      1*26    16*1      1*36     25*1
 25*1      1*26    16*1      1*36     25*1
 25*1      1*26    16*1      1*36     25*1
 25*1      1*26    16*1      1*36     25*1
 25*29     1*25    16*29     1*34     25*29
 25*17     1*26    16*17     1*34     25*17
 25*30     1*26    16*30     1*34     25*30
 25*18     1*26    16*18     1*34     25*18
 25*31     1*26    16*31     1*34     25*31
 25*19     1*26    16*19     1*34     25*19
 25*19     1*26    16*19     1*34     25*19
 25*20     1*25    16*20     1*34     25*20
 25*20     1*25    16*20     1*34     25*20                                                                  (Line 7.6)
START TIME FOR MAP 6                                                                                        (Line 7.3)
1.7356E+10                                                                                                  (Line 7.4)
MATERIAL TYPE GRID MAP                                                                                      (Line 7.5)
 22*10     3*11     1*27     19*11    23*10                                                                 (Line 7.6)
 25*10     1*27    42*10
 25*1      1*27    42*1
 25*1      1*27    42*1
 25*1      1*27    42*1
 25*1      1*27    42*1
 22*3      3*22     1*27     7*22     2*3      2*22     2*3      3*37     1*3      2*37     23*3
 22*1      3*22     1*27     7*22     2*40     2*22     2*40     3*37     1*33     2*37     23*1
 22*1      3*22     1*27     7*22     2*40     2*22     2*40     3*37     1*33     2*37     23*1
 22*1      3*21     1*27     3*21     2*41     2*32     2*39     2*32     2*39     3*15      1*33     2*16     23*1
 22*1      3*21     1*27     3*21     2*41     2*32     2*39     2*32     2*39     3*15      1*33     2*16     23*1
 22*1      3*21     1*27     3*21     2*41     2*32     2*39     2*32     2*39     3*15      1*33     2*16     23*1
 22*1      3*22     1*27     7*22     2*40     2*22     2*40     3*37     1*33     2*37     23*1
 22*4      3*22     1*27     7*22     2*4      2*22     2*4      3*37     1*4      2*37     23*4
 22*1      3*22     1*27     7*22     2*40     2*22     2*40     3*37     1*36     2*37     23*1
 22*1      3*22     1*27     7*22     2*40     2*22     2*40     3*37     1*36     2*37     23*1
```

```
  25*5       1*27     42*5
  25*1       1*27     16*1       1*36     25*1
  25*1       1*27     16*1       1*36     25*1
  25*1       1*27     16*1       1*36     25*1
  25*1       1*27     16*1       1*36     25*1
  25*1       1*27     16*1       1*36     25*1
  25*1       1*27     16*1       1*36     25*1
  25*1       1*27     16*1       1*36     25*1
  25*29      1*27     16*29      1*34     25*29
  25*17      1*27     16*17      1*34     25*17
  25*30      1*27     16*30      1*34     25*30
  25*18      1*27     16*18      1*34     25*18
  25*31      1*27     16*31      1*34     25*31
  25*19      1*27     16*19      1*34     25*19
  25*19      1*27     16*19      1*34     25*19
  25*20      1*27     16*20      1*34     25*20
  25*20      1*27     16*20      1*34     25*20                                                                                                   (Line 7.6)
 START TIME FOR MAP 7                                                                                                                              (Line 7.3)
 4.8913E+10                                                                                                                                        (Line 7.4)
 MATERIAL TYPE GRID MAP                                                                                                                            (Line 7.5)
  22*10      3*11      1*28     19*11     23*10                                                                                                   (Line 7.6)
  25*10      1*28     42*10
  25*1       1*28     42*1
  25*1       1*28     42*1
  25*1       1*28     42*1
  25*1       1*28     42*1
  22*3       3*22      1*28      7*22      2*3       2*22      2*3       3*37      1*3       2*37      23*3
  22*1       3*22      1*28      7*22      2*40      2*22      2*40      3*37      1*33      2*37      23*1
  22*1       3*22      1*28      7*22      2*40      2*22      2*40      3*37      1*33      2*37      23*1
  22*1       3*21      1*27      3*21      2*41      2*32      2*39      2*32      2*39      3*15       1*33      2*16      23*1
  22*1       3*21      1*27      3*21      2*41      2*32      2*39      2*32      2*39      3*15       1*33      2*16      23*1
  22*1       3*21      1*27      3*21      2*41      2*32      2*39      2*32      2*39      3*15       1*33      2*16      23*1
  22*1       3*22      1*27      7*22      2*40      2*22      2*40      3*37      1*33      2*37      23*1
  22*4       3*22      1*27      7*22      2*4       2*22      2*4       3*37      1*4       2*37      23*4
  22*1       3*22      1*27      7*22      2*40      2*22      2*40      3*37      1*36      2*37      23*1
  22*1       3*22      1*27      7*22      2*40      2*22      2*40      3*37      1*36      2*37      23*1
  25*5       1*27     42*5
  25*1       1*27     16*1       1*36     25*1
  25*1       1*27     16*1       1*36     25*1
  25*1       1*27     16*1       1*36     25*1
  25*1       1*27     16*1       1*36     25*1
  25*1       1*27     16*1       1*36     25*1
  25*1       1*27     16*1       1*36     25*1
  25*1       1*27     16*1       1*36     25*1
  25*29      1*27     16*29      1*34     25*29
  25*17      1*27     16*17      1*34     25*17
  25*30      1*27     16*30      1*34     25*30
  25*18      1*27     16*18      1*34     25*18
  25*31      1*27     16*31      1*34     25*31
  25*19      1*27     16*19      1*34     25*19
  25*19      1*27     16*19      1*34     25*19
```

```
  25*20     1*27    16*20     1*34    25*20
  25*20     1*27    16*20     1*34    25*20                    (Line 7.6)
  #     NAME                                                   (Line 7.7)
  1     S_HALITE                                               (Line 7.8)
  2     DRZ_0
  3     S_MB139
  4     S_ANH_AB
  5     S_MB138
  6     CAVITY_1
  7     CAVITY_2
  8     CAVITY_3
  9     CAVITY_4
 10     IMPERM_Z
 11     CASTILER
 12     DRZ_OE_0
 13     DRZ_PC_0
 14     CAVITY_5
 15     OPS_AREA
 16     EXP_AREA
 17     CULEBRA
 18     MAGENTA
 19     DEWYLAKE
 20     SANTAROS
 21     WAS_AREA
 22     DRZ_1
 23     DRZ_PC_1
 24     PCS_T1
 25     CONC_PLG
 26     BH_OPEN
 27     BH_SAND
 28     BH_CREEP
 29     UNNAMED
 30     TAMARISK
 31     FORTYNIN
 32     REPOSIT
 33     CONC_MON
 34     SHFTU
 35     SHFTL_T1
 36     SHFTL_T2
 37     DRZ_OE_1
 38     PCS_T2
 39     PCS_T3
 40     DRZ_PCS
 41     PCS_NO                                                 (Line 7.8)
 NWST                                                         (Line 7.9)
 2                                                            (Line 7.10)
 MAT_WASTEI   MAT_WASTE                                       (Line 7.11)
  6  7                                                        (Line 7.12)
 21 32                                                        (Line 7.12)
 NDRZ                                                         (Line 7.13)
 0                                                            (Line 7.14)
```

```
 NMATRESET                                                          (Line 7.17)
 5                                                                  (Line 7.18)
 MATRESET                                                           (Line 7.19)
 6  7  8  9 14                                                      (Line 7.20)
 BORE HOLE MATERIAL NUMBER                                          (Line 7.21)
 0                                                                  (Line 7.22)
 RESET TIME,  ICRESET                                               (Line 7.23)
 0.0000E+00    1                                                    (Line 7.24)
 PORESETIC                                                          (Line 7.25)
 1.013250E+05                                                       (Line 7.26)
 1.013250E+05
 1.013250E+05
 1.013250E+05
 1.013250E+05                                                       (Line 7.26)
 SORESETIC                                                          (Line 7.27)
 0.000000E+00                                                       (Line 7.28)
 0.000000E+00
 0.000000E+00
 0.000000E+00
 0.000000E+00                                                       (Line 7.28)
 PRESDRZ                                                            (Line 7.29)
                                                                    (Line 7.30)
 NBORERESET                                                         (Line 7.31)
 1                                                                  (Line 7.32)
 NBORETIME, NMATBORE, MATBORE(NMATBORE)                             (Line 7.33)
 5  2 26 25                                                         (Line 7.34)
 PORESET                                                            (Line 7.35)
-1.000000E+00                                                       (Line 7.36)
 SORESET                                                            (Line 7.37)
-1.000000E+00                                                       (Line 7.38)
 ICHEM                                                              (Line 7.39)
 1                                                                  (Line 7.40)
 # LAMBDA        SOR           SGR                                  (Line 7.41)
 1 7.000000E-01 3.000000E-01 2.000000E-01                           (Line 7.42)
 2 7.000000E-01 0.000000E+00 0.000000E+00
 3 6.879527E-01 7.296712E-02 5.495000E-02
 4 6.879527E-01 7.296712E-02 5.495000E-02
 5 6.879527E-01 7.296712E-02 5.495000E-02
 6 7.000000E-01 0.000000E+00 0.000000E+00
 7 7.000000E-01 0.000000E+00 0.000000E+00
 8 7.000000E-01 0.000000E+00 0.000000E+00
 9 7.000000E-01 0.000000E+00 0.000000E+00
10 7.000000E-01 0.000000E+00 0.000000E+00
11 7.000000E-01 2.000000E-01 2.000000E-01
12 7.000000E-01 0.000000E+00 0.000000E+00
13 7.000000E-01 0.000000E+00 0.000000E+00
14 7.000000E-01 0.000000E+00 0.000000E+00
15 7.000000E-01 0.000000E+00 0.000000E+00
16 7.000000E-01 0.000000E+00 0.000000E+00
17 6.436000E-01 8.363000E-02 7.711000E-02
18 6.436000E-01 8.363000E-02 7.711000E-02
```

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19 6.436000E-01 8.363000E-02 7.711000E-02
20 6.436000E-01 8.363000E-02 7.711000E-02
21 2.890000E+00 1.776051E-01 1.654909E-02
22 7.000000E-01 0.000000E+00 0.000000E+00
23 7.000000E-01 0.000000E+00 0.000000E+00
24 8.723522E-01 5.664186E-01 2.229369E-01
25 9.400000E-01 0.000000E+00 0.000000E+00
26 7.000000E-01 0.000000E+00 0.000000E+00
27 9.400000E-01 0.000000E+00 0.000000E+00
28 9.400000E-01 0.000000E+00 0.000000E+00
29 7.000000E-01 2.000000E-01 2.000000E-01
30 7.000000E-01 2.000000E-01 2.000000E-01
31 7.000000E-01 2.000000E-01 2.000000E-01
32 2.890000E+00 1.776051E-01 1.654909E-02
33 9.400000E-01 1.275853E-01 1.218417E-01
34 9.400000E-01 1.275853E-01 1.218417E-01
35 9.400000E-01 1.275853E-01 1.218417E-01
36 9.400000E-01 1.275853E-01 1.218417E-01
37 7.000000E-01 0.000000E+00 0.000000E+00
38 8.723522E-01 5.664186E-01 2.229369E-01
39 8.723522E-01 5.664186E-01 2.229369E-01
40 7.000000E-01 0.000000E+00 0.000000E+00
41 7.000000E-01 0.000000E+00 0.000000E+00                                                    (Line 7.42)
 # SBMIN         PBMIN         PCMAX          PCT_A        PCT_EXP      KRP KPC KTP        (Line 7.43)
 1 3.150000E-01 1.013250E+05 1.000000E+08  5.600000E-01 -3.460000E-01  4  2  0             (Line 7.44)
 2 0.000000E+00 1.013250E+05 1.000000E+08  0.000000E+00  0.000000E+00  4  1  0
 3 7.661547E-02 1.013250E+05 1.000000E+08  2.600000E-01 -3.480000E-01  4  2  0
 4 7.661547E-02 1.013250E+05 1.000000E+08  2.600000E-01 -3.480000E-01  4  2  0
 5 7.661547E-02 1.013250E+05 1.000000E+08  2.600000E-01 -3.480000E-01  4  2  0
 6 0.000000E+00 1.013250E+05 1.000000E+08  0.000000E+00  0.000000E+00 11  1  0
 7 0.000000E+00 1.013250E+05 1.000000E+08  0.000000E+00  0.000000E+00 11  1  0
 8 0.000000E+00 1.013250E+05 1.000000E+08  0.000000E+00  0.000000E+00 11  1  0
 9 0.000000E+00 1.013250E+05 1.000000E+08  0.000000E+00  0.000000E+00 11  1  0
10 0.000000E+00 1.013250E+05 1.000000E+08  0.000000E+00  0.000000E+00  4  1  0
11 2.100000E-01 1.013250E+05 1.000000E+08  5.600000E-01 -3.460000E-01  4  2  0
12 0.000000E+00 1.013250E+05 1.000000E+08  0.000000E+00  0.000000E+00  4  1  0
13 0.000000E+00 1.013250E+05 1.000000E+08  0.000000E+00  0.000000E+00  4  1  0
14 0.000000E+00 1.013250E+05 1.000000E+08  0.000000E+00  0.000000E+00 11  1  0
15 0.000000E+00 1.013250E+05 1.000000E+08  0.000000E+00  0.000000E+00 11  1  0
16 0.000000E+00 1.013250E+05 1.000000E+08  0.000000E+00  0.000000E+00 11  1  0
17 8.781150E-02 1.013250E+05 1.000000E+08  2.600000E-01 -3.480000E-01  4  2  0
18 8.781150E-02 1.013250E+05 1.000000E+08  2.600000E-01 -3.480000E-01  4  2  0
19 8.781150E-02 1.013250E+05 1.000000E+08  0.000000E+00  0.000000E+00  4  1  0
20 8.781150E-02 1.013250E+05 1.000000E+08  0.000000E+00  0.000000E+00  4  1  0
21 1.864854E-01 1.013250E+05 1.000000E+08  0.000000E+00  0.000000E+00 12  1  0
22 0.000000E+00 1.013250E+05 1.000000E+08  0.000000E+00  0.000000E+00  4  1  0
23 0.000000E+00 1.013250E+05 1.000000E+08  0.000000E+00  0.000000E+00  4  1  0
24 5.947395E-01 1.013250E+05 1.000000E+08  0.000000E+00  0.000000E+00  4  1  0
25 0.000000E+00 1.013250E+05 1.000000E+08  0.000000E+00  0.000000E+00  4  1  0
26 0.000000E+00 1.013250E+05 1.000000E+08  0.000000E+00  0.000000E+00 11  1  0
27 0.000000E+00 1.013250E+05 1.000000E+08  0.000000E+00  0.000000E+00  4  1  0
```

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28 0.000000E+00 1.013250E+05 1.000000E+08  0.000000E+00  0.000000E+00  4  1  0
29 2.100000E-01 1.013250E+05 1.000000E+08  0.000000E+00  0.000000E+00  4  1  0
30 2.100000E-01 1.013250E+05 1.000000E+08  0.000000E+00  0.000000E+00  4  1  0
31 2.100000E-01 1.013250E+05 1.000000E+08  0.000000E+00  0.000000E+00  4  1  0
32 1.864854E-01 1.013250E+05 1.000000E+08  0.000000E+00  0.000000E+00 12  1  0
33 1.339646E-01 1.013250E+05 1.000000E+08  0.000000E+00  0.000000E+00  4  1  0
34 1.339646E-01 1.010000E+05 1.000000E+08  0.000000E+00  0.000000E+00  4  1  0
35 1.339646E-01 1.010000E+05 1.000000E+08  0.000000E+00  0.000000E+00  4  1  0
36 1.339646E-01 1.010000E+05 1.000000E+08  0.000000E+00  0.000000E+00  4  1  0
37 0.000000E+00 1.013250E+05 1.000000E+08  0.000000E+00  0.000000E+00  4  1  0
38 5.947395E-01 1.013250E+05 1.000000E+08  0.000000E+00  0.000000E+00  4  1  0
39 5.947395E-01 1.013250E+05 1.000000E+08  0.000000E+00  0.000000E+00  4  1  0
40 0.000000E+00 1.013250E+05 1.000000E+08  0.000000E+00  0.000000E+00  4  1  0
41 0.000000E+00 1.013250E+05 1.000000E+08  0.000000E+00  0.000000E+00 11  1  0   (Line 7.44)
 # PERMX         PERMY         PERMZ         POROSITY     COMPRES                 (Line 7.45)
 1 1.803430E-23 1.803430E-23 1.803430E-23  4.482392E-03  2.576467E-08            (Line 7.46)
 2 1.000000E-17 1.000000E-17 1.000000E-17  7.382392E-03  1.003740E-07
 3 1.047981E-19 1.047981E-19 1.047981E-19  1.100000E-02  2.027273E-09
 4 1.047981E-19 1.047981E-19 1.047981E-19  1.100000E-02  2.027273E-09
 5 1.047981E-19 1.047981E-19 1.047981E-19  1.100000E-02  2.027273E-09
 6 1.000000E-10 1.000000E-10 1.000000E-10  1.000000E+00  0.000000E+00
 7 1.000000E-10 1.000000E-10 1.000000E-10  1.000000E+00  0.000000E+00
 8 1.000000E-10 1.000000E-10 1.000000E-10  1.000000E+00  0.000000E+00
 9 1.000000E-10 1.000000E-10 1.000000E-10  1.000000E+00  0.000000E+00
10 1.000000E-35 1.000000E-35 1.000000E-35  5.000000E-03  0.000000E+00
11 2.769151E-12 2.769151E-12 2.769151E-12  4.269250E-01  5.329202E-09
12 1.000000E-17 1.000000E-17 1.000000E-17  7.382392E-03  1.003740E-07
13 1.000000E-17 1.000000E-17 1.000000E-17  7.382392E-03  1.003740E-07
14 1.000000E-10 1.000000E-10 1.000000E-10  1.000000E+00  0.000000E+00
15 1.000000E-11 1.000000E-11 1.000000E-11  1.800000E-01  0.000000E+00
16 1.000000E-11 1.000000E-11 1.000000E-11  1.800000E-01  0.000000E+00
17 9.594006E-15 9.594006E-15 9.594006E-15  1.510000E-01  6.622517E-10
18 2.098940E-15 2.098940E-15 2.098940E-15  1.380000E-01  1.915942E-09
19 5.011872E-17 5.011872E-17 5.011872E-17  1.430000E-01  6.993007E-08
20 1.000000E-10 1.000000E-10 1.000000E-10  1.750000E-01  5.714286E-08
21 2.399938E-13 2.399938E-13 2.399938E-13  8.480000E-01  0.000000E+00
22 1.334032E-18 1.334032E-18 1.334032E-18  7.382392E-03  1.003740E-07
23 1.334032E-18 1.334032E-18 1.334032E-18  7.382392E-03  1.003740E-07
24 5.576023E-18 5.576023E-18 5.576023E-18  1.337978E-01  5.979173E-10
25 1.576825E-18 1.576825E-18 1.576825E-18  3.200000E-01  1.187500E-09
26 1.000000E-09 1.000000E-09 1.000000E-09  3.200000E-01  0.000000E+00
27 7.293741E-14 7.293741E-14 7.293741E-14  3.200000E-01  0.000000E+00
28 7.293741E-15 7.293741E-15 7.293741E-15  3.200000E-01  0.000000E+00
29 1.000000E-35 1.000000E-35 1.000000E-35  1.810000E-01  0.000000E+00
30 1.000000E-35 1.000000E-35 1.000000E-35  6.400000E-02  0.000000E+00
31 1.000000E-35 1.000000E-35 1.000000E-35  8.200000E-02  0.000000E+00
32 2.399938E-13 2.399938E-13 2.399938E-13  8.480000E-01  0.000000E+00
33 1.000000E-14 1.000000E-14 1.000000E-14  5.000000E-02  1.200000E-09
34 4.298557E-19 4.298557E-19 4.298557E-19  2.910000E-01  2.050000E-08
35 1.563232E-19 1.563232E-19 1.563232E-19  1.130000E-01  4.280000E-09
36 2.238051E-20 2.238051E-20 2.238051E-20  1.130000E-01  4.280000E-09
```

```
37 1.334032E-18 1.334032E-18 1.334032E-18  7.382392E-03  1.003740E-07
38 3.548300E-21 3.548300E-21 3.548300E-21  3.092999E-02  2.586486E-09
39 2.468482E-21 2.468482E-21 2.468482E-21  2.349192E-02  3.405426E-09
40 1.658714E-20 1.658714E-20 1.658714E-20  7.382392E-03  1.003740E-07
41 1.000000E-11 1.000000E-11 1.000000E-11  1.800000E-01  0.000000E+00                                    (Line 7.46)
 TOL AND SOCEFFMIN FOR PERMEABILITY MODELS 11 & 12                                                      (Line 7.47)
 1.000000E-02  1.000000E-03                                                                             (Line 7.48)
 NMATSP, FOR SMOOTH PERMEABILITY TRANSITION MODEL                                                       (Line 7.49)
 0                                                                                                      (Line 7.50)
 FRACTURE MODEL DATA TO FOLLOW :T OR F                                                                  (Line 7.55)
 T                                                                                                      (Line 7.56)
 NFRAC                                                                                                  (Line 7.57)
 9                                                                                                      (Line 7.58)
 # DELTA_PI    DELTA_PF      FRAC_PHI     FRAC_EXP     IFRX IFRY IFRZ LPFC                              (Line 7.59)
 3 2.000000E+05 3.800000E+06 5.000000E-02 1.518045E+01    1    1    0    F                              (Line 7.60)
 4 2.000000E+05 3.800000E+06 2.500000E-01 7.357607E+00    1    1    0    F
 5 2.000000E+05 3.800000E+06 5.000000E-02 1.518045E+01    1    1    0    F
 2 2.000000E+05 3.800000E+06 4.638239E-02 1.013380E+01    1    1    0    F
22 2.000000E+05 3.800000E+06 4.638239E-02 1.124197E+01    1    1    0    F
12 2.000000E+05 3.800000E+06 4.638239E-02 1.013380E+01    1    1    0    F
37 2.000000E+05 3.800000E+06 4.638239E-02 1.124197E+01    1    1    0    F
13 2.000000E+05 3.800000E+06 4.638239E-02 1.013380E+01    1    1    0    F
23 2.000000E+05 3.800000E+06 4.638239E-02 1.124197E+01    1    1    0    F                              (Line 7.60)
 KLINKENBERG EFFECT TO BE USED? True or False                                                           (Line 7.61)
 T                                                                                                      (Line 7.62)
 BKLINK        EXPKLINK                                                                                 (Line 7.63)
  2.71000E-01 -3.41000E-01                                                                              (Line 7.64)
 GRAVITY CONSTANT (GSTD) AND GAS CONSTANT (R)                                                            (Line 8.0)
  9.80665E+00  8.31451E+00                                                                              (Line 8.1)
 REFERENCE TEMPERATURE AND PRESSURE FOR DENSITY CALCULATIONS                                            (Line 8.2)
  3.00150E+02  1.01325E+05                                                                              (Line 8.3)
 SALT(WT.%)  DEN_BR  KGSAT  IDGAS,  COMPR_BR,  WMSALT, WMH2O                                            (Line 8.4)
 3.2400E+01 1.2200E+03    1    0    3.1000E-10 5.8442E-02 1.8015E-02                                     (Line 8.5)
 VISC_BR   VISC_GAS                                                                                     (Line 8.6)
  2.10000E-03  8.93389E-06                                                                              (Line 8.7)
 GAS DENSITY DATA: =0 OR -2 COMPUTE USING RKS OR IDEAL GAS; =1 OR -1 INTERPOLATE USING RKS OR IDEAL GAS (Line 8.8)
 1                                                                                                      (Line 8.9)
 GAS MOLE FRACTIONS FOR H2, CO2, CH4, N2, H2S, AND O2                                                  (Line 8.10)
  1.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00                         (Line 8.11)
 GAS MOLECULAR WEIGHTS FOR H2, CO2, CH4, N2, H2S, AND O2                                               (Line 8.12)
  2.01588E-03  4.40098E-02  1.60428E-02  2.80135E-02  3.40819E-02  3.19988E-02                        (Line 8.13)
 NUMBER OF GAS COMPONENTS ACTUALLY USED (NGAS) AND COMPONENT NUMBER OF GAS (N1GAS)                      (Line 8.14)
    1    1                                                                                              (Line 8.15)
 RKS SPECIFIED: TC FOR H2, CO2, CH4, N2, H2S, AND O2                                                   (Line 8.16)
  4.36000E+01  3.04150E+02  1.90630E+02  1.26150E+02  3.73550E+02  1.54770E+02                        (Line 8.17)
 RKS SPECIFIED: PC FOR H2, CO2, CH4, N2, H2S, AND O2                                                   (Line 8.18)
  2.04700E+06  7.37600E+06  4.61700E+06  3.39400E+06  9.00700E+06  5.08000E+06                        (Line 8.19)
 RKS SPECIFIED: ACEN FOR H2, CO2, CH4, N2, H2S, AND O2                                                 (Line 8.20)
  0.00000E+00  2.31000E-01  1.00000E-02  4.50000E-02  1.00000E-01  1.90000E-02                        (Line 8.21)
 RKS SPECIFIED: SPECIAL PROPERTIES FOR H2- TCH2, PCH2,AND WMH2                                         (Line 8.22)
  4.36000E+01  2.04700E+06  2.01588E-03                                                                (Line 8.23)
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RKS SPECIFIED: CONSTANTS OMEGAA AND OMEGAB                                                                    (Line 8.24)
 4.27470E-01  8.66400E-02                                                                                     (Line 8.25)
RKS SPECIFIED: BINARY INTERACTION PARAMETERS, AKIJ(1-MGAS, 1-MGAS)                                            (Line 8.26)
BINARY INTERACTION PARAMETER FOR H2                                                                           (Line 8.26.1)
 0.00000E+00 -3.42600E-01 -2.22000E-02  9.78000E-02  0.00000E+00  0.00000E+00                                 (Line 8.26.2)
BINARY INTERACTION PARAMETER FOR CO2                                                                          (Line 8.26.3)
-3.42600E-01  0.00000E+00  9.33000E-02 -3.15000E-02  9.89000E-02  0.00000E+00                                 (Line 8.26.4)
BINARY INTERACTION PARAMETER FOR CH4                                                                          (Line 8.26.5)
-2.22000E-02  9.33000E-02  0.00000E+00  2.78000E-02  8.50000E-02  0.00000E+00                                 (Line 8.26.6)
BINARY INTERACTION PARAMETER FOR N2                                                                           (Line 8.26.7)
 9.78000E-02 -3.15000E-02  2.78000E-02  0.00000E+00  1.69600E-01 -7.80000E-03                                 (Line 8.26.8)
BINARY INTERACTION PARAMETER FOR H2S                                                                          (Line 8.26.9)
 0.00000E+00  9.89000E-02  8.50000E-02  1.69600E-01  0.00000E+00  0.00000E+00                                 (Line 8.26.10)
BINARY INTERACTION PARAMETER FOR O2                                                                           (Line 8.26.11)
 0.00000E+00  0.00000E+00  0.00000E+00 -7.80000E-03  0.00000E+00  0.00000E+00                                 (Line 8.26.12)
IGASVAR (2= REACTION PATH,  1= USING AVG. STOICH. , 0= USING WELLS)                                           (Line 9.1)
1                                                                                                             (Line 9.2)
RATE CONSTANTS: CORROSION (RKCOR) AND BIODEGRADATION (RKBIO), INTRINSIC RATES                                 (Line 9.3)
 1.0541E-08   3.4165E-09   F                                                                                  (Line 9.4)
HUMIDITY FACTORS: HUMFAC_COR, HUMFAC_BIO                                                                      (Line 9.5)
 0.0000E+00   1.4203E-01                                                                                      (Line 9.6)
RATE CONSTANTS: BRUCITEI, BRUCITEH, HYMAGCON                                                                  (Line 9.7)
 5.9143E-06   2.0875E-06   6.4760E-10                                                                         (Line 9.8)
RATE COEFFICIENTS FOR EACH WASTE AREA: GAS AND CO2                                                            (Line 9.9)
 4.8907E-01   1.0000E+00                                                                                      (Line 9.10)
 4.8907E-01   1.0000E+00                                                                                      (Line 9.10)
CHEMISTRY CUTOFF SATURATION:  SOCMIN                                                                          (Line 9.11)
 1.5000E-02                                                                                                   (Line 9.12)
REACTANT/PRODUCT MOLECULAR WEIGHTS (H2, H2O, Fe, [C6-H10-O5]/6)                                               (Line 9.13)
2.015880E-03  1.801528E-02  5.584700E-02  2.702300E-02                                                        (Line 9.14)
REACTANT/PRODUCT MOLECULAR WEIGHT (Fe(OH)2, FeS, MgO, Mg(OH)2, Hydro, MgCO3)                                  (Line 9.15)
8.986000E-02  8.791100E-02  4.030400E-02  5.832000E-02  4.676360E-01  8.431400E-02                            (Line 9.16)
S_H2,S_H2O,S_Fe,S_Bio,S_FeOH2,S_FeS,S_MgO,S_MgOH2,S_Hydro,S_MgCO3                                             (Line 9.17)
1.0000E+00 -2.0000E+00 -1.0000E+00  0.0000E+00  1.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00   (Line 9.18)
0.0000E+00  8.7705E-01  0.0000E+00 -1.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
0.0000E+00 -1.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00 -1.0000E+00  1.0000E+00  0.0000E+00  0.0000E+00
0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00 -1.2500E+00  2.5000E-01  0.0000E+00
0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00 -1.0000E+00  0.0000E+00  0.0000E+00  1.0000E+00
0.0000E+00  4.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  1.0000E+00 -1.0000E+00  4.0000E+00   (Line 9.18)
REACTANT/PRODUCT DENSITIES (Fe, Fe(OH)2, FeS, Bio)                                                            (Line 9.19)
 7.8700E+03   3.4000E+03   4.7000E+03   1.1000E+03                                                            (Line 9.20)
REACTANT/PRODUCT DENSITIES (MgO, Mg(OH)2, Hydro, MgCO3, SALT)                                                 (Line 9.21)
 3.6000E+03   2.3700E+03   2.3000E+03   3.0500E+03   2.1800E+03                                               (Line 9.22)
WICKING SATURATION, HUMID RATE SMOOTHING, CONCENTRATION SMOOTHING, ALPHARXN                                   (Line 9.23)
 3.2225E-01   T   T  -1.0000E+03                                                                              (Line 9.24)
CREEP CLOSURE? IF TRUE AN EXTERNAL FILE OF CLOSURE DATA IS ALSO EXPECTED                                      (Line 10.1)
 T                                                                                                            (Line 10.2)
NKLOS, KLOSINT (0=MOLES,1=PRESSURE) KLOSAVE (1=REGION AVE,2=CELL)                                             (Line 10.3)
  1    1    2                                                                                                 (Line 10.4)
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CLOSURE PARAMETERS: PRES_LITHO, TIME_OFF, MODPERM, LIMIT POROSITY INCREASE, INCLUDE SOLID PRODUCTION                (Line 10.5)
4   5.0000E+07   3.1557E+12   1   F   F                                                                            (Line 10.6)
MODPERM PARAMETERS                                                                                               (Line 10.7)
 2.3999E-13   0.0000E+00                                                                                          (Line 10.8)
NUMBER OF MATERIAL REGIONS FOR CLOSURE                                                                           (Line 10.9)
  2                                                                                                             (Line 10.10)
#  MAT NO.   MODEL 1= WASTE-NOBACKFILL, 2=DRIFT-NOBACKFILL, 3=WASTE-BACKFILL 4=JAN_96:WASTE-NOBACKFILL          (Line 10.11)
1   21         4                                                                                                 (Line 10.12)
2   32         4                                                                                                 (Line 10.12)
WILL RADIONUCLIDE DECAY BE CALCULATED? T or F                                                                    (Line 11.1)
T                                                                                                                (Line 11.2)
WILL TRANSPORT BE CALCULATED? T or F                                                                             (Line 11.3)
F                                                                                                                (Line 11.4)
WILL RADIOLYSIS BE CALCULATED? T or F                                                                            (Line 11.5)
T                                                                                                                (Line 11.6)
NUMBER OF NUCLIDES                                                                                               (Line 11.7)
   5                                                                                                             (Line 11.8)
DECAY CONTROL PARAMETERS: XLIM, HALFMAX, T_SCALE, SRADO2, GH2AVG, GDEPFAC                                        (Line 11.9)
 1.0000E-07   5.0000E+01   3.1557E+07   0.0000E+00   1.4000E-02   6.3844E-03                                    (Line 11.10)
NUCLIDE IDs: PARENTS                                                                                             (Line 11.11)
'AM241   '   'PU238   '   'PU239   '   'PU240   '   'PU242   '                                                   (Line 11.12)
DAUGHTER IDs                                                                                                     (Line 11.13)
'NP237   '   'U234    '   'U235    '   'U236    '   'U238    '                                                   (Line 11.14)
SOLUBILITY MAPPING                                                                                               (Line 11.15)
   2    1    1    1    1                                                                                        (Line 11.16)
HALF-LIVES                                                                                                       (Line 11.17)
 1.3640E+10   2.7690E+09   7.5940E+11   2.0630E+11   1.2210E+13                                                 (Line 11.18)
ATOMIC WEIGHTS                                                                                                   (Line 11.19)
 2.4106E-01   2.3805E-01   2.3905E-01   2.4005E-01   2.4206E-01                                                 (Line 11.20)
SOLUBILITY LIMITS                                                                                                (Line 11.21)
 5.8857E-02   3.5239E-03   3.5239E-03   3.5239E-03   3.5239E-03                                                 (Line 11.22)
DISINTEGRATION ENERGIES                                                                                          (Line 11.23)
 5.6378E+00   5.5932E+00   5.2445E+00   5.2557E+00   4.9847E+00                                                 (Line 11.24)
INITIAL INVENTORY: NUCLIDE=  AM241                                                                               (Line 11.25)
 1.6893E+03                                                                                                      (Line 11.26)
INITIAL INVENTORY: NUCLIDE=  PU238                                                                               (Line 11.25)
 2.3582E+02                                                                                                      (Line 11.26)
INITIAL INVENTORY: NUCLIDE=  PU239                                                                               (Line 11.25)
 2.2640E+05                                                                                                      (Line 11.26)
INITIAL INVENTORY: NUCLIDE=  PU240                                                                               (Line 11.25)
 1.5514E+04                                                                                                      (Line 11.26)
INITIAL INVENTORY: NUCLIDE=  PU242                                                                               (Line 11.25)
 7.3758E+03                                                                                                      (Line 11.26)
BRAGFLO GAS COMPONENT TRANSPORT MODEL                                                                            (Line 12.1)
F                                                                                                                (Line 12.2)
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11.2 Appendix B: Sample BRAGFLO Closure Look-Up Table Data Input File

