Appendix E

NUCLEAR WASTE MANAGEMENT PROCEDURE Sandia National Laboratories	**Design Document Criteria**	**Form Number: NP 19-1-4** **Page 1 of 1**

1. **Software Name:** DRSPALL
2. **Software Version:** 1.24
3. **Document Version:** 1.24
4. **ERMS #:** 573906

Prior to sign-off of the DD, all items shall be appropriately addressed by the code sponsor so that "Yes" may be checked. Include this form as part of the DD.

Are the following appropriately defined and documented in the DD?

5. Major Software Components — ☒ Yes
6. Technical description of the software with respect to: theoretical basis, embodied mathematical model, major control flow, control logic, and data structures — ☒ Yes
7. Functionalities and interfaces of object components, functions, and subroutines. — ☒ Yes
8. Allowable or prescribed ranges for inputs and outputs — ☒ Yes
9. Verifiability: Is the design verifiable through testing or other means? — ☒ Yes
10. Consistency and Traceability: Is the design consistent with and traceable to the software's requirements? — ☒ Yes
11. Technical Feasibility: Is the design technically feasible? — ☒ Yes
12. Implementation: Is the design presented in sufficient detail to allow for implementation as computer software? — ☒ Yes

13.	Dwayne Kicker **Code Team/Sponsor** (*print*)	*Signature on File* Signature	4/15/21 Date
14.	Cliff Hansen **Technical Reviewer** (*print*)	*Signature on File* Signature	4/23/21 Date
15.	Shelly Nielsen **QA Reviewer** (*print*)	Shelly R. Nielsen Signature	4-5-2021 Date
16.	Steve Wagner **Responsible Manager** (*print*)	*Signature on File* Signature	4/23/21 Date
17.	Jennifer Long **SCM Coordinator** (*print*)	*Signature on File* Signature	4/15/21 Date

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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:** DRSPALL
2. **Software Version:** 1.24
3. **Document Version:** 1.24
4. **ERMS #:** 573906

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)?	☒	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.	Dwayne Kicker **Code Team/Sponsor** (*print*)	*Signature on File* Signature	4/15/2021 Date
16.	Cliff Hansen **Technical Reviewer** (*print*)	*Signature on File* Signature	4/23/2021 Date
17.	Shelly Nielsen **QA Reviewer** (*print*)	Shelly R. Nielsen Signature	4-15-2021 Date
18.	Steve Wagner **Responsible Manager** (*print*)	*Signature on File* Signature	4/23/2021 Date
19.	Jennifer Long **SCM Coordinator** (*print*)	*Signature on File* Signature	4/15/2021 Date

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WIPP PA

Design Document and User's Manual

for

DRSPALL Version 1.24

Document Version 1.24

ERMS # 573906

April 2021

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1.0 INTRODUCTION AND SCOPE

This Design Document and User's Manual for DRSPALL Version 1.24, describes the following major features of software design: software components, theoretical basis, mathematical model, control flow and logic, data structures, and functionality and the interfaces of subroutines. It also describes in detail the allowed or prescribed ranges for input data and user interface, in accordance with the Nuclear Waste Management Procedure NP 19-1 Software Requirements (Long, 2020). This code is used by the Sandia National Laboratories' Performance Assessment (PA) Department in support of the performance assessment calculations for the Waste Isolation Pilot Plant (WIPP). It is controlled under the software configuration management system Concurrent Versions System (CVS) on the Linux cluster.

1.1 Software Identification

Code Name:	DRSPALL
Version:	1.24
CVS Repository:	/data/cvs/CVSLIB/WIPP_CODES/PA_CODES/DRSPALL
Platform:	CentOS 7/Dell PowerEdge C6420
Host:	fwm.sandia.gov
Compiler:	Gfortran/GCC 8.2.0

1.2 Points of Contact

Code Sponsor:	Dwayne Kicker	dckicke@sandia.gov	(575) 620-0117

1.3 Code Overview

DRSPALL is written to calculate the spallings release, defined as the mass of waste subject to tensile failure and transport during an inadvertent drilling intrusion into a high-pressure WIPP repository. Cuttings removed by the direct action of the drillbit, and cavings removed by shear forces of the drilling mud against the drilled cavity wall are handled separately in the CUTTINGS_S code. DRSPALL uses both text-formatted and CDB input and output files, and calculates coupled repository and wellbore transient compressible fluid flow before, during, and after the drilling intrusion process. Mathematical models are included of multi-phase flow in the well, fluid expulsion at the surface, coupling of the well and the repository, repository spalling (tensile) failure associated with fluidized bed transport, and repository internal gas flow. The wellbore model is one-dimensional linear, and the repository model is one-dimensional, either spherical or cylindrical.

DRSPALL is based on the theory of one-dimensional, time-dependent compressible isothermal fluid flow. Somewhat different forms of that theory are used, depending on whether the flow is in the wellbore or the repository, and whether the wellbore currently penetrates the repository. The wellbore and repository flows are coupled at a specified boundary. Flow in the well is

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treated as a compressible, viscous, multi-phase mixture of mud, gas, salt, and possibly waste solids. Flow in the repository is treated as viscous, compressible single-phase gas flow in a porous solid. At the cavity forming the repository-wellbore boundary (following penetration), waste solids freed by drilling, tensile failure, and associated fluidization may enter the wellbore flow stream. Between the well and the repository, flow is treated according to the state of penetration.

The wellbore calculations use time-marching finite differences. These are part of a single computational loop. The numerical method is Eulerian in that zone boundaries are fixed, and fluid moves through the interfaces by convection. Quantities are zone-centered and integration is explicit in time.

The repository calculations also use time-marching finite differences that are part of a single computational loop. The method is implicit with spatial derivatives determined after the time increment.

2.0 REQUIREMENTS

The requirements for DRSPALL are listed in the *Requirements Document, Verification and Validation Plan, and Validation Document for DRSPALL Version 1.24* (Kicker, 2021a). The requirements are repeated here for the reader's convenience.

2.1 Functional Requirements

The functional requirements for DRSPALL Version 1.24 are listed below.

R.1 Compressible, viscous, isothermal, multiphase mixture flow (mud, salt, waste, repository gas) in the wellbore using one-dimensional linear geometry and assuming a Newtonian fluid. Either laminar or turbulent flow shall be modeled depending on wellbore and fluid properties.

Wellbore flow output variables will be evaluated against results from a commercial computational flow model configured to run the same test problem.

R.2 Repository gas flow as single-phase Darcy porous flow using either one dimensional cylindrical or spherical geometry.

Repository pressure distributions will be compared to independent solutions (numerical, analytic, or semi-analytic) of the governing equations obtained from published scientific literature.

R.3 Coupling of the wellbore and the repository flow models prior to and after penetration

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This requirement will be tested by reporting intermediate variables (pore velocity, gas density, cavity area) describing the mass flow between the repository and wellbore as a function of time in order to confirm mass balance.

R.4 Spalling (tensile) failure of the homogeneous waste material using an effective stress law with seepage forces.

The time-histories of the output variables pressure distribution, effective stress and tensile-failed volume will be examined for conceptually consistent behavior.

R.5 Fluidized bed transport of failed (disaggregated) waste material.

This requirement will be evaluated by comparing the DRSPALL fluidization velocity to that obtained from independent test evaluation script calculations.

R.6 Mixture expulsion at the surface.

This requirement will be evaluated by reporting the time-history of waste expelled and computing a solids mass balance to assure that waste removed from the repository is accounted for at the surface.

2.2 External Interface Requirements

The external interface requirements are listed below:

R.7 DRSPALL shall read an input control file, which may be pre-generated using a text processor. It will contain numerical control parameters and, optionally, material properties and problem geometry.

R.8 Properties and non-numerical control parameters will, optionally, be read from a CDB.

R.9 Grid, properties, parameters and spatial and time dependent results will be written to an output CDB.

DRSPALL will link to the standard WIPP code libraries, namely, CAMDAT_LIB, CAMCON_LIB, and CAMSUPES_LIB (Rechard et al., 1993). User interactions will consist of command line execution, batch files, and input files.

2.3 Other Requirements

There are no other requirements for DRSPALL.

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2.4 Functionality Not Tested

All code functionality is covered in the requirements and test cases.

3.0 MAJOR SOFTWARE COMPONENTS

The major code components consist of an input control file, an optional input CDB file, the main computational loop, and output files, as shown in Figure 1.

The use of CDB files for input and output is optional. Input parameters can be provided in the input control file or read from the input CDB. However, input parameters are always echoed to the diagnostic output file. For any run, all files have the same prefix name assigned by the user, while the suffix names denote the type of file.

DRSPALL makes use of the WIPP PA libraries CAMCON_LIB, CAMSUPES_LIB and CAMDAT_LIB to standardize common user interface and I/O functions and to simplify CDB access (Gilkey, 1995a; Gilkey, 1995b; Gilkey, 1995c). These libraries are linked to the DRSPALL executable during the build process as documented in the *Implementation Document for DRSPALL Version 1.24* (Kicker, 2021b).

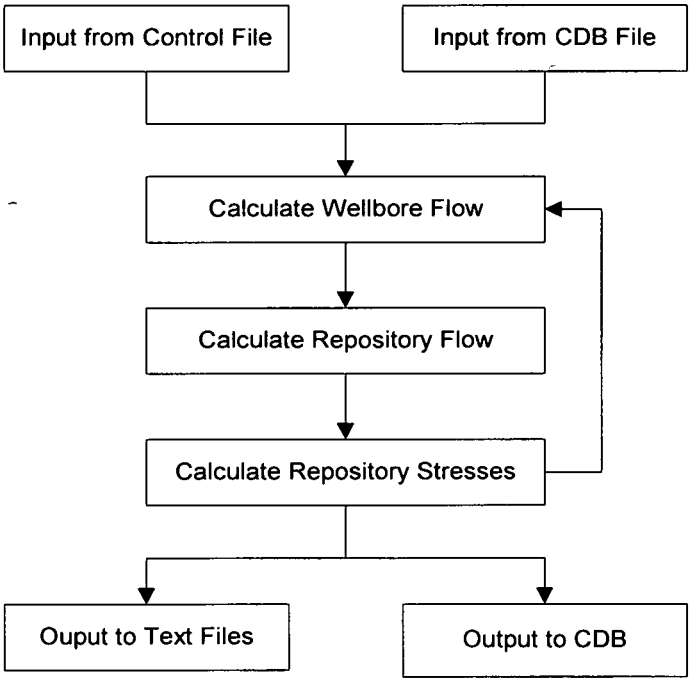


Figure 1 Flow chart of major code components.

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The CAMCON_LIB library provides a library of standardized QA and user interface routines such as a code banner with credits (authors), software ID, revision date, and current date and time; file processing routines to read and parse the command line, and to specify and open files; free-field input routines; and string processing routines.

The CAMSUPES_LIB library is a collection of machine dependent routines to access the system clock and allocate memory. However, CAMSUPES dynamic memory allocation has not been implemented in this version of DRSPALL except in the CAMDAT_LIB library. FORTRAN 90 dynamic memory allocation is used instead.

The CAMDAT_LIB library provides a programmer's interface through subroutine calls for accessing and creating CDB files.

4.0 THEORETICAL BASIS

DRSPALL is based on the theory of one-dimensional time-dependent compressible isothermal fluid flow. Somewhat different forms of that theory are used, depending on whether the flow is in the wellbore or in the repository, and whether the wellbore currently penetrates the repository or not. The wellbore and repository flows are coupled at a specified boundary by a set of conditions. Schematic diagrams of the flow geometry prior to and after penetration are shown in Figure 2 and Figure 4, respectively. Throughout the process, the drillbit can move downward as a function of time, removing salt or waste material. Flow in the well is treated as a compressible, viscous, multi-phase mixture of mud, gas, salt, and possibly waste solids. Flow in the repository is treated as viscous, compressible single-phase gas flow in a porous solid. At the cavity forming the repository-wellbore boundary (following penetration) waste solids freed by drilling, tensile failure, and associated fluidization may enter the wellbore flow stream. Between the well and the repository, flow is treated according to the state of penetration, as described later.