Below is a truncated listing (first two of four surfaces presented with selected SDATA and PDATA ommitted) of the closure file used since the 1996 CCA.

```
PHIMIN_BRAG(1:MKLOS); MKLOS=4                                                    (Line 1.0)
      4.626436E-02, 2.272370E-02, 9.461577E-02, 4.659957E-02                     (Line 2.0)
 PHIMAX_BRAG(1:MKLOS); MKLOS=4                                                   (Line 3.0)
      4*1.0D0                                                                    (Line 4.0)
 TIME_DATA_MAX(1:MKLOS); MKLOS=4                                                 (Line 5.0)
      4*3.787160E+11                                                             (Line 6.0)

 F FACTOR DATA, FDATA (1:MKLOS,1:NSDATA); MKLOS=4, NSDATA=13.                    (Line 7.0)
 FDATA(I,1),I=1,13, ALL 13 ARE USED.                                             (Line 8.0)
      0.D0,        0.025D0,     0.05D0,      0.1D0,       0.2D0,                (Line 9.0)
      0.4D0,       0.5D0,       0.6D0,       0.8D0,       1.0D0,
      1.2D0,       1.6D0,       2.0D0
 FDATA(I,2),I=1,13, ONLY FIRST 7 ARE USED.
      0.D0,        0.01D0,      0.1D0,       0.2D0,       0.4D0,
      0.6D0,       1.0D0        6*0.0D0
 FDATA(I,3),I=1,5,  ONLY FIRST 5 ARE USED.
      0.D0,        0.2D0,       0.4D0,       0.6D0,       1.0D0
      8*0.0D0
 FDATA(I,4),I=1,13, ALL 13 ARE USED.
      0.D0,        0.025D       0.05D0,      0.1D0,       0.2D0,
      0.4D0,       0.5D0,       0.6D0,       0.8D0,       1.0D0,
      1.2D0,       1.6D0,       2.0D0
 Time data, TDATA (1:NTDATA); NTDATA=214                                         (Line 10.0)
 TDATA(1:214)                                                                    (Line 11.0)
     0.000000E+00,1.579360E+07,3.158860E+07,1.895220E+08,3.474430E+08,           (Line 12.0)
     5.053850E+08,6.633280E+08,8.212710E+08,9.792140E+08,1.137120E+09,
     … (39 lines ommitted)
     6.099340E+10,6.130890E+10,6.162770E+10,6.194320E+10,6.225880E+10,
     6.257440E+10,6.288990E+10,3.155600E+11,3.787160E+11
 POROSITY SURFACE #1, FOR WASTE w/o BACKFILL. FIRST USED IN SPM2 IN JANUARY 1995. (Line 13.0)
 PDATA(1:NSDATA,1:NTDATA,1:MKLOS); NSDATA=13, NTDATA=214, MKLOS=4                (Line 14.0)
 FOR POROSITY SURFACE 1 ALL NSDATA=13 GAS GENERATION RATES ARE USED.             (Line 15.0)
    POROSITY SURFACE #1; GAS GENERATION RATE #1.                                 (Line 16.0)
    PDATA(NSDATA =1,NTDATA=1:214,MKLOS =1)                                       (Line 17.0)
       214*1.013250E+05                                                          (Line 18.0)
    POROSITY SURFACE #1; GAS GENERATION RATE #1.                                 (Line 19.0)
    SDATA(NSDATA =1,NTDATA=1:214,MKLOS =1)                                       (Line 20.0)
       8.810350E-01,7.909613E-01,7.699415E-01,6.453196E-01,5.579810E-01,         (Line 21.0)
       4.866897E-01,4.265381E-01,3.755593E-01,3.309335E-01,2.913361E-01,
      … (39 lines ommitted)
       5.142215E-02,5.139977E-02,5.137468E-02,5.135003E-02,5.132905E-02,
       5.130884E-02,5.128795E-02,4.626436E-02,4.626436E-02
    POROSITY SURFACE #1; GAS GENERATION RATE #2.
    PDATA(NSDATA =2,NTDATA=1:214,MKLOS =1)
```

```
   1.013250E+05,1.015174E+05,1.017112E+05,1.036490E+05,1.064923E+05,
   1.100090E+05,1.135256E+05,1.179715E+05,1.247003E+05,1.314275E+05,
  … (39 lines ommitted)
   2.844375E+06,2.844661E+06,2.844939E+06,2.845205E+06,2.845476E+06,
   2.845744E+06,2.845997E+06,2.910266E+06,2.910266E+06
POROSITY SURFACE #1; GAS GENERATION RATE #2.
SDATA(NSDATA =2,NTDATA=1:214,MKLOS =1)
   8.810350E-01,8.188063E-01,8.046822E-01,6.634560E-01,5.660348E-01,
   5.011425E-01,4.362498E-01,3.787115E-01,3.392426E-01,2.997831E-01,
  … (39 lines ommitted)
   6.808329E-02,6.807632E-02,6.806945E-02,6.806283E-02,6.805606E-02,
   6.804938E-02,6.804313E-02,6.648637E-02,6.648637E-02
POROSITY SURFACE #1; GAS GENERATION RATE #3.
PDATA(NSDATA =3,NTDATA=1:214,MKLOS =1)
   1.013250E+05,1.016308E+05,1.019518E+05,1.056790E+05,1.106154E+05,
   1.168006E+05,1.243913E+05,1.336190E+05,1.448739E+05,1.586777E+05,
  … (39 lines ommitted)
   4.881976E+06,4.882011E+06,4.882045E+06,4.882079E+06,4.882111E+06,
   4.882143E+06,4.882176E+06,4.885821E+06,4.885821E+06
POROSITY SURFACE #1; GAS GENERATION RATE #3.
SDATA(NSDATA =3,NTDATA=1:214,MKLOS =1)
   8.810350E-01,7.887582E-01,7.708505E-01,6.448627E-01,5.588016E-01,
   4.881833E-01,4.288228E-01,3.776416E-01,3.330553E-01,2.945655E-01,
  … (39 lines ommitted)
   7.812980E-02,7.812933E-02,7.812886E-02,7.812839E-02,7.812779E-02,
   7.812713E-02,7.812666E-02,7.806707E-02,7.806707E-02
POROSITY SURFACE #1; GAS GENERATION RATE #4.
PDATA(NSDATA =4,NTDATA=1:214,MKLOS =1)
   1.013250E+05,1.019367E+05,1.025844E+05,1.100541E+05,1.199691E+05,
   1.323559E+05,1.474737E+05,1.658334E+05,1.881738E+05,2.154314E+05,
  … (39 lines ommitted)
   8.103964E+06,8.103973E+06,8.103979E+06,8.103989E+06,8.103997E+06,
   8.104007E+06,8.104015E+06,8.105364E+06,8.105364E+06
POROSITY SURFACE #1; GAS GENERATION RATE #4.
SDATA(NSDATA =4,NTDATA=1:214,MKLOS =1)
   8.810350E-01,7.878199E-01,7.701936E-01,6.429939E-01,5.568310E-01,
   4.869273E-01,4.283253E-01,3.778764E-01,3.341083E-01,2.962066E-01,
  … (39 lines ommitted)
   9.334710E-02,9.334704E-02,9.334704E-02,9.334704E-02,9.334666E-02,
   9.334666E-02,9.334666E-02,9.333074E-02,9.333074E-02
POROSITY SURFACE #1; GAS GENERATION RATE #5.
PDATA(NSDATA =5,NTDATA=1:214,MKLOS =1)
   1.013250E+05,1.028230E+05,1.043268E+05,1.193632E+05,1.433537E+05,
   1.701278E+05,1.969022E+05,2.346395E+05,2.843196E+05,3.339881E+05,
  … (39 lines ommitted)
   1.274219E+07,1.274217E+07,1.274215E+07,1.274213E+07,1.274212E+07,
   1.274210E+07,1.274209E+07,1.274260E+07,1.274260E+07
POROSITY SURFACE #1; GAS GENERATION RATE #5.
SDATA(NSDATA =5,NTDATA=1:214,MKLOS =1)
   8.810350E-01,8.221918E-01,8.071246E-01,6.564677E-01,5.701580E-01,
   5.038119E-01,4.374655E-01,3.841511E-01,3.450336E-01,3.059252E-01,
```

```
  … (39 lines ommitted)
    1.181920E-01,1.181923E-01,1.181924E-01,1.181924E-01,1.181926E-01,
    1.181928E-01,1.181928E-01,1.181881E-01,1.181881E-01
POROSITY SURFACE #1; GAS GENERATION RATE #6.
PDATA(NSDATA =6,NTDATA=1:214,MKLOS =1)
    1.013250E+05,1.044625E+05,1.076827E+05,1.398820E+05,1.794587E+05,
    2.373400E+05,2.952216E+05,3.532305E+05,4.536252E+05,5.539963E+05,
  … (39 lines ommitted)
    1.834106E+07,1.833825E+07,1.833540E+07,1.833253E+07,1.832976E+07,
    1.832701E+07,1.832421E+07,1.784436E+07,1.784436E+07
POROSITY SURFACE #1; GAS GENERATION RATE #6.
SDATA(NSDATA =6,NTDATA=1:214,MKLOS =1)
    8.810350E-01,8.093810E-01,7.967799E-01,6.707830E-01,5.639549E-01,
    5.046195E-01,4.452838E-01,3.860223E-01,3.514972E-01,3.169802E-01,
  … (39 lines ommitted)
    1.638237E-01,1.638486E-01,1.638741E-01,1.638999E-01,1.639248E-01,
    1.639495E-01,1.639748E-01,1.684095E-01,1.684095E-01
POROSITY SURFACE #1; GAS GENERATION RATE #7.
PDATA(NSDATA =7,NTDATA=1:214,MKLOS =1)
    1.013250E+05,1.055196E+05,1.098189E+05,1.528066E+05,1.957910E+05,
    2.668437E+05,3.453648E+05,4.238860E+05,5.281031E+05,6.574334E+05,
  … (39 lines ommitted)
    1.897320E+07,1.896861E+07,1.896384E+07,1.895977E+07,1.895595E+07,
    1.895243E+07,1.894900E+07,1.842811E+07,1.842811E+07
POROSITY SURFACE #1; GAS GENERATION RATE #7.
SDATA(NSDATA =7,NTDATA=1:214,MKLOS =1)
    8.810350E-01,8.121463E-01,8.005424E-01,6.845162E-01,5.684990E-01,
    5.018084E-01,4.482483E-01,3.946883E-01,3.526027E-01,3.217522E-01,
  … (39 lines ommitted)
    1.979199E-01,1.979682E-01,1.980187E-01,1.980613E-01,1.981013E-01,
    1.981383E-01,1.981741E-01,2.038069E-01,2.038069E-01
POROSITY SURFACE #1; GAS GENERATION RATE #8.
PDATA(NSDATA =8,NTDATA=1:214,MKLOS =1)
    1.013250E+05,1.060899E+05,1.109714E+05,1.597815E+05,2.163145E+05,
    3.029852E+05,3.896565E+05,4.763278E+05,6.155277E+05,7.592791E+05,
  … (39 lines ommitted)
    1.937925E+07,1.937388E+07,1.936831E+07,1.936254E+07,1.935756E+07,
    1.935292E+07,1.934765E+07,1.869588E+07,1.869588E+07
POROSITY SURFACE #1; GAS GENERATION RATE #8.
SDATA(NSDATA =8,NTDATA=1:214,MKLOS =1)
    8.810350E-01,8.106902E-01,7.982643E-01,6.740181E-01,5.634896E-01,
    5.063996E-01,4.493093E-01,3.922190E-01,3.578168E-01,3.254026E-01,
  … (39 lines ommitted)
    2.325018E-01,2.325664E-01,2.326336E-01,2.327031E-01,2.327633E-01,
    2.328193E-01,2.328832E-01,2.410464E-01,2.410464E-01
POROSITY SURFACE #1; GAS GENERATION RATE #9.
PDATA(NSDATA =9,NTDATA=1:214,MKLOS =1)
    1.013250E+05,1.075138E+05,1.137576E+05,1.761884E+05,2.606492E+05,
    3.687214E+05,4.767943E+05,5.980646E+05,7.726453E+05,9.471851E+05,
  … (39 lines ommitted)
    1.983323E+07,1.982785E+07,1.982260E+07,1.981762E+07,1.981253E+07,
```

```
   1.980727E+07,1.980139E+07,1.900425E+07,1.900425E+07
POROSITY SURFACE #1; GAS GENERATION RATE #9.
SDATA(NSDATA =9,NTDATA=1:214,MKLOS =1)
   8.810350E-01,8.178201E-01,8.042962E-01,6.690713E-01,5.705597E-01,
   5.113449E-01,4.521297E-01,3.982915E-01,3.661736E-01,3.340631E-01,
  … (39 lines ommitted)
   3.028700E-01,3.029518E-01,3.030321E-01,3.031086E-01,3.031874E-01,
   3.032685E-01,3.033588E-01,3.161523E-01,3.161523E-01
POROSITY SURFACE #1; GAS GENERATION RATE #10.
PDATA(NSDATA =10,NTDATA=1:214,MKLOS =1)
   1.013250E+05,1.086925E+05,1.161023E+05,1.901929E+05,3.072118E+05,
   4.320126E+05,5.568141E+05,7.235048E+05,9.227972E+05,1.122043E+06,
  … (39 lines ommitted)
   2.007459E+07,2.007008E+07,2.006470E+07,2.005891E+07,2.005422E+07,
   2.004950E+07,2.004473E+07,1.918239E+07,1.918239E+07
POROSITY SURFACE #1; GAS GENERATION RATE #10.
SDATA(NSDATA =10,NTDATA=1:214,MKLOS =1)
   8.810350E-01,8.186546E-01,8.036798E-01,6.539479E-01,5.778739E-01,
   5.151116E-01,4.523489E-01,4.065616E-01,3.739860E-01,3.414181E-01,
  … (39 lines ommitted)
   3.740120E-01,3.740965E-01,3.741970E-01,3.743052E-01,3.743936E-01,
   3.744824E-01,3.745721E-01,3.915004E-01,3.915004E-01
POROSITY SURFACE #1; GAS GENERATION RATE #11.
PDATA(NSDATA =11,NTDATA=1:214,MKLOS =1)
   1.013250E+05,1.107756E+05,1.202943E+05,2.154709E+05,3.335003E+05,
   4.950159E+05,6.565325E+05,8.228237E+05,1.063589E+06,1.304297E+06,
  … (39 lines ommitted)
   2.022343E+07,2.021993E+07,2.021634E+07,2.021272E+07,2.020874E+07,
   2.020459E+07,2.019998E+07,1.929467E+07,1.929467E+07
POROSITY SURFACE #1; GAS GENERATION RATE #11.
SDATA(NSDATA =11,NTDATA=1:214,MKLOS =1)
   8.810350E-01,8.206745E-01,8.074997E-01,6.757653E-01,5.703730E-01,
   5.150381E-01,4.597029E-01,4.060090E-01,3.779154E-01,3.498283E-01,
  … (39 lines ommitted)
   4.454941E-01,4.455723E-01,4.456520E-01,4.457319E-01,4.458203E-01,
   4.459127E-01,4.460138E-01,4.670521E-01,4.670521E-01
POROSITY SURFACE #1; GAS GENERATION RATE #12.
PDATA(NSDATA =12,NTDATA=1:214,MKLOS =1)
   1.013250E+05,1.139705E+05,1.268619E+05,2.557623E+05,4.022974E+05,
   6.154264E+05,8.285568E+05,1.041687E+06,1.331579E+06,1.627615E+06,
  … (39 lines ommitted)
   2.032312E+07,2.032029E+07,2.031731E+07,2.031408E+07,2.031066E+07,
   2.030716E+07,2.030437E+07,1.942159E+07,1.942159E+07
POROSITY SURFACE #1; GAS GENERATION RATE #12.
SDATA(NSDATA =12,NTDATA=1:214,MKLOS =1)
   8.810350E-01,8.128521E-01,8.005670E-01,6.777283E-01,5.699072E-01,
   5.186972E-01,4.674869E-01,4.162765E-01,3.897323E-01,3.651903E-01,
  … (39 lines ommitted)
   5.910663E-01,5.911493E-01,5.912360E-01,5.913289E-01,5.914288E-01,
   5.915313E-01,5.916139E-01,6.186466E-01,6.186466E-01
POROSITY SURFACE #1; GAS GENERATION RATE #13.
```

```
    PDATA(NSDATA =13,NTDATA=1:214,MKLOS =1)
       1.013250E+05,1.134578E+05,1.262180E+05,2.762811E+05,4.663713E+05,
       6.930938E+05,9.537801E+05,1.245543E+06,1.565859E+06,1.905497E+06,
      … (39 lines ommitted)
       2.029380E+07,2.029190E+07,2.028993E+07,2.028801E+07,2.028575E+07,
       2.028364E+07,2.028181E+07,1.955846E+07,1.955846E+07
    POROSITY SURFACE #1; GAS GENERATION RATE #13.
    SDATA(NSDATA =13,NTDATA=1:214,MKLOS =1)
       8.810350E-01,7.875822E-01,7.691885E-01,6.495094E-01,5.695103E-01,
       5.089608E-01,4.618662E-01,4.249945E-01,3.964172E-01,3.736529E-01,
      … (39 lines ommitted)
       7.399021E-01,7.399742E-01,7.400475E-01,7.401146E-01,7.401974E-01,
       7.402756E-01,7.403433E-01,7.678674E-01,7.678674E-01
  POROSTIY SURFACE #2, FOR NORTH END w/o BACKFILL.
  PDATA(1:NSDATA,1:NTDATA,1:MKLOS); NSDATA=13, NTDATA=214, MKLOS=4
  FOR POROSITY SURFACE 2 ONLY 7 GAS GENERATION RATES ARE USED. THE OTHERS ARE SET TO 0.
    POROSITY SURFACE #2; GAS GENERATION RATE #1.
    PDATA(NSDATA =1,NTDATA=1:214,MKLOS =2)
      214*1.01325E+05
    POROSITY SURFACE #2; GAS GENERATION RATE #1.
    SDATA(NSDATA =1,NTDATA=1:214,MKLOS =2)
      1.000000E+00,9.534095E-01,9.470812E-01,8.838051E-01,8.276433E-01,
      7.861733E-01,7.484064E-01,7.173585E-01,6.885050E-01,6.631673E-01,
      … (39 lines ommitted)
      3.716311E-02,3.709546E-02,3.702772E-02,3.695971E-02,3.689402E-02,
      3.682877E-02,3.676412E-02,2.272370E-02,2.272370E-02
    POROSITY SURFACE #2; GAS GENERATION RATE #2.
    PDATA(NSDATA =2,NTDATA=1:214,MKLOS =2)
      1.013250E+05,1.014093E+05,1.015523E+05,1.031616E+05,1.048276E+05,
      1.068422E+05,1.089119E+05,1.112513E+05,1.136401E+05,1.162275E+05,
      … (39 lines ommitted)
      3.640222E+06,3.642184E+06,3.644082E+06,3.646202E+06,3.647983E+06,
      3.649877E+06,3.651749E+06,4.110656E+06,4.110656E+06
    POROSITY SURFACE #2; GAS GENERATION RATE #2.
    SDATA(NSDATA =2,NTDATA=1:214,MKLOS =2)
      1.000000E+00,9.565004E-01,9.436509E-01,8.868655E-01,8.322576E-01,
      7.909592E-01,7.512482E-01,7.193079E-01,6.888833E-01,6.645635E-01,
      … (39 lines ommitted)
      6.285289E-02,6.281804E-02,6.278440E-02,6.274686E-02,6.271534E-02,
      6.268188E-02,6.264882E-02,5.547806E-02,5.547806E-02
    POROSITY SURFACE #2; GAS GENERATION RATE #3.
    PDATA(NSDATA =3,NTDATA=1:214,MKLOS =2)
      1.013250E+05,1.015771E+05,1.018292E+05,1.147067E+05,1.306487E+05,
      1.491446E+05,1.682754E+05,1.892675E+05,2.106405E+05,2.342118E+05,
      … (39 lines ommitted)
      9.358548E+06,9.359201E+06,9.359818E+06,9.360461E+06,9.361114E+06,
      9.361724E+06,9.362368E+06,9.649179E+06,9.649179E+06
    POROSITY SURFACE #2; GAS GENERATION RATE #3.
    SDATA(NSDATA =3,NTDATA=1:214,MKLOS =2)
      1.000000E+00,9.751257E-01,9.560622E-01,8.804212E-01,8.388185E-01,
      8.082005E-01,7.803164E-01,7.558443E-01,7.320703E-01,7.097225E-01,
```

```
  … (39 lines ommitted)
  2.402771E-01,2.402602E-01,2.402441E-01,2.402274E-01,2.402105E-01,
  2.401947E-01,2.401781E-01,2.329632E-01,2.329632E-01
POROSITY SURFACE #2; GAS GENERATION RATE #4.
PDATA(NSDATA =4,NTDATA=1:214,MKLOS =2)
  1.013250E+05,1.019288E+05,1.025327E+05,1.300565E+05,1.614025E+05,
  1.986491E+05,2.367147E+05,2.781497E+05,3.199284E+05,3.662243E+05,
  … (39 lines ommitted)
  1.272395E+07,1.272395E+07,1.272395E+07,1.272391E+07,1.272390E+07,
  1.272390E+07,1.272390E+07,1.272415E+07,1.272415E+07
POROSITY SURFACE #2; GAS GENERATION RATE #4.
SDATA(NSDATA =4,NTDATA=1:214,MKLOS =2)
  1.000000E+00,9.724346E-01,9.541304E-01,8.917347E-01,8.508140E-01,
  8.181004E-01,7.865272E-01,7.634814E-01,7.413054E-01,7.199909E-01,
  … (39 lines ommitted)
  3.524306E-01,3.524306E-01,3.524306E-01,3.524318E-01,3.524320E-01,
  3.524320E-01,3.524320E-01,3.524250E-01,3.524250E-01
POROSITY SURFACE #2; GAS GENERATION RATE #5.
PDATA(NSDATA =5,NTDATA=1:214,MKLOS =2)
  1.013250E+05,1.026735E+05,1.040221E+05,1.607512E+05,2.228597E+05,
  2.965181E+05,3.712018E+05,4.545696E+05,5.384155E+05,6.316594E+05,
  … (39 lines ommitted)
  1.816319E+07,1.816101E+07,1.815881E+07,1.815663E+07,1.815451E+07,
  1.815239E+07,1.815031E+07,1.782467E+07,1.782467E+07
POROSITY SURFACE #2; GAS GENERATION RATE #5.
SDATA(NSDATA =5,NTDATA=1:214,MKLOS =2)
  1.000000E+00,9.748433E-01,9.570604E-01,8.993860E-01,8.566730E-01,
  8.261634E-01,7.967376E-01,7.714288E-01,7.463467E-01,7.237408E-01,
  … (39 lines ommitted)
  4.925956E-01,4.926553E-01,4.927153E-01,4.927746E-01,4.928326E-01,
  4.928905E-01,4.929473E-01,5.020043E-01,5.020043E-01
POROSITY SURFACE #2; GAS GENERATION RATE #6.
PDATA(NSDATA =6,NTDATA=1:214,MKLOS =2)
  1.013250E+05,1.041277E+05,1.069304E+05,1.997906E+05,2.942560E+05,
  4.081954E+05,5.225804E+05,6.487903E+05,7.756826E+05,9.122583E+05,
  … (39 lines ommitted)
  2.032416E+07,2.031420E+07,2.030426E+07,2.029450E+07,2.028483E+07,
  2.027529E+07,2.026586E+07,1.869941E+07,1.869941E+07
POROSITY SURFACE #2; GAS GENERATION RATE #6.
SDATA(NSDATA =6,NTDATA=1:214,MKLOS =2)
  1.000000E+00,9.725971E-01,9.501980E-01,8.946068E-01,8.430061E-01,
  8.128133E-01,7.828748E-01,7.597040E-01,7.368370E-01,7.182998E-01,
  … (39 lines ommitted)
  6.599369E-01,6.602622E-01,6.605868E-01,6.609063E-01,6.612228E-01,
  6.615354E-01,6.618451E-01,7.175897E-01,7.175897E-01
POROSITY SURFACE #2; GAS GENERATION RATE #7.
PDATA(NSDATA =7,NTDATA=1:214,MKLOS =2)
  1.013250E+05,1.164545E+05,1.328637E+05,2.969381E+05,4.678443E+05,
  6.583228E+05,8.551700E+05,1.067707E+06,1.285569E+06,1.514794E+06,
  … (39 lines ommitted)
  2.091650E+07,2.090379E+07,2.089115E+07,2.087875E+07,2.086650E+07,
```

```
  2.085438E+07,2.084242E+07,1.886452E+07,1.886452E+07
POROSITY SURFACE #2; GAS GENERATION RATE #7.
SDATA(NSDATA =7,NTDATA=1:214,MKLOS =2)
  1.000000E+00,9.478489E-01,9.426141E-01,8.902719E-01,8.428811E-01,
  8.096146E-01,7.787077E-01,7.536157E-01,7.304598E-01,7.114597E-01,
  … (39 lines ommitted)
  1.068595E+00,1.069248E+00,1.069898E+00,1.070537E+00,1.071168E+00,
  1.071794E+00,1.072411E+00,1.185459E+00,1.185459E+00
POROSITY SURFACE #2; GAS GENERATION RATE #8.
PDATA(NSDATA =8,NTDATA=1:214,MKLOS =2)
  214*0.0D0
POROSITY SURFACE #2; GAS GENERATION RATE #8.
SDATA(NSDATA =8,NTDATA=1:214,MKLOS =2)
  214*0.0D0
POROSITY SURFACE #2; GAS GENERATION RATE #9.
PDATA(NSDATA =9,NTDATA=1:214,MKLOS =2)
  214*0.0D0
POROSITY SURFACE #2; GAS GENERATION RATE #9.
SDATA(NSDATA =9,NTDATA=1:214,MKLOS =2)
  214*0.0D0
POROSITY SURFACE #2; GAS GENERATION RATE #10.
PDATA(NSDATA =10,NTDATA=1:214,MKLOS =2)
  214*0.0D0
POROSITY SURFACE #2; GAS GENERATION RATE #10.
SDATA(NSDATA =10,NTDATA=1:214,MKLOS =2)
  214*0.0D0
POROSITY SURFACE #2; GAS GENERATION RATE #11.
PDATA(NSDATA =11,NTDATA=1:214,MKLOS =2)
  214*0.0D0
POROSITY SURFACE #2; GAS GENERATION RATE #11.
SDATA(NSDATA =11,NTDATA=1:214,MKLOS =2)
  214*0.0D0
POROSITY SURFACE #2; GAS GENERATION RATE #12.
PDATA(NSDATA =12,NTDATA=1:214,MKLOS =2)
  214*0.0D0
POROSITY SURFACE #2; GAS GENERATION RATE #12.
SDATA(NSDATA =12,NTDATA=1:214,MKLOS =2)
  214*0.0D0
POROSITY SURFACE #2; GAS GENERATION RATE #13.
PDATA(NSDATA =13,NTDATA=1:214,MKLOS =2)
  214*0.0D0
POROSITY SURFACE #2; GAS GENERATION RATE #13.
SDATA(NSDATA =13,NTDATA=1:214,MKLOS =2)
  214*0.0D0
  … (surfaces 3 and 4 ommitted)
```

11.3 Appendix C: Sample Output File

Below is listed an example BRAGFLO ASCII .xout file. This file is a truncated version (only brine pressure data from first and last time steps included) of output generated by the input file given in Section 11.1, Appendix A.

```
*****************************************************************************
 ** Beginning of BRAGFLO        Version: 7.00          Revised: 08/14/18      **
 ** Begun on: 11/27/18 at 09:29:33    Run on: i86pc santana SunOS 5.11        **
 *****************************************************************************


  BBBBBB   RRRRRR    AAAAA    GGGGG   FFFFFFF  LL         OOOOO
  BB   BB  RR   RR  AA   AA  GG   GG  FF       LL        OO   OO
  BB   BB  RR   RR  AA   AA  GG       FF       LL        OO   OO
  BBBBBB   RRRRRR   AAAAAAA  GG       FFFFF    LL        OO   OO
  BB   BB  RRRRR    AA   AA  GG  GGG  FF       LL        OO   OO
  BB   BB  RR  RR   AA   AA  GG   GG  FF       LL        OO   OO
  BBBBBB   RR   RR  AA   AA   GGGGG   FF       LLLLLLL    OOOOO


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                           Ali A. Shinta, API
                           John Wormeck, Ecodynamics


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                        Disclaimer
                        ----------

This computer program was prepared as  an  account  of  work
sponsored  by  an  agency  of  the United States Government.
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product,  process,  or  service  by  trade  name,  trademark,
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        manufacturer,  or otherwise, does not necessarily constitute
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        United States Government, any agency thereof or any of their
        contractors  or  subcontractors.   The  views  and  opinions
        expressed  herein  do not necessarily state or reflect those
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        of their contractors or subcontractors.

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 **QA**    -- QA info for:
 PREBRAG   -- program name;
 9.00      -- PREBRAG version number;
 08/16/18  -- PREBRAG revision date;
 10/02/18  -- PREBRAG run date;
 10:52:56  -- PREBRAG run time.



Number of file names to follow =   6

*******************************************************************************
Input File Name:
bf2_EX_r1_s2_v001.inp
*******************************************************************************

*******************************************************************************
Closure Input File Name:
bf2_EX_closure.dat
*******************************************************************************

*******************************************************************************
ASCII Output File Name:
bf2_EX_r1_s2_v001.xout
*******************************************************************************

*******************************************************************************
ASCII Summary File Name:
bf2_EX_r1_s2_v001.sum
*******************************************************************************

*******************************************************************************
Binary Output File Name:
bf2_EX_r1_s2_v001.xbin
*******************************************************************************

*******************************************************************************
Restart Output File Name:
```

```
bf2_bf2_EX_r1_s2_v001.xrot
********************************************************************************


 Simulation title:
 BRAGFLO S2-BF FOR EXAMPLE IO

 Size parameters:   NX,   NY,   NZ
                    68    33     1

 Number of grid blocks = 2244

 Model Type  (MODTYPE) =  2-Dimensional

*************************************************************************************************************************************************
 Parameters for adjusting DELT:
     Number of times to fix DELT  (NDTFIX) =     6
     TIMEDTFIX = Time for fixing DELT, s
     DTFIX     = DELT to be used when TIMEDTFIX is exceeded, s
        K   TIMEDTFIX(K)      DTFIX(K)
        1   0.000000E+00 8.640000E+02
        2   3.155700E+09 8.640000E+02
        3   6.311400E+09 8.640000E+02
        4   1.104500E+10 8.640000E+02
        5   1.735600E+10 8.640000E+02
        6   4.891300E+10 8.640000E+02

 UNITS used in input:
    SI

 UNITS used in output:
    SI

*************************************************************************************************************************************************

 Start time of simulation     (START) =-1.57780E+08 s
 End time for simulation     (FINISH) = 3.15570E+11 s
 Max no. time steps allowed  (MAXITF) = 30000
 Initial time step             (DELT) = 8.64000E+00 s
 Minimum time step allowed  (DELTMIN) = 8.64000E-04 s
 Maximum time step allowed  (DELTMAX) = 3.15570E+08 s
 Max fractional increase in time step allowed    (DTIMEMAX) = 1.25000E+00
 Flag for auto time step control (0=No,1=Yes)  (ITIMECNTRL) = 1
 Switch from relative to absolute change
     in variable for determining time step size   (TSWITCH) = 1.00000E+00

*************************************************************************************************************************************************

 ASCII print control type         (IPRTYPEASC) =  2
 Binary print control type        (IPRTYPEBIN) =  0
 Restart print control type       (IPRTYPERST) =  2
```

```
 ASCII output at  9 specified times:
     1    0.00000E+00 s
     2    3.15570E+09 s
     3    1.10450E+10 s
     4    3.15570E+10 s
     5    9.46710E+10 s
     6    1.57780E+11 s
     7    2.20900E+11 s
     8    2.84010E+11 s
     9    3.15570E+11 s

 Binary output timestep interval    (IPRNTBIN) =   5

 Restart output at  1 specified times:
     1    3.15570E+11 s
```

****

**** Variable Output Flags ****
0 = Do NOT Print to Designated Output File
1 = DO Print to Designated Output File

I	ASC	BIN	Variable	Description	Units
1	1	1	PO	Brine pressure	Pa
2	1	1	PG	Gas pressure	Pa
3	0	0	POTO	Brine rho*g*potentiometric head	Pa
4	0	0	POTG	Gas rho*g*potentiometric head	Pa
5	0	0	PBUB	Brine bubble pressure	Pa
6	1	1	PHI	Porosity	dimensionless
7	0	0	RKO	Relative permeability to brine	dimensionless
8	0	0	RKG	Relative permeability to gas	dimensionless
9	0	0	RHOB	Brine density	kg/m^3
10	0	1	RHOG	Gas density	kg/m^3
11	0	1	PERMBX	Permeability to brine, x-direction	m^2
12	0	0	PERMBY	Permeability to brine, y-direction	m^2
13	0	0	PERMBZ	Permeability to brine, z-direction	m^2
14	0	1	PERMGX	Permeability to gas, x-direction	m^2
15	0	0	PERMGY	Permeability to gas, y-direction	m^2
16	0	0	PERMGZ	Permeability to gas, z-direction	m^2
17	0	0	SO	Brine saturation	fraction void volume
18	1	1	SG	Gas saturation	fraction void volume
19	0	0	COO	Brine component of brine phase	mass fr brine phase
20	0	0	CGO	Gas component of brine phase	mass fr brine phase
21	0	0	QOREFAVE	Time-average well brine flow rate	m^3/s (ref conds)
22	0	0	QGREFAVE	Time-average well gas flow rate	m^3/s (ref conds)
23	0	0	QOCUM	Cumulative well brine flow	m^3 (ref conds)
24	0	0	QGCUM	Cumulative well gas flow	m^3 (ref conds)
25	0	0	VODAVEI	Time-avg brine Darcy velocity, x-dir	m/s

26	0	0	VODAVEJ	Time-avg brine Darcy velocity, y-dir	m/s
27	0	0	VODAVEK	Time-avg brine Darcy velocity, z-dir	m/s
28	0	0	VGDAVEI	Time-avg gas Darcy velocity, x-dir	m/s
29	0	0	VGDAVEJ	Time-avg gas Darcy velocity, y-dir	m/s
30	0	0	VGDAVEK	Time-avg gas Darcy velocity, z-dir	m/s
31	0	1	QODAVEI	Time-avg interblock brine flow, x-dir	m^3/s (@ ref conds)
32	0	1	QODAVEJ	Time-avg interblock brine flow, y-dir	m^3/s (@ ref conds)
33	0	0	QODAVEK	Time-avg interblock brine flow, z-dir	m^3/s (@ ref conds)
34	0	1	QGDAVEI	Time-avg interblock gas flow, x-dir	m^3/s (@ ref conds)
35	0	1	QGDAVEJ	Time-avg interblock gas flow, y-dir	m^3/s (@ ref conds)
36	0	0	QGDAVEK	Time-avg interblock gas flow, z-dir	m^3/s (@ ref conds)
37	0	0	BRNBALREL	Relative Brine mass balance	dimensionless
38	0	0	GASBALREL	Relative Gas mass balance	dimensionless
39	0	0	RXNR(I,J,K,1)	Inundated corrosion rate	mol/s
40	0	0	RXNR(I,J,K,2)	Humid corrosion rate	mol/s
41	0	0	RXNR(I,J,K,3)	Inundated biodegradation rate	mol/s
42	0	0	RXNR(I,J,K,4)	Humid biodegradation rate	mol/s
43	0	0	RXNR(I,J,K,5)	Fe(OH)2 sulfidation rate	mol/s
44	0	0	RXNR(I,J,K,6)	Fe sulfidation rate	mol/s
45	0	0	RXNR(I,J,K,7)	MgO hydration rate	mol/s
46	0	0	RXNR(I,J,K,8)	Mg(OH)2 carbonation rate	mol/s
47	0	0	RXNR(I,J,K,9)	MgO carbonation rate	mol/s
48	0	0	RXNR(I,J,K,10)	Hydromagnesite conversion rate	mol/s
49	1	1	QR(I,J,K,1)	H2 generation rate -- simple model	kg/(s*m^3)
50	0	1	QR(I,J,K,2)	Brine consumption rate -- simple model	kg/(s*m^3)
51	0	0	QR(I,J,K,3)	Fe consumption rate -- simple model	kg/(s*m^3)
52	0	0	QR(I,J,K,4)	C6-H10-O5 consumption rate -- simple model	kg/(s*m^3)
53	0	0	QR(I,J,K,5)	Fe(OH)2 generation rate -- simple model	kg/(s*m^3)
54	0	0	QR(I,J,K,6)	FeS generation rate -- simple model	kg/(s*m^3)
55	0	0	QR(I,J,K,7)	MgO generation rate -- simple model	kg/(s*m^3)
56	0	0	QR(I,J,K,8)	Mg(OH)2 generation rate -- simple model	kg/(s*m^3)
57	0	0	QR(I,J,K,9)	Hydromagnesite generation rate -- simple model	kg/(s*m^3)
58	0	0	QR(I,J,K,10)	MgCO3 generation rate -- simple model	kg/(s*m^3)
59	1	1	CONCFE(I,J,K,1)	Fe concentration -- simple model	kg/m^3
60	1	1	CONCBIO	C6-H10-O5 concentration -- simple model	kg/m^3
61	0	0	CONCFE(I,J,K,2)	Fe(OH)2 concentration -- simple model	kg/m^3
62	0	0	CONCFE(I,J,K,3)	FeS concentration -- simple model	kg/m^3
63	1	1	CONCMG(I,J,K,1)	MgO concentration -- simple model	kg/m^3
64	0	0	CONCMG(I,J,K,2)	Mg(OH)2 concentration -- simple model	kg/m^3
65	0	0	CONCMG(I,J,K,3)	Hydromagnesite concentration -- simple model	kg/m^3
66	0	0	CONCMG(I,J,K,4)	MgCO3 concentration -- simple model	kg/m^3
67	0	0	CONCST	Salt concentration -- simple model	kg/m^3
68	0	0	PORSOLID	Volume fraction of generated solids	dimensionless
69	0	0	GENRAT(1,I,J,K)	H2 generation rate -- reaction path model	kg/(s*m^3)
70	0	0	GENRAT(2,I,J,K)	CO2 generation rate -- reaction path model	kg/(s*m^3)
71	0	0	GENRAT(3,I,J,K)	CH4 generation rate -- reaction path model	kg/(s*m^3)
72	0	0	GENRAT(4,I,J,K)	N2 generation rate -- reaction path model	kg/(s*m^3)
73	0	0	GENRAT(5,I,J,K)	H2S generation rate -- reaction path model	kg/(s*m^3)
74	0	0	GENRAT(6,I,J,K)	O2 generation rate -- reaction path model	kg/(s*m^3)
75	0	0	GENRAT(7,I,J,K)	H2O generation rate -- reaction path model	kg/(s*m^3)
76	0	0	GENRAT(8,I,J,K)	H2SO4 generation rate -- reaction path model	kg/(s*m^3)

77	0	0	GENRAT(9,I,J,K)	HNO3 generation rate -- reaction path model	kg/(s*m^3)
78	0	0	GENRAT(10,I,J,K)	C6-H10-O5 consumption rate -- reaction path model	kg/(s*m^3)
79	0	0	GENRAT(11,I,J,K)	Fe consumption rate -- reaction path model	kg/(s*m^3)
80	0	0	GENRAT(12,I,J,K)	FeS2_F generation rate -- reaction path model	kg/(s*m^3)
81	0	0	GENRAT(13,I,J,K)	FeS2_O generation rate -- reaction path model	kg/(s*m^3)
82	0	0	GENRAT(14,I,J,K)	FeCO3_F generation rate -- reaction path model	kg/(s*m^3)
83	0	0	GENRAT(15,I,J,K)	FeCO3_O generation rate -- reaction path model	kg/(s*m^3)
84	0	0	GENRAT(16,I,J,K)	Fe(OH)2 generation rate -- reaction path model	kg/(s*m^3)
85	0	0	GENRAT(17,I,J,K)	FeO(OH) generation rate -- reaction path model	kg/(s*m^3)
86	0	0	GENRAT(18,I,J,K)	Fe3O4 generation rate -- reaction path model	kg/(s*m^3)
87	0	0	GENRAT(19,I,J,K)	FeS generation rate -- reaction path model	kg/(s*m^3)
88	0	0	GENRAT(20,I,J,K)	CaO generation rate -- reaction path model	kg/(s*m^3)
89	0	0	GENRAT(21,I,J,K)	Ca(OH)2 generation rate -- reaction path model	kg/(s*m^3)
90	0	0	GENRAT(22,I,J,K)	CaCO3 generation rate -- reaction path model	kg/(s*m^3)
91	1	1	GENRAT(23,I,J,K)	H2 generation rate -- radiolysis	kg/(s*m^3)
92	0	0	CONCRXN(1,I,J,K)	H2 concentration -- reaction path model	kg/m^3
93	0	0	CONCRXN(2,I,J,K)	CO2 concentration -- reaction path model	kg/m^3
94	0	0	CONCRXN(3,I,J,K)	CH4 concentration -- reaction path model	kg/m^3
95	0	0	CONCRXN(4,I,J,K)	N2 concentration -- reaction path model	kg/m^3
96	0	0	CONCRXN(5,I,J,K)	H2S concentration -- reaction path model	kg/m^3
97	0	0	CONCRXN(6,I,J,K)	O2 concentration -- reaction path model	kg/m^3
98	0	0	CONCRXN(7,I,J,K)	H2O concentration -- reaction path model	kg/m^3
99	0	0	CONCRXN(8,I,J,K)	H2SO4 concentration -- reaction path model	kg/m^3
100	0	0	CONCRXN(9,I,J,K)	HNO3 concentration -- reaction path model	kg/m^3
101	0	0	CONCRXN(10,I,J,K)	C6-H10-O5 concentration -- reaction path model	kg/m^3
102	0	0	CONCRXN(11,I,J,K)	Fe concentration -- reaction path model	kg/m^3
103	0	0	CONCRXN(12,I,J,K)	FeS2_F concentration -- reaction path model	kg/m^3
104	0	0	CONCRXN(13,I,J,K)	FeS2_O concentration -- reaction path model	kg/m^3
105	0	0	CONCRXN(14,I,J,K)	FeCO3_F concentration -- reaction path model	kg/m^3
106	0	0	CONCRXN(15,I,J,K)	FeCO3_O concentration -- reaction path model	kg/m^3
107	0	0	CONCRXN(16,I,J,K)	Fe(OH)2 concentration -- reaction path model	kg/m^3
108	0	0	CONCRXN(17,I,J,K)	FeO(OH) concentration -- reaction path model	kg/m^3
109	0	0	CONCRXN(18,I,J,K)	Fe3O4 concentration -- reaction path model	kg/m^3
110	0	0	CONCRXN(19,I,J,K)	FeS concentration -- reaction path model	kg/m^3
111	0	0	CONCRXN(20,I,J,K)	CaO concentration -- reaction path model	kg/m^3
112	0	0	CONCRXN(21,I,J,K)	Ca(OH)2 concentration -- reaction path model	kg/m^3
113	0	0	CONCRXN(22,I,J,K)	CaCO3 concentration -- reaction path model	kg/m^3
114	0	0	CONCRXN(23,I,J,K)	H2 concentration -- radiolysis	kg/m^3
115	0	0	H2OFLOWIN	Water inflow rate	kg/s
116	1	1	S_MASS(1,1)	Amount of isotope 1 from Waste Region 1	mol
117	1	1	S_MASS(1,2)	Amount of isotope 1 from Waste Region 2	mol
118	1	1	S_MASS(2,1)	Amount of isotope 2 from Waste Region 1	mol
119	1	1	S_MASS(2,2)	Amount of isotope 2 from Waste Region 2	mol
120	1	1	S_MASS(3,1)	Amount of isotope 3 from Waste Region 1	mol
121	1	1	S_MASS(3,2)	Amount of isotope 3 from Waste Region 2	mol
122	1	1	S_MASS(4,1)	Amount of isotope 4 from Waste Region 1	mol
123	1	1	S_MASS(4,2)	Amount of isotope 4 from Waste Region 2	mol
124	1	1	S_MASS(5,1)	Amount of isotope 5 from Waste Region 1	mol
125	1	1	S_MASS(5,2)	Amount of isotope 5 from Waste Region 2	mol