4.1 Wellbore Flow Prior to Penetration

Flow in the well prior to drillbit penetration into the repository is treated as shown in Figure 4. In concept this model is similar to that proposed by Podio and Yang (1986) and now in use in the oil and gas industry. The pump input is controlled by volume flow rate (with a maximum pressure), and may be stopped or started. Flow is one dimensional pipe flow with cross sectional areas corresponding to the appropriate flow area at a given position in the well. The drillbit is treated as a choke with cross-sectional area appropriate to the bit nozzle area. Immediately below the bit, gas from the repository can flow through drilling-damaged salt into the well, as described in Section 4.3. After the bit, return flow to the surface is treated as pipe flow in the annulus separating the drill string and the outer hole boundary. At the annulus output to the surface, mud ejection is to a constant atmospheric pressure. The gravitational body force acts in its appropriate direction based on position before or after the bit. The well fluid is Newtonian. Viscosity of the phase mixture is determined by an approximation as discussed in Section 5.1. Flow friction may be either laminar or turbulent, also based on an approximation given in Section 5.1.

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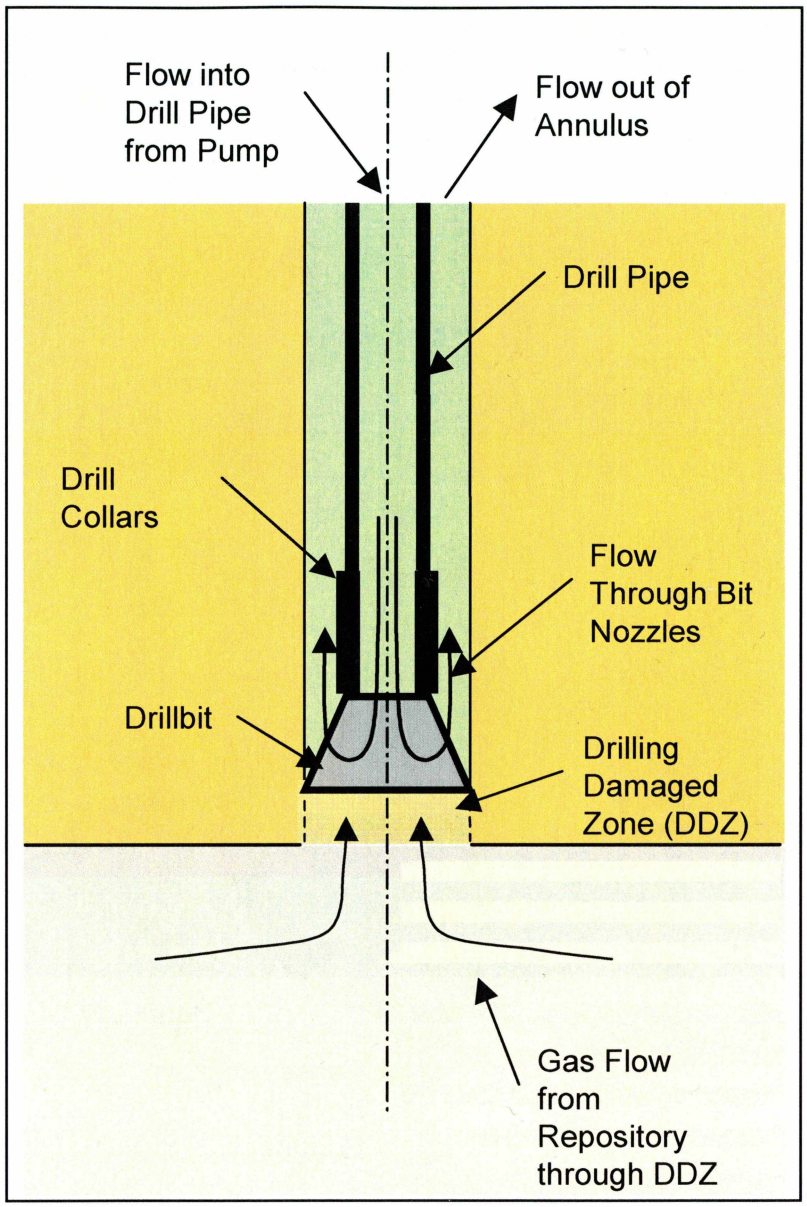


Figure 2 Schematic diagram of the flow geometry prior to repository penetration.