****

```
Number of variables to be printed as History Variables  (NHIV) =  0
NOTE:  History variables printed only to Binary output file.

Monitor key parameters  (MONITOR):  T
   Number of Monitor Blocks  (NMON) =  3
   I-index of grid block 1 to be monitored  (IMONITOR) = 26
   J-index of grid block 1 to be monitored  (JMONITOR) = 12
   K-index of grid block 1 to be monitored  (KMONITOR) =  1
   I-index of grid block 2 to be monitored  (IMONITOR) = 32
   J-index of grid block 2 to be monitored  (JMONITOR) = 12
   K-index of grid block 2 to be monitored  (KMONITOR) =  1
   I-index of grid block 3 to be monitored  (IMONITOR) = 36
   J-index of grid block 3 to be monitored  (JMONITOR) = 12
   K-index of grid block 3 to be monitored  (KMONITOR) =  1

Geometry Flags -- Specifies how block thicknesses are to be read.
   IDXFLAG    =  1
   IDYFLAG    =  2
   IDZFLAG    =  1
   IDEPTHFLAG =  7

Grid block dimensions in I-direction, m
  1.220383E+04 3.126850E+03 2.156450E+03 1.487210E+03 1.025660E+03
  7.073500E+02 5.266800E+02 3.632300E+02 2.505000E+02 1.727600E+02
  1.191500E+02 8.217000E+01 5.667000E+01 3.908000E+01 2.695000E+01
  1.859000E+01 1.282000E+01 8.840000E+00 6.100000E+00 4.200000E+00
  2.900000E+00 2.000000E+00 4.380000E+01 1.000000E+01 2.000000E+00
  2.757500E-01 2.000000E+00 1.000000E+01 4.380000E+01 1.524000E+01
  1.524000E+01 1.402000E+02 1.402000E+02 1.524000E+01 1.524000E+01
  1.402000E+02 1.402000E+02 3.048000E+01 3.048000E+01 9.870000E+01
  9.870000E+01 9.870000E+01 1.000000E+01 3.616500E+02 3.616500E+02
  2.000000E+00 2.900000E+00 4.200000E+00 6.100000E+00 8.840000E+00
  1.282000E+01 1.859000E+01 2.695000E+01 3.908000E+01 5.667000E+01
  8.217000E+01 1.191500E+02 1.727600E+02 2.505000E+02 3.632300E+02
  5.266800E+02 7.073500E+02 1.025660E+03 1.487210E+03 2.156450E+03
  3.126850E+03 4.533940E+03 7.669890E+03

Grid block dimensions in J-direction, m
  1.258300E+02 5.227000E+01 6.672000E+01 6.672000E+01 6.572000E+01
  1.000000E+00 8.500000E-01 6.900000E-01 6.900000E-01 1.320000E+00
  1.320000E+00 1.320000E+00 2.620000E+00 2.700000E-01 4.530000E+00
  4.530000E+00 1.800000E-01 5.473000E+01 5.473000E+01 5.473000E+01
  5.473000E+01 5.473000E+01 5.473000E+01 5.473000E+01 3.600000E+01
  7.700000E+00 2.480000E+01 8.500000E+00 1.730000E+01 1.060000E+02
  4.330000E+01 1.566000E+01 1.000000E-01

Grid block dimensions in K-direction, m
  6.617707E+04 3.551571E+04 2.494910E+04 1.766178E+04 1.263605E+04
  9.170020E+03 6.701950E+03 4.922120E+03 3.694660E+03 2.848130E+03
  2.264310E+03 1.861680E+03 1.584010E+03 1.392510E+03 1.260440E+03
```

```
  1.169360E+03 1.106540E+03 1.063220E+03 1.033340E+03 1.012740E+03
  9.985300E+02 9.887300E+02 1.262000E+02 2.880000E+01 4.800000E+00
  2.757500E-01 4.800000E+00 2.880000E+01 1.262000E+02 2.000000E+01
  2.000000E+01 1.569040E+02 1.569040E+02 4.000000E+01 4.000000E+01
  1.961300E+02 1.961300E+02 4.000000E+01 4.000000E+01 3.218000E+01
  3.218000E+01 3.218000E+01 9.500000E+00 5.167000E+01 5.168000E+01
  2.839580E+03 2.849380E+03 2.863590E+03 2.884190E+03 2.914070E+03
  2.957390E+03 3.020200E+03 3.111290E+03 3.243360E+03 3.434860E+03
  3.712530E+03 4.115160E+03 4.698980E+03 5.545500E+03 6.772970E+03
  8.552800E+03 1.102087E+04 1.448690E+04 1.951263E+04 2.679995E+04
  3.736656E+04 5.268814E+04 7.709580E+04

Elevations to grid block centers in IJK-direction, m
  6.291500E+01 6.291500E+01 6.291500E+01 6.291500E+01 6.291500E+01
  6.291500E+01 6.291500E+01 6.291500E+01 6.291500E+01 6.291500E+01
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3.777470E+02 3.782164E+02 3.783212E+02 3.783410E+02 3.783609E+02
3.784656E+02 3.789351E+02 3.794502E+02 3.797162E+02 3.810726E+02
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3.904344E+02 3.909664E+02 3.920936E+02 3.938162E+02 3.955387E+02
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4.093200E+02 4.094099E+02 4.095403E+02 4.097293E+02 4.100034E+02
4.104008E+02 4.109770E+02 4.118125E+02 4.130241E+02 4.147808E+02
4.173281E+02 4.210215E+02 4.263771E+02 4.341426E+02 4.449110E+02
4.600336E+02 4.819614E+02 5.137567E+02 5.598599E+02 6.267095E+02
7.332026E+02 1.203749E+02 2.541536E+02 3.002567E+02 3.320520E+02
3.539799E+02 3.691025E+02 3.798708E+02 3.876364E+02 3.929919E+02
3.966854E+02 3.992326E+02 4.009894E+02 4.022009E+02 4.030365E+02
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 Dirichlet BCs to be specified? (T/F)                  (DIRICHLET) =   T
 Number of grid blocks where Dirichlet BCs specified (NO_DIRGRID) =  72
   N      I    J    K     DIRGRIDP  DIRGRIDS     DIR_PRES [Pa]      DIR_SATB
   1      1   26    1        T         F          9.333000E+05   0.000000E+00
   2     68   26    1        T         F          9.333000E+05   0.000000E+00
   3      1   28    1        T         F          9.631000E+05   0.000000E+00
   4     68   28    1        T         F          9.631000E+05   0.000000E+00
   5      1   33    1        T         T          1.013250E+05   8.363000E-02
   6      2   33    1        T         T          1.013250E+05   8.363000E-02
   7      3   33    1        T         T          1.013250E+05   8.363000E-02
   8      4   33    1        T         T          1.013250E+05   8.363000E-02
   9      5   33    1        T         T          1.013250E+05   8.363000E-02
  10      6   33    1        T         T          1.013250E+05   8.363000E-02
  11      7   33    1        T         T          1.013250E+05   8.363000E-02
  12      8   33    1        T         T          1.013250E+05   8.363000E-02
  13      9   33    1        T         T          1.013250E+05   8.363000E-02
  14     10   33    1        T         T          1.013250E+05   8.363000E-02
  15     11   33    1        T         T          1.013250E+05   8.363000E-02
  16     12   33    1        T         T          1.013250E+05   8.363000E-02
  17     13   33    1        T         T          1.013250E+05   8.363000E-02
  18     14   33    1        T         T          1.013250E+05   8.363000E-02
  19     15   33    1        T         T          1.013250E+05   8.363000E-02
  20     16   33    1        T         T          1.013250E+05   8.363000E-02
  21     17   33    1        T         T          1.013250E+05   8.363000E-02
  22     18   33    1        T         T          1.013250E+05   8.363000E-02
  23     19   33    1        T         T          1.013250E+05   8.363000E-02
  24     20   33    1        T         T          1.013250E+05   8.363000E-02
  25     21   33    1        T         T          1.013250E+05   8.363000E-02
  26     22   33    1        T         T          1.013250E+05   8.363000E-02
  27     23   33    1        T         T          1.013250E+05   8.363000E-02
  28     24   33    1        T         T          1.013250E+05   8.363000E-02
  29     25   33    1        T         T          1.013250E+05   8.363000E-02
  30     26   33    1        T         T          1.013250E+05   8.363000E-02
  31     27   33    1        T         T          1.013250E+05   8.363000E-02
  32     28   33    1        T         T          1.013250E+05   8.363000E-02
  33     29   33    1        T         T          1.013250E+05   8.363000E-02
  34     30   33    1        T         T          1.013250E+05   8.363000E-02
  35     31   33    1        T         T          1.013250E+05   8.363000E-02
  36     32   33    1        T         T          1.013250E+05   8.363000E-02
  37     33   33    1        T         T          1.013250E+05   8.363000E-02
  38     34   33    1        T         T          1.013250E+05   8.363000E-02
  39     35   33    1        T         T          1.013250E+05   8.363000E-02
  40     36   33    1        T         T          1.013250E+05   8.363000E-02
  41     37   33    1        T         T          1.013250E+05   8.363000E-02
  42     38   33    1        T         T          1.013250E+05   8.363000E-02
  43     39   33    1        T         T          1.013250E+05   8.363000E-02
  44     40   33    1        T         T          1.013250E+05   8.363000E-02
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  45     41   33    1        T          T          1.013250E+05   8.363000E-02
  46     42   33    1        T          T          1.013250E+05   8.363000E-02
  47     43   33    1        T          F          1.013250E+05   0.000000E+00
  48     44   33    1        T          T          1.013250E+05   8.363000E-02
  49     45   33    1        T          T          1.013250E+05   8.363000E-02
  50     46   33    1        T          T          1.013250E+05   8.363000E-02
  51     47   33    1        T          T          1.013250E+05   8.363000E-02
  52     48   33    1        T          T          1.013250E+05   8.363000E-02
  53     49   33    1        T          T          1.013250E+05   8.363000E-02
  54     50   33    1        T          T          1.013250E+05   8.363000E-02
  55     51   33    1        T          T          1.013250E+05   8.363000E-02
  56     52   33    1        T          T          1.013250E+05   8.363000E-02
  57     53   33    1        T          T          1.013250E+05   8.363000E-02
  58     54   33    1        T          T          1.013250E+05   8.363000E-02
  59     55   33    1        T          T          1.013250E+05   8.363000E-02
  60     56   33    1        T          T          1.013250E+05   8.363000E-02
  61     57   33    1        T          T          1.013250E+05   8.363000E-02
  62     58   33    1        T          T          1.013250E+05   8.363000E-02
  63     59   33    1        T          T          1.013250E+05   8.363000E-02
  64     60   33    1        T          T          1.013250E+05   8.363000E-02
  65     61   33    1        T          T          1.013250E+05   8.363000E-02
  66     62   33    1        T          T          1.013250E+05   8.363000E-02
  67     63   33    1        T          T          1.013250E+05   8.363000E-02
  68     64   33    1        T          T          1.013250E+05   8.363000E-02
  69     65   33    1        T          T          1.013250E+05   8.363000E-02
  70     66   33    1        T          T          1.013250E+05   8.363000E-02
  71     67   33    1        T          T          1.013250E+05   8.363000E-02
  72     68   33    1        T          T          1.013250E+05   8.363000E-02

SATLIMIT and DEPLIMIT for 2 equations:
    SATLIMIT    = 1.000E-03
    DEPLIMIT(1) = 2.000E-01
    DEPLIMIT(2) =-1.000E+08 Pa

Variable change allowed to keep same time step  (DELTADEPNORM):
    DELTADEPNORM(1) = 3.000E-01
    DELTADEPNORM(2) = 5.000E+05 Pa

Max variable change allowed over time step  (DDEPMAX):
    DDEPMAX(1) = 1.000E+00
    DDEPMAX(2) = 1.000E+07 Pa

NORMAL Newton-Raphson convergence criteria (EPSNORM):
    EPSNORM(1) = 3.000E+00
    EPSNORM(2) = 1.000E-02

LOOSE Newton-Raphson convergence criteria (EPSLOOSE):
    EPSLOOSE(1) = 3.000E+00
    EPSLOOSE(2) = 1.000E-02

NORMAL Min. value of RHS function vector below which
```

```
    convergence is accepted regardless of EPS (FTOLNORM):
    FTOLNORM(1) = 1.000E-02
    FTOLNORM(2) = 1.000E-02

LOOSE Min. value of RHS function vector below which
    convergence is accepted regardless of EPS (FTOLLOOSE):
    FTOLLOOSE(1) = 1.000E-02
    FTOLLOOSE(2) = 1.000E-02

Convergence criteria for gas component transport:
    EPSGAS(1) =-1.000E-05
    EPSGAS(2) = 1.000E-05
    EPSGAS(3) = 1.000E-05
    EPSGAS(4) = 1.000E-05

Solver to be used (CHSOLVER):  LU

Newton-Raphson control parameters:
    Maximum number of Newton-Raphson iterations      (ITMAX) =   8
    Maximum number of interval halvings
        if Newton-Raphson encounters errors      (IRESETMAX) =  40
    Interval frequency for updating Jacobian     (IJACINPUT) =   1
    Scaling of matrix to be done before solution    (LSCALE) =   T
    Pressure scaling factor                        (P_SCALE) = 1.000E+07
    Variable switching allowed                    (LVARSWTCH) =   F
    Upstream weighting update frequency for
        relative permeabilities                   (IUPRPFLAG) =   9
    Upstream weighting update frequency for
        mass fractions                            (IUPMFFLAG) =   9
    Timestep reduction factor if error occurs   (DELTFACTOR) = 5.000E-01
    Transmissivity averaging method                  (ITRAVE) =   1
    Mass fraction averaging method                  (IMFRAVE) =   0

Jacobian reevaluation control parameters:
    Number of time step reductions allowed
       before Jacobian starts to be reevaluated
       every IJACMINth iteration     (IJACSWITCH) = 41
    New number of iterations allowed before
       Jacobian is reevaluated           (IJACMIN) =  1
    Number of time steps IJACMIN is in effect
       after violation of IJACSWITCH (IJACRESET) =  5
    Upstream weighting update frequency for
       relative permeabilities while
       IJACMIN is in effect          (IUPRPLOOSE) =  9
    Upstream weighting update frequency for dissolved gas
       while IJACMIN is in effect    (IUPMFLOOSE) =  9

Relative change in variable for Jacobian element derivative calculations (DH):
    DH(1) = 1.000E-08
    DH(2) = 1.000E-08
```

```
 Minimum variable change allowed for Jacobian element derivative calculations (HMIN):
     HMIN(1) = 1.000E-10
     HMIN(2) = 1.000E-02 Pa

*****************************************************************************************************************************************************

 Number of times to specify material grid (NMATTIMES) =   7
-----------------------------------------------------------------------------------------------------------------------------------------------------
 Material time number =  1          Starting at time =-1.577800E+08 s
     Layer    1
 1    10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 11 11 11 11 11 11 11 11 11 11 11 11 11 11 11 11 11
      11 11 11 11 11 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10
 2    10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10
      10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10
 3     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
       1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 4     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
       1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 5     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
       1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 6     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
       1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 7     3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  2  2  2  2  2  2  2  3  3  2  2  3  3  2  2  3  3 12
      12 12  3 12 12  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3
 8     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  2  2  2  2  2  2  2 13 13  2  2 13 13  2  2 13 13 12
      12 12  9 12 12  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 9     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  2  2  2  2  2  2  2 13 13  2  2 13 13  2  2 13 13 12
      12 12  9 12 12  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
10     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  6  6  6  6  6  6  6 14 14  7  7 14 14  7  7 14 14  8
       8  8  9  8  8  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
11     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  6  6  6  6  6  6  6 14 14  7  7 14 14  7  7 14 14  8
       8  8  9  8  8  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
12     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  6  6  6  6  6  6  6 14 14  7  7 14 14  7  7 14 14  8
       8  8  9  8  8  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
13     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  2  2  2  2  2  2  2 13 13  2  2 13 13  2  2 13 13 12
      12 12  9 12 12  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
14     4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  2  2  2  2  2  2  2  4  4  2  2  4  4  2  2  4  4 12
      12 12  4 12 12  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4
15     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  2  2  2  2  2  2  2 13 13  2  2 13 13  2  2 13 13 12
      12 12  9 12 12  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
16     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  2  2  2  2  2  2  2 13 13  2  2 13 13  2  2 13 13 12
      12 12  9 12 12  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
17     5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5
       5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5
18     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
       1  1  9  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
19     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
       1  1  9  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
20     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
       1  1  9  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
21     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
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```
       1  1  9  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
22     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
       1  1  9  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
23     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
       1  1  9  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
24     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
       1  1  9  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
25    10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10
      10 10  9 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10
26    10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10
      10 10  9 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10
27    10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10
      10 10  9 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10
28    10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10
      10 10  9 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10
29    10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10
      10 10  9 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10
30    10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10
      10 10  9 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10
31    10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10
      10 10  9 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10
32    10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10
      10 10  9 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10
33    10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10
      10 10  9 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10
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      11 11 11 11 11 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10
 2    10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10
      10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10
 3     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
       1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
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       1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
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       1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 6     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
       1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 7     3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3 22 22 22 22 22 22 22 22 22 22 22  3  3 22 22  3  3 37
      37 37  3 37 37  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3
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      37 37 33 37 37  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
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      37 37 33 37 37  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
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      15 15 33 16 16  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
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      15 15 33 16 16  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
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```

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      15 15 33 16 16  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
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      37 37 33 37 37  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 14    4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4 22 22 22 22 22 22 22 22 22 22 22  4  4 22 22  4  4 37
      37 37  4 37 37  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4
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      37 37 35 37 37  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 16    1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 22 22 22 22 22 22 22 22 22 22 22 23 23 22 22 23 23 37
      37 37 35 37 37  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
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      1  1 35  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
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      1  1 35  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
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      1  1 35  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
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      1  1 35  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 25   29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29
      29 29 34 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29
 26   17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17
      17 17 34 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17
 27   30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30
      30 30 34 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30
 28   18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18
      18 18 34 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18
 29   31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31
      31 31 34 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31
 30   19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19
      19 19 34 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19
 31   19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19
      19 19 34 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19
 32   20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20
      20 20 34 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20
 33   20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20
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 2    10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10
      10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10
 3     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
```

```
      1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
  4   1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
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  7   3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3 22 22 22 22 22 22 22 22 22 22 22  3  3 22 22  3  3 37
     37 37  3 37 37  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3
  8   1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 22 22 22 22 22 22 23 23 22 22 23 23 37
     37 37 33 37 37  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
  9   1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 22 22 22 22 22 22 22 22 22 22 22 23 23 22 22 23 23 37
     37 37 33 37 37  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
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     15 15 33 16 16  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 11   1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 21 21 21 21 21 21 21 41 41 32 32 38 38 32 32 38 38 15
     15 15 33 16 16  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
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     15 15 33 16 16  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 13   1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 22 22 22 22 22 22 22 22 22 22 22 23 23 22 22 23 23 37
     37 37 33 37 37  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
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     37 37  4 37 37  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4
 15   1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 22 22 22 22 22 22 22 22 22 22 22 23 23 22 22 23 23 37
     37 37 35 37 37  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 16   1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 22 22 22 22 22 22 22 22 22 22 22 23 23 22 22 23 23 37
     37 37 35 37 37  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
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      5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5
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      1  1 35  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
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      1  1 35  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
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      1  1 35  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
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      1  1 35  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 22   1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
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      1  1 35  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
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 25  29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29
     29 29 34 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29
 26  17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17
     17 17 34 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17
 27  30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30
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       19 19 34 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19
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       19 19 34 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19
 32    20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20
       20 20 34 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20
 33    20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20
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       11 11 11 11 11 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10
 2     10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10
       10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10
 3      1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
        1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
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        1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 5      1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
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       37 37  3 37 37  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3
 8      1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
       37 37 33 37 37  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 9      1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
       37 37 33 37 37  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
10     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
       15 15 33 16 16  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
11     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
       15 15 33 16 16  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
12     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
       15 15 33 16 16  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
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       37 37 33 37 37  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
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       37 37 36 37 37  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
16     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
       37 37 36 37 37  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
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       1  1 36  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
19     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
       1  1 36  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
```

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20     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
       1  1 36  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
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       1  1 36  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
22     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
       1  1 36  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
23     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
       1  1 36  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
24     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
       1  1 36  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
25    29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29
      29 29 34 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29
26    17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17
      17 17 34 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17
27    30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30
      30 30 34 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30
28    18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18
      18 18 34 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18
29    31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31
      31 31 34 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31
30    19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19
      19 19 34 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19
31    19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19
      19 19 34 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19
32    20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20
      20 20 34 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20
33    20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20
      20 20 34 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20
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      11 11 11 11 11 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10
 2    10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 26 10 10 10 10 10 10 10 10 10 10 10 10 10
      10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10
 3     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 26  1  1  1  1  1  1  1  1  1  1  1  1  1  1
       1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 4     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 26  1  1  1  1  1  1  1  1  1  1  1  1  1
       1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 5     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 26  1  1  1  1  1  1  1  1  1  1  1  1  1
       1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 6     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 26  1  1  1  1  1  1  1  1  1  1  1  1
       1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 7     3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3 22 22 22 26 22 22 22 22 22 22 22  3  3 22 22  3  3 37
      37 37  3 37 37  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3
 8     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 22 22 22 26 22 22 22 22 22 22 22 40 40 22 22 40 40 37
      37 37 33 37 37  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 9     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 22 22 22 26 22 22 22 22 22 22 22 40 40 22 22 40 40 37
      37 37 33 37 37  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
10     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 21 21 21 26 21 21 21 41 41 32 32 39 39 32 32 39 39 15
      15 15 33 16 16  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
```

```
11     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 21 21 21 26 21 21 21 41 41 32 32 39 39 32 32 39 39 15
      15 15 33 16 16  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
12     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 21 21 21 26 21 21 21 41 41 32 32 39 39 32 32 39 39 15
      15 15 33 16 16  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
13     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 22 22 22 26 22 22 22 22 22 22 22 22 40 40 22 22 40 40 37
      37 37 33 37 37  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
14     4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4 22 22 22 26 22 22 22 22 22 22 22 22  4  4 22 22  4  4 37
      37 37  4 37 37  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4
15     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 22 22 22 26 22 22 22 22 22 22 22 22 40 40 22 22 40 40 37
      37 37 36 37 37  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
16     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 22 22 22 26 22 22 22 22 22 22 22 22 40 40 22 22 40 40 37
      37 37 36 37 37  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
17     5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5 26  5  5  5  5  5  5  5  5  5  5  5  5  5
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18     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 26  1  1  1  1  1  1  1  1  1  1  1  1  1
       1  1 36  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
19     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 26  1  1  1  1  1  1  1  1  1  1  1  1  1
       1  1 36  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
20     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 26  1  1  1  1  1  1  1  1  1  1  1  1  1
       1  1 36  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
21     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 26  1  1  1  1  1  1  1  1  1  1  1  1  1
       1  1 36  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
22     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 26  1  1  1  1  1  1  1  1  1  1  1  1  1
       1  1 36  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
23     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 26  1  1  1  1  1  1  1  1  1  1  1  1  1
       1  1 36  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
24     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 26  1  1  1  1  1  1  1  1  1  1  1  1  1
       1  1 36  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
25    29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 25 29 29 29 29 29 29 29 29 29 29 29 29 29
      29 29 34 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29
26    17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 26 17 17 17 17 17 17 17 17 17 17 17 17 17
      17 17 34 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17
27    30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 26 30 30 30 30 30 30 30 30 30 30 30 30 30
      30 30 34 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30
28    18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 26 18 18 18 18 18 18 18 18 18 18 18 18 18
      18 18 34 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18
29    31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 26 31 31 31 31 31 31 31 31 31 31 31 31 31
      31 31 34 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31
30    19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 26 19 19 19 19 19 19 19 19 19 19 19 19 19
      19 19 34 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19
31    19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 26 19 19 19 19 19 19 19 19 19 19 19 19 19
      19 19 34 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19
32    20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 25 20 20 20 20 20 20 20 20 20 20 20 20 20
      20 20 34 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20
33    20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 25 20 20 20 20 20 20 20 20 20 20 20 20 20
      20 20 34 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20
```

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    Layer    1
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      11 11 11 11 11 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10
```

```
 2   10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 27 10 10 10 10 10 10 10 10 10 10 10 10 10
     10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10
 3    1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 27  1  1  1  1  1  1  1  1  1  1  1  1
      1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 4    1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 27  1  1  1  1  1  1  1  1  1  1  1  1
      1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 5    1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 27  1  1  1  1  1  1  1  1  1  1  1  1
      1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 6    1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 27  1  1  1  1  1  1  1  1  1  1  1  1
      1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 7    3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3 22 22 22 27 22 22 22 22 22 22 22  3  3 22 22  3  3 37
     37 37  3 37 37  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3
 8    1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 22 22 22 27 22 22 22 22 22 22 22 22 40 40 22 22 40 40 37
     37 37 33 37 37  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 9    1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 22 22 22 27 22 22 22 22 22 22 22 22 40 40 22 22 40 40 37
     37 37 33 37 37  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
10    1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 21 21 21 27 21 21 21 41 41 32 32 39 39 32 32 39 39 15
     15 15 33 16 16  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
11    1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 21 21 21 27 21 21 21 41 41 32 32 39 39 32 32 39 39 15
     15 15 33 16 16  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
12    1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 21 21 21 27 21 21 21 41 41 32 32 39 39 32 32 39 39 15
     15 15 33 16 16  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
13    1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 22 22 22 27 22 22 22 22 22 22 22 22 40 40 22 22 40 40 37
     37 37 33 37 37  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
14    4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4 22 22 22 27 22 22 22 22 22 22 22  4  4 22 22  4  4 37
     37 37  4 37 37  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4
15    1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 22 22 22 27 22 22 22 22 22 22 22 22 40 40 22 22 40 40 37
     37 37 36 37 37  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
16    1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 22 22 22 27 22 22 22 22 22 22 22 22 40 40 22 22 40 40 37
     37 37 36 37 37  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
17    5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5 27  5  5  5  5  5  5  5  5  5  5  5  5
      5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5
18    1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 27  1  1  1  1  1  1  1  1  1  1  1  1
      1  1 36  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
19    1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 27  1  1  1  1  1  1  1  1  1  1  1  1
      1  1 36  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
20    1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 27  1  1  1  1  1  1  1  1  1  1  1  1
      1  1 36  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
21    1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 27  1  1  1  1  1  1  1  1  1  1  1  1
      1  1 36  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
22    1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 27  1  1  1  1  1  1  1  1  1  1  1  1
      1  1 36  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
23    1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 27  1  1  1  1  1  1  1  1  1  1  1  1
      1  1 36  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
24    1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 27  1  1  1  1  1  1  1  1  1  1  1  1
      1  1 36  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
25   29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 27 29 29 29 29 29 29 29 29 29 29 29 29 29
     29 29 34 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29
26   17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 27 17 17 17 17 17 17 17 17 17 17 17 17 17
     17 17 34 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17
27   30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 27 30 30 30 30 30 30 30 30 30 30 30 30 30
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      30 30 34 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30
 28   18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 27 18 18 18 18 18 18 18 18 18 18 18 18
      18 18 34 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18
 29   31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 27 31 31 31 31 31 31 31 31 31 31 31 31
      31 31 34 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31
 30   19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 27 19 19 19 19 19 19 19 19 19 19 19 19
      19 19 34 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19
 31   19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 27 19 19 19 19 19 19 19 19 19 19 19 19
      19 19 34 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19
 32   20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 27 20 20 20 20 20 20 20 20 20 20 20 20
      20 20 34 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20
 33   20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 27 20 20 20 20 20 20 20 20 20 20 20 20
      20 20 34 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20
 ------------------------------------------------------------------------------------------------------------------------------------------------------
 Material time number =  7          Starting at time = 4.891300E+10 s
     Layer    1
 1    10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 11 11 11 28 11 11 11 11 11 11 11 11 11 11 11 11 11
      11 11 11 11 11 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10
 2    10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 28 10 10 10 10 10 10 10 10 10 10 10 10
      10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10
 3     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 28  1  1  1  1  1  1  1  1  1  1  1  1
       1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 4     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 28  1  1  1  1  1  1  1  1  1  1  1  1
       1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 5     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 28  1  1  1  1  1  1  1  1  1  1  1  1
       1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 6     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 28  1  1  1  1  1  1  1  1  1  1  1  1
       1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 7     3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3 22 22 22 28 22 22 22 22 22 22 22  3  3 22 22  3  3 37
      37 37  3 37 37  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3  3
 8     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 22 22 22 28 22 22 22 22 22 22 22 40 40 22 22 40 40 37
      37 37 33 37 37  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
 9     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 22 22 22 28 22 22 22 22 22 40 40 22 22 40 40 37
      37 37 33 37 37  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
10     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 21 21 21 27 21 21 21 41 41 32 32 39 39 32 32 39 39 15
      15 15 33 16 16  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
11     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 21 21 21 27 21 21 21 41 41 32 32 39 39 32 32 39 39 15
      15 15 33 16 16  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
12     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 21 21 21 27 21 21 21 41 41 32 32 39 39 32 32 39 39 15
      15 15 33 16 16  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
13     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 22 22 22 27 22 22 22 22 22 22 22 40 40 22 22 40 40 37
      37 37 33 37 37  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
14     4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4 22 22 22 27 22 22 22 22 22 22 22  4  4 22 22  4  4 37
      37 37  4 37 37  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4  4
15     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 22 22 22 27 22 22 22 22 22 40 40 22 22 40 40 37
      37 37 36 37 37  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
16     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 22 22 22 27 22 22 22 22 22 22 22 40 40 22 22 40 40 37
      37 37 36 37 37  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
17     5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5 27  5  5  5  5  5  5  5  5  5  5  5  5
       5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5  5
18     1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 27  1  1  1  1  1  1  1  1  1  1  1  1
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      1  1 36  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
19    1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 27  1  1  1  1  1  1  1  1  1  1  1  1
      1  1 36  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
20    1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 27  1  1  1  1  1  1  1  1  1  1  1  1
      1  1 36  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
21    1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 27  1  1  1  1  1  1  1  1  1  1  1  1
      1  1 36  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
22    1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 27  1  1  1  1  1  1  1  1  1  1  1  1
      1  1 36  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
23    1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 27  1  1  1  1  1  1  1  1  1  1  1  1
      1  1 36  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
24    1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1 27  1  1  1  1  1  1  1  1  1  1  1  1
      1  1 36  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1  1
25   29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 27 29 29 29 29 29 29 29 29 29 29 29 29
     29 29 34 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29 29
26   17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 27 17 17 17 17 17 17 17 17 17 17 17 17
     17 17 34 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17 17
27   30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 27 30 30 30 30 30 30 30 30 30 30 30 30
     30 30 34 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30 30
28   18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 27 18 18 18 18 18 18 18 18 18 18 18 18
     18 18 34 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18 18
29   31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 27 31 31 31 31 31 31 31 31 31 31 31 31
     31 31 34 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31 31
30   19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 27 19 19 19 19 19 19 19 19 19 19 19 19
     19 19 34 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19
31   19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 27 19 19 19 19 19 19 19 19 19 19 19 19
     19 19 34 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19 19
32   20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 27 20 20 20 20 20 20 20 20 20 20 20 20
     20 20 34 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20
33   20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 27 20 20 20 20 20 20 20 20 20 20 20 20
     20 20 34 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20 20

 Material type number and name of material:
      1     S_HALITE
      2     DRZ_0
      3     S_MB139
      4     S_ANH_AB
      5     S_MB138
      6     CAVITY_1
      7     CAVITY_2
      8     CAVITY_3
      9     CAVITY_4
     10     IMPERM_Z
     11     CASTILER
     12     DRZ_OE_0
     13     DRZ_PC_0
     14     CAVITY_5
     15     OPS_AREA
     16     EXP_AREA
     17     CULEBRA
     18     MAGENTA
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      19     DEWYLAKE
      20     SANTAROS
      21     WAS_AREA
      22     DRZ_1
      23     DRZ_PC_1
      24     PCS_T1
      25     CONC_PLG
      26     BH_OPEN
      27     BH_SAND
      28     BH_CREEP
      29     UNNAMED
      30     TAMARISK
      31     FORTYNIN
      32     REPOSIT
      33     CONC_MON
      34     SHFTU
      35     SHFTL_T1
      36     SHFTL_T2
      37     DRZ_OE_1
      38     PCS_T2
      39     PCS_T3
      40     DRZ_PCS
      41     PCS_NO

  Special material index numbers:
      Number of waste regions              (NWST) =  2
      Initial waste matl index nos. (MAT_WASTEI) =  6  7

      Final waste matl index numbers (MAT_WASTE) = 21 32

      Number of MAT_DRZ regions            (NDRZ) =  0
      Material type index for DRZ before
          IC's are reset                (MAT_DRZ) =

      Material type index for DRZ after
          IC's are reset             (MAT_DRZNEW) =

      Number of material regions
          where IC's will be reset    (NMATRESET) =  5
      Material type indexes of material regions
          where IC's will be reset     (MATRESET) =  6  7  8  9 14

      Borehole matl index number (MAT_BOREHOLE)   =  0

  Initial Conditions reset parameters:
      Time when IC's are reset          (TIMEICRESET) =  0.00000E+00 s
      Startup Initial Conditions will be used
          instead of Input IC's for the Cavities
          [0=No, 1=Yes]                      (ICWASTE) =  1

          Uniform Cavity Region  1 Startup Pressure   (POWASTEIC) =  1.01325E+05 Pa
```

```
        Uniform Cavity Region  2 Startup Pressure    (POWASTEIC) =  1.01325E+05 Pa
        Uniform Cavity Region  3 Startup Pressure    (POWASTEIC) =  1.01325E+05 Pa
        Uniform Cavity Region  4 Startup Pressure    (POWASTEIC) =  1.01325E+05 Pa
        Uniform Cavity Region  5 Startup Pressure    (POWASTEIC) =  1.01325E+05 Pa
        Uniform Cavity Region  1 Startup Brine Satn (SOWASTEIC) =  0.00000E+00
        Uniform Cavity Region  2 Startup Brine Satn (SOWASTEIC) =  0.00000E+00
        Uniform Cavity Region  3 Startup Brine Satn (SOWASTEIC) =  0.00000E+00
        Uniform Cavity Region  4 Startup Brine Satn (SOWASTEIC) =  0.00000E+00
        Uniform Cavity Region  5 Startup Brine Satn (SOWASTEIC) =  0.00000E+00

Borehole Conditions reset #  1
        Reset Time  (TIMEBORE) =  1.10450E+10 s
        Material #  1(MATBORE) = 26
        Material #  2(MATBORE) = 25
        Pressure is not reset
        Brine Satn is not reset
        Chemistry      (ICHEM) =  1

-------------------------------------------------------------------------------------------------------------------------------
Material properties:
    XLAMDA     = Brooks-Corey parameter "lambda,"
                 for calculating relative permeability
    SBR        = Residual brine saturation
    SGR        = Residual gas saturation
    XKX        = X-direction permeability, m^2
    YKY        = Y-direction permeability, m^2
    ZKZ        = Z-direction permeability, m^2
    PORROCKMAT = Rock porosity
    CROCK      = Rock compressibility, 1/Pa
    SBMIN      = Min brine satn at which Pc will be
                 computed using char curve params
    POMIN      = Min brine pressure used to adjust cap
                 pressure when variable model used, Pa
    PCMAX      = Max Pc that can be used, Pa
    PCTA       = Constant in threshold cap press (PCT) correlation, Pa
    PCTEXP     = Exponent in PCT correlation:
                    PCT = PCTA*PERMBX**PCTEXP
    KRP        = Relative permeability model number
    KPC        = Capillary pressure model number
    KPT        = Threshold capillary pressure (PCT) flag:
                 0 = PCT constant
                 1 = PCT function of dynamic permeability
-------------------------------------------------------------------------------------------------------------------------------

I  XLAMDA     SBR      SGR      XKX      YKY      ZKZ   PORREFROCK CROCK    SBMIN    POMIN    PCMAX     PCTA     PCTEXP   KRP KPC KPT
-------------------------------------------------------------------------------------------------------------------------------
1 7.00E-01 3.00E-01 2.00E-01 1.80E-23 1.80E-23 1.80E-23 4.48E-03 2.58E-08 3.15E-01 1.01E+05 1.00E+08 5.60E-01-3.46E-01   4   2   0
2 7.00E-01 0.00E+00 0.00E+00 1.00E-17 1.00E-17 1.00E-17 7.38E-03 1.00E-07 0.00E+00 1.01E+05 1.00E+08 0.00E+00 0.00E+00   4   1   0
3 6.88E-01 7.30E-02 5.49E-02 1.05E-19 1.05E-19 1.05E-19 1.10E-02 2.03E-09 7.66E-02 1.01E+05 1.00E+08 2.60E-01-3.48E-01   4   2   0
4 6.88E-01 7.30E-02 5.49E-02 1.05E-19 1.05E-19 1.05E-19 1.10E-02 2.03E-09 7.66E-02 1.01E+05 1.00E+08 2.60E-01-3.48E-01   4   2   0
5 6.88E-01 7.30E-02 5.49E-02 1.05E-19 1.05E-19 1.05E-19 1.10E-02 2.03E-09 7.66E-02 1.01E+05 1.00E+08 2.60E-01-3.48E-01   4   2   0
```

```
  6 7.00E-01 0.00E+00 0.00E+00 1.00E-10 1.00E-10 1.00E-10 1.00E+00 0.00E+00 0.00E+00 1.01E+05 1.00E+08 0.00E+00 0.00E+00  11   1   0
  7 7.00E-01 0.00E+00 0.00E+00 1.00E-10 1.00E-10 1.00E-10 1.00E+00 0.00E+00 0.00E+00 1.01E+05 1.00E+08 0.00E+00 0.00E+00  11   1   0
  8 7.00E-01 0.00E+00 0.00E+00 1.00E-10 1.00E-10 1.00E-10 1.00E+00 0.00E+00 0.00E+00 1.01E+05 1.00E+08 0.00E+00 0.00E+00  11   1   0
  9 7.00E-01 0.00E+00 0.00E+00 1.00E-10 1.00E-10 1.00E-10 1.00E+00 0.00E+00 0.00E+00 1.01E+05 1.00E+08 0.00E+00 0.00E+00  11   1   0
 10 7.00E-01 0.00E+00 0.00E+00 1.00E-35 1.00E-35 1.00E-35 5.00E-03 0.00E+00 0.00E+00 1.01E+05 1.00E+08 0.00E+00 0.00E+00   4   1   0
 11 7.00E-01 2.00E-01 2.00E-01 2.77E-12 2.77E-12 2.77E-12 4.27E-01 5.33E-09 2.10E-01 1.01E+05 1.00E+08 5.60E-01-3.46E-01   4   2   0
 12 7.00E-01 0.00E+00 0.00E+00 1.00E-17 1.00E-17 1.00E-17 7.38E-03 1.00E-07 0.00E+00 1.01E+05 1.00E+08 0.00E+00 0.00E+00   4   1   0
 13 7.00E-01 0.00E+00 0.00E+00 1.00E-17 1.00E-17 1.00E-17 7.38E-03 1.00E-07 0.00E+00 1.01E+05 1.00E+08 0.00E+00 0.00E+00   4   1   0
 14 7.00E-01 0.00E+00 0.00E+00 1.00E-10 1.00E-10 1.00E-10 1.00E+00 0.00E+00 0.00E+00 1.01E+05 1.00E+08 0.00E+00 0.00E+00  11   1   0
 15 7.00E-01 0.00E+00 0.00E+00 1.00E-11 1.00E-11 1.00E-11 1.80E-01 0.00E+00 0.00E+00 1.01E+05 1.00E+08 0.00E+00 0.00E+00  11   1   0
 16 7.00E-01 0.00E+00 0.00E+00 1.00E-11 1.00E-11 1.00E-11 1.80E-01 0.00E+00 0.00E+00 1.01E+05 1.00E+08 0.00E+00 0.00E+00  11   1   0
 17 6.44E-01 8.36E-02 7.71E-02 9.59E-15 9.59E-15 9.59E-15 1.51E-01 6.62E-10 8.78E-02 1.01E+05 1.00E+08 2.60E-01-3.48E-01   4   2   0
 18 6.44E-01 8.36E-02 7.71E-02 2.10E-15 2.10E-15 2.10E-15 1.38E-01 1.92E-09 8.78E-02 1.01E+05 1.00E+08 2.60E-01-3.48E-01   4   2   0
 19 6.44E-01 8.36E-02 7.71E-02 5.01E-17 5.01E-17 5.01E-17 1.43E-01 6.99E-08 8.78E-02 1.01E+05 1.00E+08 0.00E+00 0.00E+00   4   1   0
 20 6.44E-01 8.36E-02 7.71E-02 1.00E-10 1.00E-10 1.00E-10 1.75E-01 5.71E-08 8.78E-02 1.01E+05 1.00E+08 0.00E+00 0.00E+00   4   1   0
 21 2.89E+00 1.78E-01 1.65E-02 2.40E-13 2.40E-13 2.40E-13 8.48E-01 0.00E+00 1.86E-01 1.01E+05 1.00E+08 0.00E+00 0.00E+00  12   1   0
 22 7.00E-01 0.00E+00 0.00E+00 1.33E-18 1.33E-18 1.33E-18 7.38E-03 1.00E-07 0.00E+00 1.01E+05 1.00E+08 0.00E+00 0.00E+00   4   1   0
 23 7.00E-01 0.00E+00 0.00E+00 1.33E-18 1.33E-18 1.33E-18 7.38E-03 1.00E-07 0.00E+00 1.01E+05 1.00E+08 0.00E+00 0.00E+00   4   1   0
 24 8.72E-01 5.66E-01 2.23E-01 5.58E-18 5.58E-18 5.58E-18 1.34E-01 5.98E-10 5.95E-01 1.01E+05 1.00E+08 0.00E+00 0.00E+00   4   1   0
 25 9.40E-01 0.00E+00 0.00E+00 1.58E-18 1.58E-18 1.58E-18 3.20E-01 1.19E-09 0.00E+00 1.01E+05 1.00E+08 0.00E+00 0.00E+00   4   1   0
 26 7.00E-01 0.00E+00 0.00E+00 1.00E-09 1.00E-09 1.00E-09 3.20E-01 0.00E+00 0.00E+00 1.01E+05 1.00E+08 0.00E+00 0.00E+00  11   1   0
 27 9.40E-01 0.00E+00 0.00E+00 7.29E-14 7.29E-14 7.29E-14 3.20E-01 0.00E+00 0.00E+00 1.01E+05 1.00E+08 0.00E+00 0.00E+00   4   1   0
 28 9.40E-01 0.00E+00 0.00E+00 7.29E-15 7.29E-15 7.29E-15 3.20E-01 0.00E+00 0.00E+00 1.01E+05 1.00E+08 0.00E+00 0.00E+00   4   1   0
 29 7.00E-01 2.00E-01 2.00E-01 1.00E-35 1.00E-35 1.00E-35 1.81E-01 0.00E+00 2.10E-01 1.01E+05 1.00E+08 0.00E+00 0.00E+00   4   1   0
 30 7.00E-01 2.00E-01 2.00E-01 1.00E-35 1.00E-35 1.00E-35 6.40E-02 0.00E+00 2.10E-01 1.01E+05 1.00E+08 0.00E+00 0.00E+00   4   1   0
 31 7.00E-01 2.00E-01 2.00E-01 1.00E-35 1.00E-35 1.00E-35 8.20E-02 0.00E+00 2.10E-01 1.01E+05 1.00E+08 0.00E+00 0.00E+00   4   1   0
 32 2.89E+00 1.78E-01 1.65E-02 2.40E-13 2.40E-13 2.40E-13 8.48E-01 0.00E+00 1.86E-01 1.01E+05 1.00E+08 0.00E+00 0.00E+00  12   1   0
 33 9.40E-01 1.28E-01 1.22E-01 1.00E-14 1.00E-14 1.00E-14 5.00E-02 1.20E-09 1.34E-01 1.01E+05 1.00E+08 0.00E+00 0.00E+00   4   1   0
 34 9.40E-01 1.28E-01 1.22E-01 4.30E-19 4.30E-19 4.30E-19 2.91E-01 2.05E-08 1.34E-01 1.01E+05 1.00E+08 0.00E+00 0.00E+00   4   1   0
 35 9.40E-01 1.28E-01 1.22E-01 1.56E-19 1.56E-19 1.56E-19 1.13E-01 4.28E-09 1.34E-01 1.01E+05 1.00E+08 0.00E+00 0.00E+00   4   1   0
 36 9.40E-01 1.28E-01 1.22E-01 2.24E-20 2.24E-20 2.24E-20 1.13E-01 4.28E-09 1.34E-01 1.01E+05 1.00E+08 0.00E+00 0.00E+00   4   1   0
 37 7.00E-01 0.00E+00 0.00E+00 1.33E-18 1.33E-18 1.33E-18 7.38E-03 1.00E-07 0.00E+00 1.01E+05 1.00E+08 0.00E+00 0.00E+00   4   1   0
 38 8.72E-01 5.66E-01 2.23E-01 3.55E-21 3.55E-21 3.55E-21 3.09E-02 2.59E-09 5.95E-01 1.01E+05 1.00E+08 0.00E+00 0.00E+00   4   1   0
 39 8.72E-01 5.66E-01 2.23E-01 2.47E-21 2.47E-21 2.47E-21 2.35E-02 3.41E-09 5.95E-01 1.01E+05 1.00E+08 0.00E+00 0.00E+00   4   1   0
 40 7.00E-01 0.00E+00 0.00E+00 1.66E-20 1.66E-20 1.66E-20 7.38E-03 1.00E-07 0.00E+00 1.01E+05 1.00E+08 0.00E+00 0.00E+00   4   1   0
 41 7.00E-01 0.00E+00 0.00E+00 1.00E-11 1.00E-11 1.00E-11 1.80E-01 0.00E+00 0.00E+00 1.01E+05 1.00E+08 0.00E+00 0.00E+00  11   1   0
TOL       =    1.0000E-02
SOCEFFMIN =    1.0000E-03

 Fracture model will be used?  (KFRACTURE): T

 Fracture model parameters:
     Index for material in which fracturing occurs (IFRCMAT) =   3
     Fracture initiation pressure increment        (FRPIINC) = 2.00000E+05 Pa
     Fully-developed fracture pressure increment   (FRPFINC) = 3.80000E+06 Pa
     Maximum fracture porosity                    (FRPHIMAX) = 5.00000E-02
     Fracture permeability function exponent      (FRPRMEXP) = 1.51805E+01
     Flag to calc x-direction perm as fractured       (IFRX) =   1  (yes)
     Flag to calc y-direction perm as fractured       (IFRY) =   1  (yes)
     Flag to calc z-direction perm as fractured       (IFRZ) =   0  (no)
     Flag to hold pressure constant during fracturing       (LFPC) =(no)
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Fracture model parameters:
    Index for material in which fracturing occurs (IFRCMAT) =   4
    Fracture initiation pressure increment        (FRPIINC) = 2.00000E+05 Pa
    Fully-developed fracture pressure increment   (FRPFINC) = 3.80000E+06 Pa
    Maximum fracture porosity                    (FRPHIMAX) = 2.50000E-01
    Fracture permeability function exponent      (FRPRMEXP) = 7.35761E+00
    Flag to calc x-direction perm as fractured       (IFRX) =   1  (yes)
    Flag to calc y-direction perm as fractured       (IFRY) =   1  (yes)
    Flag to calc z-direction perm as fractured       (IFRZ) =   0  (no)
    Flag to hold pressure constant during fracturing       (LFPC) =(no)

Fracture model parameters:
    Index for material in which fracturing occurs (IFRCMAT) =   5
    Fracture initiation pressure increment        (FRPIINC) = 2.00000E+05 Pa
    Fully-developed fracture pressure increment   (FRPFINC) = 3.80000E+06 Pa
    Maximum fracture porosity                    (FRPHIMAX) = 5.00000E-02
    Fracture permeability function exponent      (FRPRMEXP) = 1.51805E+01
    Flag to calc x-direction perm as fractured       (IFRX) =   1  (yes)
    Flag to calc y-direction perm as fractured       (IFRY) =   1  (yes)
    Flag to calc z-direction perm as fractured       (IFRZ) =   0  (no)
    Flag to hold pressure constant during fracturing       (LFPC) =(no)

Fracture model parameters:
    Index for material in which fracturing occurs (IFRCMAT) =   2
    Fracture initiation pressure increment        (FRPIINC) = 2.00000E+05 Pa
    Fully-developed fracture pressure increment   (FRPFINC) = 3.80000E+06 Pa
    Maximum fracture porosity                    (FRPHIMAX) = 4.63824E-02
    Fracture permeability function exponent      (FRPRMEXP) = 1.01338E+01
    Flag to calc x-direction perm as fractured       (IFRX) =   1  (yes)
    Flag to calc y-direction perm as fractured       (IFRY) =   1  (yes)
    Flag to calc z-direction perm as fractured       (IFRZ) =   0  (no)
    Flag to hold pressure constant during fracturing       (LFPC) =(no)

Fracture model parameters:
    Index for material in which fracturing occurs (IFRCMAT) =  22
    Fracture initiation pressure increment        (FRPIINC) = 2.00000E+05 Pa
    Fully-developed fracture pressure increment   (FRPFINC) = 3.80000E+06 Pa
    Maximum fracture porosity                    (FRPHIMAX) = 4.63824E-02
    Fracture permeability function exponent      (FRPRMEXP) = 1.12420E+01
    Flag to calc x-direction perm as fractured       (IFRX) =   1  (yes)
    Flag to calc y-direction perm as fractured       (IFRY) =   1  (yes)
    Flag to calc z-direction perm as fractured       (IFRZ) =   0  (no)
    Flag to hold pressure constant during fracturing       (LFPC) =(no)

Fracture model parameters:
    Index for material in which fracturing occurs (IFRCMAT) =  12
    Fracture initiation pressure increment        (FRPIINC) = 2.00000E+05 Pa
    Fully-developed fracture pressure increment   (FRPFINC) = 3.80000E+06 Pa
    Maximum fracture porosity                    (FRPHIMAX) = 4.63824E-02
    Fracture permeability function exponent      (FRPRMEXP) = 1.01338E+01
```

```
    Flag to calc x-direction perm as fractured       (IFRX) =   1  (yes)
    Flag to calc y-direction perm as fractured       (IFRY) =   1  (yes)
    Flag to calc z-direction perm as fractured       (IFRZ) =   0  (no)
    Flag to hold pressure constant during fracturing       (LFPC) =(no)

Fracture model parameters:
    Index for material in which fracturing occurs (IFRCMAT) =  37
    Fracture initiation pressure increment        (FRPIINC) = 2.00000E+05 Pa
    Fully-developed fracture pressure increment   (FRPFINC) = 3.80000E+06 Pa
    Maximum fracture porosity                     (FRPHIMAX) = 4.63824E-02
    Fracture permeability function exponent       (FRPRMEXP) = 1.12420E+01
    Flag to calc x-direction perm as fractured       (IFRX) =   1  (yes)
    Flag to calc y-direction perm as fractured       (IFRY) =   1  (yes)
    Flag to calc z-direction perm as fractured       (IFRZ) =   0  (no)
    Flag to hold pressure constant during fracturing       (LFPC) =(no)

Fracture model parameters:
    Index for material in which fracturing occurs (IFRCMAT) =  13
    Fracture initiation pressure increment        (FRPIINC) = 2.00000E+05 Pa
    Fully-developed fracture pressure increment   (FRPFINC) = 3.80000E+06 Pa
    Maximum fracture porosity                     (FRPHIMAX) = 4.63824E-02
    Fracture permeability function exponent       (FRPRMEXP) = 1.01338E+01
    Flag to calc x-direction perm as fractured       (IFRX) =   1  (yes)
    Flag to calc y-direction perm as fractured       (IFRY) =   1  (yes)
    Flag to calc z-direction perm as fractured       (IFRZ) =   0  (no)
    Flag to hold pressure constant during fracturing       (LFPC) =(no)

Fracture model parameters:
    Index for material in which fracturing occurs (IFRCMAT) =  23
    Fracture initiation pressure increment        (FRPIINC) = 2.00000E+05 Pa
    Fully-developed fracture pressure increment   (FRPFINC) = 3.80000E+06 Pa
    Maximum fracture porosity                     (FRPHIMAX) = 4.63824E-02
    Fracture permeability function exponent       (FRPRMEXP) = 1.12420E+01
    Flag to calc x-direction perm as fractured       (IFRX) =   1  (yes)
    Flag to calc y-direction perm as fractured       (IFRY) =   1  (yes)
    Flag to calc z-direction perm as fractured       (IFRZ) =   0  (no)
    Flag to hold pressure constant during fracturing       (LFPC) =(no)

Klinkenberg effect will be included?  (KLINK): T

Klinkenberg equation parameters:
     Linear factor    (BKLINK) = 2.71000E-01 Pa
     Exponent       (EXPKLINK) =-3.41000E-01


Constants           :
    Gravity constant        (GSTD) = 9.80665E+00 m/s^2
    Gas constant            (R   ) = 8.31451E+00 J/(mol*K)


Reference conditions:
```

```
     Reference temperature  (TREF) = 3.00150E+02 K
     Reference pressure     (PREF) = 1.01325E+05 Pa

  Brine salinity                              (SALT) = 3.2400E+01 wt %
  Brine density at ref. conditions           (DENOSC) = 1.2200E+03 kg/m^3
  Gas-free (=0) or gas-sat'd brine (=1)       (KGSAT) = 1
  Dissolved gas (=1) or no dissolved gas (=0) (IDGAS) = 0
  Brine compressibility                      (BRCOMP) = 3.1000E-10 1/Pa
  Salt Molecular Weight                      (WMSALT) = 5.8442E-02 kg/mol
  Water Molecular Weight                     (WMSALT) = 1.8015E-02 kg/mol

  Brine viscosity  (VISO) =  2.1000E-03 Pa*s
  Gas viscosity    (VISG) =  8.9339E-06 Pa*s

  Flag for calculating gas density (INTERPDENG):
     INTERPDENG = 1:  Interpolate from table with RKS EOS.

  Gas parameters:
     Gas mole fraction  (YGAS)
         H2:    1.000E+00      CO2:   0.000E+00
         CH4:   0.000E+00      N2:    0.000E+00
         H2S:   0.000E+00      O2:    0.000E+00
     Gas component molecular weights (WMGAS) kg/mol
         H2:    2.016E-03      CO2:   4.401E-02
         CH4:   1.604E-02      N2:    2.801E-02
         H2S:   3.408E-02      O2:    3.200E-02
     Number of gases actually used    (NGAS) = 1
     Gas number used if NGAS=1;
         (1=H2, 2=CO2, 3=CH4, 4=N2
          5=H2S, 6=O2)               (NGAS1) = 1

  Additional RKS EOS Gas parameters:
     Gas component Critical Temperatures  (TC) K
         H2:    4.360E+01      CO2:   3.041E+02
         CH4:   1.906E+02      N2:    1.262E+02
         H2S:   3.736E+02      O2:    1.548E+02
     Gas component Critical Pressures     (PC) Pa
         H2:    2.047E+06      CO2:   7.376E+06
         CH4:   4.617E+06      N2:    3.394E+06
         H2S:   9.007E+06      O2:    5.080E+06
     Gas component Acentric Factors     (ACEN)
         H2:    0.000E+00      CO2:   2.310E-01
         CH4:   1.000E-02      N2:    4.500E-02
         H2S:   1.000E-01      O2:    1.900E-02

  Additional RKS EOS Gas parameters:
     H2 Special Critical Temperatures  (TCH2) K
         H2:    4.360E+01
     H2 Special Critical Pressures     (PCH2) Pa
         H2:    2.047E+06
     H2 Special Molecular Weight       (WMH2) Pa
```

```
         H2:    2.016E-03

 Additional RKS EOS Constants:
     OMEGAA Constant  (OMEGAA)  4.275E-01
     OMEGAB Constant  (OMEGAB)  8.664E-02

 Binary Interaction Parameters for RKS EOS:
     H2 interaction with
         H2:    0.000E+00      CO2:  -3.426E-01
         CH4:  -2.220E-02      N2:    9.780E-02
         H2S:   0.000E+00      O2:    0.000E+00
     CO2 interaction with
         H2:   -3.426E-01      CO2:   0.000E+00
         CH4:   9.330E-02      N2:  -3.150E-02
         H2S:   9.890E-02      O2:    0.000E+00
     CH4 interaction with
         H2:   -2.220E-02      CO2:   9.330E-02
         CH4:   0.000E+00      N2:    2.780E-02
         H2S:   8.500E-02      O2:    0.000E+00
     N2  interaction with
         H2:    9.780E-02      CO2:  -3.150E-02
         CH4:   2.780E-02      N2:    0.000E+00
         H2S:   1.696E-01      O2:   -7.800E-03
     H2S interaction with
         H2:    0.000E+00      CO2:   9.890E-02
         CH4:   8.500E-02      N2:    1.696E-01
         H2S:   0.000E+00      O2:    0.000E+00
     O2 interaction with
         H2:    0.000E+00      CO2:   0.000E+00
         CH4:   0.000E+00      N2:   -7.800E-03
         H2S:   0.000E+00      O2:    0.000E+00

*************************************************************************************************************************************

 Gas generation model (IGASVAR) = 1
     Original model:  Zeroth-order corrosion & biodegradation.

 Intrinsic reaction rate constants?  (LINTRIN): F

 Reaction rate constants  (RK):
     Corrosion reaction rate constant      = 1.054100E-08 mol Fe/(s*m^3)
     Biodegradation reaction rate constant = 3.416500E-09 mol cell/(s*m^3)

 Factor for humid reaction rate constants  (HF):
     Corrosion reaction      = 0.000000E+00
     Biodegradation reaction = 1.420300E-01

 MgO hydration reaction rate constants:
     Inundated reaction (BRUCITEI) = 5.914300E-06 mol MgO/(s*m^3)
     Humid reaction     (BRUCITEH) = 2.087500E-06 mol MgO/(s*m^3)
```

```
Hydromagnesite reaction rate constant (HYMAGCON) = 6.476000E-10 mol MgO/(s*m^3)

Gas generation factors for biodegradation reaction:
    Waste Area # 1
    H2/H2S production     (RXH2S) = 4.890700E-01
    CO2 production        (RXCO2) = 1.000000E+00

Gas generation factors for biodegradation reaction:
    Waste Area # 2
    H2/H2S production     (RXH2S) = 4.890700E-01
    CO2 production        (RXCO2) = 1.000000E+00

Saturation cutoff value  (SOCMIN): 1.500000E-02

Stoichiometric coeff's for Rxn 1:
    H2       coefficient =  1.000000E+00
    H2O      coefficient = -2.000000E+00
    Fe       coefficient = -1.000000E+00
    Bio      coefficient =  0.000000E+00
    Fe(OH)2  coefficient =  1.000000E+00
    FeS      coefficient =  0.000000E+00
    MgO      coefficient =  0.000000E+00
    Mg(OH)2  coefficient =  0.000000E+00
    Hydromagnesite coefficient =  0.000000E+00
    MgCO3    coefficient =  0.000000E+00

Stoichiometric coeff's for Rxn 2:
    H2       coefficient =  4.890700E-01
    H2O      coefficient =  8.770500E-01
    Fe       coefficient =  0.000000E+00
    Bio      coefficient = -1.000000E+00
    Fe(OH)2  coefficient =  0.000000E+00
    FeS      coefficient =  0.000000E+00
    MgO      coefficient =  0.000000E+00
    Mg(OH)2  coefficient =  0.000000E+00
    Hydromagnesite coefficient =  0.000000E+00
    MgCO3    coefficient =  0.000000E+00

Stoichiometric coeff's for Rxn 3:
    H2       coefficient =  0.000000E+00
    H2O      coefficient =  0.000000E+00
    Fe       coefficient =  0.000000E+00
    Bio      coefficient =  0.000000E+00
    Fe(OH)2  coefficient =  0.000000E+00
    FeS      coefficient =  0.000000E+00
    MgO      coefficient =  0.000000E+00
    Mg(OH)2  coefficient =  0.000000E+00
    Hydromagnesite coefficient =  0.000000E+00
    MgCO3    coefficient =  0.000000E+00

Stoichiometric coeff's for Rxn 4:
```

```
      H2       coefficient =  0.000000E+00
      H2O      coefficient =  0.000000E+00
      Fe       coefficient =  0.000000E+00
      Bio      coefficient =  0.000000E+00
      Fe(OH)2  coefficient =  0.000000E+00
      FeS      coefficient =  0.000000E+00
      MgO      coefficient =  0.000000E+00
      Mg(OH)2  coefficient =  0.000000E+00
      Hydromagnesite coefficient =  0.000000E+00
      MgCO3    coefficient =  0.000000E+00

  Stoichiometric coeff's for Rxn 5:
      H2       coefficient =  0.000000E+00
      H2O      coefficient = -1.000000E+00
      Fe       coefficient =  0.000000E+00
      Bio      coefficient =  0.000000E+00
      Fe(OH)2  coefficient =  0.000000E+00
      FeS      coefficient =  0.000000E+00
      MgO      coefficient = -1.000000E+00
      Mg(OH)2  coefficient =  1.000000E+00
      Hydromagnesite coefficient =  0.000000E+00
      MgCO3    coefficient =  0.000000E+00

  Stoichiometric coeff's for Rxn 6:
      H2       coefficient =  0.000000E+00
      H2O      coefficient =  0.000000E+00
      Fe       coefficient =  0.000000E+00
      Bio      coefficient =  0.000000E+00
      Fe(OH)2  coefficient =  0.000000E+00
      FeS      coefficient =  0.000000E+00
      MgO      coefficient =  0.000000E+00
      Mg(OH)2  coefficient = -1.250000E+00
      Hydromagnesite coefficient =  2.500000E-01
      MgCO3    coefficient =  0.000000E+00

  Stoichiometric coeff's for Rxn 7:
      H2       coefficient =  0.000000E+00
      H2O      coefficient =  0.000000E+00
      Fe       coefficient =  0.000000E+00
      Bio      coefficient =  0.000000E+00
      Fe(OH)2  coefficient =  0.000000E+00
      FeS      coefficient =  0.000000E+00
      MgO      coefficient = -1.000000E+00
      Mg(OH)2  coefficient =  0.000000E+00
      Hydromagnesite coefficient =  0.000000E+00
      MgCO3    coefficient =  1.000000E+00

  Stoichiometric coeff's for Rxn 8:
      H2       coefficient =  0.000000E+00
      H2O      coefficient =  4.000000E+00
      Fe       coefficient =  0.000000E+00
```

```
      Bio      coefficient =  0.000000E+00
      Fe(OH)2  coefficient =  0.000000E+00
      FeS      coefficient =  0.000000E+00
      MgO      coefficient =  0.000000E+00
      Mg(OH)2  coefficient =  1.000000E+00
      Hydromagnesite coefficient = -1.000000E+00
      MgCO3    coefficient =  4.000000E+00

 Wicking term                        (SATWICK) = 3.222500E-01
 Humid rates to be smoothed?           (LARXN) = T
 Concentration rates to be smoothed? (LARXN2) = T
 Humid rate smoothing factor        (ALPHARXN) =-1.000000E+03

  Molecular weights  (WM):
      H2:    2.0159E-03 kg/mol
      H2O:   1.8015E-02 kg/mol
      Fe:    5.5847E-02 kg/mol
      Bio:   2.7023E-02 kg/mol

  Molecular weights  (WM):
      Fe(OH)2:  8.9860E-02 kg/mol
      FeS:      8.7911E-02 kg/mol
      MgO:      4.0304E-02 kg/mol
      Mg(OH)2:  5.8320E-02 kg/mol
      Hydromagnesite:  4.6764E-01 kg/mol
      MgCO3:    8.4314E-02 kg/mol

  Densities  (DEN(1-4)):
      Fe:       7.8700E+03 kg/m3
      Fe(OH)2:  3.4000E+03 kg/m3
      FeS:      4.7000E+03 kg/m3
      Bio:      1.1000E+03 kg/m3

  Densities  (DEN(5-9)):
      MgO:      3.6000E+03 kg/m3
      Mg(OH)2:  2.3700E+03 kg/m3
      Hydromagnesite:    2.3000E+03 kg/m3
      MgCO3:    3.0500E+03 kg/m3
      SALT:     2.1800E+03 kg/m3

  Will creep closure be used  (CLOSURE):  T

  Number of closure surfaces  (NKLOS) =    1
  Closure surface interpolation basis (KLOSINT):  1
      [Gas generation rate:     KLOSINT=0]
      [Average waste pressure:  KLOSINT=1]
  Pressure averaging method for closure (KLOSAVG):  2
      [Average all closure surface blocks:  KLOSAVG=1]
      [No averaging; use PO in (I,J,K):     KLOSAVG=2]

  PLITHO       = Maximum pressure for closure
```

```
  TIME_CLOSOFF = Time limit for closure
  CLOSPERMFACT = Constant factor in permeability-porosity expression
  CLOSPERMEXP  = Exponent in permeability-porosity expression
  PHIUPPER     = Upper porosity limit in permeability-porosity expression
  PHILOWER     = Lower porosity limit in permeability-porosity expression
     Model Number    (PLITHO) [Pa]     (TIME_CLOSOFF) [s]   (MODPERM) [-]
 Refer to the Closure LOOK-UP TABLE DATA FILE for values
           4          5.000000E+07       3.155700E+12             1        F  F
  MODPERM Parameters
     Model Number    (CLOSPERMFACT) [m^2]   (CLOSPERMEXP) [-]
           4          2.399900E-13          0.000000E+00

  Number of materials using closure (NMATCLOS) =    2
         Material Index    Model Number
     #       (MATCLOS)       (MODELCLOS)
     1          21               4
     2          32               4

  Radionuclide decay will be calculated? (LRADDK):  T

  Solute transport will be calculated?    (LTRANS):  F
  Solute radiolysis will be calculated? (LRADLSIS):  T

  Number of radionuclide species to be transported (NRAD) =  5

  Radionuclide decay control parameters:
      Minimum decay factor                    (XLIM) = 1.0000E-07
      Max number of half-lives              (HALFMAX) = 5.0000E+01
      Max time for computing decay          (T_SCALE) = 3.1557E+07 s
      Radiolysis stoichiometric coef for O2 (SRADO2) = 0.0000E+00 mol O2/mol H2
      Average "G" value for H2               (GH2AVG) = 1.4000E-02
      Deposition factor for wetted solids   (GDEPFAC) = 6.3844E-03

  Radionuclide IDs and Properties
  ===============================

      Isotope     Daughter      Element      Half life    Atomic wt.   Solub. limit    Disint. Energy
   I    ID          ID           Index          s          kg/mol        mol/m^3           MeV/dis
  --  -------     --------      -------     ----------   ----------  ------------   --------------
   1   AM241       NP237             2    1.36400E+10   0.241060   5.88570E-02         5.638
   2   PU238       U234              1    2.76900E+09   0.238050   3.52390E-03         5.593
   3   PU239       U235              1    7.59400E+11   0.239050   3.52390E-03         5.245
   4   PU240       U236              1    2.06300E+11   0.240050   3.52390E-03         5.256
   5   PU242       U238              1    1.22100E+13   0.242060   3.52390E-03         4.985

  Initial radionuclide inventory in waste (mol):
     1    AM241        1.689300E+03
     2    PU238        2.358200E+02
     3    PU239        2.264000E+05
     4    PU240        1.551400E+04
     5    PU242        7.375800E+03
```

```
 Will gas component transport be calculated?  (LRXGAST):   F

*** Cavity Region  1 is initialized with PO & SO =   1.013250E+05   0.000000E+00

*** Cavity Region  2 is initialized with PO & SO =   1.013250E+05   0.000000E+00

*** Cavity Region  3 is initialized with PO & SO =   1.013250E+05   0.000000E+00

*** Cavity Region  4 is initialized with PO & SO =   1.013250E+05   0.000000E+00

*** Cavity Region  5 is initialized with PO & SO =   1.013250E+05   0.000000E+00


*************************************************************************************************************************************
 Total mesh volume  = 2.174500E+12 m^3
 Total waste volume = 4.381389E+05 m^3
 Density of initial brine at ref cond = 1.220000E+03 kg/m^3
 Density of initial gas at ref cond   = 8.179988E-02 kg/m^3
 Mass fraction of initial brine in brine phase at ref. cond = 1.000000E+00
 Mass fraction of initial gas in brine phase at ref. cond   = 0.000000E+00
 Original brine in place at ref. cond = 9.709693E+09 m^3
 Original brine in place              = 1.184583E+13 kg
 Original gas in place at ref. cond   = 5.670309E+08 m^3
 Original gas in place                = 4.638306E+07 kg


 Number of element variables printed to ASCII output =   19

 Number of global  variables printed to ASCII output =   10
```

No.	CAMCON Vbl Name	Element Variable Description	Units Label	Units Conv Factor
1	PRESBRIN	Brine pressure	Pa	1.000000E+00
2	PRESGAS	Gas pressure	Pa	1.000000E+00
6	POROS	Porosity	dimensionless	1.000000E+00
18	SATGAS	Gas saturation	fraction void volume	1.000000E+00
49	H2RATE	H2 generation rate -- simple model	kg/(s*m^3)	1.000000E+00
59	FECONC	Fe concentration -- simple model	kg/m^3	1.000000E+00
60	CELLCONC	C6-H10-O5 concentration -- simple model	kg/m^3	1.000000E+00
63	MGOC	MgO concentration -- simple model	kg/m^3	1.000000E+00
91	H2_RAD_R	H2 generation rate -- radiolysis	kg/(s*m^3)	1.000000E+00
116	SM1AM241	Amount of isotope 1 from Waste Region 1	mol	1.000000E+00
117	SM2AM241	Amount of isotope 1 from Waste Region 2	mol	1.000000E+00

118	SM1PU238	Amount of isotope 2 from Waste Region 1	mol	1.000000E+00
119	SM2PU238	Amount of isotope 2 from Waste Region 2	mol	1.000000E+00
120	SM1PU239	Amount of isotope 3 from Waste Region 1	mol	1.000000E+00
121	SM2PU239	Amount of isotope 3 from Waste Region 2	mol	1.000000E+00
122	SM1PU240	Amount of isotope 4 from Waste Region 1	mol	1.000000E+00
123	SM2PU240	Amount of isotope 4 from Waste Region 2	mol	1.000000E+00
124	SM1PU242	Amount of isotope 5 from Waste Region 1	mol	1.000000E+00
125	SM2PU242	Amount of isotope 5 from Waste Region 2	mol	1.000000E+00

No.	CAMCON Vbl Name	Global Variable Description	Units Label	Units Conv Factor
1	BRNMBCUM	Cumulative brine mass balance	dimensionless	1.000000E+00
2	GASMBCUM	Cumulative gas mass balance	dimensionless	1.000000E+00
3	BRNMBMAX	Maximum brine mass balance	dimensionless	1.000000E+00
4	GASMBMAX	Maximum gas mass balance	dimensionless	1.000000E+00
5	IBRNMBMX	I-index, location of maximum brine mass balance	dimensionless	1.000000E+00
6	JBRNMBMX	J-index, location of maximum brine mass balance	dimensionless	1.000000E+00
7	KBRNMBMX	K-index, location of maximum brine mass balance	dimensionless	1.000000E+00
8	IGASMBMX	I-index, location of maximum gas mass balance	dimensionless	1.000000E+00
9	JGASMBMX	J-index, location of maximum gas mass balance	dimensionless	1.000000E+00
10	KGASMBMX	K-index, location of maximum gas mass balance	dimensionless	1.000000E+00

Grid block dimensions

Grid block dimensions in X-direction m

Layer 1										
1	1.22038E+04	3.12685E+03	2.15645E+03	1.48721E+03	1.02566E+03	7.07350E+02	5.26680E+02	3.63230E+02	2.50500E+02	1.72760E+02
	1.19150E+02	8.21700E+01	5.66700E+01	3.90800E+01	2.69500E+01	1.85900E+01	1.28200E+01	8.84000E+00	6.10000E+00	4.20000E+00
	2.90000E+00	2.00000E+00	4.38000E+01	1.00000E+01	2.00000E+00	2.75750E-01	2.00000E+00	1.00000E+01	4.38000E+01	1.52400E+01
	1.52400E+01	1.40200E+02	1.40200E+02	1.52400E+01	1.52400E+01	1.40200E+02	1.40200E+02	3.04800E+01	3.04800E+01	9.87000E+01
	9.87000E+01	9.87000E+01	1.00000E+01	3.61650E+02	3.61650E+02	2.00000E+00	2.90000E+00	4.20000E+00	6.10000E+00	8.84000E+00
	1.28200E+01	1.85900E+01	2.69500E+01	3.90800E+01	5.66700E+01	8.21700E+01	1.19150E+02	1.72760E+02	2.50500E+02	3.63230E+02
	5.26680E+02	7.07350E+02	1.02566E+03	1.48721E+03	2.15645E+03	3.12685E+03	4.53394E+03	7.66989E+03		
2	1.22038E+04	3.12685E+03	2.15645E+03	1.48721E+03	1.02566E+03	7.07350E+02	5.26680E+02	3.63230E+02	2.50500E+02	1.72760E+02
	1.19150E+02	8.21700E+01	5.66700E+01	3.90800E+01	2.69500E+01	1.85900E+01	1.28200E+01	8.84000E+00	6.10000E+00	4.20000E+00
	2.90000E+00	2.00000E+00	4.38000E+01	1.00000E+01	2.00000E+00	2.75750E-01	2.00000E+00	1.00000E+01	4.38000E+01	1.52400E+01
	1.52400E+01	1.40200E+02	1.40200E+02	1.52400E+01	1.52400E+01	1.40200E+02	1.40200E+02	3.04800E+01	3.04800E+01	9.87000E+01
	9.87000E+01	9.87000E+01	1.00000E+01	3.61650E+02	3.61650E+02	2.00000E+00	2.90000E+00	4.20000E+00	6.10000E+00	8.84000E+00
	1.28200E+01	1.85900E+01	2.69500E+01	3.90800E+01	5.66700E+01	8.21700E+01	1.19150E+02	1.72760E+02	2.50500E+02	3.63230E+02
	5.26680E+02	7.07350E+02	1.02566E+03	1.48721E+03	2.15645E+03	3.12685E+03	4.53394E+03	7.66989E+03		
3	1.22038E+04	3.12685E+03	2.15645E+03	1.48721E+03	1.02566E+03	7.07350E+02	5.26680E+02	3.63230E+02	2.50500E+02	1.72760E+02
	1.19150E+02	8.21700E+01	5.66700E+01	3.90800E+01	2.69500E+01	1.85900E+01	1.28200E+01	8.84000E+00	6.10000E+00	4.20000E+00
	2.90000E+00	2.00000E+00	4.38000E+01	1.00000E+01	2.00000E+00	2.75750E-01	2.00000E+00	1.00000E+01	4.38000E+01	1.52400E+01
	1.52400E+01	1.40200E+02	1.40200E+02	1.52400E+01	1.52400E+01	1.40200E+02	1.40200E+02	3.04800E+01	3.04800E+01	9.87000E+01
	9.87000E+01	9.87000E+01	1.00000E+01	3.61650E+02	3.61650E+02	2.00000E+00	2.90000E+00	4.20000E+00	6.10000E+00	8.84000E+00
	1.28200E+01	1.85900E+01	2.69500E+01	3.90800E+01	5.66700E+01	8.21700E+01	1.19150E+02	1.72760E+02	2.50500E+02	3.63230E+02
	5.26680E+02	7.07350E+02	1.02566E+03	1.48721E+03	2.15645E+03	3.12685E+03	4.53394E+03	7.66989E+03		
4	1.22038E+04	3.12685E+03	2.15645E+03	1.48721E+03	1.02566E+03	7.07350E+02	5.26680E+02	3.63230E+02	2.50500E+02	1.72760E+02
	1.19150E+02	8.21700E+01	5.66700E+01	3.90800E+01	2.69500E+01	1.85900E+01	1.28200E+01	8.84000E+00	6.10000E+00	4.20000E+00

```
    2.90000E+00  2.00000E+00  4.38000E+01  1.00000E+01  2.00000E+00  2.75750E-01  2.00000E+00  1.00000E+01  4.38000E+01  1.52400E+01
    1.52400E+01  1.40200E+02  1.40200E+02  1.52400E+01  1.52400E+01  1.40200E+02  1.40200E+02  3.04800E+01  3.04800E+01  9.87000E+01
    9.87000E+01  9.87000E+01  1.00000E+01  3.61650E+02  3.61650E+02  2.00000E+00  2.90000E+00  4.20000E+00  6.10000E+00  8.84000E+00
    1.28200E+01  1.85900E+01  2.69500E+01  3.90800E+01  5.66700E+01  8.21700E+01  1.19150E+02  1.72760E+02  2.50500E+02  3.63230E+02
    5.26680E+02  7.07350E+02  1.02566E+03  1.48721E+03  2.15645E+03  3.12685E+03  4.53394E+03  7.66989E+03
5   1.22038E+04  3.12685E+03  2.15645E+03  1.48721E+03  1.02566E+03  7.07350E+02  5.26680E+02  3.63230E+02  2.50500E+02  1.72760E+02
    1.19150E+02  8.21700E+01  5.66700E+01  3.90800E+01  2.69500E+01  1.85900E+01  1.28200E+01  8.84000E+00  6.10000E+00  4.20000E+00
    2.90000E+00  2.00000E+00  4.38000E+01  1.00000E+01  2.00000E+00  2.75750E-01  2.00000E+00  1.00000E+01  4.38000E+01  1.52400E+01
    1.52400E+01  1.40200E+02  1.40200E+02  1.52400E+01  1.52400E+01  1.40200E+02  1.40200E+02  3.04800E+01  3.04800E+01  9.87000E+01
    9.87000E+01  9.87000E+01  1.00000E+01  3.61650E+02  3.61650E+02  2.00000E+00  2.90000E+00  4.20000E+00  6.10000E+00  8.84000E+00
    1.28200E+01  1.85900E+01  2.69500E+01  3.90800E+01  5.66700E+01  8.21700E+01  1.19150E+02  1.72760E+02  2.50500E+02  3.63230E+02
    5.26680E+02  7.07350E+02  1.02566E+03  1.48721E+03  2.15645E+03  3.12685E+03  4.53394E+03  7.66989E+03
6   1.22038E+04  3.12685E+03  2.15645E+03  1.48721E+03  1.02566E+03  7.07350E+02  5.26680E+02  3.63230E+02  2.50500E+02  1.72760E+02
    1.19150E+02  8.21700E+01  5.66700E+01  3.90800E+01  2.69500E+01  1.85900E+01  1.28200E+01  8.84000E+00  6.10000E+00  4.20000E+00
    2.90000E+00  2.00000E+00  4.38000E+01  1.00000E+01  2.00000E+00  2.75750E-01  2.00000E+00  1.00000E+01  4.38000E+01  1.52400E+01
    1.52400E+01  1.40200E+02  1.40200E+02  1.52400E+01  1.52400E+01  1.40200E+02  1.40200E+02  3.04800E+01  3.04800E+01  9.87000E+01
    9.87000E+01  9.87000E+01  1.00000E+01  3.61650E+02  3.61650E+02  2.00000E+00  2.90000E+00  4.20000E+00  6.10000E+00  8.84000E+00
    1.28200E+01  1.85900E+01  2.69500E+01  3.90800E+01  5.66700E+01  8.21700E+01  1.19150E+02  1.72760E+02  2.50500E+02  3.63230E+02
    5.26680E+02  7.07350E+02  1.02566E+03  1.48721E+03  2.15645E+03  3.12685E+03  4.53394E+03  7.66989E+03
7   1.22038E+04  3.12685E+03  2.15645E+03  1.48721E+03  1.02566E+03  7.07350E+02  5.26680E+02  3.63230E+02  2.50500E+02  1.72760E+02
    1.19150E+02  8.21700E+01  5.66700E+01  3.90800E+01  2.69500E+01  1.85900E+01  1.28200E+01  8.84000E+00  6.10000E+00  4.20000E+00
    2.90000E+00  2.00000E+00  4.38000E+01  1.00000E+01  2.00000E+00  2.75750E-01  2.00000E+00  1.00000E+01  4.38000E+01  1.52400E+01
    1.52400E+01  1.40200E+02  1.40200E+02  1.52400E+01  1.52400E+01  1.40200E+02  1.40200E+02  3.04800E+01  3.04800E+01  9.87000E+01
    9.87000E+01  9.87000E+01  1.00000E+01  3.61650E+02  3.61650E+02  2.00000E+00  2.90000E+00  4.20000E+00  6.10000E+00  8.84000E+00
    1.28200E+01  1.85900E+01  2.69500E+01  3.90800E+01  5.66700E+01  8.21700E+01  1.19150E+02  1.72760E+02  2.50500E+02  3.63230E+02
    5.26680E+02  7.07350E+02  1.02566E+03  1.48721E+03  2.15645E+03  3.12685E+03  4.53394E+03  7.66989E+03
8   1.22038E+04  3.12685E+03  2.15645E+03  1.48721E+03  1.02566E+03  7.07350E+02  5.26680E+02  3.63230E+02  2.50500E+02  1.72760E+02
    1.19150E+02  8.21700E+01  5.66700E+01  3.90800E+01  2.69500E+01  1.85900E+01  1.28200E+01  8.84000E+00  6.10000E+00  4.20000E+00
    2.90000E+00  2.00000E+00  4.38000E+01  1.00000E+01  2.00000E+00  2.75750E-01  2.00000E+00  1.00000E+01  4.38000E+01  1.52400E+01
    1.52400E+01  1.40200E+02  1.40200E+02  1.52400E+01  1.52400E+01  1.40200E+02  1.40200E+02  3.04800E+01  3.04800E+01  9.87000E+01
    9.87000E+01  9.87000E+01  1.00000E+01  3.61650E+02  3.61650E+02  2.00000E+00  2.90000E+00  4.20000E+00  6.10000E+00  8.84000E+00
    1.28200E+01  1.85900E+01  2.69500E+01  3.90800E+01  5.66700E+01  8.21700E+01  1.19150E+02  1.72760E+02  2.50500E+02  3.63230E+02
    5.26680E+02  7.07350E+02  1.02566E+03  1.48721E+03  2.15645E+03  3.12685E+03  4.53394E+03  7.66989E+03
9   1.22038E+04  3.12685E+03  2.15645E+03  1.48721E+03  1.02566E+03  7.07350E+02  5.26680E+02  3.63230E+02  2.50500E+02  1.72760E+02
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    2.90000E+00  2.00000E+00  4.38000E+01  1.00000E+01  2.00000E+00  2.75750E-01  2.00000E+00  1.00000E+01  4.38000E+01  1.52400E+01
    1.52400E+01  1.40200E+02  1.40200E+02  1.52400E+01  1.52400E+01  1.40200E+02  1.40200E+02  3.04800E+01  3.04800E+01  9.87000E+01
    9.87000E+01  9.87000E+01  1.00000E+01  3.61650E+02  3.61650E+02  2.00000E+00  2.90000E+00  4.20000E+00  6.10000E+00  8.84000E+00
    1.28200E+01  1.85900E+01  2.69500E+01  3.90800E+01  5.66700E+01  8.21700E+01  1.19150E+02  1.72760E+02  2.50500E+02  3.63230E+02
    5.26680E+02  7.07350E+02  1.02566E+03  1.48721E+03  2.15645E+03  3.12685E+03  4.53394E+03  7.66989E+03
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    1.52400E+01  1.40200E+02  1.40200E+02  1.52400E+01  1.52400E+01  1.40200E+02  1.40200E+02  3.04800E+01  3.04800E+01  9.87000E+01
    9.87000E+01  9.87000E+01  1.00000E+01  3.61650E+02  3.61650E+02  2.00000E+00  2.90000E+00  4.20000E+00  6.10000E+00  8.84000E+00
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    5.26680E+02  7.07350E+02  1.02566E+03  1.48721E+03  2.15645E+03  3.12685E+03  4.53394E+03  7.66989E+03
11  1.22038E+04  3.12685E+03  2.15645E+03  1.48721E+03  1.02566E+03  7.07350E+02  5.26680E+02  3.63230E+02  2.50500E+02  1.72760E+02
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    2.90000E+00  2.00000E+00  4.38000E+01  1.00000E+01  2.00000E+00  2.75750E-01  2.00000E+00  1.00000E+01  4.38000E+01  1.52400E+01
    1.52400E+01  1.40200E+02  1.40200E+02  1.52400E+01  1.52400E+01  1.40200E+02  1.40200E+02  3.04800E+01  3.04800E+01  9.87000E+01
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    9.87000E+01  9.87000E+01  1.00000E+01  3.61650E+02  3.61650E+02  2.00000E+00  2.90000E+00  4.20000E+00  6.10000E+00  8.84000E+00
    1.28200E+01  1.85900E+01  2.69500E+01  3.90800E+01  5.66700E+01  8.21700E+01  1.19150E+02  1.72760E+02  2.50500E+02  3.63230E+02
    5.26680E+02  7.07350E+02  1.02566E+03  1.48721E+03  2.15645E+03  3.12685E+03  4.53394E+03  7.66989E+03
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    1.52400E+01  1.40200E+02  1.40200E+02  1.52400E+01  1.52400E+01  1.40200E+02  1.40200E+02  3.04800E+01  3.04800E+01  9.87000E+01
    9.87000E+01  9.87000E+01  1.00000E+01  3.61650E+02  3.61650E+02  2.00000E+00  2.90000E+00  4.20000E+00  6.10000E+00  8.84000E+00
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13  1.22038E+04  3.12685E+03  2.15645E+03  1.48721E+03  1.02566E+03  7.07350E+02  5.26680E+02  3.63230E+02  2.50500E+02  1.72760E+02
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    1.52400E+01  1.40200E+02  1.40200E+02  1.52400E+01  1.52400E+01  1.40200E+02  1.40200E+02  3.04800E+01  3.04800E+01  9.87000E+01
    9.87000E+01  9.87000E+01  1.00000E+01  3.61650E+02  3.61650E+02  2.00000E+00  2.90000E+00  4.20000E+00  6.10000E+00  8.84000E+00
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    1.52400E+01  1.40200E+02  1.40200E+02  1.52400E+01  1.52400E+01  1.40200E+02  1.40200E+02  3.04800E+01  3.04800E+01  9.87000E+01
    9.87000E+01  9.87000E+01  1.00000E+01  3.61650E+02  3.61650E+02  2.00000E+00  2.90000E+00  4.20000E+00  6.10000E+00  8.84000E+00
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    1.52400E+01  1.40200E+02  1.40200E+02  1.52400E+01  1.52400E+01  1.40200E+02  1.40200E+02  3.04800E+01  3.04800E+01  9.87000E+01
    9.87000E+01  9.87000E+01  1.00000E+01  3.61650E+02  3.61650E+02  2.00000E+00  2.90000E+00  4.20000E+00  6.10000E+00  8.84000E+00
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    1.52400E+01  1.40200E+02  1.40200E+02  1.52400E+01  1.52400E+01  1.40200E+02  1.40200E+02  3.04800E+01  3.04800E+01  9.87000E+01
    9.87000E+01  9.87000E+01  1.00000E+01  3.61650E+02  3.61650E+02  2.00000E+00  2.90000E+00  4.20000E+00  6.10000E+00  8.84000E+00
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    9.87000E+01  9.87000E+01  1.00000E+01  3.61650E+02  3.61650E+02  2.00000E+00  2.90000E+00  4.20000E+00  6.10000E+00  8.84000E+00
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    5.26680E+02  7.07350E+02  1.02566E+03  1.48721E+03  2.15645E+03  3.12685E+03  4.53394E+03  7.66989E+03
19  1.22038E+04  3.12685E+03  2.15645E+03  1.48721E+03  1.02566E+03  7.07350E+02  5.26680E+02  3.63230E+02  2.50500E+02  1.72760E+02
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    9.87000E+01  9.87000E+01  1.00000E+01  3.61650E+02  3.61650E+02  2.00000E+00  2.90000E+00  4.20000E+00  6.10000E+00  8.84000E+00
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    1.19150E+02  8.21700E+01  5.66700E+01  3.90800E+01  2.69500E+01  1.85900E+01  1.28200E+01  8.84000E+00  6.10000E+00  4.20000E+00
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    9.87000E+01  9.87000E+01  1.00000E+01  3.61650E+02  3.61650E+02  2.00000E+00  2.90000E+00  4.20000E+00  6.10000E+00  8.84000E+00
    1.28200E+01  1.85900E+01  2.69500E+01  3.90800E+01  5.66700E+01  8.21700E+01  1.19150E+02  1.72760E+02  2.50500E+02  3.63230E+02
    5.26680E+02  7.07350E+02  1.02566E+03  1.48721E+03  2.15645E+03  3.12685E+03  4.53394E+03  7.66989E+03
21  1.22038E+04  3.12685E+03  2.15645E+03  1.48721E+03  1.02566E+03  7.07350E+02  5.26680E+02  3.63230E+02  2.50500E+02  1.72760E+02
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    1.52400E+01  1.40200E+02  1.40200E+02  1.52400E+01  1.52400E+01  1.40200E+02  1.40200E+02  3.04800E+01  3.04800E+01  9.87000E+01
    9.87000E+01  9.87000E+01  1.00000E+01  3.61650E+02  3.61650E+02  2.00000E+00  2.90000E+00  4.20000E+00  6.10000E+00  8.84000E+00
    1.28200E+01  1.85900E+01  2.69500E+01  3.90800E+01  5.66700E+01  8.21700E+01  1.19150E+02  1.72760E+02  2.50500E+02  3.63230E+02
    5.26680E+02  7.07350E+02  1.02566E+03  1.48721E+03  2.15645E+03  3.12685E+03  4.53394E+03  7.66989E+03
22  1.22038E+04  3.12685E+03  2.15645E+03  1.48721E+03  1.02566E+03  7.07350E+02  5.26680E+02  3.63230E+02  2.50500E+02  1.72760E+02
    1.19150E+02  8.21700E+01  5.66700E+01  3.90800E+01  2.69500E+01  1.85900E+01  1.28200E+01  8.84000E+00  6.10000E+00  4.20000E+00
    2.90000E+00  2.00000E+00  4.38000E+01  1.00000E+01  2.00000E+00  2.75750E-01  2.00000E+00  1.00000E+01  4.38000E+01  1.52400E+01
    1.52400E+01  1.40200E+02  1.40200E+02  1.52400E+01  1.52400E+01  1.40200E+02  1.40200E+02  3.04800E+01  3.04800E+01  9.87000E+01
    9.87000E+01  9.87000E+01  1.00000E+01  3.61650E+02  3.61650E+02  2.00000E+00  2.90000E+00  4.20000E+00  6.10000E+00  8.84000E+00
    1.28200E+01  1.85900E+01  2.69500E+01  3.90800E+01  5.66700E+01  8.21700E+01  1.19150E+02  1.72760E+02  2.50500E+02  3.63230E+02
    5.26680E+02  7.07350E+02  1.02566E+03  1.48721E+03  2.15645E+03  3.12685E+03  4.53394E+03  7.66989E+03
23  1.22038E+04  3.12685E+03  2.15645E+03  1.48721E+03  1.02566E+03  7.07350E+02  5.26680E+02  3.63230E+02  2.50500E+02  1.72760E+02
    1.19150E+02  8.21700E+01  5.66700E+01  3.90800E+01  2.69500E+01  1.85900E+01  1.28200E+01  8.84000E+00  6.10000E+00  4.20000E+00
    2.90000E+00  2.00000E+00  4.38000E+01  1.00000E+01  2.00000E+00  2.75750E-01  2.00000E+00  1.00000E+01  4.38000E+01  1.52400E+01
    1.52400E+01  1.40200E+02  1.40200E+02  1.52400E+01  1.52400E+01  1.40200E+02  1.40200E+02  3.04800E+01  3.04800E+01  9.87000E+01
    9.87000E+01  9.87000E+01  1.00000E+01  3.61650E+02  3.61650E+02  2.00000E+00  2.90000E+00  4.20000E+00  6.10000E+00  8.84000E+00
    1.28200E+01  1.85900E+01  2.69500E+01  3.90800E+01  5.66700E+01  8.21700E+01  1.19150E+02  1.72760E+02  2.50500E+02  3.63230E+02
    5.26680E+02  7.07350E+02  1.02566E+03  1.48721E+03  2.15645E+03  3.12685E+03  4.53394E+03  7.66989E+03
24  1.22038E+04  3.12685E+03  2.15645E+03  1.48721E+03  1.02566E+03  7.07350E+02  5.26680E+02  3.63230E+02  2.50500E+02  1.72760E+02
    1.19150E+02  8.21700E+01  5.66700E+01  3.90800E+01  2.69500E+01  1.85900E+01  1.28200E+01  8.84000E+00  6.10000E+00  4.20000E+00
    2.90000E+00  2.00000E+00  4.38000E+01  1.00000E+01  2.00000E+00  2.75750E-01  2.00000E+00  1.00000E+01  4.38000E+01  1.52400E+01
    1.52400E+01  1.40200E+02  1.40200E+02  1.52400E+01  1.52400E+01  1.40200E+02  1.40200E+02  3.04800E+01  3.04800E+01  9.87000E+01
    9.87000E+01  9.87000E+01  1.00000E+01  3.61650E+02  3.61650E+02  2.00000E+00  2.90000E+00  4.20000E+00  6.10000E+00  8.84000E+00
    1.28200E+01  1.85900E+01  2.69500E+01  3.90800E+01  5.66700E+01  8.21700E+01  1.19150E+02  1.72760E+02  2.50500E+02  3.63230E+02
    5.26680E+02  7.07350E+02  1.02566E+03  1.48721E+03  2.15645E+03  3.12685E+03  4.53394E+03  7.66989E+03
25  1.22038E+04  3.12685E+03  2.15645E+03  1.48721E+03  1.02566E+03  7.07350E+02  5.26680E+02  3.63230E+02  2.50500E+02  1.72760E+02
    1.19150E+02  8.21700E+01  5.66700E+01  3.90800E+01  2.69500E+01  1.85900E+01  1.28200E+01  8.84000E+00  6.10000E+00  4.20000E+00
    2.90000E+00  2.00000E+00  4.38000E+01  1.00000E+01  2.00000E+00  2.75750E-01  2.00000E+00  1.00000E+01  4.38000E+01  1.52400E+01
    1.52400E+01  1.40200E+02  1.40200E+02  1.52400E+01  1.52400E+01  1.40200E+02  1.40200E+02  3.04800E+01  3.04800E+01  9.87000E+01
    9.87000E+01  9.87000E+01  1.00000E+01  3.61650E+02  3.61650E+02  2.00000E+00  2.90000E+00  4.20000E+00  6.10000E+00  8.84000E+00
    1.28200E+01  1.85900E+01  2.69500E+01  3.90800E+01  5.66700E+01  8.21700E+01  1.19150E+02  1.72760E+02  2.50500E+02  3.63230E+02
    5.26680E+02  7.07350E+02  1.02566E+03  1.48721E+03  2.15645E+03  3.12685E+03  4.53394E+03  7.66989E+03
26  1.22038E+04  3.12685E+03  2.15645E+03  1.48721E+03  1.02566E+03  7.07350E+02  5.26680E+02  3.63230E+02  2.50500E+02  1.72760E+02
```