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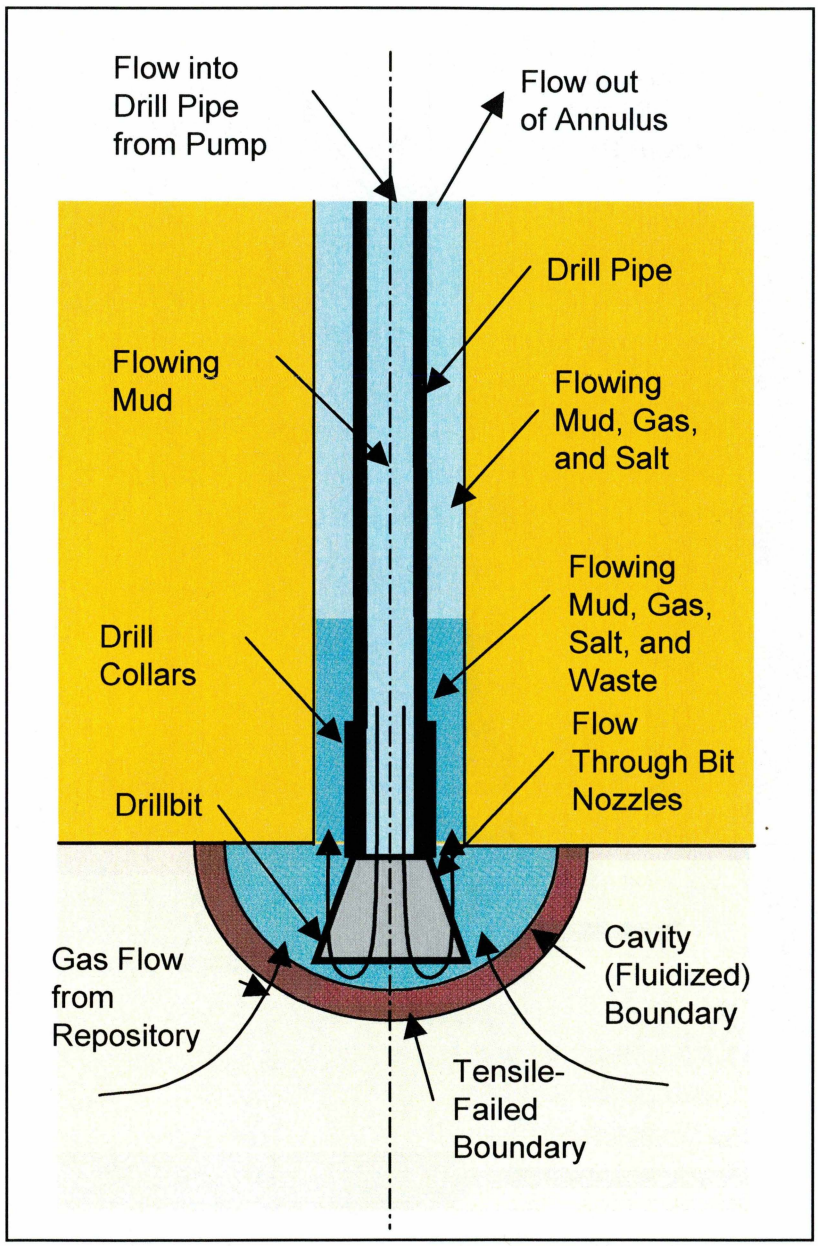


Figure 3 Schematic diagram of the flow geometry after repository penetration. Spherical case is shown.

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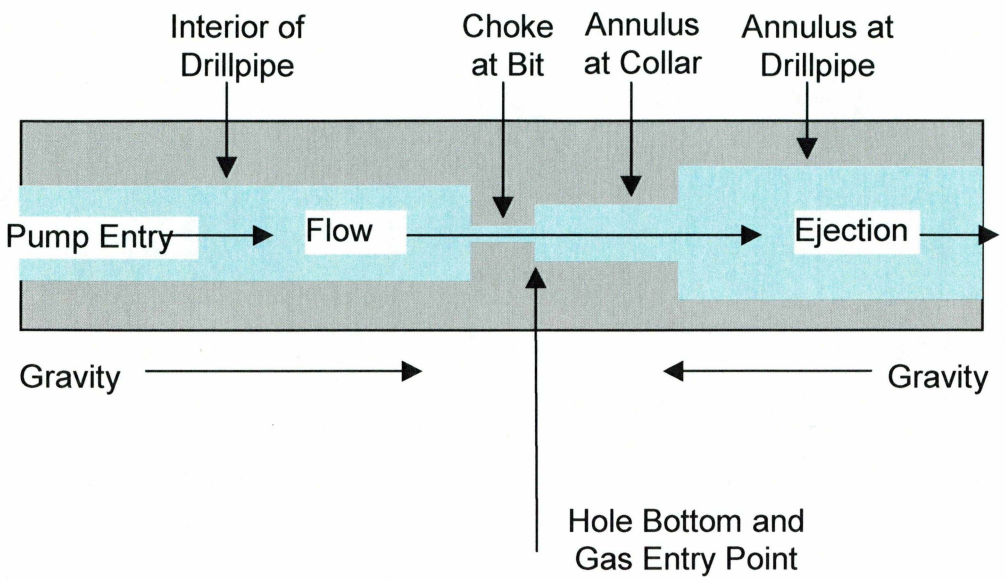


Figure 4 Effective wellbore flow geometry before bit penetration.

4.2 Repository Flow Prior to Penetration

The flow in the repository is one-dimensional radial, either hemispherical or cylindrical with its origin at the centerline of the well. Darcy flow of an isothermal ideal gas in a porous medium allows the simplifying pseudopressure approach to be taken, as is commonly done in the field of petroleum reservoir engineering. A modification allowing for non-Darcy inertial effects at high flow velocities is included. Near the well, the boundary pressure is determined as discussed in the next section on coupling. The outer boundary of the repository is set to a no flow condition, consistent with repository far-field conditions.

Solid stresses in the repository are treated as elastic and with an effective stress law. Flow-related forces are included. A homogeneous solid is assumed. Solid stresses are not relevant prior to penetration, but play a key role in determining failure and fluidization after penetration, as discussed later.

4.3 Coupling of Wellbore and Repository Flow Prior to Penetration

Prior to penetration, it is assumed that the drilling action creates a cylinder of altered-permeability salt material with diameter equal to the drillbit that moves ahead of the drillbit. This material allows limited porous gas flow from the repository to the wellbore. This is shown simply as the drilling damaged zone (DDZ) in Figure 2. Additional conceptual detail is shown in Figure 5. The permeability of this altered zone is greater than that of the intact salt and the disturbed rock zone (DRZ), and is based on a composite model as described in the Section 5.2.

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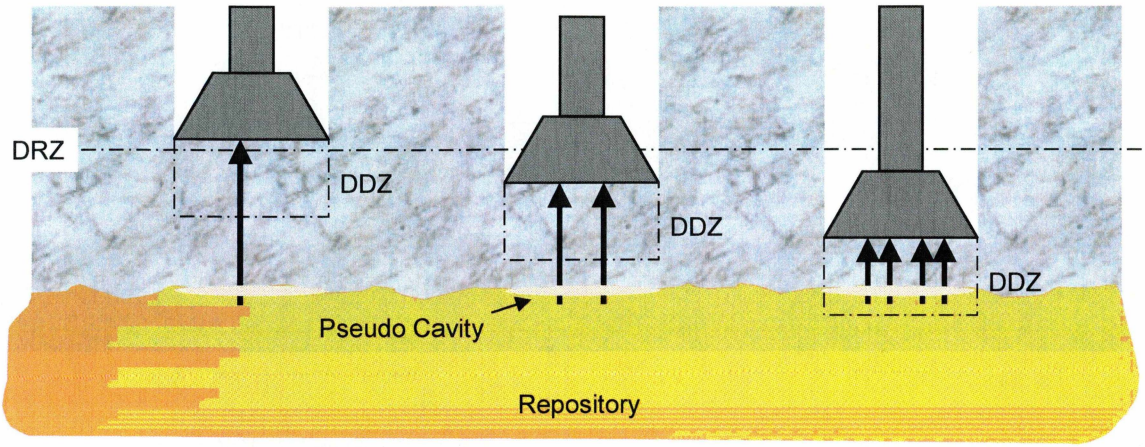


Figure 5 Coupling of the repository and wellbore prior to drillbit penetration.

Porous flow through this cylindrical volume is determined by the boundary pressures and flow areas of the volume. The boundary pressure on the well side is the pressure immediately below the bit. The area is the bit cross-sectional area (also assumed to be the wellbore area). The boundary pressure on the repository side is the pressure in a small pseudo-cavity at the wellbore face of the waste with the same surface area as the end of the drillbit. The pseudo-cavity provides continuity between the wellbore and repository and does not play a material role in total flow.

The main effect of the DDZ is to smooth the step function in pressure and flow rate that would otherwise occur upon bit penetration of the repository.

4.4 Wellbore Flow After Penetration

After drillbit penetration, the pseudo-cavity at the waste face becomes a real cavity and is connected to the flow area of the wellbore as shown in Figure 6. The cavity is now representative of the material removed from the repository by drilling, material failure, and subsequent fluidization.

After penetration, the cavity is treated as a mixing volume connecting the wellbore and the repository, and is used to provide the pressure boundary conditions at the inner wall of the repository. The volume of the cavity zone shown in Figure 6 is constantly adjusted so that it is equal to the growing volume of the actual hemispherical or cylindrical cavity. Fluidized waste solids mix with the mud/gas/salt flow and are moved up the wellbore and possibly out at the surface. An approximate model for the viscosity of the multi-phase mixture is used. All phases in the wellbore are assumed to move at the same velocity. The assumption of a single phase velocity greatly simplifies the mathematics and speeds numerical execution time. This assumption should be conservative with respect to waste release to the surface because a lagging waste particle velocity is expected in the wellbore, leading to a lower surface release rate and lower total release. The viscosity model causes the mixed fluid to act as a dense slurry for high solids concentrations, and there is a relative solids volume which causes complete choking.

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Treating the fluidized cavity as a region in one-dimensional series with the wellbore flow is a simplification. However, it is consistent with the one-dimensional nature of the flows in both wellbore and repository, and is a simple and convenient way of introducing the boundary coupling without introducing more complexity than knowledge of parameters justifies.

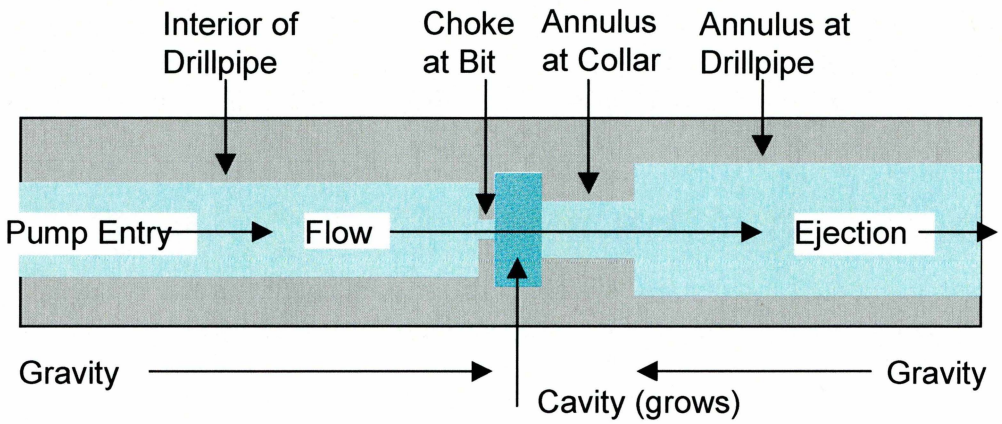


Figure 6 Effective wellbore flow geometry after bit penetration.

4.5 Repository Flow After Penetration

The flow model is basically the same after penetration as before. Without failure, the inner surface area of the repository is maintained at the same as the surface area of the true drilled borehole cavity. If radial tensile failure occurs as a result of pressure relief at the inner boundary and flow-related forces, the waste material is deemed susceptible to fluidization in the region of tensile failure. Then the pore fluid flow velocity is compared to a limiting velocity based on fluidized bed theory. If this fluidization velocity is exceeded, material is assumed to disaggregate and move into the cavity, thus enlarging the cavity and adding waste solids to it. The cavity volume is determined by cavity radius. The cavity radius is the sum of two components: the drilling radius and the spallings depth. The drilling radius is the radius of the volume with surface area equivalent to the surface area of the cylinder removed by drilling, as explained in Section 5.4. The spallings depth is the depth to which fluidization extends beyond the current cavity radius, as explained in Section 5.3.3.