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    1.19150E+02  8.21700E+01  5.66700E+01  3.90800E+01  2.69500E+01  1.85900E+01  1.28200E+01  8.84000E+00  6.10000E+00  4.20000E+00
    2.90000E+00  2.00000E+00  4.38000E+01  1.00000E+01  2.00000E+00  2.75750E-01  2.00000E+00  1.00000E+01  4.38000E+01  1.52400E+01
    1.52400E+01  1.40200E+02  1.40200E+02  1.52400E+01  1.52400E+01  1.40200E+02  1.40200E+02  3.04800E+01  3.04800E+01  9.87000E+01
    9.87000E+01  9.87000E+01  1.00000E+01  3.61650E+02  3.61650E+02  2.00000E+00  2.90000E+00  4.20000E+00  6.10000E+00  8.84000E+00
    1.28200E+01  1.85900E+01  2.69500E+01  3.90800E+01  5.66700E+01  8.21700E+01  1.19150E+02  1.72760E+02  2.50500E+02  3.63230E+02
    5.26680E+02  7.07350E+02  1.02566E+03  1.48721E+03  2.15645E+03  3.12685E+03  4.53394E+03  7.66989E+03
27  1.22038E+04  3.12685E+03  2.15645E+03  1.48721E+03  1.02566E+03  7.07350E+02  5.26680E+02  3.63230E+02  2.50500E+02  1.72760E+02
    1.19150E+02  8.21700E+01  5.66700E+01  3.90800E+01  2.69500E+01  1.85900E+01  1.28200E+01  8.84000E+00  6.10000E+00  4.20000E+00
    2.90000E+00  2.00000E+00  4.38000E+01  1.00000E+01  2.00000E+00  2.75750E-01  2.00000E+00  1.00000E+01  4.38000E+01  1.52400E+01
    1.52400E+01  1.40200E+02  1.40200E+02  1.52400E+01  1.52400E+01  1.40200E+02  1.40200E+02  3.04800E+01  3.04800E+01  9.87000E+01
    9.87000E+01  9.87000E+01  1.00000E+01  3.61650E+02  3.61650E+02  2.00000E+00  2.90000E+00  4.20000E+00  6.10000E+00  8.84000E+00
    1.28200E+01  1.85900E+01  2.69500E+01  3.90800E+01  5.66700E+01  8.21700E+01  1.19150E+02  1.72760E+02  2.50500E+02  3.63230E+02
    5.26680E+02  7.07350E+02  1.02566E+03  1.48721E+03  2.15645E+03  3.12685E+03  4.53394E+03  7.66989E+03
28  1.22038E+04  3.12685E+03  2.15645E+03  1.48721E+03  1.02566E+03  7.07350E+02  5.26680E+02  3.63230E+02  2.50500E+02  1.72760E+02
    1.19150E+02  8.21700E+01  5.66700E+01  3.90800E+01  2.69500E+01  1.85900E+01  1.28200E+01  8.84000E+00  6.10000E+00  4.20000E+00
    2.90000E+00  2.00000E+00  4.38000E+01  1.00000E+01  2.00000E+00  2.75750E-01  2.00000E+00  1.00000E+01  4.38000E+01  1.52400E+01
    1.52400E+01  1.40200E+02  1.40200E+02  1.52400E+01  1.52400E+01  1.40200E+02  1.40200E+02  3.04800E+01  3.04800E+01  9.87000E+01
    9.87000E+01  9.87000E+01  1.00000E+01  3.61650E+02  3.61650E+02  2.00000E+00  2.90000E+00  4.20000E+00  6.10000E+00  8.84000E+00
    1.28200E+01  1.85900E+01  2.69500E+01  3.90800E+01  5.66700E+01  8.21700E+01  1.19150E+02  1.72760E+02  2.50500E+02  3.63230E+02
    5.26680E+02  7.07350E+02  1.02566E+03  1.48721E+03  2.15645E+03  3.12685E+03  4.53394E+03  7.66989E+03
29  1.22038E+04  3.12685E+03  2.15645E+03  1.48721E+03  1.02566E+03  7.07350E+02  5.26680E+02  3.63230E+02  2.50500E+02  1.72760E+02
    1.19150E+02  8.21700E+01  5.66700E+01  3.90800E+01  2.69500E+01  1.85900E+01  1.28200E+01  8.84000E+00  6.10000E+00  4.20000E+00
    2.90000E+00  2.00000E+00  4.38000E+01  1.00000E+01  2.00000E+00  2.75750E-01  2.00000E+00  1.00000E+01  4.38000E+01  1.52400E+01
    1.52400E+01  1.40200E+02  1.40200E+02  1.52400E+01  1.52400E+01  1.40200E+02  1.40200E+02  3.04800E+01  3.04800E+01  9.87000E+01
    9.87000E+01  9.87000E+01  1.00000E+01  3.61650E+02  3.61650E+02  2.00000E+00  2.90000E+00  4.20000E+00  6.10000E+00  8.84000E+00
    1.28200E+01  1.85900E+01  2.69500E+01  3.90800E+01  5.66700E+01  8.21700E+01  1.19150E+02  1.72760E+02  2.50500E+02  3.63230E+02
    5.26680E+02  7.07350E+02  1.02566E+03  1.48721E+03  2.15645E+03  3.12685E+03  4.53394E+03  7.66989E+03
30  1.22038E+04  3.12685E+03  2.15645E+03  1.48721E+03  1.02566E+03  7.07350E+02  5.26680E+02  3.63230E+02  2.50500E+02  1.72760E+02
    1.19150E+02  8.21700E+01  5.66700E+01  3.90800E+01  2.69500E+01  1.85900E+01  1.28200E+01  8.84000E+00  6.10000E+00  4.20000E+00
    2.90000E+00  2.00000E+00  4.38000E+01  1.00000E+01  2.00000E+00  2.75750E-01  2.00000E+00  1.00000E+01  4.38000E+01  1.52400E+01
    1.52400E+01  1.40200E+02  1.40200E+02  1.52400E+01  1.52400E+01  1.40200E+02  1.40200E+02  3.04800E+01  3.04800E+01  9.87000E+01
    9.87000E+01  9.87000E+01  1.00000E+01  3.61650E+02  3.61650E+02  2.00000E+00  2.90000E+00  4.20000E+00  6.10000E+00  8.84000E+00
    1.28200E+01  1.85900E+01  2.69500E+01  3.90800E+01  5.66700E+01  8.21700E+01  1.19150E+02  1.72760E+02  2.50500E+02  3.63230E+02
    5.26680E+02  7.07350E+02  1.02566E+03  1.48721E+03  2.15645E+03  3.12685E+03  4.53394E+03  7.66989E+03
31  1.22038E+04  3.12685E+03  2.15645E+03  1.48721E+03  1.02566E+03  7.07350E+02  5.26680E+02  3.63230E+02  2.50500E+02  1.72760E+02
    1.19150E+02  8.21700E+01  5.66700E+01  3.90800E+01  2.69500E+01  1.85900E+01  1.28200E+01  8.84000E+00  6.10000E+00  4.20000E+00
    2.90000E+00  2.00000E+00  4.38000E+01  1.00000E+01  2.00000E+00  2.75750E-01  2.00000E+00  1.00000E+01  4.38000E+01  1.52400E+01
    1.52400E+01  1.40200E+02  1.40200E+02  1.52400E+01  1.52400E+01  1.40200E+02  1.40200E+02  3.04800E+01  3.04800E+01  9.87000E+01
    9.87000E+01  9.87000E+01  1.00000E+01  3.61650E+02  3.61650E+02  2.00000E+00  2.90000E+00  4.20000E+00  6.10000E+00  8.84000E+00
    1.28200E+01  1.85900E+01  2.69500E+01  3.90800E+01  5.66700E+01  8.21700E+01  1.19150E+02  1.72760E+02  2.50500E+02  3.63230E+02
    5.26680E+02  7.07350E+02  1.02566E+03  1.48721E+03  2.15645E+03  3.12685E+03  4.53394E+03  7.66989E+03
32  1.22038E+04  3.12685E+03  2.15645E+03  1.48721E+03  1.02566E+03  7.07350E+02  5.26680E+02  3.63230E+02  2.50500E+02  1.72760E+02
    1.19150E+02  8.21700E+01  5.66700E+01  3.90800E+01  2.69500E+01  1.85900E+01  1.28200E+01  8.84000E+00  6.10000E+00  4.20000E+00
    2.90000E+00  2.00000E+00  4.38000E+01  1.00000E+01  2.00000E+00  2.75750E-01  2.00000E+00  1.00000E+01  4.38000E+01  1.52400E+01
    1.52400E+01  1.40200E+02  1.40200E+02  1.52400E+01  1.52400E+01  1.40200E+02  1.40200E+02  3.04800E+01  3.04800E+01  9.87000E+01
    9.87000E+01  9.87000E+01  1.00000E+01  3.61650E+02  3.61650E+02  2.00000E+00  2.90000E+00  4.20000E+00  6.10000E+00  8.84000E+00
    1.28200E+01  1.85900E+01  2.69500E+01  3.90800E+01  5.66700E+01  8.21700E+01  1.19150E+02  1.72760E+02  2.50500E+02  3.63230E+02
    5.26680E+02  7.07350E+02  1.02566E+03  1.48721E+03  2.15645E+03  3.12685E+03  4.53394E+03  7.66989E+03
33  1.22038E+04  3.12685E+03  2.15645E+03  1.48721E+03  1.02566E+03  7.07350E+02  5.26680E+02  3.63230E+02  2.50500E+02  1.72760E+02
    1.19150E+02  8.21700E+01  5.66700E+01  3.90800E+01  2.69500E+01  1.85900E+01  1.28200E+01  8.84000E+00  6.10000E+00  4.20000E+00
    2.90000E+00  2.00000E+00  4.38000E+01  1.00000E+01  2.00000E+00  2.75750E-01  2.00000E+00  1.00000E+01  4.38000E+01  1.52400E+01
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    1.52400E+01  1.40200E+02  1.40200E+02  1.52400E+01  1.52400E+01  1.40200E+02  1.40200E+02  3.04800E+01  3.04800E+01  9.87000E+01
    9.87000E+01  9.87000E+01  1.00000E+01  3.61650E+02  3.61650E+02  2.00000E+00  2.90000E+00  4.20000E+00  6.10000E+00  8.84000E+00
    1.28200E+01  1.85900E+01  2.69500E+01  3.90800E+01  5.66700E+01  8.21700E+01  1.19150E+02  1.72760E+02  2.50500E+02  3.63230E+02
    5.26680E+02  7.07350E+02  1.02566E+03  1.48721E+03  2.15645E+03  3.12685E+03  4.53394E+03  7.66989E+03
-------------------------------------------------------------------------------------------------------------------------------
 Grid block dimensions in Y-direction              m
    Layer    1
 1  1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02
    1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02
    1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02
    1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02
    1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02
    1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02
    1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02  1.25830E+02
 2  5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01
    5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01
    5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01
    5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01
    5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01
    5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01
    5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01  5.22700E+01
 3  6.67200E+01  6.67200E+01  6.67200E+01  6.67200E+01  6.67200E+01  6.67200E+01  6.67200E+01  6.67200E+01  6.67200E+01  6.67200E+01
    6.67200E+01  6.67200E+01  6.67200E+01  6.67200E+01  6.67200E+01  6.67200E+01  6.67200E+01  6.67200E+01  6.67200E+01  6.67200E+01
    6.67200E+01  6.67200E+01  6.67200E+01  6.67200E+01  6.67200E+01  6.67200E+01  6.67200E+01  6.67200E+01  6.67200E+01  6.67200E+01
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16  4.53000E+00 4.53000E+00 4.53000E+00 4.53000E+00 4.53000E+00 4.53000E+00 4.53000E+00 4.53000E+00 4.53000E+00 4.53000E+00
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18  5.47300E+01 5.47300E+01 5.47300E+01 5.47300E+01 5.47300E+01 5.47300E+01 5.47300E+01 5.47300E+01 5.47300E+01 5.47300E+01
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19  5.47300E+01 5.47300E+01 5.47300E+01 5.47300E+01 5.47300E+01 5.47300E+01 5.47300E+01 5.47300E+01 5.47300E+01 5.47300E+01
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21  5.47300E+01 5.47300E+01 5.47300E+01 5.47300E+01 5.47300E+01 5.47300E+01 5.47300E+01 5.47300E+01 5.47300E+01 5.47300E+01
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    1.56600E+01  1.56600E+01  1.56600E+01  1.56600E+01  1.56600E+01  1.56600E+01  1.56600E+01  1.56600E+01  1.56600E+01  1.56600E+01
    1.56600E+01  1.56600E+01  1.56600E+01  1.56600E+01  1.56600E+01  1.56600E+01  1.56600E+01  1.56600E+01  1.56600E+01  1.56600E+01
    1.56600E+01  1.56600E+01  1.56600E+01  1.56600E+01  1.56600E+01  1.56600E+01  1.56600E+01  1.56600E+01
33  1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01
    1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01
    1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01
    1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01
    1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01
    1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01
    1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01  1.00000E-01
----------------------------------------------------------------------------------------------------------------------------------
 Grid block dimensions in Z-direction                 m
    Layer   1
 1  6.61771E+04  3.55157E+04  2.49491E+04  1.76618E+04  1.26360E+04  9.17002E+03  6.70195E+03  4.92212E+03  3.69466E+03  2.84813E+03
    2.26431E+03  1.86168E+03  1.58401E+03  1.39251E+03  1.26044E+03  1.16936E+03  1.10654E+03  1.06322E+03  1.03334E+03  1.01274E+03
    9.98530E+02  9.88730E+02  1.26200E+02  2.88000E+01  4.80000E+00  2.75750E-01  4.80000E+00  2.88000E+01  1.26200E+02  2.00000E+01
    2.00000E+01  1.56904E+02  1.56904E+02  4.00000E+01  4.00000E+01  1.96130E+02  1.96130E+02  4.00000E+01  4.00000E+01  3.21800E+01
    3.21800E+01  3.21800E+01  9.50000E+00  5.16700E+01  5.16800E+01  2.83958E+03  2.84938E+03  2.86359E+03  2.88419E+03  2.91407E+03
    2.95739E+03  3.02020E+03  3.11129E+03  3.24336E+03  3.43486E+03  3.71253E+03  4.11516E+03  4.69898E+03  5.54550E+03  6.77297E+03
    8.55280E+03  1.10209E+04  1.44869E+04  1.95126E+04  2.68000E+04  3.73666E+04  5.26881E+04  7.70958E+04
 2  6.61771E+04  3.55157E+04  2.49491E+04  1.76618E+04  1.26360E+04  9.17002E+03  6.70195E+03  4.92212E+03  3.69466E+03  2.84813E+03
    2.26431E+03  1.86168E+03  1.58401E+03  1.39251E+03  1.26044E+03  1.16936E+03  1.10654E+03  1.06322E+03  1.03334E+03  1.01274E+03
    9.98530E+02  9.88730E+02  1.26200E+02  2.88000E+01  4.80000E+00  2.75750E-01  4.80000E+00  2.88000E+01  1.26200E+02  2.00000E+01
    2.00000E+01  1.56904E+02  1.56904E+02  4.00000E+01  4.00000E+01  1.96130E+02  1.96130E+02  4.00000E+01  4.00000E+01  3.21800E+01
    3.21800E+01  3.21800E+01  9.50000E+00  5.16700E+01  5.16800E+01  2.83958E+03  2.84938E+03  2.86359E+03  2.88419E+03  2.91407E+03
    2.95739E+03  3.02020E+03  3.11129E+03  3.24336E+03  3.43486E+03  3.71253E+03  4.11516E+03  4.69898E+03  5.54550E+03  6.77297E+03
    8.55280E+03  1.10209E+04  1.44869E+04  1.95126E+04  2.68000E+04  3.73666E+04  5.26881E+04  7.70958E+04
```

3	6.61771E+04	3.55157E+04	2.49491E+04	1.76618E+04	1.26360E+04	9.17002E+03	6.70195E+03	4.92212E+03	3.69466E+03	2.84813E+03
	2.26431E+03	1.86168E+03	1.58401E+03	1.39251E+03	1.26044E+03	1.16936E+03	1.10654E+03	1.06322E+03	1.03334E+03	1.01274E+03
	9.98530E+02	9.88730E+02	1.26200E+02	2.88000E+01	4.80000E+00	2.75750E-01	4.80000E+00	2.88000E+01	1.26200E+02	2.00000E+01
	2.00000E+01	1.56904E+02	1.56904E+02	4.00000E+01	4.00000E+01	1.96130E+02	1.96130E+02	4.00000E+01	4.00000E+01	3.21800E+01
	3.21800E+01	3.21800E+01	9.50000E+00	5.16700E+01	5.16800E+01	2.83958E+03	2.84938E+03	2.86359E+03	2.88419E+03	2.91407E+03
	2.95739E+03	3.02020E+03	3.11129E+03	3.24336E+03	3.43486E+03	3.71253E+03	4.11516E+03	4.69898E+03	5.54550E+03	6.77297E+03
	8.55280E+03	1.10209E+04	1.44869E+04	1.95126E+04	2.68000E+04	3.73666E+04	5.26881E+04	7.70958E+04		
4	6.61771E+04	3.55157E+04	2.49491E+04	1.76618E+04	1.26360E+04	9.17002E+03	6.70195E+03	4.92212E+03	3.69466E+03	2.84813E+03
	2.26431E+03	1.86168E+03	1.58401E+03	1.39251E+03	1.26044E+03	1.16936E+03	1.10654E+03	1.06322E+03	1.03334E+03	1.01274E+03
	9.98530E+02	9.88730E+02	1.26200E+02	2.88000E+01	4.80000E+00	2.75750E-01	4.80000E+00	2.88000E+01	1.26200E+02	2.00000E+01
	2.00000E+01	1.56904E+02	1.56904E+02	4.00000E+01	4.00000E+01	1.96130E+02	1.96130E+02	4.00000E+01	4.00000E+01	3.21800E+01
	3.21800E+01	3.21800E+01	9.50000E+00	5.16700E+01	5.16800E+01	2.83958E+03	2.84938E+03	2.86359E+03	2.88419E+03	2.91407E+03
	2.95739E+03	3.02020E+03	3.11129E+03	3.24336E+03	3.43486E+03	3.71253E+03	4.11516E+03	4.69898E+03	5.54550E+03	6.77297E+03
	8.55280E+03	1.10209E+04	1.44869E+04	1.95126E+04	2.68000E+04	3.73666E+04	5.26881E+04	7.70958E+04		
5	6.61771E+04	3.55157E+04	2.49491E+04	1.76618E+04	1.26360E+04	9.17002E+03	6.70195E+03	4.92212E+03	3.69466E+03	2.84813E+03
	2.26431E+03	1.86168E+03	1.58401E+03	1.39251E+03	1.26044E+03	1.16936E+03	1.10654E+03	1.06322E+03	1.03334E+03	1.01274E+03
	9.98530E+02	9.88730E+02	1.26200E+02	2.88000E+01	4.80000E+00	2.75750E-01	4.80000E+00	2.88000E+01	1.26200E+02	2.00000E+01
	2.00000E+01	1.56904E+02	1.56904E+02	4.00000E+01	4.00000E+01	1.96130E+02	1.96130E+02	4.00000E+01	4.00000E+01	3.21800E+01
	3.21800E+01	3.21800E+01	9.50000E+00	5.16700E+01	5.16800E+01	2.83958E+03	2.84938E+03	2.86359E+03	2.88419E+03	2.91407E+03
	2.95739E+03	3.02020E+03	3.11129E+03	3.24336E+03	3.43486E+03	3.71253E+03	4.11516E+03	4.69898E+03	5.54550E+03	6.77297E+03
	8.55280E+03	1.10209E+04	1.44869E+04	1.95126E+04	2.68000E+04	3.73666E+04	5.26881E+04	7.70958E+04		
6	6.61771E+04	3.55157E+04	2.49491E+04	1.76618E+04	1.26360E+04	9.17002E+03	6.70195E+03	4.92212E+03	3.69466E+03	2.84813E+03
	2.26431E+03	1.86168E+03	1.58401E+03	1.39251E+03	1.26044E+03	1.16936E+03	1.10654E+03	1.06322E+03	1.03334E+03	1.01274E+03
	9.98530E+02	9.88730E+02	1.26200E+02	2.88000E+01	4.80000E+00	2.75750E-01	4.80000E+00	2.88000E+01	1.26200E+02	2.00000E+01
	2.00000E+01	1.56904E+02	1.56904E+02	4.00000E+01	4.00000E+01	1.96130E+02	1.96130E+02	4.00000E+01	4.00000E+01	3.21800E+01
	3.21800E+01	3.21800E+01	9.50000E+00	5.16700E+01	5.16800E+01	2.83958E+03	2.84938E+03	2.86359E+03	2.88419E+03	2.91407E+03
	2.95739E+03	3.02020E+03	3.11129E+03	3.24336E+03	3.43486E+03	3.71253E+03	4.11516E+03	4.69898E+03	5.54550E+03	6.77297E+03
	8.55280E+03	1.10209E+04	1.44869E+04	1.95126E+04	2.68000E+04	3.73666E+04	5.26881E+04	7.70958E+04		
7	6.61771E+04	3.55157E+04	2.49491E+04	1.76618E+04	1.26360E+04	9.17002E+03	6.70195E+03	4.92212E+03	3.69466E+03	2.84813E+03
	2.26431E+03	1.86168E+03	1.58401E+03	1.39251E+03	1.26044E+03	1.16936E+03	1.10654E+03	1.06322E+03	1.03334E+03	1.01274E+03
	9.98530E+02	9.88730E+02	1.26200E+02	2.88000E+01	4.80000E+00	2.75750E-01	4.80000E+00	2.88000E+01	1.26200E+02	2.00000E+01
	2.00000E+01	1.56904E+02	1.56904E+02	4.00000E+01	4.00000E+01	1.96130E+02	1.96130E+02	4.00000E+01	4.00000E+01	3.21800E+01
	3.21800E+01	3.21800E+01	9.50000E+00	5.16700E+01	5.16800E+01	2.83958E+03	2.84938E+03	2.86359E+03	2.88419E+03	2.91407E+03
	2.95739E+03	3.02020E+03	3.11129E+03	3.24336E+03	3.43486E+03	3.71253E+03	4.11516E+03	4.69898E+03	5.54550E+03	6.77297E+03
	8.55280E+03	1.10209E+04	1.44869E+04	1.95126E+04	2.68000E+04	3.73666E+04	5.26881E+04	7.70958E+04		
8	6.61771E+04	3.55157E+04	2.49491E+04	1.76618E+04	1.26360E+04	9.17002E+03	6.70195E+03	4.92212E+03	3.69466E+03	2.84813E+03
	2.26431E+03	1.86168E+03	1.58401E+03	1.39251E+03	1.26044E+03	1.16936E+03	1.10654E+03	1.06322E+03	1.03334E+03	1.01274E+03
	9.98530E+02	9.88730E+02	1.26200E+02	2.88000E+01	4.80000E+00	2.75750E-01	4.80000E+00	2.88000E+01	1.26200E+02	2.00000E+01
	2.00000E+01	1.56904E+02	1.56904E+02	4.00000E+01	4.00000E+01	1.96130E+02	1.96130E+02	4.00000E+01	4.00000E+01	3.21800E+01
	3.21800E+01	3.21800E+01	9.50000E+00	5.16700E+01	5.16800E+01	2.83958E+03	2.84938E+03	2.86359E+03	2.88419E+03	2.91407E+03
	2.95739E+03	3.02020E+03	3.11129E+03	3.24336E+03	3.43486E+03	3.71253E+03	4.11516E+03	4.69898E+03	5.54550E+03	6.77297E+03
	8.55280E+03	1.10209E+04	1.44869E+04	1.95126E+04	2.68000E+04	3.73666E+04	5.26881E+04	7.70958E+04		
9	6.61771E+04	3.55157E+04	2.49491E+04	1.76618E+04	1.26360E+04	9.17002E+03	6.70195E+03	4.92212E+03	3.69466E+03	2.84813E+03
	2.26431E+03	1.86168E+03	1.58401E+03	1.39251E+03	1.26044E+03	1.16936E+03	1.10654E+03	1.06322E+03	1.03334E+03	1.01274E+03
	9.98530E+02	9.88730E+02	1.26200E+02	2.88000E+01	4.80000E+00	2.75750E-01	4.80000E+00	2.88000E+01	1.26200E+02	2.00000E+01
	2.00000E+01	1.56904E+02	1.56904E+02	4.00000E+01	4.00000E+01	1.96130E+02	1.96130E+02	4.00000E+01	4.00000E+01	3.21800E+01
	3.21800E+01	3.21800E+01	9.50000E+00	5.16700E+01	5.16800E+01	2.83958E+03	2.84938E+03	2.86359E+03	2.88419E+03	2.91407E+03
	2.95739E+03	3.02020E+03	3.11129E+03	3.24336E+03	3.43486E+03	3.71253E+03	4.11516E+03	4.69898E+03	5.54550E+03	6.77297E+03
	8.55280E+03	1.10209E+04	1.44869E+04	1.95126E+04	2.68000E+04	3.73666E+04	5.26881E+04	7.70958E+04		
10	6.61771E+04	3.55157E+04	2.49491E+04	1.76618E+04	1.26360E+04	9.17002E+03	6.70195E+03	4.92212E+03	3.69466E+03	2.84813E+03
	2.26431E+03	1.86168E+03	1.58401E+03	1.39251E+03	1.26044E+03	1.16936E+03	1.10654E+03	1.06322E+03	1.03334E+03	1.01274E+03

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    9.98530E+02  9.88730E+02  1.26200E+02  2.88000E+01  4.80000E+00  2.75750E-01  4.80000E+00  2.88000E+01  1.26200E+02  2.00000E+01
    2.00000E+01  1.56904E+02  1.56904E+02  4.00000E+01  4.00000E+01  1.96130E+02  1.96130E+02  4.00000E+01  4.00000E+01  3.21800E+01
    3.21800E+01  3.21800E+01  9.50000E+00  5.16700E+01  5.16800E+01  2.83958E+03  2.84938E+03  2.86359E+03  2.88419E+03  2.91407E+03
    2.95739E+03  3.02020E+03  3.11129E+03  3.24336E+03  3.43486E+03  3.71253E+03  4.11516E+03  4.69898E+03  5.54550E+03  6.77297E+03
    8.55280E+03  1.10209E+04  1.44869E+04  1.95126E+04  2.68000E+04  3.73666E+04  5.26881E+04  7.70958E+04
11  6.61771E+04  3.55157E+04  2.49491E+04  1.76618E+04  1.26360E+04  9.17002E+03  6.70195E+03  4.92212E+03  3.69466E+03  2.84813E+03
    2.26431E+03  1.86168E+03  1.58401E+03  1.39251E+03  1.26044E+03  1.16936E+03  1.10654E+03  1.06322E+03  1.03334E+03  1.01274E+03
    9.98530E+02  9.88730E+02  1.26200E+02  2.88000E+01  4.80000E+00  2.75750E-01  4.80000E+00  2.88000E+01  1.26200E+02  2.00000E+01
    2.00000E+01  1.56904E+02  1.56904E+02  4.00000E+01  4.00000E+01  1.96130E+02  1.96130E+02  4.00000E+01  4.00000E+01  3.21800E+01
    3.21800E+01  3.21800E+01  9.50000E+00  5.16700E+01  5.16800E+01  2.83958E+03  2.84938E+03  2.86359E+03  2.88419E+03  2.91407E+03
    2.95739E+03  3.02020E+03  3.11129E+03  3.24336E+03  3.43486E+03  3.71253E+03  4.11516E+03  4.69898E+03  5.54550E+03  6.77297E+03
    8.55280E+03  1.10209E+04  1.44869E+04  1.95126E+04  2.68000E+04  3.73666E+04  5.26881E+04  7.70958E+04
12  6.61771E+04  3.55157E+04  2.49491E+04  1.76618E+04  1.26360E+04  9.17002E+03  6.70195E+03  4.92212E+03  3.69466E+03  2.84813E+03
    2.26431E+03  1.86168E+03  1.58401E+03  1.39251E+03  1.26044E+03  1.16936E+03  1.10654E+03  1.06322E+03  1.03334E+03  1.01274E+03
    9.98530E+02  9.88730E+02  1.26200E+02  2.88000E+01  4.80000E+00  2.75750E-01  4.80000E+00  2.88000E+01  1.26200E+02  2.00000E+01
    2.00000E+01  1.56904E+02  1.56904E+02  4.00000E+01  4.00000E+01  1.96130E+02  1.96130E+02  4.00000E+01  4.00000E+01  3.21800E+01
    3.21800E+01  3.21800E+01  9.50000E+00  5.16700E+01  5.16800E+01  2.83958E+03  2.84938E+03  2.86359E+03  2.88419E+03  2.91407E+03
    2.95739E+03  3.02020E+03  3.11129E+03  3.24336E+03  3.43486E+03  3.71253E+03  4.11516E+03  4.69898E+03  5.54550E+03  6.77297E+03
    8.55280E+03  1.10209E+04  1.44869E+04  1.95126E+04  2.68000E+04  3.73666E+04  5.26881E+04  7.70958E+04
13  6.61771E+04  3.55157E+04  2.49491E+04  1.76618E+04  1.26360E+04  9.17002E+03  6.70195E+03  4.92212E+03  3.69466E+03  2.84813E+03
    2.26431E+03  1.86168E+03  1.58401E+03  1.39251E+03  1.26044E+03  1.16936E+03  1.10654E+03  1.06322E+03  1.03334E+03  1.01274E+03
    9.98530E+02  9.88730E+02  1.26200E+02  2.88000E+01  4.80000E+00  2.75750E-01  4.80000E+00  2.88000E+01  1.26200E+02  2.00000E+01
    2.00000E+01  1.56904E+02  1.56904E+02  4.00000E+01  4.00000E+01  1.96130E+02  1.96130E+02  4.00000E+01  4.00000E+01  3.21800E+01
    3.21800E+01  3.21800E+01  9.50000E+00  5.16700E+01  5.16800E+01  2.83958E+03  2.84938E+03  2.86359E+03  2.88419E+03  2.91407E+03
    2.95739E+03  3.02020E+03  3.11129E+03  3.24336E+03  3.43486E+03  3.71253E+03  4.11516E+03  4.69898E+03  5.54550E+03  6.77297E+03
    8.55280E+03  1.10209E+04  1.44869E+04  1.95126E+04  2.68000E+04  3.73666E+04  5.26881E+04  7.70958E+04
14  6.61771E+04  3.55157E+04  2.49491E+04  1.76618E+04  1.26360E+04  9.17002E+03  6.70195E+03  4.92212E+03  3.69466E+03  2.84813E+03
    2.26431E+03  1.86168E+03  1.58401E+03  1.39251E+03  1.26044E+03  1.16936E+03  1.10654E+03  1.06322E+03  1.03334E+03  1.01274E+03
    9.98530E+02  9.88730E+02  1.26200E+02  2.88000E+01  4.80000E+00  2.75750E-01  4.80000E+00  2.88000E+01  1.26200E+02  2.00000E+01
    2.00000E+01  1.56904E+02  1.56904E+02  4.00000E+01  4.00000E+01  1.96130E+02  1.96130E+02  4.00000E+01  4.00000E+01  3.21800E+01
    3.21800E+01  3.21800E+01  9.50000E+00  5.16700E+01  5.16800E+01  2.83958E+03  2.84938E+03  2.86359E+03  2.88419E+03  2.91407E+03
    2.95739E+03  3.02020E+03  3.11129E+03  3.24336E+03  3.43486E+03  3.71253E+03  4.11516E+03  4.69898E+03  5.54550E+03  6.77297E+03
    8.55280E+03  1.10209E+04  1.44869E+04  1.95126E+04  2.68000E+04  3.73666E+04  5.26881E+04  7.70958E+04
15  6.61771E+04  3.55157E+04  2.49491E+04  1.76618E+04  1.26360E+04  9.17002E+03  6.70195E+03  4.92212E+03  3.69466E+03  2.84813E+03
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    2.00000E+01  1.56904E+02  1.56904E+02  4.00000E+01  4.00000E+01  1.96130E+02  1.96130E+02  4.00000E+01  4.00000E+01  3.21800E+01
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16  6.61771E+04  3.55157E+04  2.49491E+04  1.76618E+04  1.26360E+04  9.17002E+03  6.70195E+03  4.92212E+03  3.69466E+03  2.84813E+03
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17  6.61771E+04  3.55157E+04  2.49491E+04  1.76618E+04  1.26360E+04  9.17002E+03  6.70195E+03  4.92212E+03  3.69466E+03  2.84813E+03
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    2.00000E+01  1.56904E+02  1.56904E+02  4.00000E+01  4.00000E+01  1.96130E+02  1.96130E+02  4.00000E+01  4.00000E+01  3.21800E+01
```