4.6 Coupling of Wellbore and Repository After Penetration

As mentioned above, the coupling of the wellbore and the repository following penetration is achieved by treating the cavity as a mixing volume (Figure 6). If no fluidization occurs but drilling continues, the cavity grows at a rate equivalent to the volume being drilled. If fluidization occurs, the cavity volume may be greater than the drilled volume. Waste moves into the cavity when it is fluidized. Mass balance is maintained at all times. Mud flows into the cavity through the nozzles at the bit. Gas, waste and salt are moved into the cavity as drilling and fluidization occur. Subsequently, all components progress up the well. Salt and waste solids

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are treated as incompressible. Volumes of the compressible phases (gas and mud) are calculated based on their equations of state and the current pressure.

4.7 Preparation for Verification and Validation Testing

Isolation of model components for testing requires special code logic for each test case. To facilitate testing using the production executable without modifications, the special logic is incorporated prior to the production build and is activated via user-controllable input switches. Warning messages are generated that clearly indicate that DRSPALL is being executed in the testing mode.

5.0 MODELS AND METHODS

DRSPALL is implemented as a coupled system of differential equations and evaluated by time-marching integration. This section describes the system of equations used and the numerical techniques involved.

5.1 Wellbore Equations

Nomenclature is given in Table 5-1.

Table 5-1– Nomenclature for Wellbore Equations.

Symbol	Definition	Units
A	Flow area	m^2
A_p	Inlet area of mud pump	m^2
A_{out}	Outlet area of well	m^2
c_m	Compressibility of mud	Pa^{-1}
d_h	Hydraulic diameter	m
D_i, D_o	Inner and outer diameters	m
g	Acceleration of gravity	m/s^2
i	Zone index	--
m_w, m_s	Mass of waste and salt	kg
n	Timestep index	--
P	Pressure	Pa
$R_{mud\ pump}$	Volumetric rate of mud pump	m^3/s
Re	Reynold's number	--
S	Exponent in slurry viscosity formula	--
S_{mass}	Mass source term	kg/s
S_{mom}	Momentum source term	$kg\ m/s^2$
ss_m	Sound speed in mud	m/s
t	Time	s
u	Velocity	m/s

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Symbol	Definition	Units
u_{out}	Fluid velocity at outlet boundary	m/s
V	Volume	m^3
V_w, V_s, V_g, V_m,	Volumes of waste, salt, gas, and mud	m^3
w	Volume fraction of waste solids	--
w_{max}	Maximum allowed value of w	--
z	Distance from pump inlet	m
ε	Roughness of wall	m
F	Friction loss term	kg / m^2s^2
f	Darcy-Weisbach friction factor	--
η	Viscosity	kg /m s
ρ	Density	kg /m^3
0	Sub or superscript denoting initial value	--

Flow in the well is transient, compressible, isothermal, viscous, and multi-phase, including a mixture of mud, gas, salt, and possibly waste solids. Leakoff to the walls is ignored. All equations are adaptations of the well-known Navier-Stokes equations for compressible fluid flow. For example, see Oran and Boris (1987). The one-dimensional conservation equations that apply in this case are, for mass balance:

$$\frac{\partial}{\partial t}(\rho V)+\frac{\partial}{\partial z}(\rho V u)=S_{mass} \tag{5.1}$$

and for momentum balance:

$$\frac{\partial}{\partial t}(\rho V u)+\frac{\partial}{\partial z}\left(\rho V u^2\right)=-V\left(\frac{\partial P}{\partial z}-\rho g+F\right)+S_{mom} \tag{5.2}$$

where the value of the dissipation term in F cannot exceed the total momentum in the current flow direction. (That is, local dissipation can slow or stop the flow, but not reverse it.) To complete the system, an equation of state relating pressure and density and the friction loss term must be defined. Also, the source term and boundary conditions must be specified.

Density ρ in Equations 5.1 and 5.2 is the mixture density, computed as the sum of the masses of individual phase components in a representative volume, divided by that volume. The mixture equation of state must account for the four possible mass components in the well: mud, salt, gas, and waste. Because of known initial conditions, mud pumping rate, surface effluent rate, and the gas and solids exchange rate at the cavity-wellbore interface, the convection equations result in a known mass of each component in a given total volume. Then the individual volumes occupied by each component are determined, where

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$$V = V_s + V_w + V_m + V_g . \tag{5.3}$$

The salt and waste components are treated as incompressible, so their volumes are independent of pressure and determined from their initial user-specified densities by

$$V_s = \frac{m_s}{\rho_{0(s)}} \tag{5.4a}$$

and

$$V_w = \frac{m_w}{\rho_{0(w)}} . \tag{5.4b}$$

The gas is treated as isothermal and ideal, so

$$\rho_g = \rho_{0(g)} \frac{P}{P_0} . \tag{5.5}$$

The mud is assumed to be a compressible liquid, so

$$\rho_m = \rho_{0(m)} \left[1 + c_m (P - P_0) \right] \tag{5.6}$$

where P_0 is atmospheric pressure. To calculate pressure at a given location, note that the masses and total volume will always be known. Also, the volumes of salt and waste will be known, since they are considered incompressible. This means the total combined volume of gas and mud are known. This allows Equations 5.5 and 5.6 to be combined, resulting in a quadratic equation for gas volume:

$$a V_g^2 + b V_g - c = 0 \tag{5.7}$$

where

$$a = 1 - c_m P^0$$
$$b = \left(c_m P^0 V_g^0 - a V^* + V_m^0 \right)$$
$$c = V^* c_m P^0 V_g^0$$

and

$$V^* = V_m + V_g = V - V_s - V_w .$$

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Once gas volume is known, densities can be determined and pressure can be evaluated from either the gas (Equation 5.5) or mud equation of state (Equation 5.6).

For friction loss, a standard formulation for pipe flow is used (Fox and McDonald, 1985), where the head loss per unit length is given as:

$$F = f\frac{\rho}{d_h}\frac{u^2}{2}. \tag{5.8}$$

The hydraulic diameter d_h is given by

$$d_h = \frac{4A}{\pi(D_i + D_o)}. \tag{5.9}$$

Note that for flow in the drill pipe, $D_i = 0$. For annular flow up the wellbore, D_i is the outer diameter of the drill pipe and D_o is the wellbore diameter.

5.1.1 Wellbore Friction Factor

The friction factor f is determined by the method of Colebrook (Fox and MacDonald, 1985). In the laminar regime (Re < 2100)

$$f = \frac{64}{\mathrm{Re}} \qquad \text{where} \qquad \mathrm{Re} = \frac{u\rho d_h}{\eta}. \tag{5.10}$$

In the turbulent regime (Re > 2100)

$$\frac{1}{\sqrt{f}} = 2.0\log\left(\frac{\varepsilon/d_h}{3.7} + \frac{2.51}{\mathrm{Re}\sqrt{f}}\right). \tag{5.11}$$

An approximate solution for Colebrook's f in the turbulent regime is given by Serghides (1984):

$$f = \left[a - \frac{(b-a)^2}{c+a-2b}\right]^{-2} \tag{5.12}$$

$$a = -2\log\left[\frac{\varepsilon/d_h}{3.7} + \frac{12}{\mathrm{Re}}\right] \tag{5.13}$$

$$b = -2\log\left[\frac{\varepsilon/d_h}{3.7} + \frac{2.51a}{\mathrm{Re}}\right] \tag{5.14}$$

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$$c = -2\log\left[\frac{\varepsilon / d_h}{3.7} + \frac{2.51b}{\mathrm{Re}}\right]. \tag{5.15}$$

5.1.2 Viscosity of Wellbore Slurry

As the wellbore mixture becomes particle-laden, the viscosity of the mixture is determined from an empirical relationship developed for proppant slurry flows in channels for the oil and gas industry (Barree and Conway, 1995). First, a base fluid viscosity η_0 is determined by relative volume-weighting of the user-specified viscosities of the mud and gas. Then this viscosity is modified by an approximate slurry formula based on the volume fraction of waste solids.

$$\eta = \eta_0\left(1 - \frac{w}{w_{\max}}\right)^S. \tag{5.16}$$

An important assumption is that the particle diameter of the solids is always less than the channel width. If w reaches or exceeds its maximum value w_{max}, effective viscosity becomes large, and the flow chokes. Both w_{max} and s are empirically determined.

5.1.3 Wellbore Boundary Conditions

At the pump inlet, the source terms S_{mass} and S_{mom} are set by the volume flow rate of the pump and the density of the mud at the inlet such that

$$S_{mass} = \rho_{0(m)} R_{mudpump} \tag{5.17}$$

and

$$S_{mom} = \frac{\rho_{0(m)}}{A_p} R^2{}_{mudpump}. \tag{5.18}$$

The outlet boundary at the surface uses a specified pressure, usually set to atmospheric pressure. This contributes to setting dP/dz at the outlet boundary in Equation 5.2 and the resulting outlet boundary velocity sets the outlet source terms as

$$S_{mass} = -\rho A_{out} u_{out} \tag{5.19}$$

and

$$S_{mom} = -\rho A_{out} u_{out}^2. \tag{5.20}$$

Additionally, mass input sources, as specified in Sections 5.2 and 5.4, occur at a point corresponding to the porous flow across the drilling damaged zone prior to penetration and at a

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point corresponding to the cavity wall after penetration. No momentum is assumed to be contributed by these inputs.

5.2 Wellbore-Repository Coupling Equations Prior to Penetration

Nomenclature is given in Table 5-2.

Table 5-2– Nomenclature for Wellbore-Repository Coupling Equations.

Symbol	Definition	Units
A_{cav}	Outer area of pseudo cavity	m^2
d_{bit}	Diameter of drillbit	m
H_o	Thickness of repository prior to closure	m
H	Current thickness of repository	m
k_{eff}	Effective permeability of cylinder	m^2
k_{DDZ}	Permeability of DDZ	m^2
k_{DRZ}	Permeability of DRZ	m^2
L	Total length of cylinder	m
L_{DDZ}	Length of cylinder in DDZ	m
L_{DRZ}	Length of cylinder in DRZ	m
m_{cav}	Mass of gas in pseudo cavity	kg
m_{cyl}	Mass of gas flowing from cylinder	kg
P_{cav}	Pressure in repository pseudo cavity	Pa
P_{BH}	Pressure in bore hole just ahead of bit	Pa
T	Temperature	K
R_0	Ideal gas constant	J/kg·K
η	Gas viscosity	kg /m s
ϕ_o	Porosity of a waste-filled room prior to closure	--
ϕ	Current repository porosity	--
ρ_g	Density of gas	kg/m^3

Prior to penetration, the cylinder of altered permeable salt connecting the wellbore and the repository has a permeability and gas flow rate determined by the series connection of the salt, DRZ, and DDZ permeability (Gross and Thompson, 1998). Since the DDZ permeability is the greatest of these, and the DRZ boundary is fixed while the DDZ boundary advances with drilling, and L is decreasing with time, the permeability of this zone increases with time and becomes unbounded as the repository is penetrated. However, since the cavity and borehole pressures converge as the repository is penetrated, the overall mass flow remains bounded. If we start the process at the moment the DRZ or DDZ is contacted (whichever is most above the

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repository) the mass flow rate thus defined is determined by an incrementally steady-state solution to Darcy's equation for compressible flow (Gross and Thompson, 1998):

$$\frac{dm_{cyl}}{dt} = \frac{k_{eff}\pi\left(\frac{d_{bit}}{2}\right)^2}{2\eta R_0 TL}(P_{cav}^2 - P_{BH}^2) \tag{5.21}$$

where

$$k_{eff} = \frac{L}{\frac{L_{DDZ}}{k_{DDZ}} + \frac{L_{DRZ}}{k_{DRZ}}}. \tag{5.22}$$

There is no need to start this process while there is intact salt between the DDZ and repository, as the flow is too small to have noticeable effect. In the numerical analysis, a series of steady-states (one for each timestep) is used with time-varying pressure boundary conditions. The wellbore pressure boundary is the pressure at the point of entry (just below the bit) and the repository pressure is that of the small pseudo cavity at the face of the repository. Although the flow is not truly steady-state, this approach is justified as follows: When the distance L is large (that is, drilling is at or above the DRZ) the steady state assumption will somewhat overestimate the flow, but the flow itself is so small that the error is small. When the distance L becomes small, the steady-state assumption becomes more and more accurate, since equilibrium is rapidly achieved. Thus the stepwise steady state approach becomes sufficiently accurate at the time and position of the bit where accuracy is most required. These conclusions are established by inspection of the results of (Gross and Thompson, 1998).