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    3.21800E+01  3.21800E+01  9.50000E+00  5.16700E+01  5.16800E+01  2.83958E+03  2.84938E+03  2.86359E+03  2.88419E+03  2.91407E+03
    2.95739E+03  3.02020E+03  3.11129E+03  3.24336E+03  3.43486E+03  3.71253E+03  4.11516E+03  4.69898E+03  5.54550E+03  6.77297E+03
    8.55280E+03  1.10209E+04  1.44869E+04  1.95126E+04  2.68000E+04  3.73666E+04  5.26881E+04  7.70958E+04
18  6.61771E+04  3.55157E+04  2.49491E+04  1.76618E+04  1.26360E+04  9.17002E+03  6.70195E+03  4.92212E+03  3.69466E+03  2.84813E+03
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19  6.61771E+04  3.55157E+04  2.49491E+04  1.76618E+04  1.26360E+04  9.17002E+03  6.70195E+03  4.92212E+03  3.69466E+03  2.84813E+03
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25  6.61771E+04  3.55157E+04  2.49491E+04  1.76618E+04  1.26360E+04  9.17002E+03  6.70195E+03  4.92212E+03  3.69466E+03  2.84813E+03
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    8.55280E+03  1.10209E+04  1.44869E+04  1.95126E+04  2.68000E+04  3.73666E+04  5.26881E+04  7.70958E+04
28  6.61771E+04  3.55157E+04  2.49491E+04  1.76618E+04  1.26360E+04  9.17002E+03  6.70195E+03  4.92212E+03  3.69466E+03  2.84813E+03
    2.26431E+03  1.86168E+03  1.58401E+03  1.39251E+03  1.26044E+03  1.16936E+03  1.10654E+03  1.06322E+03  1.03334E+03  1.01274E+03
    9.98530E+02  9.88730E+02  1.26200E+02  2.88000E+01  4.80000E+00  2.75750E-01  4.80000E+00  2.88000E+01  1.26200E+02  2.00000E+01
    2.00000E+01  1.56904E+02  1.56904E+02  4.00000E+01  4.00000E+01  1.96130E+02  1.96130E+02  4.00000E+01  4.00000E+01  3.21800E+01
    3.21800E+01  3.21800E+01  9.50000E+00  5.16700E+01  5.16800E+01  2.83958E+03  2.84938E+03  2.86359E+03  2.88419E+03  2.91407E+03
    2.95739E+03  3.02020E+03  3.11129E+03  3.24336E+03  3.43486E+03  3.71253E+03  4.11516E+03  4.69898E+03  5.54550E+03  6.77297E+03
    8.55280E+03  1.10209E+04  1.44869E+04  1.95126E+04  2.68000E+04  3.73666E+04  5.26881E+04  7.70958E+04
29  6.61771E+04  3.55157E+04  2.49491E+04  1.76618E+04  1.26360E+04  9.17002E+03  6.70195E+03  4.92212E+03  3.69466E+03  2.84813E+03
    2.26431E+03  1.86168E+03  1.58401E+03  1.39251E+03  1.26044E+03  1.16936E+03  1.10654E+03  1.06322E+03  1.03334E+03  1.01274E+03
    9.98530E+02  9.88730E+02  1.26200E+02  2.88000E+01  4.80000E+00  2.75750E-01  4.80000E+00  2.88000E+01  1.26200E+02  2.00000E+01
    2.00000E+01  1.56904E+02  1.56904E+02  4.00000E+01  4.00000E+01  1.96130E+02  1.96130E+02  4.00000E+01  4.00000E+01  3.21800E+01
    3.21800E+01  3.21800E+01  9.50000E+00  5.16700E+01  5.16800E+01  2.83958E+03  2.84938E+03  2.86359E+03  2.88419E+03  2.91407E+03
    2.95739E+03  3.02020E+03  3.11129E+03  3.24336E+03  3.43486E+03  3.71253E+03  4.11516E+03  4.69898E+03  5.54550E+03  6.77297E+03
    8.55280E+03  1.10209E+04  1.44869E+04  1.95126E+04  2.68000E+04  3.73666E+04  5.26881E+04  7.70958E+04
30  6.61771E+04  3.55157E+04  2.49491E+04  1.76618E+04  1.26360E+04  9.17002E+03  6.70195E+03  4.92212E+03  3.69466E+03  2.84813E+03
    2.26431E+03  1.86168E+03  1.58401E+03  1.39251E+03  1.26044E+03  1.16936E+03  1.10654E+03  1.06322E+03  1.03334E+03  1.01274E+03
    9.98530E+02  9.88730E+02  1.26200E+02  2.88000E+01  4.80000E+00  2.75750E-01  4.80000E+00  2.88000E+01  1.26200E+02  2.00000E+01
    2.00000E+01  1.56904E+02  1.56904E+02  4.00000E+01  4.00000E+01  1.96130E+02  1.96130E+02  4.00000E+01  4.00000E+01  3.21800E+01
    3.21800E+01  3.21800E+01  9.50000E+00  5.16700E+01  5.16800E+01  2.83958E+03  2.84938E+03  2.86359E+03  2.88419E+03  2.91407E+03
    2.95739E+03  3.02020E+03  3.11129E+03  3.24336E+03  3.43486E+03  3.71253E+03  4.11516E+03  4.69898E+03  5.54550E+03  6.77297E+03
    8.55280E+03  1.10209E+04  1.44869E+04  1.95126E+04  2.68000E+04  3.73666E+04  5.26881E+04  7.70958E+04
31  6.61771E+04  3.55157E+04  2.49491E+04  1.76618E+04  1.26360E+04  9.17002E+03  6.70195E+03  4.92212E+03  3.69466E+03  2.84813E+03
    2.26431E+03  1.86168E+03  1.58401E+03  1.39251E+03  1.26044E+03  1.16936E+03  1.10654E+03  1.06322E+03  1.03334E+03  1.01274E+03
    9.98530E+02  9.88730E+02  1.26200E+02  2.88000E+01  4.80000E+00  2.75750E-01  4.80000E+00  2.88000E+01  1.26200E+02  2.00000E+01
    2.00000E+01  1.56904E+02  1.56904E+02  4.00000E+01  4.00000E+01  1.96130E+02  1.96130E+02  4.00000E+01  4.00000E+01  3.21800E+01
    3.21800E+01  3.21800E+01  9.50000E+00  5.16700E+01  5.16800E+01  2.83958E+03  2.84938E+03  2.86359E+03  2.88419E+03  2.91407E+03
    2.95739E+03  3.02020E+03  3.11129E+03  3.24336E+03  3.43486E+03  3.71253E+03  4.11516E+03  4.69898E+03  5.54550E+03  6.77297E+03
    8.55280E+03  1.10209E+04  1.44869E+04  1.95126E+04  2.68000E+04  3.73666E+04  5.26881E+04  7.70958E+04
32  6.61771E+04  3.55157E+04  2.49491E+04  1.76618E+04  1.26360E+04  9.17002E+03  6.70195E+03  4.92212E+03  3.69466E+03  2.84813E+03
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	2.26431E+03	1.86168E+03	1.58401E+03	1.39251E+03	1.26044E+03	1.16936E+03	1.10654E+03	1.06322E+03	1.03334E+03	1.01274E+03
	9.98530E+02	9.88730E+02	1.26200E+02	2.88000E+01	4.80000E+00	2.75750E-01	4.80000E+00	2.88000E+01	1.26200E+02	2.00000E+01
	2.00000E+01	1.56904E+02	1.56904E+02	4.00000E+01	4.00000E+01	1.96130E+02	1.96130E+02	4.00000E+01	4.00000E+01	3.21800E+01
	3.21800E+01	3.21800E+01	9.50000E+00	5.16700E+01	5.16800E+01	2.83958E+03	2.84938E+03	2.86359E+03	2.88419E+03	2.91407E+03
	2.95739E+03	3.02020E+03	3.11129E+03	3.24336E+03	3.43486E+03	3.71253E+03	4.11516E+03	4.69898E+03	5.54550E+03	6.77297E+03
	8.55280E+03	1.10209E+04	1.44869E+04	1.95126E+04	2.68000E+04	3.73666E+04	5.26881E+04	7.70958E+04		
33	6.61771E+04	3.55157E+04	2.49491E+04	1.76618E+04	1.26360E+04	9.17002E+03	6.70195E+03	4.92212E+03	3.69466E+03	2.84813E+03
	2.26431E+03	1.86168E+03	1.58401E+03	1.39251E+03	1.26044E+03	1.16936E+03	1.10654E+03	1.06322E+03	1.03334E+03	1.01274E+03
	9.98530E+02	9.88730E+02	1.26200E+02	2.88000E+01	4.80000E+00	2.75750E-01	4.80000E+00	2.88000E+01	1.26200E+02	2.00000E+01
	2.00000E+01	1.56904E+02	1.56904E+02	4.00000E+01	4.00000E+01	1.96130E+02	1.96130E+02	4.00000E+01	4.00000E+01	3.21800E+01
	3.21800E+01	3.21800E+01	9.50000E+00	5.16700E+01	5.16800E+01	2.83958E+03	2.84938E+03	2.86359E+03	2.88419E+03	2.91407E+03
	2.95739E+03	3.02020E+03	3.11129E+03	3.24336E+03	3.43486E+03	3.71253E+03	4.11516E+03	4.69898E+03	5.54550E+03	6.77297E+03
	8.55280E+03	1.10209E+04	1.44869E+04	1.95126E+04	2.68000E+04	3.73666E+04	5.26881E+04	7.70958E+04		

Grid Block Volumes m^3

	Layer 1									
1	1.01622E+11	1.39737E+10	6.76984E+09	3.30515E+09	1.63079E+09	8.16185E+08	4.44153E+08	2.24967E+08	1.16457E+08	6.19138E+07
	3.39480E+07	1.92487E+07	1.12952E+07	6.84758E+06	4.27430E+06	2.73534E+06	1.78500E+06	1.18266E+06	7.93154E+05	5.35219E+05
	3.64371E+05	2.48824E+05	6.95533E+05	3.62390E+04	1.20797E+03	9.56787E+00	1.20797E+03	3.62390E+04	6.95533E+05	3.83530E+04
	3.83530E+04	2.76800E+06	2.76800E+06	7.67060E+04	7.67060E+04	3.46000E+06	3.46000E+06	1.53412E+05	1.53412E+05	3.99657E+05
	3.99657E+05	3.99657E+05	1.19539E+04	2.35132E+06	2.35177E+06	7.14609E+05	1.03976E+06	1.51337E+06	2.21380E+06	3.24143E+06
	4.77069E+06	7.06479E+06	1.05508E+07	1.59490E+07	2.44933E+07	3.83855E+07	6.16971E+07	1.02148E+08	1.74796E+08	3.09560E+08
	5.66812E+08	9.80922E+08	1.86966E+09	3.65151E+09	7.27206E+09	1.47019E+10	3.00589E+10	7.44053E+10		
2	4.22140E+10	5.80470E+09	2.81220E+09	1.37296E+09	6.77434E+08	3.39045E+08	1.84502E+08	9.34515E+07	4.83765E+07	2.57191E+07
	1.41021E+07	7.99596E+06	4.69206E+06	2.84450E+06	1.77555E+06	1.13627E+06	7.41494E+05	4.91279E+05	3.29477E+05	2.22331E+05
	1.51360E+05	1.03362E+05	2.88926E+05	1.50538E+04	5.01792E+02	3.97451E+00	5.01792E+02	1.50538E+04	2.88926E+05	1.59319E+04
	1.59319E+04	1.14983E+06	1.14983E+06	3.18638E+04	3.18638E+04	1.43729E+06	1.43729E+06	6.37276E+04	6.37276E+04	1.66018E+05
	1.66018E+05	1.66018E+05	4.96565E+03	9.76741E+05	9.76930E+05	2.96850E+05	4.31918E+05	6.28655E+05	9.19615E+05	1.34649E+06
	1.98175E+06	2.93473E+06	4.38280E+06	6.62525E+06	1.01745E+07	1.59454E+07	2.56291E+07	4.24326E+07	7.26108E+07	1.28592E+08
	2.35455E+08	4.07477E+08	7.76661E+08	1.51684E+09	3.02083E+09	6.10721E+09	1.24865E+10	3.09081E+10		
3	5.38840E+10	7.40941E+09	3.58964E+09	1.75252E+09	8.64711E+08	4.32774E+08	2.35507E+08	1.19286E+08	6.17502E+07	3.28291E+07
	1.80006E+07	1.02064E+07	5.98918E+06	3.63086E+06	2.26640E+06	1.45039E+06	9.46479E+05	6.27092E+05	4.20561E+05	2.83794E+05
	1.93204E+05	1.31936E+05	3.68799E+05	1.92154E+04	6.40512E+02	5.07326E+00	6.40512E+02	1.92154E+04	3.68799E+05	2.03363E+04
	2.03363E+04	1.46770E+06	1.46770E+06	4.06725E+04	4.06725E+04	1.83463E+06	1.83463E+06	8.13450E+04	8.13450E+04	2.11914E+05
	2.11914E+05	2.11914E+05	6.33840E+03	1.24676E+06	1.24700E+06	3.78914E+05	5.51321E+05	8.02447E+05	1.17384E+06	1.71873E+06
	2.52960E+06	3.74603E+06	5.59442E+06	8.45679E+06	1.29873E+07	2.03535E+07	3.27142E+07	5.41630E+07	9.26839E+07	1.64141E+08
	3.00546E+08	5.20123E+08	9.91368E+08	1.93617E+09	3.85593E+09	7.79554E+09	1.59384E+10	3.94526E+10		
4	5.38840E+10	7.40941E+09	3.58964E+09	1.75252E+09	8.64711E+08	4.32774E+08	2.35507E+08	1.19286E+08	6.17502E+07	3.28291E+07
	1.80006E+07	1.02064E+07	5.98918E+06	3.63086E+06	2.26640E+06	1.45039E+06	9.46479E+05	6.27092E+05	4.20561E+05	2.83794E+05
	1.93204E+05	1.31936E+05	3.68799E+05	1.92154E+04	6.40512E+02	5.07326E+00	6.40512E+02	1.92154E+04	3.68799E+05	2.03363E+04
	2.03363E+04	1.46770E+06	1.46770E+06	4.06725E+04	4.06725E+04	1.83463E+06	1.83463E+06	8.13450E+04	8.13450E+04	2.11914E+05
	2.11914E+05	2.11914E+05	6.33840E+03	1.24676E+06	1.24700E+06	3.78914E+05	5.51321E+05	8.02447E+05	1.17384E+06	1.71873E+06
	2.52960E+06	3.74603E+06	5.59442E+06	8.45679E+06	1.29873E+07	2.03535E+07	3.27142E+07	5.41630E+07	9.26839E+07	1.64141E+08
	3.00546E+08	5.20123E+08	9.91368E+08	1.93617E+09	3.85593E+09	7.79554E+09	1.59384E+10	3.94526E+10		
5	5.30764E+10	7.29836E+09	3.53583E+09	1.72625E+09	8.51750E+08	4.26287E+08	2.31977E+08	1.17498E+08	6.08247E+07	3.23371E+07
	1.77308E+07	1.00535E+07	5.89941E+06	3.57644E+06	2.23243E+06	1.42865E+06	9.32294E+05	6.17693E+05	4.14258E+05	2.79541E+05
	1.90308E+05	1.29959E+05	3.63271E+05	1.89274E+04	6.30912E+02	4.99722E+00	6.30912E+02	1.89274E+04	3.63271E+05	2.00315E+04
	2.00315E+04	1.44570E+06	1.44570E+06	4.00629E+04	4.00629E+04	1.80713E+06	1.80713E+06	8.01258E+04	8.01258E+04	2.08738E+05
	2.08738E+05	2.08738E+05	6.24340E+03	1.22807E+06	1.22831E+06	3.73234E+05	5.43058E+05	7.90420E+05	1.15625E+06	1.69297E+06
	2.49169E+06	3.68988E+06	5.51057E+06	8.33004E+06	1.27926E+07	2.00485E+07	3.22239E+07	5.33512E+07	9.12948E+07	1.61681E+08
	2.96042E+08	5.12328E+08	9.76509E+08	1.90715E+09	3.79814E+09	7.67870E+09	1.56995E+10	3.88613E+10		

6	8.07614E+08	1.11052E+08	5.38015E+07	2.62668E+07	1.29603E+07	6.48641E+06	3.52978E+06	1.78786E+06	9.25512E+05	4.92043E+05
	2.69793E+05	1.52974E+05	8.97658E+04	5.44193E+04	3.39689E+04	2.17384E+04	1.41858E+04	9.39886E+03	6.30337E+03	4.25351E+03
	2.89574E+03	1.97746E+03	5.52756E+03	2.88000E+02	9.60000E+00	7.60381E-02	9.60000E+00	2.88000E+02	5.52756E+03	3.04800E+02
	3.04800E+02	2.19979E+04	2.19979E+04	6.09600E+02	6.09600E+02	2.74974E+04	2.74974E+04	1.21920E+03	1.21920E+03	3.17617E+03
	3.17617E+03	3.17617E+03	9.50000E+01	1.86865E+04	1.86901E+04	5.67916E+03	8.26320E+03	1.20271E+04	1.75936E+04	2.57604E+04
	3.79137E+04	5.61455E+04	8.38493E+04	1.26751E+05	1.94654E+05	3.05059E+05	4.90321E+05	8.11796E+05	1.38915E+06	2.46015E+06
	4.50459E+06	7.79561E+06	1.48586E+07	2.90194E+07	5.77928E+07	1.16840E+08	2.38885E+08	5.91316E+08		
7	6.86472E+08	9.43945E+07	4.57313E+07	2.23268E+07	1.10162E+07	5.51345E+06	3.00032E+06	1.51968E+06	7.86685E+05	4.18236E+05
	2.29324E+05	1.30028E+05	7.63010E+04	4.62564E+04	2.88735E+04	1.84776E+04	1.20580E+04	7.98904E+03	5.35787E+03	3.61548E+03
	2.46138E+03	1.68084E+03	4.69843E+03	2.44800E+02	8.16000E+00	6.46324E-02	8.16000E+00	2.44800E+02	4.69843E+03	2.59080E+02
	2.59080E+02	1.86982E+04	1.86982E+04	5.18160E+02	5.18160E+02	2.33728E+04	2.33728E+04	1.03632E+03	1.03632E+03	2.69974E+03
	2.69974E+03	2.69974E+03	8.07500E+01	1.58835E+04	1.58866E+04	4.82729E+03	7.02372E+03	1.02230E+04	1.49545E+04	2.18963E+04
	3.22267E+04	4.77237E+04	7.12719E+04	1.07738E+05	1.65455E+05	2.59300E+05	4.16773E+05	6.90026E+05	1.18078E+06	2.09112E+06
	3.82890E+06	6.62627E+06	1.26298E+07	2.46665E+07	4.91238E+07	9.93137E+07	2.03052E+08	5.02619E+08		
8	5.57253E+08	7.66261E+07	3.71230E+07	1.81241E+07	8.94260E+06	4.47563E+06	2.43555E+06	1.23362E+06	6.38604E+05	3.39510E+05
	1.86157E+05	1.05552E+05	6.19384E+04	3.75493E+04	2.34385E+04	1.49995E+04	9.78823E+03	6.48522E+03	4.34933E+03	2.93492E+03
	1.99806E+03	1.36445E+03	3.81402E+03	1.98720E+02	6.62400E+00	5.24663E-02	6.62400E+00	1.98720E+02	3.81402E+03	2.10312E+02
	2.10312E+02	1.51786E+04	1.51786E+04	4.20624E+02	4.20624E+02	1.89732E+04	1.89732E+04	8.41248E+02	8.41248E+02	2.19155E+03
	2.19155E+03	2.19155E+03	6.55500E+01	1.28937E+04	1.28961E+04	3.91862E+03	5.70161E+03	8.29868E+03	1.21396E+04	1.77747E+04
	2.61605E+04	3.87404E+04	5.78560E+04	8.74579E+04	1.34311E+05	2.10490E+05	3.38322E+05	5.60139E+05	9.58512E+05	1.69750E+06
	3.10817E+06	5.37897E+06	1.02525E+07	2.00234E+07	3.98770E+07	8.01693E+07	1.64831E+08	4.08008E+08		
9	5.57253E+08	7.66261E+07	3.71230E+07	1.81241E+07	8.94260E+06	4.47563E+06	2.43555E+06	1.23362E+06	6.38604E+05	3.39510E+05
	1.86157E+05	1.05552E+05	6.19384E+04	3.75493E+04	2.34385E+04	1.49995E+04	9.78823E+03	6.48522E+03	4.34933E+03	2.93492E+03
	1.99806E+03	1.36445E+03	3.81402E+03	1.98720E+02	6.62400E+00	5.24663E-02	6.62400E+00	1.98720E+02	3.81402E+03	2.10312E+02
	2.10312E+02	1.51786E+04	1.51786E+04	4.20624E+02	4.20624E+02	1.89732E+04	1.89732E+04	8.41248E+02	8.41248E+02	2.19155E+03
	2.19155E+03	2.19155E+03	6.55500E+01	1.28937E+04	1.28961E+04	3.91862E+03	5.70161E+03	8.29868E+03	1.21396E+04	1.77747E+04
	2.61605E+04	3.87404E+04	5.78560E+04	8.74579E+04	1.34311E+05	2.10490E+05	3.38322E+05	5.60139E+05	9.58512E+05	1.69750E+06
	3.10817E+06	5.37897E+06	1.02525E+07	2.00234E+07	3.98770E+07	8.06193E+07	1.64831E+08	4.08008E+08		
10	1.06605E+09	1.46589E+08	7.10180E+07	3.46721E+07	1.71076E+07	8.56207E+06	4.65931E+06	2.35998E+06	1.22168E+06	6.49497E+05
	3.56126E+05	2.01926E+05	1.18491E+05	7.18335E+04	4.48389E+04	2.86947E+04	1.87253E+04	1.24065E+04	8.32045E+03	5.61463E+03
	3.82237E+03	2.61025E+03	7.29638E+03	3.80160E+02	1.26720E+01	1.00370E-01	1.26720E+01	3.80160E+02	7.29638E+03	4.02336E+02
	4.02336E+02	2.90373E+04	2.90373E+04	8.04672E+02	8.04672E+02	3.62966E+04	3.62966E+04	1.60934E+03	1.60934E+03	4.19254E+03
	4.19254E+03	4.19254E+03	1.25400E+02	2.46661E+04	2.46709E+04	7.49649E+03	1.09074E+04	1.58757E+04	2.32235E+04	3.40037E+04
	5.00461E+04	7.41121E+04	1.10681E+05	1.67311E+05	2.56943E+05	4.02677E+05	6.47224E+05	1.07157E+06	1.83368E+06	3.24739E+06
	5.94606E+06	1.02902E+07	1.96134E+07	3.83056E+07	7.62864E+07	1.54228E+08	3.15328E+08	7.80538E+08		
11	1.06605E+09	1.46589E+08	7.10180E+07	3.46721E+07	1.71076E+07	8.56207E+06	4.65931E+06	2.35998E+06	1.22168E+06	6.49497E+05
	3.56126E+05	2.01926E+05	1.18491E+05	7.18335E+04	4.48389E+04	2.86947E+04	1.87253E+04	1.24065E+04	8.32045E+03	5.61463E+03
	3.82237E+03	2.61025E+03	7.29638E+03	3.80160E+02	1.26720E+01	1.00370E-01	1.26720E+01	3.80160E+02	7.29638E+03	4.02336E+02
	4.02336E+02	2.90373E+04	2.90373E+04	8.04672E+02	8.04672E+02	3.62966E+04	3.62966E+04	1.60934E+03	1.60934E+03	4.19254E+03
	4.19254E+03	4.19254E+03	1.25400E+02	2.46661E+04	2.46709E+04	7.49649E+03	1.09074E+04	1.58757E+04	2.32235E+04	3.40037E+04
	5.00461E+04	7.41121E+04	1.10681E+05	1.67311E+05	2.56943E+05	4.02677E+05	6.47224E+05	1.07157E+06	1.83368E+06	3.24739E+06
	5.94606E+06	1.02902E+07	1.96134E+07	3.83056E+07	7.62864E+07	1.54228E+08	3.15328E+08	7.80538E+08		
12	1.06605E+09	1.46589E+08	7.10180E+07	3.46721E+07	1.71076E+07	8.56207E+06	4.65931E+06	2.35998E+06	1.22168E+06	6.49497E+05
	3.56126E+05	2.01926E+05	1.18491E+05	7.18335E+04	4.48389E+04	2.86947E+04	1.87253E+04	1.24065E+04	8.32045E+03	5.61463E+03
	3.82237E+03	2.61025E+03	7.29638E+03	3.80160E+02	1.26720E+01	1.00370E-01	1.26720E+01	3.80160E+02	7.29638E+03	4.02336E+02
	4.02336E+02	2.90373E+04	2.90373E+04	8.04672E+02	8.04672E+02	3.62966E+04	3.62966E+04	1.60934E+03	1.60934E+03	4.19254E+03
	4.19254E+03	4.19254E+03	1.25400E+02	2.46661E+04	2.46709E+04	7.49649E+03	1.09074E+04	1.58757E+04	2.32235E+04	3.40037E+04
	5.00461E+04	7.41121E+04	1.10681E+05	1.67311E+05	2.56943E+05	4.02677E+05	6.47224E+05	1.07157E+06	1.83368E+06	3.24739E+06
	5.94606E+06	1.02902E+07	1.96134E+07	3.83056E+07	7.62864E+07	1.54228E+08	3.15328E+08	7.80538E+08		
13	2.11595E+09	2.90957E+08	1.40960E+08	6.88190E+07	3.39560E+07	1.69944E+07	9.24803E+06	4.68420E+06	2.42484E+06	1.28915E+06
	7.06856E+05	4.00793E+05	2.35187E+05	1.42579E+05	8.89984E+04	5.69546E+04	3.71669E+04	2.46250E+04	1.65148E+04	1.11442E+04

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    7.58683E+03  5.18095E+03  1.44822E+04  7.54560E+02  2.51520E+01  1.99220E-01  2.51520E+01  7.54560E+02  1.44822E+04  7.98576E+02
    7.98576E+02  5.76346E+04  5.76346E+04  1.59715E+03  1.59715E+03  7.20433E+04  7.20433E+04  3.19430E+03  3.19430E+03  8.32155E+03
    8.32155E+03  8.32155E+03  2.48900E+02  4.89585E+04  4.89680E+04  1.48794E+04  2.16496E+04  3.15109E+04  4.60951E+04  6.74922E+04
    9.93340E+04  1.47101E+05  2.19685E+05  3.32086E+05  5.09992E+05  7.99254E+05  1.28464E+06  2.12690E+06  3.63957E+06  6.44558E+06
    1.18020E+07  2.04245E+07  3.89296E+07  7.60308E+07  1.51417E+08  3.06120E+08  6.25878E+08  1.54925E+09
14  2.18056E+08  2.99841E+07  1.45264E+07  7.09203E+06  3.49928E+06  1.75133E+06  9.53041E+05  4.82723E+05  2.49888E+05  1.32852E+05
    7.28440E+04  4.13030E+04  2.42368E+04  1.46932E+04  9.17159E+03  5.86937E+03  3.83018E+03  2.53769E+03  1.70191E+03  1.14845E+03
    7.81849E+02  5.33914E+02  1.49244E+03  7.77600E+01  2.59200E+00  2.05303E-02  2.59200E+00  7.77600E+01  1.49244E+03  8.22960E+01
    8.22960E+01  5.93944E+03  5.93944E+03  1.64592E+02  1.64592E+02  7.42431E+03  7.42431E+03  3.29184E+02  3.29184E+02  8.57565E+02
    8.57565E+02  8.57565E+02  2.56500E+01  5.04534E+03  5.04632E+03  1.53337E+03  2.23106E+03  3.24731E+03  4.75026E+03  6.95530E+03
    1.02367E+04  1.51593E+04  2.26393E+04  3.42226E+04  5.25564E+04  8.23658E+04  1.32387E+05  2.19185E+05  3.75070E+05  6.64239E+05
    1.21624E+06  2.10482E+06  4.01183E+06  7.83523E+06  1.56040E+07  3.15467E+07  6.44989E+07  1.59655E+08
15  3.65849E+09  5.03067E+08  2.43721E+08  1.18988E+08  5.87101E+07  2.93835E+07  1.59899E+07  8.09901E+06  4.19257E+06  2.22895E+06
    1.22216E+06  6.92973E+05  4.06639E+05  2.46519E+05  1.53879E+05  9.84750E+04  6.42619E+04  4.25769E+04  2.85543E+04  1.92684E+04
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    1.43880E+04  1.43880E+04  4.30350E+02  8.46496E+04  8.46660E+04  2.57266E+04  3.74323E+04  5.44827E+04  7.96988E+04  1.16695E+05
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    2.04058E+07  3.53141E+07  6.73096E+07  1.31458E+08  2.61801E+08  5.29284E+08  1.08215E+09  2.67866E+09
16  3.65849E+09  5.03067E+08  2.43721E+08  1.18988E+08  5.87101E+07  2.93835E+07  1.59899E+07  8.09901E+06  4.19257E+06  2.22895E+06
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18  4.42007E+10  6.07789E+09  2.94456E+09  1.43758E+09  7.09317E+08  3.55001E+08  1.93185E+08  9.78497E+07  5.06533E+07  2.69295E+07
    1.47657E+07  8.37228E+06  4.91288E+06  2.97837E+06  1.85912E+06  1.18974E+06  7.76391E+05  5.14400E+05  3.44984E+05  2.32794E+05
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    1.73832E+05  1.73832E+05  5.19935E+03  1.02271E+06  1.02291E+06  3.10820E+05  4.52245E+05  6.58242E+05  9.62895E+05  1.40987E+06
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    2.46536E+08  4.26654E+08  8.13213E+08  1.58823E+09  3.16300E+09  6.39463E+09  1.30742E+10  3.23627E+10
19  4.42007E+10  6.07789E+09  2.94456E+09  1.43758E+09  7.09317E+08  3.55001E+08  1.93185E+08  9.78497E+07  5.06533E+07  2.69295E+07
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    1.66817E+04  1.20395E+06  1.20395E+06  3.33634E+04  3.33634E+04  1.50493E+06  1.50493E+06  6.67268E+04  6.67268E+04  1.73832E+05
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21  4.42007E+10  6.07789E+09  2.94456E+09  1.43758E+09  7.09317E+08  3.55001E+08  1.93185E+08  9.78497E+07  5.06533E+07  2.69295E+07
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22  4.42007E+10  6.07789E+09  2.94456E+09  1.43758E+09  7.09317E+08  3.55001E+08  1.93185E+08  9.78497E+07  5.06533E+07  2.69295E+07
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    1.47657E+07  8.37228E+06  4.91288E+06  2.97837E+06  1.85912E+06  1.18974E+06  7.76391E+05  5.14400E+05  3.44984E+05  2.32794E+05
    1.58484E+05  1.08226E+05  3.02523E+05  1.57622E+04  5.25408E+02  4.16156E+00  5.25408E+02  1.57622E+04  3.02523E+05  1.66817E+04
    1.66817E+04  1.20395E+06  1.20395E+06  3.33634E+04  3.33634E+04  1.50493E+06  1.50493E+06  6.67268E+04  6.67268E+04  1.73832E+05
    1.73832E+05  1.73832E+05  5.19935E+03  1.02271E+06  1.02291E+06  3.10820E+05  4.52245E+05  6.58242E+05  9.62895E+05  1.40987E+06
    2.07502E+06  3.07284E+06  4.58907E+06  6.93706E+06  1.06534E+07  1.66959E+07  2.68353E+07  4.44296E+07  7.60281E+07  1.34644E+08
    2.46536E+08  4.26654E+08  8.13213E+08  1.58823E+09  3.16300E+09  6.39463E+09  1.30742E+10  3.23627E+10
24  4.42007E+10  6.07789E+09  2.94456E+09  1.43758E+09  7.09317E+08  3.55001E+08  1.93185E+08  9.78497E+07  5.06533E+07  2.69295E+07
    1.47657E+07  8.37228E+06  4.91288E+06  2.97837E+06  1.85912E+06  1.18974E+06  7.76391E+05  5.14400E+05  3.44984E+05  2.32794E+05
    1.58484E+05  1.08226E+05  3.02523E+05  1.57622E+04  5.25408E+02  4.16156E+00  5.25408E+02  1.57622E+04  3.02523E+05  1.66817E+04
    1.66817E+04  1.20395E+06  1.20395E+06  3.33634E+04  3.33634E+04  1.50493E+06  1.50493E+06  6.67268E+04  6.67268E+04  1.73832E+05
    1.73832E+05  1.73832E+05  5.19935E+03  1.02271E+06  1.02291E+06  3.10820E+05  4.52245E+05  6.58242E+05  9.62895E+05  1.40987E+06
    2.07502E+06  3.07284E+06  4.58907E+06  6.93706E+06  1.06534E+07  1.66959E+07  2.68353E+07  4.44296E+07  7.60281E+07  1.34644E+08
    2.46536E+08  4.26654E+08  8.13213E+08  1.58823E+09  3.16300E+09  6.39463E+09  1.30742E+10  3.23627E+10
25  2.90741E+10  3.99788E+09  1.93685E+09  9.45604E+08  4.66570E+08  2.33511E+08  1.27072E+08  6.43630E+07  3.33184E+07  1.77135E+07
    9.71253E+06  5.50707E+06  3.23157E+06  1.95909E+06  1.22288E+06  7.82582E+05  5.10690E+05  3.38359E+05  2.26921E+05  1.53126E+05
    1.04247E+05  7.11886E+04  1.98992E+05  1.03680E+04  3.45600E+02  2.73737E+00  3.45600E+02  1.03680E+04  1.98992E+05  1.09728E+04
    1.09728E+04  7.91926E+05  7.91926E+05  2.19456E+04  2.19456E+04  9.89907E+05  9.89907E+05  4.38912E+04  4.38912E+04  1.14342E+05
    1.14342E+05  1.14342E+05  3.42000E+03  6.72712E+05  6.72843E+05  2.04450E+05  2.97475E+05  4.32975E+05  6.33368E+05  9.27374E+05
    1.36489E+06  2.02124E+06  3.01857E+06  4.56302E+06  7.00753E+06  1.09821E+07  1.76516E+07  2.92246E+07  5.00093E+07  8.85653E+07
    1.62165E+08  2.80642E+08  5.34911E+08  1.04470E+09  2.08054E+09  4.20623E+09  8.59986E+09  2.12874E+10
26  6.21863E+09  8.55103E+08  4.14271E+08  2.02254E+08  9.97942E+07  4.99454E+07  2.71793E+07  1.37665E+07  7.12644E+06  3.78873E+06
    2.07740E+06  1.17790E+06  6.91197E+05  4.19029E+05  2.61560E+05  1.67386E+05  1.09231E+05  7.23713E+04  4.85360E+04  3.27520E+04
    2.22972E+04  1.52264E+04  4.25622E+04  2.21760E+03  7.39200E+01  5.85493E-01  7.39200E+01  2.21760E+03  4.25622E+04  2.34696E+03
    2.34696E+03  1.69384E+05  1.69384E+05  4.69392E+03  4.69392E+03  2.11730E+05  2.11730E+05  9.38784E+03  9.38784E+03  2.44565E+04
    2.44565E+04  2.44565E+04  7.31500E+02  1.43886E+05  1.43914E+05  4.37295E+04  6.36267E+04  9.26085E+04  1.35470E+05  1.98355E+05
    2.91936E+05  4.32320E+05  6.45639E+05  9.75979E+05  1.49883E+06  2.34895E+06  3.77547E+06  6.25083E+06  1.06964E+07  1.89431E+07
    3.46853E+07  6.00262E+07  1.14411E+08  2.23449E+08  4.45004E+08  8.99665E+08  1.83941E+09  4.55314E+09
27  2.00288E+10  2.75410E+09  1.33428E+09  6.51416E+08  3.21415E+08  1.60863E+08  8.75386E+07  4.43390E+07  2.29527E+07  1.22027E+07
    6.69085E+06  3.79376E+06  2.22619E+06  1.34960E+06  8.42428E+05  5.39112E+05  3.51809E+05  2.33092E+05  1.56324E+05  1.05487E+05
    7.18143E+04  4.90410E+04  1.37083E+05  7.14240E+03  2.38080E+02  1.88574E+00  2.38080E+02  7.14240E+03  1.37083E+05  7.55904E+03
    7.55904E+03  5.45549E+05  5.45549E+05  1.51181E+04  1.51181E+04  6.81936E+05  6.81936E+05  3.02362E+04  3.02362E+04  7.87689E+04
    7.87689E+04  7.87689E+04  2.35600E+03  4.63424E+05  4.63514E+05  1.40843E+05  2.04927E+05  2.98272E+05  4.36320E+05  6.38857E+05
    9.40261E+05  1.39241E+06  2.07946E+06  3.14341E+06  4.82741E+06  7.56545E+06  1.21600E+07  2.01325E+07  3.44509E+07  6.10116E+07
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    1.11714E+08  1.93331E+08  3.68494E+08  7.19681E+08  1.43326E+09  2.89762E+09  5.92434E+09  1.46646E+10
28  6.86472E+09  9.43945E+08  4.57313E+08  2.23268E+08  1.10162E+08  5.51345E+07  3.00032E+07  1.51968E+07  7.86685E+06  4.18236E+06
    2.29324E+06  1.30028E+06  7.63010E+05  4.62564E+05  2.88735E+05  1.84776E+05  1.20580E+05  7.98904E+04  5.35787E+04  3.61548E+04
    2.46138E+04  1.68084E+04  4.69843E+04  2.44800E+03  8.16000E+01  6.46324E-01  8.16000E+01  2.44800E+03  4.69843E+04  2.59080E+03
    2.59080E+03  1.86982E+05  1.86982E+05  5.18160E+03  5.18160E+03  2.33728E+05  2.33728E+05  1.03632E+04  1.03632E+04  2.69974E+04
    2.69974E+04  2.69974E+04  8.07500E+02  1.58835E+05  1.58866E+05  4.82729E+04  7.02372E+04  1.02230E+05  1.49545E+05  2.18963E+05
    3.22267E+05  4.77237E+05  7.12719E+05  1.07738E+06  1.65455E+06  2.59300E+06  4.16773E+06  6.90026E+06  1.18078E+07  2.09112E+07
    3.82890E+07  6.62627E+07  1.26298E+08  2.46665E+08  4.91238E+08  9.93137E+08  2.03052E+09  5.02619E+09
29  1.39717E+10  1.92120E+09  9.30766E+08  4.54415E+08  2.24213E+08  1.12215E+08  6.10652E+07  3.09300E+07  1.60114E+07  8.51234E+06
    4.66741E+06  2.64645E+06  1.55295E+06  9.41454E+05  5.87661E+05  3.76074E+05  2.45415E+05  1.62600E+05  1.09048E+05  7.35857E+04
    5.00963E+04  3.42101E+04  9.56268E+04  4.98240E+03  1.66080E+02  1.31546E+00  1.66080E+02  4.98240E+03  9.56268E+04  5.27304E+03
    5.27304E+03  3.80564E+05  3.80564E+05  1.05461E+04  1.05461E+04  4.75705E+05  4.75705E+05  2.10922E+04  2.10922E+04  5.49477E+04
    5.49477E+04  5.49477E+04  1.64350E+03  3.23276E+05  3.23338E+05  9.82495E+04  1.42953E+05  2.08068E+05  3.04369E+05  4.45655E+05
    6.55908E+05  9.71317E+05  1.45059E+06  2.19278E+06  3.36751E+06  5.27751E+06  8.48256E+06  1.40441E+07  2.40323E+07  4.25605E+07
    7.79294E+07  1.34864E+08  2.57054E+08  5.02035E+08  9.99815E+08  2.02133E+09  4.13271E+09  1.02298E+10
30  8.56071E+10  1.17715E+10  5.70296E+09  2.78428E+09  1.37379E+09  6.87560E+08  3.74157E+08  1.89513E+08  9.81043E+07  5.21566E+07
    2.85980E+07  1.62153E+07  9.51518E+06  5.76844E+06  3.60070E+06  2.30427E+06  1.50370E+06  9.96280E+05  6.68158E+05  4.50872E+05
    3.06948E+05  2.09611E+05  5.85921E+05  3.05280E+04  1.01760E+03  8.06003E+00  1.01760E+03  3.05280E+04  5.85921E+05  3.23088E+04
    3.23088E+04  2.33178E+06  2.33178E+06  6.46176E+04  6.46176E+04  2.91473E+06  2.91473E+06  1.29235E+05  1.29235E+05  3.36674E+05
    3.36674E+05  3.36674E+05  1.00700E+04  1.98076E+06  1.98115E+06  6.01991E+05  8.75899E+05  1.27487E+06  1.86492E+06  2.73060E+06
    4.01886E+06  5.95142E+06  8.88802E+06  1.34356E+07  2.06333E+07  3.23362E+07  5.19741E+07  8.60504E+07  1.47250E+08  2.60775E+08
    4.77486E+08  8.26335E+08  1.57502E+09  3.07605E+09  6.12603E+09  1.23850E+10  2.53218E+10  6.26795E+10
31  3.49697E+10  4.80856E+09  2.32960E+09  1.13735E+09  5.61181E+08  2.80862E+08  1.52840E+08  7.74144E+07  4.00747E+07  2.13055E+07
    1.16820E+07  6.62378E+06  3.88686E+06  2.35636E+06  1.47085E+06  9.41273E+05  6.14247E+05  4.06971E+05  2.72936E+05  1.84177E+05
    1.25385E+05  8.56240E+04  2.39343E+05  1.24704E+04  4.15680E+02  3.29245E+00  4.15680E+02  1.24704E+04  2.39343E+05  1.31978E+04
    1.31978E+04  9.52511E+05  9.52511E+05  2.63957E+04  2.63957E+04  1.19064E+06  1.19064E+06  5.27914E+04  5.27914E+04  1.37528E+05
    1.37528E+05  1.37528E+05  4.11350E+03  8.09124E+05  8.09280E+05  2.45908E+05  3.57797E+05  5.20772E+05  7.61801E+05  1.11542E+06
    1.64166E+06  2.43110E+06  3.63067E+06  5.48830E+06  8.42850E+06  1.32090E+07  2.12309E+07  3.51508E+07  6.01501E+07  1.06524E+08
    1.95049E+08  3.37550E+08  6.43379E+08  1.25654E+09  2.50243E+09  5.05916E+09  1.03437E+10  2.56040E+10
32  1.26472E+10  1.73908E+09  8.42531E+08  4.11338E+08  2.02958E+08  1.01577E+08  5.52764E+07  2.79979E+07  1.44935E+07  7.70539E+06
    4.22495E+06  2.39558E+06  1.40573E+06  8.52206E+05  5.31952E+05  3.40423E+05  2.22150E+05  1.47186E+05  9.87108E+04  6.66099E+04
    4.53472E+04  3.09670E+04  8.65616E+04  4.51008E+03  1.50336E+02  1.19076E+00  1.50336E+02  4.51008E+03  8.65616E+04  4.77317E+03
    4.77317E+03  3.44488E+05  3.44488E+05  9.54634E+03  9.54634E+03  4.30610E+05  4.30610E+05  1.90927E+04  1.90927E+04  4.97388E+04
    4.97388E+04  4.97388E+04  1.48770E+03  2.92630E+05  2.92687E+05  8.89356E+04  1.29402E+05  1.88344E+05  2.75515E+05  4.03408E+05
    5.93729E+05  8.79239E+05  1.31308E+06  1.98491E+06  3.04827E+06  4.77722E+06  7.67843E+06  1.27127E+07  2.17541E+07  3.85259E+07
    7.05419E+07  1.22079E+08  2.32686E+08  4.54443E+08  9.05034E+08  1.82971E+09  3.74094E+09  9.26001E+09
33  8.07614E+07  1.11052E+07  5.38015E+06  2.62668E+06  1.29603E+06  6.48641E+05  3.52978E+05  1.78786E+05  9.25512E+04  4.92043E+04
    2.69793E+04  1.52974E+04  8.97658E+03  5.44193E+03  3.39689E+03  2.17384E+03  1.41858E+03  9.39886E+02  6.30337E+02  4.25351E+02
    2.89574E+02  1.97746E+02  5.52756E+02  2.88000E+01  9.60000E-01  7.60381E-03  9.60000E-01  2.88000E+01  5.52756E+02  3.04800E+01
    3.04800E+01  2.19979E+03  2.19979E+03  6.09600E+01  6.09600E+01  2.74974E+03  2.74974E+03  1.21920E+02  1.21920E+02  3.17617E+02
    3.17617E+02  3.17617E+02  9.50000E+00  1.86865E+03  1.86901E+03  5.67916E+02  8.26320E+02  1.20271E+03  1.75936E+03  2.57604E+03
    3.79137E+03  5.61455E+03  8.38493E+03  1.26751E+04  1.94654E+04  3.05059E+04  4.90321E+04  8.11796E+04  1.38915E+05  2.46015E+05
    4.50459E+05  7.79561E+05  1.48586E+06  2.90194E+06  5.77928E+06  1.16840E+07  2.38885E+07  5.91316E+07

*******************************************************************************
    Elapsed Time
     0.000000E+00 sec = 0.000000E+00 day = 0.000000E+00 yr
    DELT
     1.595385E+07 sec = 1.846510E+02 day = 5.055578E-01 yr
    Time Step Number  =   342
    Total Newton-Raphson Iterations          =    711
```

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    Avg Newton-Raphson Iterations/Time Step  =  2.079
********************************************************************************

    Cumulative Mass Balance
       Brine:    5.231511E-18
       Gas:     -5.757813E-17

    Maximum Relative Mass Balance (Current Time Step)
       Brine:    4.101704E-01 at (I,J,K) =   30   11    1
       Gas:      7.330456E-04 at (I,J,K) =   26   11    1
-------------------------------------------------------------------------------------------------------------------------------------
 Brine pressure                                     Pa
    Layer    1
 1  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07
    1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07
    1.59919E+07  1.59919E+07  1.33122E+07  1.33122E+07  1.33122E+07  1.33122E+07  1.33122E+07  1.33122E+07  1.33122E+07  1.33122E+07
    1.33122E+07  1.33122E+07  1.33122E+07  1.33122E+07  1.33122E+07  1.33122E+07  1.33122E+07  1.33122E+07  1.33122E+07  1.33122E+07
    1.33122E+07  1.33122E+07  1.33122E+07  1.33122E+07  1.33122E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07
    1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07
    1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07
 2  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07
    1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07
    1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07
    1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07
    1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07
    1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07
    1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07
 3  1.78561E+07  1.62469E+07  1.56926E+07  1.53104E+07  1.50468E+07  1.48650E+07  1.47356E+07  1.46423E+07  1.45779E+07  1.45335E+07
    1.45029E+07  1.44818E+07  1.44673E+07  1.44572E+07  1.44503E+07  1.44455E+07  1.44422E+07  1.44399E+07  1.44384E+07  1.44373E+07
    1.44366E+07  1.44360E+07  1.44312E+07  1.44256E+07  1.44243E+07  1.44241E+07  1.44239E+07  1.44226E+07  1.44170E+07  1.44108E+07
    1.44076E+07  1.43913E+07  1.43619E+07  1.43456E+07  1.43424E+07  1.43261E+07  1.42967E+07  1.42788E+07  1.42724E+07  1.42588E+07
    1.42381E+07  1.42174E+07  1.42060E+07  1.41671E+07  1.40912E+07  1.40531E+07  1.40526E+07  1.40518E+07  1.40508E+07  1.40492E+07
    1.40469E+07  1.40436E+07  1.40389E+07  1.40319E+07  1.40219E+07  1.40073E+07  1.39862E+07  1.39556E+07  1.39112E+07  1.38469E+07
    1.37536E+07  1.36242E+07  1.34425E+07  1.31791E+07  1.27972E+07  1.22435E+07  1.14408E+07  1.01625E+07
 4  1.70537E+07  1.54449E+07  1.48907E+07  1.45086E+07  1.42451E+07  1.40634E+07  1.39340E+07  1.38407E+07  1.37763E+07  1.37319E+07
    1.37013E+07  1.36802E+07  1.36657E+07  1.36556E+07  1.36487E+07  1.36439E+07  1.36406E+07  1.36384E+07  1.36368E+07  1.36357E+07
    1.36350E+07  1.36345E+07  1.36297E+07  1.36240E+07  1.36228E+07  1.36225E+07  1.36223E+07  1.36210E+07  1.36154E+07  1.36092E+07
    1.36060E+07  1.35897E+07  1.35603E+07  1.35440E+07  1.35408E+07  1.35245E+07  1.34951E+07  1.34772E+07  1.34708E+07  1.34573E+07
    1.34366E+07  1.34159E+07  1.34045E+07  1.33656E+07  1.32897E+07  1.32516E+07  1.32511E+07  1.32504E+07  1.32493E+07  1.32477E+07
    1.32454E+07  1.32421E+07  1.32374E+07  1.32304E+07  1.32204E+07  1.32059E+07  1.31848E+07  1.31542E+07  1.31098E+07  1.30455E+07
    1.29522E+07  1.28228E+07  1.26412E+07  1.23778E+07  1.19960E+07  1.14424E+07  1.06399E+07  9.36200E+06
 5  1.62575E+07  1.46491E+07  1.40950E+07  1.37130E+07  1.34495E+07  1.32679E+07  1.31385E+07  1.30452E+07  1.29809E+07  1.29365E+07
    1.29059E+07  1.28848E+07  1.28703E+07  1.28602E+07  1.28533E+07  1.28485E+07  1.28453E+07  1.28430E+07  1.28414E+07  1.28403E+07
    1.28396E+07  1.28391E+07  1.28343E+07  1.28286E+07  1.28274E+07  1.28271E+07  1.28269E+07  1.28257E+07  1.28200E+07  1.28138E+07
    1.28106E+07  1.27943E+07  1.27649E+07  1.27487E+07  1.27455E+07  1.27292E+07  1.26998E+07  1.26819E+07  1.26755E+07  1.26620E+07
    1.26413E+07  1.26206E+07  1.26092E+07  1.25702E+07  1.24944E+07  1.24563E+07  1.24558E+07  1.24551E+07  1.24540E+07  1.24524E+07
    1.24502E+07  1.24469E+07  1.24421E+07  1.24352E+07  1.24251E+07  1.24106E+07  1.23895E+07  1.23589E+07  1.23145E+07  1.22502E+07
    1.21570E+07  1.20276E+07  1.18461E+07  1.15828E+07  1.12010E+07  1.06476E+07  9.84531E+06  8.56768E+06
 6  1.58564E+07  1.42482E+07  1.36942E+07  1.33123E+07  1.30488E+07  1.28672E+07  1.27378E+07  1.26446E+07  1.25802E+07  1.25359E+07
    1.25053E+07  1.24842E+07  1.24696E+07  1.24596E+07  1.24523E+07  1.24440E+07  1.24260E+07  1.23916E+07  1.23443E+07  1.22933E+07
    1.22464E+07  1.22072E+07  1.21519E+07  1.21462E+07  1.21450E+07  1.21448E+07  1.21445E+07  1.21433E+07  1.21377E+07  1.21318E+07
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	1.21287E+07	1.21126E+07	1.20839E+07	1.20681E+07	1.20650E+07	1.20489E+07	1.20202E+07	1.20029E+07	1.19967E+07	1.19833E+07
	1.19631E+07	1.19429E+07	1.19317E+07	1.18937E+07	1.18196E+07	1.20280E+07	1.20324E+07	1.20375E+07	1.20425E+07	1.20463E+07
	1.20476E+07	1.20459E+07	1.20415E+07	1.20346E+07	1.20245E+07	1.20100E+07	1.19889E+07	1.19583E+07	1.19140E+07	1.18497E+07
	1.17564E+07	1.16271E+07	1.14455E+07	1.11823E+07	1.08006E+07	1.02472E+07	9.44504E+06	8.16757E+06		
7	1.58453E+07	1.42371E+07	1.36831E+07	1.33011E+07	1.30377E+07	1.28561E+07	1.27267E+07	1.26335E+07	1.25691E+07	1.25248E+07
	1.24942E+07	1.24731E+07	1.24584E+07	1.24450E+07	1.23791E+07	1.19517E+07	1.06348E+07	8.53736E+06	6.29282E+06	4.32195E+06
	2.75607E+06	1.57570E+06	1.48525E+05	1.41471E+05	1.40198E+05	1.39955E+05	1.39710E+05	1.38456E+05	1.32840E+05	1.34537E+05
	1.34667E+05	1.32840E+05	1.32831E+05	1.34487E+05	1.34638E+05	1.32835E+05	1.32826E+05	1.34524E+05	1.34554E+05	1.32829E+05
	1.32824E+05	1.32820E+05	1.34632E+05	1.32819E+05	1.33053E+05	1.03582E+07	1.05774E+07	1.08568E+07	1.11883E+07	1.15352E+07
	1.18241E+07	1.19820E+07	1.20240E+07	1.20231E+07	1.20134E+07	1.19989E+07	1.19778E+07	1.19472E+07	1.19029E+07	1.18386E+07
	1.17453E+07	1.16160E+07	1.14344E+07	1.11712E+07	1.07895E+07	1.02361E+07	9.43395E+06	8.15648E+06		
8	1.58360E+07	1.42278E+07	1.36739E+07	1.32919E+07	1.30285E+07	1.28468E+07	1.27175E+07	1.26242E+07	1.25599E+07	1.25155E+07
	1.24849E+07	1.24638E+07	1.24493E+07	1.24392E+07	1.24315E+07	1.24194E+07	1.23858E+07	1.23172E+07	1.22215E+07	1.21181E+07
	1.20226E+07	1.18743E+07	1.38657E+05	1.32217E+05	1.30951E+05	1.30708E+05	1.30466E+05	1.29211E+05	1.23596E+05	1.23572E+05
	1.23642E+05	1.23594E+05	1.23589E+05	1.23561E+05	1.23623E+05	1.23589E+05	1.23584E+05	1.23571E+05	1.23582E+05	1.23584E+05
	1.23580E+05	1.23578E+05	1.01325E+05	1.23575E+05	1.23709E+05	1.19124E+07	1.19879E+07	1.19991E+07	1.20106E+07	1.20201E+07
	1.20252E+07	1.20251E+07	1.20211E+07	1.20142E+07	1.20042E+07	1.19896E+07	1.19686E+07	1.19380E+07	1.18936E+07	1.18293E+07
	1.17361E+07	1.16068E+07	1.14252E+07	1.11619E+07	1.07803E+07	1.02269E+07	9.42471E+06	8.14724E+06		
9	1.58278E+07	1.42196E+07	1.36656E+07	1.32836E+07	1.30202E+07	1.28385E+07	1.27092E+07	1.26159E+07	1.25516E+07	1.25072E+07
	1.24767E+07	1.24556E+07	1.24410E+07	1.24310E+07	1.24240E+07	1.24192E+07	1.24157E+07	1.24128E+07	1.24101E+07	1.24077E+07
	1.24056E+07	1.23331E+07	1.29812E+05	1.23921E+05	1.22663E+05	1.22422E+05	1.22181E+05	1.20927E+05	1.15311E+05	1.15299E+05
	1.15334E+05	1.15309E+05	1.15306E+05	1.15291E+05	1.15322E+05	1.15304E+05	1.15301E+05	1.15294E+05	1.15298E+05	1.15299E+05
	1.15296E+05	1.15295E+05	1.01325E+05	1.15291E+05	1.15334E+05	1.19587E+07	1.20260E+07	1.20255E+07	1.20246E+07	1.20231E+07
	1.20209E+07	1.20176E+07	1.20129E+07	1.20059E+07	1.19959E+07	1.19814E+07	1.19603E+07	1.19297E+07	1.18853E+07	1.18210E+07
	1.17278E+07	1.15985E+07	1.14169E+07	1.11537E+07	1.07720E+07	1.02186E+07	9.41643E+06	8.13897E+06		
10	1.58157E+07	1.42075E+07	1.36535E+07	1.32715E+07	1.30081E+07	1.28265E+07	1.26971E+07	1.26039E+07	1.25395E+07	1.24952E+07
	1.24646E+07	1.24435E+07	1.24289E+07	1.24189E+07	1.24120E+07	1.24072E+07	1.24039E+07	1.24016E+07	1.24001E+07	1.23990E+07
	1.23982E+07	1.23268E+07	1.28039E+05	1.28039E+05	1.28039E+05	1.28039E+05	1.28039E+05	1.28039E+05	1.28039E+05	1.01325E+05
	1.01325E+05	1.28039E+05	1.28039E+05	1.01325E+05	1.01325E+05	1.28039E+05	1.28039E+05	1.01325E+05	1.01325E+05	1.01325E+05
	1.01325E+05	1.01325E+05	1.01325E+05	1.01325E+05	1.01325E+05	1.19460E+07	1.20145E+07	1.20138E+07	1.20127E+07	1.20111E+07
	1.20089E+07	1.20056E+07	1.20008E+07	1.19939E+07	1.19838E+07	1.19693E+07	1.19482E+07	1.19176E+07	1.18733E+07	1.18090E+07
	1.17157E+07	1.15864E+07	1.14048E+07	1.11416E+07	1.07599E+07	1.02066E+07	9.40437E+06	8.12692E+06		
11	1.57998E+07	1.41916E+07	1.36377E+07	1.32557E+07	1.29923E+07	1.28106E+07	1.26813E+07	1.25880E+07	1.25237E+07	1.24793E+07
	1.24487E+07	1.24276E+07	1.24131E+07	1.24030E+07	1.23961E+07	1.23914E+07	1.23881E+07	1.23858E+07	1.23842E+07	1.23831E+07
	1.23823E+07	1.23110E+07	1.28039E+05	1.28039E+05	1.28039E+05	1.28039E+05	1.28039E+05	1.28039E+05	1.28039E+05	1.01325E+05
	1.01325E+05	1.28039E+05	1.28039E+05	1.01325E+05	1.01325E+05	1.28039E+05	1.28039E+05	1.01325E+05	1.01325E+05	1.01325E+05
	1.01325E+05	1.01325E+05	1.01325E+05	1.01325E+05	1.01325E+05	1.19303E+07	1.19986E+07	1.19979E+07	1.19968E+07	1.19953E+07
	1.19930E+07	1.19897E+07	1.19849E+07	1.19780E+07	1.19680E+07	1.19534E+07	1.19324E+07	1.19018E+07	1.18574E+07	1.17931E+07
	1.16999E+07	1.15706E+07	1.13890E+07	1.11257E+07	1.07441E+07	1.01907E+07	9.38854E+06	8.11109E+06		
12	1.57839E+07	1.41758E+07	1.36218E+07	1.32398E+07	1.29764E+07	1.27948E+07	1.26654E+07	1.25722E+07	1.25078E+07	1.24635E+07
	1.24329E+07	1.24118E+07	1.23972E+07	1.23872E+07	1.23803E+07	1.23755E+07	1.23722E+07	1.23699E+07	1.23684E+07	1.23673E+07
	1.23664E+07	1.22952E+07	1.28039E+05	1.28039E+05	1.28039E+05	1.28039E+05	1.28039E+05	1.28039E+05	1.28039E+05	1.01325E+05
	1.01325E+05	1.28039E+05	1.28039E+05	1.01325E+05	1.01325E+05	1.28039E+05	1.28039E+05	1.01325E+05	1.01325E+05	1.01325E+05
	1.01325E+05	1.01325E+05	1.01325E+05	1.01325E+05	1.01325E+05	1.19145E+07	1.19828E+07	1.19821E+07	1.19810E+07	1.19794E+07
	1.19772E+07	1.19739E+07	1.19691E+07	1.19622E+07	1.19522E+07	1.19376E+07	1.19165E+07	1.18859E+07	1.18416E+07	1.17773E+07
	1.16840E+07	1.15547E+07	1.13732E+07	1.11099E+07	1.07282E+07	1.01749E+07	9.37270E+06	8.09526E+06		
13	1.57603E+07	1.41521E+07	1.35981E+07	1.32162E+07	1.29528E+07	1.27711E+07	1.26418E+07	1.25485E+07	1.24842E+07	1.24398E+07
	1.24092E+07	1.23881E+07	1.23736E+07	1.23635E+07	1.23566E+07	1.23513E+07	1.23458E+07	1.23389E+07	1.23307E+07	1.23224E+07
	1.23150E+07	1.22392E+07	1.03242E+05	1.03238E+05	1.03226E+05	1.03240E+05	1.03251E+05	1.03242E+05	1.03240E+05	1.03266E+05
	1.03265E+05	1.03238E+05	1.03236E+05	1.03259E+05	1.03259E+05	1.03234E+05	1.03232E+05	1.03251E+05	1.03249E+05	1.03229E+05
	1.03228E+05	1.03231E+05	1.01325E+05	1.03223E+05	1.03218E+05	1.18889E+07	1.19558E+07	1.19560E+07	1.19558E+07	1.19550E+07

	1.19532E+07	1.19502E+07	1.19454E+07	1.19385E+07	1.19285E+07	1.19139E+07	1.18929E+07	1.18623E+07	1.18179E+07	1.17536E+07
	1.16604E+07	1.15311E+07	1.13495E+07	1.10863E+07	1.07046E+07	1.01512E+07	9.34907E+06	8.07163E+06		
14	1.57429E+07	1.41347E+07	1.35808E+07	1.31988E+07	1.29354E+07	1.27537E+07	1.26244E+07	1.25311E+07	1.24668E+07	1.24225E+07
	1.23919E+07	1.23708E+07	1.23561E+07	1.23427E+07	1.22758E+07	1.18408E+07	1.04992E+07	8.37227E+06	6.11929E+06	4.16458E+06
	2.62835E+06	1.48054E+06	1.01949E+05	1.01964E+05	1.01825E+05	1.01988E+05	1.02140E+05	1.01989E+05	1.01971E+05	1.08677E+05
	1.09096E+05	1.01994E+05	1.01980E+05	1.05471E+05	1.06488E+05	1.01976E+05	1.01964E+05	9.93009E+04	9.52331E+04	1.01899E+05
	1.01985E+05	1.02223E+05	1.06623E+05	1.01999E+05	1.01951E+05	1.02433E+07	1.04615E+07	1.07408E+07	1.10740E+07	1.14247E+07
	1.17182E+07	1.18789E+07	1.19216E+07	1.19208E+07	1.19111E+07	1.18966E+07	1.18755E+07	1.18449E+07	1.18006E+07	1.17363E+07
	1.16430E+07	1.15137E+07	1.13322E+07	1.10689E+07	1.06872E+07	1.01339E+07	9.33173E+06	8.05431E+06		
15	1.57140E+07	1.41059E+07	1.35519E+07	1.31700E+07	1.29066E+07	1.27249E+07	1.25956E+07	1.25023E+07	1.24380E+07	1.23936E+07
	1.23631E+07	1.23420E+07	1.23274E+07	1.23174E+07	1.23104E+07	1.23055E+07	1.23015E+07	1.22976E+07	1.22939E+07	1.22904E+07
	1.22874E+07	1.22166E+07	9.59324E+04	9.67434E+04	9.66825E+04	9.66610E+04	9.66398E+04	9.65057E+04	9.64728E+04	1.04449E+05
	1.05221E+05	9.66708E+04	9.65639E+04	9.78674E+04	9.98524E+04	9.65489E+04	9.64537E+04	8.50063E+04	7.64862E+04	9.58982E+04
	9.66514E+04	9.88634E+04	1.01325E+05	9.68310E+04	9.63812E+04	1.18468E+07	1.19118E+07	1.19114E+07	1.19106E+07	1.19094E+07
	1.19073E+07	1.19040E+07	1.18993E+07	1.18924E+07	1.18823E+07	1.18678E+07	1.18467E+07	1.18161E+07	1.17718E+07	1.17074E+07
	1.16142E+07	1.14849E+07	1.13034E+07	1.10401E+07	1.06584E+07	1.01051E+07	9.30294E+06	8.02552E+06		
16	1.56596E+07	1.40515E+07	1.34975E+07	1.31156E+07	1.28522E+07	1.26705E+07	1.25412E+07	1.24479E+07	1.23836E+07	1.23393E+07
	1.23087E+07	1.22876E+07	1.22730E+07	1.22630E+07	1.22561E+07	1.22513E+07	1.22479E+07	1.22456E+07	1.22438E+07	1.22426E+07
	1.22416E+07	1.21735E+07	8.40600E+04	8.64075E+04	8.63962E+04	8.56865E+04	8.49621E+04	8.45570E+04	8.45393E+04	6.17844E+04
	6.07829E+04	8.56017E+04	8.50499E+04	5.23989E+04	5.45901E+04	8.49893E+04	8.45113E+04	3.56245E+04	2.51305E+04	8.13954E+04
	8.55308E+04	9.54096E+04	1.01325E+05	8.65885E+04	8.45168E+04	1.17947E+07	1.18586E+07	1.18579E+07	1.18568E+07	1.18552E+07
	1.18530E+07	1.18497E+07	1.18449E+07	1.18380E+07	1.18279E+07	1.18134E+07	1.17923E+07	1.17617E+07	1.17174E+07	1.16531E+07
	1.15598E+07	1.14305E+07	1.12490E+07	1.09857E+07	1.06041E+07	1.00507E+07	9.24860E+06	7.97120E+06		
17	1.56313E+07	1.40232E+07	1.34692E+07	1.30873E+07	1.28239E+07	1.26423E+07	1.25129E+07	1.24197E+07	1.23553E+07	1.23110E+07
	1.22804E+07	1.22593E+07	1.22447E+07	1.22345E+07	1.22238E+07	1.21895E+07	1.20815E+07	1.18868E+07	1.16535E+07	1.14316E+07
	1.12455E+07	1.11003E+07	5.61288E+04	5.82421E+04	5.82167E+04	5.75179E+04	5.68028E+04	5.63925E+04	5.63736E+04	3.36202E+04
	3.26198E+04	5.74374E+04	5.68843E+04	2.42332E+04	2.64266E+04	5.68249E+04	5.63456E+04	7.46066E+03	-3.03177E+03	5.32306E+04
	5.73664E+04	6.72472E+04	2.51138E+05	5.84230E+04	5.63560E+04	1.18096E+07	1.18119E+07	1.18147E+07	1.18178E+07	1.18207E+07
	1.18221E+07	1.18208E+07	1.18165E+07	1.18097E+07	1.17997E+07	1.17851E+07	1.17640E+07	1.17334E+07	1.16891E+07	1.16248E+07
	1.15316E+07	1.14023E+07	1.12207E+07	1.09575E+07	1.05758E+07	1.00225E+07	9.22035E+06	7.94296E+06		
18	1.53013E+07	1.36934E+07	1.31395E+07	1.27576E+07	1.24942E+07	1.23126E+07	1.21833E+07	1.20900E+07	1.20257E+07	1.19813E+07
	1.19507E+07	1.19296E+07	1.19151E+07	1.19051E+07	1.18981E+07	1.18934E+07	1.18901E+07	1.18878E+07	1.18862E+07	1.18852E+07
	1.18844E+07	1.18839E+07	1.18790E+07	1.18734E+07	1.18721E+07	1.18719E+07	1.18717E+07	1.18704E+07	1.18648E+07	1.18586E+07
	1.18554E+07	1.18391E+07	1.18097E+07	1.17934E+07	1.17902E+07	1.17740E+07	1.17446E+07	1.17267E+07	1.17203E+07	1.17068E+07
	1.16861E+07	1.16654E+07	1.01325E+05	1.16151E+07	1.15393E+07	1.15013E+07	1.15008E+07	1.15000E+07	1.14989E+07	1.14974E+07
	1.14951E+07	1.14918E+07	1.14870E+07	1.14801E+07	1.14701E+07	1.14555E+07	1.14344E+07	1.14039E+07	1.13595E+07	1.12952E+07
	1.12020E+07	1.10727E+07	1.08912E+07	1.06280E+07	1.02463E+07	9.69309E+06	8.89103E+06	7.61377E+06		
19	1.46436E+07	1.30360E+07	1.24822E+07	1.21004E+07	1.18370E+07	1.16555E+07	1.15262E+07	1.14329E+07	1.13686E+07	1.13243E+07
	1.12937E+07	1.12726E+07	1.12581E+07	1.12480E+07	1.12411E+07	1.12364E+07	1.12331E+07	1.12308E+07	1.12292E+07	1.12282E+07
	1.12274E+07	1.12269E+07	1.12221E+07	1.12165E+07	1.12152E+07	1.12150E+07	1.12147E+07	1.12135E+07	1.12078E+07	1.12016E+07
	1.11985E+07	1.11822E+07	1.11528E+07	1.11365E+07	1.11333E+07	1.11170E+07	1.10877E+07	1.10698E+07	1.10634E+07	1.10499E+07
	1.10292E+07	1.10085E+07	1.01325E+05	1.09582E+07	1.08824E+07	1.08443E+07	1.08438E+07	1.08431E+07	1.08420E+07	1.08404E+07
	1.08382E+07	1.08349E+07	1.08301E+07	1.08232E+07	1.08131E+07	1.07986E+07	1.07775E+07	1.07469E+07	1.07026E+07	1.06383E+07
	1.05451E+07	1.04159E+07	1.02344E+07	9.97120E+06	9.58966E+06	9.03651E+06	8.23461E+06	6.95762E+06		
20	1.39860E+07	1.23787E+07	1.18251E+07	1.14433E+07	1.11800E+07	1.09985E+07	1.08692E+07	1.07760E+07	1.07117E+07	1.06674E+07
	1.06368E+07	1.06157E+07	1.06012E+07	1.05911E+07	1.05842E+07	1.05795E+07	1.05762E+07	1.05739E+07	1.05723E+07	1.05713E+07
	1.05705E+07	1.05700E+07	1.05652E+07	1.05596E+07	1.05583E+07	1.05581E+07	1.05578E+07	1.05566E+07	1.05509E+07	1.05448E+07
	1.05416E+07	1.05253E+07	1.04959E+07	1.04796E+07	1.04764E+07	1.04602E+07	1.04308E+07	1.04129E+07	1.04065E+07	1.03930E+07
	1.03723E+07	1.03516E+07	1.01325E+05	1.03013E+07	1.02256E+07	1.01875E+07	1.01870E+07	1.01863E+07	1.01852E+07	1.01836E+07
	1.01813E+07	1.01781E+07	1.01733E+07	1.01664E+07	1.01563E+07	1.01418E+07	1.01207E+07	1.00901E+07	1.00458E+07	9.98155E+06
	9.88836E+06	9.75914E+06	9.57767E+06	9.31456E+06	8.93310E+06	8.38006E+06	7.57833E+06	6.30159E+06		

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21  1.33285E+07  1.17216E+07  1.11680E+07  1.07864E+07  1.05232E+07  1.03416E+07  1.02124E+07  1.01192E+07  1.00549E+07  1.00106E+07
    9.98003E+06  9.95895E+06  9.94441E+06  9.93438E+06  9.92747E+06  9.92270E+06  9.91941E+06  9.91714E+06  9.91558E+06  9.91450E+06
    9.91376E+06  9.91324E+06  9.90845E+06  9.90281E+06  9.90156E+06  9.90132E+06  9.90108E+06  9.89982E+06  9.89419E+06  9.88801E+06
    9.88482E+06  9.86854E+06  9.83918E+06  9.82290E+06  9.81971E+06  9.80343E+06  9.77407E+06  9.75619E+06  9.74981E+06  9.73628E+06
    9.71561E+06  9.69492E+06  1.01325E+05  9.64464E+06  9.56891E+06  9.53083E+06  9.53032E+06  9.52957E+06  9.52850E+06  9.52693E+06
    9.52467E+06  9.52138E+06  9.51661E+06  9.50969E+06  9.49967E+06  9.48513E+06  9.46405E+06  9.43349E+06  9.38917E+06  9.32491E+06
    9.23174E+06  9.10254E+06  8.92112E+06  8.65806E+06  8.27668E+06  7.72375E+06  6.92218E+06  5.64570E+06
22  1.26712E+07  1.10646E+07  1.05112E+07  1.01296E+07  9.86640E+06  9.68493E+06  9.55571E+06  9.46254E+06  9.39828E+06  9.35396E+06
    9.32340E+06  9.30232E+06  9.28778E+06  9.27776E+06  9.27084E+06  9.26607E+06  9.26279E+06  9.26052E+06  9.25895E+06  9.25788E+06
    9.25713E+06  9.25662E+06  9.25182E+06  9.24619E+06  9.24494E+06  9.24470E+06  9.24446E+06  9.24320E+06  9.23757E+06  9.23139E+06
    9.22820E+06  9.21192E+06  9.18257E+06  9.16629E+06  9.16310E+06  9.14683E+06  9.11747E+06  9.09960E+06  9.09322E+06  9.07970E+06
    9.05903E+06  9.03834E+06  1.01325E+05  8.98807E+06  8.91236E+06  8.87429E+06  8.87377E+06  8.87303E+06  8.87195E+06  8.87039E+06
    8.86812E+06  8.86483E+06  8.86006E+06  8.85315E+06  8.84313E+06  8.82859E+06  8.80752E+06  8.77696E+06  8.73265E+06  8.66841E+06
    8.57525E+06  8.44608E+06  8.26469E+06  8.00169E+06  7.62039E+06  7.06757E+06  6.26616E+06  4.98995E+06
23  1.20140E+07  1.04077E+07  9.85443E+06  9.47289E+06  9.20979E+06  9.02835E+06  8.89916E+06  8.80600E+06  8.74176E+06  8.69745E+06
    8.66689E+06  8.64582E+06  8.63128E+06  8.62126E+06  8.61435E+06  8.60958E+06  8.60630E+06  8.60403E+06  8.60246E+06  8.60139E+06
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    8.57171E+06  8.55544E+06  8.52609E+06  8.50982E+06  8.50663E+06  8.49036E+06  8.46101E+06  8.44314E+06  8.43676E+06  8.42324E+06
    8.40258E+06  8.38190E+06  1.01325E+05  8.33164E+06  8.25594E+06  8.21787E+06  8.21736E+06  8.21662E+06  8.21554E+06  8.21398E+06
    8.21171E+06  8.20842E+06  8.20365E+06  8.19674E+06  8.18672E+06  8.17219E+06  8.15112E+06  8.12057E+06  8.07627E+06  8.01204E+06
    7.91890E+06  7.78976E+06  7.60841E+06  7.34546E+06  6.96423E+06  6.41153E+06  5.61028E+06  4.33433E+06
24  1.13570E+07  9.75101E+06  9.19781E+06  8.81636E+06  8.55331E+06  8.37191E+06  8.24275E+06  8.14960E+06  8.08537E+06  8.04107E+06
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25  2.28313E+06  2.28313E+06  2.28313E+06  2.28313E+06  2.28313E+06  2.28313E+06  2.28313E+06  2.28313E+06  2.28313E+06  2.28313E+06
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27  1.82702E+06  1.82702E+06  1.82702E+06  1.82702E+06  1.82702E+06  1.82702E+06  1.82702E+06  1.82702E+06  1.82702E+06  1.82702E+06
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28  9.63100E+05  9.63100E+05  9.63100E+05  9.63100E+05  9.63100E+05  9.63100E+05  9.63100E+05  9.63100E+05  9.63100E+05  9.63100E+05
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31  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05
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32  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05
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    1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05
    1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05
    1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05
    1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05
    1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05
33  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05
    1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05
    1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05
    1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05
    1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05
    1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05
    1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05
----------------------------------------------------------------------------------------------------------------------------------

********************************************************************************
    Elapsed Time
     3.155700E+11 sec = 3.652431E+06 day = 1.000003E+04 yr
    DELT
     3.000000E+06 sec = 3.472222E+01 day = 9.506631E-02 yr
    Time Step Number  =  2381
    Total Newton-Raphson Iterations            =    6811
    Avg Newton-Raphson Iterations/Time Step    =   2.861
********************************************************************************
```

```
    Cumulative Mass Balance
       Brine:   -1.092837E-18
       Gas:     -8.412219E-16

    Maximum Relative Mass Balance (Current Time Step)
       Brine:   -9.221946E+00 at (I,J,K) =    44    12     1
       Gas:      1.234699E-01 at (I,J,K) =    40    11     1
------------------------------------------------------------------------------------------------------------------------------------
 Brine pressure                                   Pa
    Layer    1
 1  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07
    1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07
    1.59919E+07  1.59919E+07  1.24245E+07  1.24245E+07  1.24245E+07  1.24245E+07  1.24245E+07  1.24245E+07  1.24245E+07  1.24245E+07
    1.24245E+07  1.24245E+07  1.24245E+07  1.24245E+07  1.24245E+07  1.24245E+07  1.24245E+07  1.24245E+07  1.24245E+07  1.24245E+07
    1.24245E+07  1.24245E+07  1.24245E+07  1.24245E+07  1.24245E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07
    1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07
    1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07  1.59919E+07
 2  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07
    1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07
    1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.22005E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07
    1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07
    1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07
    1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07
    1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07  1.49213E+07
 3  1.78561E+07  1.62469E+07  1.56926E+07  1.53104E+07  1.50468E+07  1.48650E+07  1.47356E+07  1.46423E+07  1.45779E+07  1.45335E+07
    1.45029E+07  1.44818E+07  1.44673E+07  1.44572E+07  1.44503E+07  1.44455E+07  1.44422E+07  1.44399E+07  1.44384E+07  1.44373E+07
    1.44366E+07  1.44360E+07  1.44302E+07  1.42526E+07  1.30538E+07  1.22685E+07  1.30533E+07  1.42496E+07  1.44159E+07  1.44107E+07
    1.44076E+07  1.43913E+07  1.43619E+07  1.43456E+07  1.43424E+07  1.43261E+07  1.42967E+07  1.42788E+07  1.42724E+07  1.42588E+07
    1.42381E+07  1.42174E+07  1.42060E+07  1.41671E+07  1.40912E+07  1.40531E+07  1.40526E+07  1.40518E+07  1.40508E+07  1.40492E+07
    1.40469E+07  1.40436E+07  1.40389E+07  1.40319E+07  1.40219E+07  1.40073E+07  1.39862E+07  1.39556E+07  1.39112E+07  1.38469E+07
    1.37536E+07  1.36242E+07  1.34425E+07  1.31791E+07  1.27972E+07  1.22435E+07  1.14408E+07  1.01625E+07
 4  1.70537E+07  1.54449E+07  1.48907E+07  1.45086E+07  1.42451E+07  1.40634E+07  1.39340E+07  1.38407E+07  1.37763E+07  1.37319E+07
    1.37013E+07  1.36802E+07  1.36657E+07  1.36556E+07  1.36487E+07  1.36439E+07  1.36406E+07  1.36384E+07  1.36368E+07  1.36357E+07
    1.36350E+07  1.36345E+07  1.36292E+07  1.35424E+07  1.27307E+07  1.20998E+07  1.27302E+07  1.35394E+07  1.36149E+07  1.36092E+07
    1.36060E+07  1.35897E+07  1.35603E+07  1.35440E+07  1.35407E+07  1.35243E+07  1.34949E+07  1.34770E+07  1.34706E+07  1.34570E+07
    1.34363E+07  1.34156E+07  1.34042E+07  1.33653E+07  1.32894E+07  1.32516E+07  1.32511E+07  1.32503E+07  1.32492E+07  1.32477E+07
    1.32454E+07  1.32421E+07  1.32374E+07  1.32304E+07  1.32204E+07  1.32059E+07  1.31847E+07  1.31541E+07  1.31098E+07  1.30455E+07
    1.29522E+07  1.28228E+07  1.26412E+07  1.23778E+07  1.19960E+07  1.14424E+07  1.06399E+07  9.36200E+06
 5  1.62575E+07  1.46491E+07  1.40950E+07  1.37130E+07  1.34495E+07  1.32679E+07  1.31385E+07  1.30452E+07  1.29809E+07  1.29365E+07
    1.29059E+07  1.28850E+07  1.28708E+07  1.28613E+07  1.28549E+07  1.28504E+07  1.28473E+07  1.28450E+07  1.28434E+07  1.28422E+07
    1.28414E+07  1.28409E+07  1.28351E+07  1.28385E+07  1.24112E+07  1.19322E+07  1.24107E+07  1.28356E+07  1.28209E+07  1.28147E+07
    1.28115E+07  1.27952E+07  1.27659E+07  1.27358E+07  1.27056E+07  1.26727E+07  1.26431E+07  1.26088E+07  1.25769E+07  1.25486E+07
    1.25279E+07  1.25074E+07  1.24962E+07  1.24576E+07  1.23826E+07  1.24396E+07  1.24392E+07  1.24388E+07  1.24384E+07  1.24379E+07
    1.24369E+07  1.24354E+07  1.24328E+07  1.24283E+07  1.24208E+07  1.24084E+07  1.23887E+07  1.23587E+07  1.23145E+07  1.22502E+07
    1.21570E+07  1.20276E+07  1.18461E+07  1.15828E+07  1.12010E+07  1.06476E+07  9.84531E+06  8.56768E+06
 6  1.58564E+07  1.42482E+07  1.36942E+07  1.33123E+07  1.30488E+07  1.28672E+07  1.27378E+07  1.26445E+07  1.25806E+07  1.25440E+07
    1.25472E+07  1.25852E+07  1.26174E+07  1.26077E+07  1.25528E+07  1.24739E+07  1.23920E+07  1.23189E+07  1.22592E+07  1.22132E+07
    1.21791E+07  1.21561E+07  1.20024E+07  1.19964E+07  1.19609E+07  1.18480E+07  1.19605E+07  1.19934E+07  1.19879E+07  1.19817E+07
    1.19785E+07  1.19622E+07  1.19616E+07  1.13388E+07  9.96502E+06  9.22437E+06  9.21459E+06  6.86823E+06  4.12128E+06  3.07182E+06
    3.05107E+06  3.03888E+06  3.05052E+06  3.04871E+06  3.04855E+06  1.01375E+07  1.01612E+07  1.02002E+07  1.02573E+07  1.03384E+07
```

	1.04518E+07	1.06066E+07	1.08103E+07	1.10631E+07	1.13478E+07	1.16217E+07	1.18239E+07	1.19137E+07	1.19075E+07	1.18492E+07
	1.17564E+07	1.16271E+07	1.14455E+07	1.11823E+07	1.08006E+07	1.02472E+07	9.44505E+06	8.16758E+06		
7	1.58453E+07	1.42371E+07	1.36831E+07	1.33011E+07	1.30377E+07	1.28561E+07	1.27267E+07	1.26334E+07	1.25696E+07	1.25334E+07
	1.25362E+07	1.25692E+07	1.25888E+07	1.25618E+07	1.24908E+07	1.23982E+07	1.23048E+07	1.22224E+07	1.21557E+07	1.21044E+07
	1.20663E+07	1.20387E+07	1.18703E+07	1.18643E+07	1.18564E+07	1.18456E+07	1.18559E+07	1.18613E+07	1.18558E+07	1.18496E+07
	1.18464E+07	1.18302E+07	1.18299E+07	1.12314E+07	9.89702E+06	9.18230E+06	9.17292E+06	6.79302E+06	4.03467E+06	3.00088E+06
	2.98022E+06	2.96817E+06	2.98020E+06	2.97899E+06	2.98007E+06	1.00983E+07	1.01241E+07	1.01634E+07	1.02207E+07	1.03022E+07
	1.04161E+07	1.05717E+07	1.07770E+07	1.10323E+07	1.13208E+07	1.15996E+07	1.18070E+07	1.19006E+07	1.18960E+07	1.18381E+07
	1.17453E+07	1.16160E+07	1.14344E+07	1.11712E+07	1.07895E+07	1.02361E+07	9.43395E+06	8.15648E+06		
8	1.58361E+07	1.42278E+07	1.36739E+07	1.32919E+07	1.30285E+07	1.28468E+07	1.27175E+07	1.26242E+07	1.25602E+07	1.25229E+07
	1.25237E+07	1.25586E+07	1.25911E+07	1.25884E+07	1.25460E+07	1.24810E+07	1.24109E+07	1.23469E+07	1.22940E+07	1.22529E+07
	1.22074E+07	1.21050E+07	1.18609E+07	1.18551E+07	1.18494E+07	1.18435E+07	1.18489E+07	1.18521E+07	1.18466E+07	1.18404E+07
	1.18372E+07	1.18209E+07	1.18207E+07	1.12540E+07	9.88742E+06	9.17306E+06	9.17287E+06	8.22306E+06	5.23020E+06	2.99165E+06
	2.97100E+06	2.95895E+06	2.97093E+06	2.96977E+06	2.97078E+06	8.67551E+06	9.76312E+06	1.00824E+07	1.02249E+07	1.03247E+07
	1.04447E+07	1.06052E+07	1.08136E+07	1.10681E+07	1.13501E+07	1.16170E+07	1.18112E+07	1.18957E+07	1.18875E+07	1.18289E+07
	1.17361E+07	1.16068E+07	1.14252E+07	1.11619E+07	1.07803E+07	1.02269E+07	9.42471E+06	8.14725E+06		
9	1.58278E+07	1.42196E+07	1.36656E+07	1.32836E+07	1.30202E+07	1.28385E+07	1.27092E+07	1.26159E+07	1.25517E+07	1.25125E+07
	1.25085E+07	1.25423E+07	1.25894E+07	1.26205E+07	1.26216E+07	1.25997E+07	1.25666E+07	1.25312E+07	1.25002E+07	1.24751E+07
	1.24139E+07	1.21959E+07	1.18525E+07	1.18468E+07	1.18439E+07	1.18416E+07	1.18434E+07	1.18438E+07	1.18382E+07	1.18321E+07
	1.18289E+07	1.18126E+07	1.18124E+07	1.12591E+07	9.88432E+06	9.17299E+06	9.17282E+06	8.22300E+06	5.23013E+06	2.98338E+06
	2.96275E+06	2.95070E+06	2.96267E+06	2.96152E+06	2.96246E+06	6.95769E+06	9.11454E+06	9.93867E+06	1.02441E+07	1.03789E+07
	1.05099E+07	1.06788E+07	1.08922E+07	1.11442E+07	1.14128E+07	1.16569E+07	1.18268E+07	1.18948E+07	1.18804E+07	1.18207E+07
	1.17278E+07	1.15985E+07	1.14169E+07	1.11537E+07	1.07720E+07	1.02186E+07	9.41643E+06	8.13897E+06		
10	1.58157E+07	1.42075E+07	1.36535E+07	1.32715E+07	1.30081E+07	1.28265E+07	1.26971E+07	1.26038E+07	1.25394E+07	1.24979E+07
	1.24866E+07	1.25141E+07	1.25702E+07	1.26329E+07	1.26802E+07	1.27064E+07	1.27152E+07	1.27124E+07	1.27060E+07	1.26990E+07
	1.26175E+07	1.22767E+07	1.18404E+07	1.18348E+07	1.18335E+07	1.18333E+07	1.18330E+07	1.18318E+07	1.18262E+07	1.18200E+07
	1.18168E+07	1.18005E+07	1.18003E+07	1.12622E+07	9.88478E+06	9.17292E+06	9.17276E+06	8.22137E+06	5.23013E+06	2.97134E+06
	2.95072E+06	2.95068E+06	2.95064E+06	2.95054E+06	2.95039E+06	5.43250E+06	8.33807E+06	9.75647E+06	1.02711E+07	1.04513E+07
	1.05969E+07	1.07770E+07	1.09966E+07	1.12445E+07	1.14945E+07	1.17075E+07	1.18449E+07	1.18918E+07	1.18698E+07	1.18087E+07
	1.17157E+07	1.15864E+07	1.14049E+07	1.11416E+07	1.07599E+07	1.02066E+07	9.40438E+06	8.12692E+06		
11	1.57998E+07	1.41916E+07	1.36377E+07	1.32557E+07	1.29923E+07	1.28106E+07	1.26813E+07	1.25880E+07	1.25234E+07	1.24799E+07
	1.24607E+07	1.24761E+07	1.25271E+07	1.26012E+07	1.26761E+07	1.27359E+07	1.27750E+07	1.27956E+07	1.28065E+07	1.28121E+07
	1.27180E+07	1.23079E+07	1.18246E+07	1.18189E+07	1.18177E+07	1.18174E+07	1.18172E+07	1.18159E+07	1.18103E+07	1.18041E+07
	1.18009E+07	1.18004E+07	1.18002E+07	1.12665E+07	9.88749E+06	9.17283E+06	9.17266E+06	8.22115E+06	5.23044E+06	2.95554E+06
	2.95069E+06	2.95065E+06	2.95061E+06	2.95051E+06	2.95036E+06	4.76646E+06	7.84219E+06	9.62894E+06	1.02971E+07	1.05153E+07
	1.06768E+07	1.08704E+07	1.10984E+07	1.13435E+07	1.15744E+07	1.17547E+07	1.18585E+07	1.18844E+07	1.18552E+07	1.17930E+07
	1.16999E+07	1.15706E+07	1.13890E+07	1.11258E+07	1.07441E+07	1.01907E+07	9.38854E+06	8.11109E+06		
12	1.57839E+07	1.41758E+07	1.36218E+07	1.32398E+07	1.29764E+07	1.27948E+07	1.26654E+07	1.25721E+07	1.25075E+07	1.24630E+07
	1.24383E+07	1.24428E+07	1.24837E+07	1.25545E+07	1.26340E+07	1.27020E+07	1.27482E+07	1.27730E+07	1.27862E+07	1.27926E+07
	1.26993E+07	1.22914E+07	1.18087E+07	1.18031E+07	1.18018E+07	1.18015E+07	1.18013E+07	1.18005E+07	1.18005E+07	1.18004E+07
	1.18004E+07	1.18003E+07	1.18001E+07	1.12745E+07	9.89146E+06	9.17274E+06	9.17257E+06	8.22276E+06	5.23851E+06	2.95070E+06
	2.95066E+06	2.95062E+06	2.95058E+06	2.95048E+06	2.95033E+06	4.81557E+06	7.85904E+06	9.63631E+06	1.03078E+07	1.05359E+07
	1.07105E+07	1.09178E+07	1.11566E+07	1.14045E+07	1.16253E+07	1.17834E+07	1.18631E+07	1.18741E+07	1.18402E+07	1.17772E+07
	1.16840E+07	1.15547E+07	1.13732E+07	1.11099E+07	1.07282E+07	1.01749E+07	9.37270E+06	8.09526E+06		
13	1.57603E+07	1.41521E+07	1.35981E+07	1.32162E+07	1.29528E+07	1.27711E+07	1.26418E+07	1.25485E+07	1.24839E+07	1.24387E+07
	1.24093E+07	1.24027E+07	1.24287E+07	1.24819E+07	1.25397E+07	1.25818E+07	1.26001E+07	1.25990E+07	1.25892E+07	1.25763E+07
	1.25011E+07	1.22005E+07	1.17854E+07	1.17781E+07	1.17719E+07	1.17681E+07	1.17774E+07	1.17981E+07	1.18002E+07	1.18002E+07
	1.18002E+07	1.18001E+07	1.17999E+07	1.12810E+07	9.89292E+06	9.17264E+06	9.17242E+06	8.22334E+06	5.23972E+06	2.95131E+06
	2.95061E+06	2.95057E+06	2.95053E+06	2.95043E+06	2.95029E+06	6.03247E+06	8.63480E+06	9.84140E+06	1.02949E+07	1.04961E+07
	1.06856E+07	1.09141E+07	1.11741E+07	1.14367E+07	1.16581E+07	1.18007E+07	1.18587E+07	1.18556E+07	1.18172E+07	1.17536E+07
	1.16604E+07	1.15311E+07	1.13495E+07	1.10863E+07	1.07046E+07	1.01512E+07	9.34907E+06	8.07163E+06		

14	1.57429E+07	1.41347E+07	1.35808E+07	1.31988E+07	1.29354E+07	1.27538E+07	1.26244E+07	1.25311E+07	1.24666E+07	1.24216E+07
	1.23924E+07	1.23847E+07	1.24015E+07	1.24229E+07	1.24184E+07	1.23760E+07	1.23059E+07	1.22262E+07	1.21510E+07	1.20873E+07
	1.20370E+07	1.19992E+07	1.17684E+07	1.17595E+07	1.17488E+07	1.17427E+07	1.17586E+07	1.17917E+07	1.17999E+07	1.18001E+07
	1.18001E+07	1.18000E+07	1.17997E+07	9.33224E+06	9.09062E+06	9.17256E+06	9.17231E+06	6.54913E+06	4.07432E+06	2.95184E+06
	2.95058E+06	2.95053E+06	2.93362E+06	2.95040E+06	2.95025E+06	1.00309E+07	1.00689E+07	1.01374E+07	1.02422E+07	1.03880E+07
	1.05800E+07	1.08201E+07	1.10978E+07	1.13827E+07	1.16258E+07	1.17815E+07	1.18427E+07	1.18389E+07	1.17999E+07	1.17362E+07
	1.16430E+07	1.15137E+07	1.13322E+07	1.10689E+07	1.06872E+07	1.01339E+07	9.33174E+06	8.05431E+06		
15	1.57140E+07	1.41059E+07	1.35520E+07	1.31700E+07	1.29066E+07	1.27249E+07	1.25956E+07	1.25023E+07	1.24379E+07	1.23929E+07
	1.23612E+07	1.23433E+07	1.23474E+07	1.23779E+07	1.24263E+07	1.24775E+07	1.25177E+07	1.25412E+07	1.25520E+07	1.25665E+07
	1.25193E+07	1.21857E+07	1.17399E+07	1.17285E+07	1.17104E+07	1.17005E+07	1.17285E+07	1.17807E+07	1.17993E+07	1.17998E+07
	1.17999E+07	1.17998E+07	1.17995E+07	1.12608E+07	9.96155E+06	9.17244E+06	9.17211E+06	8.20675E+06	5.38587E+06	2.95264E+06
	2.95053E+06	2.95048E+06	2.94966E+06	2.95034E+06	2.95019E+06	5.06797E+06	7.81357E+06	9.66324E+06	1.05290E+07	1.08186E+07
	1.09905E+07	1.11795E+07	1.13855E+07	1.15814E+07	1.17318E+07	1.18138E+07	1.18333E+07	1.18140E+07	1.17716E+07	1.17074E+07
	1.16142E+07	1.14849E+07	1.13034E+07	1.10401E+07	1.06584E+07	1.01051E+07	9.30294E+06	8.02553E+06		
16	1.56596E+07	1.40515E+07	1.34975E+07	1.31156E+07	1.28522E+07	1.26705E+07	1.25412E+07	1.24479E+07	1.23836E+07	1.23390E+07
	1.23078E+07	1.22880E+07	1.22830E+07	1.22963E+07	1.23242E+07	1.23582E+07	1.23897E+07	1.24129E+07	1.24263E+07	1.24425E+07
	1.24160E+07	1.21274E+07	1.16861E+07	1.16714E+07	1.16350E+07	1.16130E+07	1.16698E+07	1.17655E+07	1.17985E+07	1.17993E+07
	1.17995E+07	1.17994E+07	1.17991E+07	1.12546E+07	9.97512E+06	9.17216E+06	9.17177E+06	8.20381E+06	5.43546E+06	2.95312E+06
	2.95042E+06	2.95037E+06	2.94857E+06	2.95023E+06	2.95008E+06	5.23392E+06	8.11744E+06	1.00067E+07	1.08558E+07	1.11061E+07
	1.12267E+07	1.13547E+07	1.14945E+07	1.16276E+07	1.17287E+07	1.17801E+07	1.17852E+07	1.17608E+07	1.17173E+07	1.16531E+07
	1.15598E+07	1.14305E+07	1.12490E+07	1.09857E+07	1.06041E+07	1.00507E+07	9.24860E+06	7.97121E+06		
17	1.56313E+07	1.40232E+07	1.34693E+07	1.30873E+07	1.28239E+07	1.26423E+07	1.25129E+07	1.24197E+07	1.23553E+07	1.23107E+07
	1.22802E+07	1.22625E+07	1.22587E+07	1.22631E+07	1.22657E+07	1.22606E+07	1.22484E+07	1.22329E+07	1.22176E+07	1.22043E+07
	1.21937E+07	1.21856E+07	1.16578E+07	1.16431E+07	1.16057E+07	1.15615E+07	1.16190E+07	1.17216E+07	1.17701E+07	1.17709E+07
	1.17712E+07	1.17711E+07	1.16351E+07	1.07369E+07	9.94968E+06	9.14392E+06	9.14352E+06	7.39519E+06	5.41060E+06	2.92496E+06
	2.92224E+06	2.92219E+06	2.81730E+06	2.92205E+06	2.92191E+06	1.08239E+07	1.08368E+07	1.08668E+07	1.09175E+07	1.09906E+07
	1.10889E+07	1.12144E+07	1.13629E+07	1.15183E+07	1.16511E+07	1.17312E+07	1.17517E+07	1.17319E+07	1.16890E+07	1.16248E+07
	1.15316E+07	1.14023E+07	1.12207E+07	1.09575E+07	1.05758E+07	1.00225E+07	9.22035E+06	7.94297E+06		
18	1.53013E+07	1.36934E+07	1.31395E+07	1.27576E+07	1.24942E+07	1.23126E+07	1.21833E+07	1.20900E+07	1.20257E+07	1.19813E+07
	1.19507E+07	1.19296E+07	1.19152E+07	1.19053E+07	1.18987E+07	1.18943E+07	1.18913E+07	1.18893E+07	1.18880E+07	1.18871E+07
	1.18864E+07	1.18859E+07	1.18803E+07	1.18690E+07	1.14455E+07	1.09568E+07	1.14452E+07	1.18666E+07	1.18670E+07	1.18612E+07
	1.18584E+07	1.18424E+07	1.18067E+07	1.17675E+07	1.17374E+07	1.16922E+07	1.16632E+07	1.16240E+07	1.15908E+07	1.15386E+07
	1.15180E+07	1.14461E+07	1.78766E+06	1.14443E+07	1.13735E+07	1.14904E+07	1.14901E+07	1.14897E+07	1.14893E+07	1.14887E+07
	1.14878E+07	1.14861E+07	1.14830E+07	1.14777E+07	1.14690E+07	1.14552E+07	1.14344E+07	1.14039E+07	1.13595E+07	1.12952E+07
	1.12020E+07	1.10727E+07	1.08912E+07	1.06280E+07	1.02463E+07	9.69309E+06	8.89103E+06	7.61377E+06		
19	1.46436E+07	1.30360E+07	1.24822E+07	1.21004E+07	1.18370E+07	1.16555E+07	1.15262E+07	1.14329E+07	1.13686E+07	1.13243E+07
	1.12937E+07	1.12726E+07	1.12581E+07	1.12480E+07	1.12411E+07	1.12364E+07	1.12331E+07	1.12308E+07	1.12292E+07	1.12282E+07
	1.12274E+07	1.12269E+07	1.12217E+07	1.11605E+07	1.03919E+07	9.74268E+06	1.03914E+07	1.11575E+07	1.12075E+07	1.12016E+07
	1.11984E+07	1.11822E+07	1.11527E+07	1.11364E+07	1.11331E+07	1.11166E+07	1.10873E+07	1.10693E+07	1.10628E+07	1.10492E+07
	1.10284E+07	1.09577E+07	9.91177E+05	1.09538E+07	1.08817E+07	1.08443E+07	1.08438E+07	1.08430E+07	1.08420E+07	1.08404E+07
	1.08381E+07	1.08348E+07	1.08301E+07	1.08232E+07	1.08131E+07	1.07986E+07	1.07775E+07	1.07469E+07	1.07026E+07	1.06383E+07
	1.05451E+07	1.04159E+07	1.02344E+07	9.97120E+06	9.58966E+06	9.03651E+06	8.23461E+06	6.95762E+06		
20	1.39860E+07	1.23787E+07	1.18251E+07	1.14433E+07	1.11800E+07	1.09985E+07	1.08692E+07	1.07760E+07	1.07117E+07	1.06674E+07
	1.06368E+07	1.06157E+07	1.06012E+07	1.05911E+07	1.05842E+07	1.05795E+07	1.05762E+07	1.05739E+07	1.05723E+07	1.05713E+07
	1.05705E+07	1.05700E+07	1.05645E+07	1.04380E+07	9.31927E+06	8.50858E+06	9.31879E+06	1.04350E+07	1.05503E+07	1.05447E+07
	1.05416E+07	1.05253E+07	1.04959E+07	1.04796E+07	1.04764E+07	1.04602E+07	1.04308E+07	1.04129E+07	1.04065E+07	1.03930E+07
	1.03723E+07	1.03044E+07	7.34072E+05	1.02978E+07	1.02256E+07	1.01875E+07	1.01870E+07	1.01863E+07	1.01852E+07	1.01836E+07
	1.01813E+07	1.01781E+07	1.01733E+07	1.01664E+07	1.01563E+07	1.01418E+07	1.01207E+07	1.00901E+07	1.00458E+07	9.98155E+06
	9.88836E+06	9.75914E+06	9.57767E+06	9.31456E+06	8.93310E+06	8.38006E+06	7.57833E+06	6.30159E+06		
21	1.33285E+07	1.17216E+07	1.11680E+07	1.07864E+07	1.05232E+07	1.03416E+07	1.02124E+07	1.01192E+07	1.00549E+07	1.00106E+07
	9.98003E+06	9.95895E+06	9.94441E+06	9.93438E+06	9.92747E+06	9.92270E+06	9.91941E+06	9.91714E+06	9.91558E+06	9.91450E+06

	9.91375E+06	9.91323E+06	9.90735E+06	9.70776E+06	8.22705E+06	7.24898E+06	8.22657E+06	9.70477E+06	9.89309E+06	9.88796E+06
	9.88481E+06	9.86854E+06	9.83918E+06	9.82290E+06	9.81971E+06	9.80343E+06	9.77407E+06	9.75619E+06	9.74981E+06	9.73628E+06
	9.71556E+06	9.65076E+06	6.93613E+05	9.64134E+06	9.56891E+06	9.53083E+06	9.53032E+06	9.52957E+06	9.52850E+06	9.52693E+06
	9.52466E+06	9.52138E+06	9.51661E+06	9.50969E+06	9.49967E+06	9.48513E+06	9.46405E+06	9.43349E+06	9.38917E+06	9.32491E+06
	9.23174E+06	9.10254E+06	8.92112E+06	8.65806E+06	8.27668E+06	7.72375E+06	6.92218E+06	5.64570E+06		
22	1.26712E+07	1.10646E+07	1.05112E+07	1.01296E+07	9.86640E+06	9.68493E+06	9.55571E+06	9.46254E+06	9.39828E+06	9.35396E+06
	9.32340E+06	9.30232E+06	9.28778E+06	9.27776E+06	9.27084E+06	9.26607E+06	9.26279E+06	9.26052E+06	9.25895E+06	9.25787E+06
	9.25713E+06	9.25660E+06	9.25030E+06	8.97279E+06	7.11042E+06	5.95511E+06	7.10994E+06	8.96980E+06	9.23603E+06	9.23133E+06
	9.22820E+06	9.21192E+06	9.18257E+06	9.16629E+06	9.16310E+06	9.14683E+06	9.11747E+06	9.09960E+06	9.09322E+06	9.07970E+06
	9.05898E+06	8.99752E+06	7.80096E+05	8.98502E+06	8.91235E+06	8.87429E+06	8.87377E+06	8.87303E+06	8.87195E+06	8.87039E+06
	8.86812E+06	8.86483E+06	8.86006E+06	8.85315E+06	8.84313E+06	8.82859E+06	8.80752E+06	8.77696E+06	8.73265E+06	8.66841E+06
	8.57525E+06	8.44608E+06	8.26469E+06	8.00169E+06	7.62039E+06	7.06757E+06	6.26616E+06	4.98995E+06		
23	1.20140E+07	1.04077E+07	9.85443E+06	9.47289E+06	9.20979E+06	9.02835E+06	8.89916E+06	8.80600E+06	8.74176E+06	8.69745E+06
	8.66689E+06	8.64582E+06	8.63128E+06	8.62126E+06	8.61435E+06	8.60958E+06	8.60630E+06	8.60403E+06	8.60246E+06	8.60138E+06
	8.60063E+06	8.60011E+06	8.59333E+06	8.23067E+06	5.95808E+06	4.61143E+06	5.95760E+06	8.22768E+06	8.57906E+06	8.57482E+06
	8.57171E+06	8.55544E+06	8.52609E+06	8.50982E+06	8.50663E+06	8.49036E+06	8.46101E+06	8.44314E+06	8.43676E+06	8.42324E+06
	8.40254E+06	8.34492E+06	9.91888E+05	8.32888E+06	8.25593E+06	8.21787E+06	8.21736E+06	8.21662E+06	8.21554E+06	8.21398E+06
	8.21171E+06	8.20842E+06	8.20365E+06	8.19674E+06	8.18672E+06	8.17219E+06	8.15112E+06	8.12057E+06	8.07627E+06	8.01204E+06
	7.91890E+06	7.78976E+06	7.60841E+06	7.34546E+06	6.96423E+06	6.41153E+06	5.61028E+06	4.33433E+06		
24	1.13570E+07	9.75101E+06	9.19781E+06	8.81636E+06	8.55331E+06	8.37191E+06	8.24275E+06	8.14960E+06	8.08537E+06	8.04107E+06
	8.01052E+06	7.98945E+06	7.97492E+06	7.96490E+06	7.95799E+06	7.95322E+06	7.94994E+06	7.94767E+06	7.94611E+06	7.94503E+06
	7.94427E+06	7.94374E+06	7.93641E+06	7.47606E+06	4.74571E+06	3.18421E+06	4.74524E+06	7.47307E+06	7.92215E+06	7.91845E+06
	7.91536E+06	7.89910E+06	7.86975E+06	7.85348E+06	7.85029E+06	7.83403E+06	7.80468E+06	7.78682E+06	7.78044E+06	7.76692E+06
	7.74622E+06	7.69349E+06	1.30144E+06	7.67294E+06	7.59965E+06	7.56159E+06	7.56108E+06	7.56034E+06	7.55926E+06	7.55770E+06
	7.55543E+06	7.55214E+06	7.54738E+06	7.54047E+06	7.53045E+06	7.51592E+06	7.49486E+06	7.46431E+06	7.42002E+06	7.35580E+06
	7.26269E+06	7.13357E+06	6.95225E+06	6.68936E+06	6.30821E+06	5.75562E+06	4.95453E+06	3.67884E+06		
25	2.28313E+06	2.28313E+06	2.28313E+06	2.28313E+06	2.28313E+06	2.28313E+06	2.28313E+06	2.28313E+06	2.28313E+06	2.28313E+06
	2.28313E+06	2.28313E+06	2.28313E+06	2.28313E+06	2.28313E+06	2.28313E+06	2.28313E+06	2.28313E+06	2.28313E+06	2.28313E+06
	2.28313E+06	2.28313E+06	2.28313E+06	2.28313E+06	2.28313E+06	1.70345E+06	2.28313E+06	2.28313E+06	2.28313E+06	2.28313E+06
	2.28313E+06	2.28313E+06	2.28313E+06	2.28313E+06	2.28313E+06	2.28313E+06	2.28313E+06	2.28313E+06	2.28313E+06	2.28313E+06
	2.28313E+06	2.28313E+06	1.23746E+06	2.28313E+06	2.28313E+06	2.28313E+06	2.28313E+06	2.28313E+06	2.28313E+06	2.28313E+06
	2.28313E+06	2.28313E+06	2.28313E+06	2.28313E+06	2.28313E+06	2.28313E+06	2.28313E+06	2.28313E+06	2.28313E+06	2.28313E+06
	2.28313E+06	2.28313E+06	2.28313E+06	2.28313E+06	2.28313E+06	2.28313E+06	2.28313E+06	2.28313E+06		
26	9.33300E+05	9.38106E+05	9.41180E+05	9.44185E+05	9.47096E+05	9.49881E+05	9.52620E+05	9.57156E+05	9.57736E+05	9.57864E+05
	9.57871E+05	9.57865E+05	9.57875E+05	9.57898E+05	9.57926E+05	9.57951E+05	9.57973E+05	9.57990E+05	9.58003E+05	9.58013E+05
	9.58020E+05	9.58024E+05	9.58408E+05	9.59296E+05	9.60363E+05	9.89501E+05	9.89501E+05	9.89501E+05	9.89502E+05	9.89502E+05
	9.89502E+05	9.89503E+05	9.89503E+05	9.89504E+05	9.89504E+05	9.89504E+05	9.89504E+05	9.89505E+05	9.89505E+05	9.89506E+05
	9.89507E+05	9.89508E+05	9.94878E+05	9.33358E+05	9.33322E+05	9.33304E+05	9.33304E+05	9.33304E+05	9.33304E+05	9.33304E+05
	9.33304E+05	9.33304E+05	9.33304E+05	9.33304E+05	9.33304E+05	9.33304E+05	9.33304E+05	9.33304E+05	9.33303E+05	9.33303E+05
	9.33303E+05	9.33302E+05	9.33302E+05	9.33302E+05	9.33301E+05	9.33301E+05	9.33300E+05	9.33300E+05		
27	1.82702E+06	1.82702E+06	1.82702E+06	1.82702E+06	1.82702E+06	1.82702E+06	1.82702E+06	1.82702E+06	1.82702E+06	1.82702E+06
	1.82702E+06	1.82702E+06	1.82702E+06	1.82702E+06	1.82702E+06	1.82702E+06	1.82702E+06	1.82702E+06	1.82702E+06	1.82702E+06
	1.82702E+06	1.82702E+06	1.82702E+06	1.82702E+06	1.82702E+06	9.82009E+05	1.82702E+06	1.82702E+06	1.82702E+06	1.82702E+06
	1.82702E+06	1.82702E+06	1.82702E+06	1.82702E+06	1.82702E+06	1.82702E+06	1.82702E+06	1.82702E+06	1.82702E+06	1.82702E+06
	1.82702E+06	1.82702E+06	9.77726E+05	1.82702E+06	1.82702E+06	1.82702E+06	1.82702E+06	1.82702E+06	1.82702E+06	1.82702E+06
	1.82702E+06	1.82702E+06	1.82702E+06	1.82702E+06	1.82702E+06	1.82702E+06	1.82702E+06	1.82702E+06	1.82702E+06	1.82702E+06
	1.82702E+06	1.82702E+06	1.82702E+06	1.82702E+06	1.82702E+06	1.82702E+06	1.82702E+06	1.82702E+06		
28	9.63100E+05	9.63151E+05	9.63184E+05	9.63216E+05	9.63246E+05	9.63276E+05	9.63305E+05	9.63333E+05	9.63360E+05	9.63384E+05
	9.63405E+05	9.63423E+05	9.63438E+05	9.63449E+05	9.63459E+05	9.63466E+05	9.63471E+05	9.63474E+05	9.63477E+05	9.63479E+05
	9.63480E+05	9.63481E+05	9.63566E+05	9.63794E+05	9.64037E+05	9.66779E+05	9.66770E+05	9.66769E+05	9.66768E+05	9.66767E+05
	9.66766E+05	9.66764E+05	9.66763E+05	9.66761E+05	9.66760E+05	9.66759E+05	9.66757E+05	9.66755E+05	9.66753E+05	9.66748E+05

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    9.66739E+05  9.66730E+05  9.59889E+05  9.63082E+05  9.63093E+05  9.63099E+05  9.63099E+05  9.63099E+05  9.63099E+05  9.63099E+05
    9.63099E+05  9.63099E+05  9.63099E+05  9.63099E+05  9.63099E+05  9.63099E+05  9.63099E+05  9.63099E+05  9.63099E+05  9.63099E+05
    9.63099E+05  9.63099E+05  9.63099E+05  9.63100E+05  9.63100E+05  9.63100E+05  9.63100E+05  9.63100E+05
29  1.47330E+06  1.47330E+06  1.47330E+06  1.47330E+06  1.47330E+06  1.47330E+06  1.47330E+06  1.47330E+06  1.47330E+06  1.47330E+06
    1.47330E+06  1.47330E+06  1.47330E+06  1.47330E+06  1.47330E+06  1.47330E+06  1.47330E+06  1.47330E+06  1.47330E+06  1.47330E+06
    1.47330E+06  1.47330E+06  1.47330E+06  1.47330E+06  1.47330E+06  9.54508E+05  1.47330E+06  1.47330E+06  1.47330E+06  1.47330E+06
    1.47330E+06  1.47330E+06  1.47330E+06  1.47330E+06  1.47330E+06  1.47330E+06  1.47330E+06  1.47330E+06  1.47330E+06  1.47330E+06
    1.47330E+06  1.47330E+06  9.20234E+05  1.47330E+06  1.47330E+06  1.47330E+06  1.47330E+06  1.47330E+06  1.47330E+06  1.47330E+06
    1.47330E+06  1.47330E+06  1.47330E+06  1.47330E+06  1.47330E+06  1.47330E+06  1.47330E+06  1.47330E+06  1.47330E+06  1.47330E+06
    1.47330E+06  1.47330E+06  1.47330E+06  1.47330E+06  1.47330E+06  1.47330E+06  1.47330E+06  1.47330E+06
30  7.35548E+05  7.35548E+05  7.35548E+05  7.35543E+05  7.35487E+05  7.35268E+05  7.34908E+05  7.34564E+05  7.34307E+05  7.34119E+05
    7.33977E+05  7.33868E+05  7.33782E+05  7.33717E+05  7.33667E+05  7.33630E+05  7.33602E+05  7.33583E+05  7.33569E+05  7.33559E+05
    7.33552E+05  7.33547E+05  7.33206E+05  7.32528E+05  7.31782E+05  7.31374E+05  7.30979E+05  7.29969E+05  7.29863E+05  7.29426E+05
    7.28921E+05  7.28373E+05  7.27850E+05  7.27548E+05  7.27369E+05  7.27114E+05  7.26919E+05  7.26872E+05  7.26831E+05  7.26746E+05
    7.26694E+05  7.26728E+05  7.30248E+05  7.34492E+05  7.35168E+05  7.35524E+05  7.35524E+05  7.35525E+05  7.35525E+05  7.35525E+05
    7.35525E+05  7.35526E+05  7.35527E+05  7.35528E+05  7.35529E+05  7.35531E+05  7.35533E+05  7.35536E+05  7.35540E+05  7.35543E+05
    7.35546E+05  7.35547E+05  7.35548E+05  7.35548E+05  7.35548E+05  7.35548E+05  7.35548E+05  7.35548E+05
31  1.01355E+05  1.01355E+05  1.01355E+05  1.01355E+05  1.01355E+05  1.01355E+05  1.01355E+05  1.01355E+05  1.01355E+05  1.01355E+05
    1.01355E+05  1.01355E+05  1.01355E+05  1.01355E+05  1.01356E+05  1.01357E+05  1.01359E+05  1.01361E+05  1.01363E+05  1.01364E+05
    1.01365E+05  1.01366E+05  1.01435E+05  1.01735E+05  1.02110E+05  1.02327E+05  1.02218E+05  1.01984E+05  1.01547E+05  1.01478E+05
    1.01413E+05  1.01358E+05  1.01355E+05  1.01355E+05  1.01355E+05  1.01355E+05  1.01355E+05  1.01355E+05  1.01355E+05  1.01355E+05
    1.01355E+05  1.01355E+05  1.07398E+05  1.01355E+05  1.01355E+05  1.01355E+05  1.01355E+05  1.01355E+05  1.01355E+05  1.01355E+05
    1.01355E+05  1.01355E+05  1.01355E+05  1.01355E+05  1.01355E+05  1.01355E+05  1.01355E+05  1.01355E+05  1.01355E+05  1.01355E+05
    1.01355E+05  1.01355E+05  1.01355E+05  1.01355E+05  1.01355E+05  1.01355E+05  1.01355E+05  1.01355E+05
32  1.01331E+05  1.01331E+05  1.01331E+05  1.01331E+05  1.01331E+05  1.01331E+05  1.01331E+05  1.01331E+05  1.01331E+05  1.01331E+05
    1.01331E+05  1.01331E+05  1.01331E+05  1.01331E+05  1.01331E+05  1.01331E+05  1.01331E+05  1.01331E+05  1.01331E+05  1.01331E+05
    1.01331E+05  1.01331E+05  1.01331E+05  1.01331E+05  1.01331E+05  1.01331E+05  1.01331E+05  1.01331E+05  1.01331E+05  1.01331E+05
    1.01331E+05  1.01331E+05  1.01331E+05  1.01331E+05  1.01331E+05  1.01331E+05  1.01331E+05  1.01331E+05  1.01331E+05  1.01331E+05
    1.01331E+05  1.01331E+05  1.02170E+05  1.01331E+05  1.01331E+05  1.01331E+05  1.01331E+05  1.01331E+05  1.01331E+05  1.01331E+05
    1.01331E+05  1.01331E+05  1.01331E+05  1.01331E+05  1.01331E+05  1.01331E+05  1.01331E+05  1.01331E+05  1.01331E+05  1.01331E+05
    1.01331E+05  1.01331E+05  1.01331E+05  1.01331E+05  1.01331E+05  1.01331E+05  1.01331E+05  1.01331E+05
33  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05
    1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05
    1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05
    1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05
    1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05
    1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05
    1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05  1.01325E+05
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 Time Step No. = 2381   Elapsed Time = 3.652431E+06 days


 ******************************************************************************
 * End of BRAGFLO             Version: 7.00               Revised: 08/14/18    *
 * Completed: 11/27/18 at 09:38:49     Run on: i86pc santana SunOS 5.11        *
 ******************************************************************************



 Normal Completion of BRAGFLO.  Total CPU Time =  0.154 hr
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11.4 Appendix D: Functionality Not Tested

For BRAGFLO, Version 7.00, the following features are not tested nor to be used as part of the WIPP compliance calculations:

1. Radionuclide transport.
2. Gas dissolution.
3. Reaction path gas generation model.
4. Multicomponent gas transport.
5. Three-dimensional calculations.
6. Alternative equation solvers (i.e., Linpack LU solver and point-SOR iterative solver).
7. Capillary pressure treatment to allow the maximum capillary pressure to vary automatically.
8. Multicomponent gas properties.
9. Restart capability.
10. Selected mesh input options (i.e., For parameter IDZFLAG, options 2, 3, and 4 are not tested. For parameter IDEPTHFLAG, options 1, 2, 3, 4, 5, 6, and -1 are not tested).
11. Permeability versus porosity models for closure materials.
12. A fracture model which effectively holds the pressure constant during fracturing.
13. Option to limit the increase in porosity.

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