Repository thickness H at the time of intrusion is determined from the current repository porosity ϕ, and the height H_o and porosity ϕ_o of a waste-filled room prior to closure:

$$H = \frac{(1-\phi_o)H_o}{1-\phi}. \tag{5.23}$$

To couple to the wellbore, Equation 5.21 is used as the source term, S_{mass}, in Equation 5.1 for the wellbore, at the leading edge of the bit. To couple to the repository, the pseudo cavity is created below the bit centered at the point where penetration will eventually occur. The geometry of the pseudo cavity is a hemisphere with outer area equal to the bit area in the spherical case, or a cylinder with outer area equal to the bit area in the cylindrical case. The volume of this cavity is thus, for example, in the spherical case

$$V_{cav} = \left(\frac{\pi}{24\sqrt{2}}\right)d_{bit}^3 \tag{5.24}$$

and in the cylindrical case

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$$V_{cav} = \left(\frac{\pi}{64H}\right) d_{bit}^4 . \tag{5.25}$$

If the pseudo cavity volume is small compared to physical volumes in the system, it will act to provide compatible boundary conditions prior to penetration and should have no other effect on the solution. For example, once the bit has penetrated the repository by about 1/10 its diameter, the volume actually drilled in the repository exceeds that volume of the pseudo cavity. The pseudo cavity starts at repository pressure and contains gas. Mass flow out of the pseudo cavity is defined by Equation 5.21. Mass flow into the cavity is defined by the pressure gradient at the repository cavity wall and other permeable flow parameters

$$\frac{dm_{cav}}{dt} = \rho_{g(repos)} u_{repos} \phi A_{cav} \tag{5.26}$$

where the density and velocity are defined in the repository at the cavity wall boundary. Once the net mass flow into/out of the cavity is determined, the pressure in the cavity is determined from the ideal gas law.

5.3 Repository Equations

Nomenclature is given in Table 5-3.

Table 5-3– Nomenclature for Repository Equations.

Symbol	Definition	Units
a	Particle shape factor	--
C_0	Cohesion	Pa
d_p	Diameter of particles (mean)	m
F_f	Fraction of material fluidized	--
F_0	Forchheimer number	--
g	Acceleration of gravity	m/s^2
i, j	Zone indices	--
k,	Permeability	m^2
k'	Velocity dependent permeability	m^2
k_f	Permeability in failed material	m^2
L_t	Characteristic length for tensile failure	m
m	Geometry exponent (m=3 for spherical, m=2 for cylindrical)	--
p	Pressure in gas	Pa
p_c	Pressure at cavity face	Pa
p_{ff}	Pressure in far-field	Pa
p_m'	Mean normal effective stress	Pa
r	Radius	m

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Symbol	Definition	Units
r_{cl}	Radius at center of first intact cell	m
r_c, r_{cequiv}	Radius at cavity face	m
S_0	Shear strength	Pa
t	Time	S
t_f	Fluidization time	s
t_m	Mixing time from store to cavity	s
T_0	Tensile strength	Pa
U_f	Fluidization velocity	m/s
U_s	Superficial gas velocity	m/s
β	Biot's constant (near 1.0)	--
β_{nd}	Non-Darcy coefficient	1/m
ΔH	Current bit penetration	m
η	Viscosity of gas	kg /m s
ψ	Pseudopressure	Pa m^2/s
ρ	Density of gas	kg/m^3
ρ_w	Density of waste solids	kg/m^3
σ_{ff}	Stress in far-field	Pa
σ_{sr} , $\sigma_{s\theta}$	Radial and tangential seepage stresses	Pa
σ_r' , σ_θ'	Radial and tangential effective stresses	Pa
τ	Maximum shear stress	Pa
θ	Angle of internal friction	rad
μ	Friction coefficient	--
υ	Poisson's ratio	--
ζ_m, ζ_p	Numerical diffusion coefficient for mass and momentum, respectively	--

5.3.1 Non-Darcy Flow

Flow in the repository is transient, compressible, viscous, and single phase for a porous diffusive solid. The gas flow rates near the cavity boundary may be quite high and cause an inertial resistance to flow (Belhaj et al., 2003). (Some early authors used turbulence as an explanation for the effect but most recent authors confirm that the flow is laminar, but tortuous (Hassanizadeh and Gray, 1987).) To account for the effect, we use a modification to the Darcy flow equation commonly called the Forchheimer effect, which we express as a velocity-dependent permeability reduction. A second term in velocity squared is added to the Darcy equation:

$$-\frac{\partial p}{\partial x} = \frac{\eta}{k} u + \beta_{nd} \rho u^2 . \qquad (5.27)$$

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This equation can be expressed in the form

$$-\frac{\partial p}{\partial x} = \frac{\eta}{k'} u \tag{5.28}$$

where

$$k' = \frac{k}{1 + F_0} \quad \text{and} \quad F_0 = \frac{\beta_{nd} \rho k u}{\eta}. \tag{5.29}$$

The Forchheimer number F_0 has sometimes been called the Reynold's number for porous flow. The non-Darcy coefficient β_{nd}, which depends on material properties such as the tortuosity and area of internal flow channels, is empirically determined. We choose a study by Li et al. (2001), which used high-velocity nitrogen flow through porous sandstone wafers, giving the result

$$\beta_{nd} = \frac{1.15 x 10^{-6}}{k\phi}. \tag{5.30}$$

Other published values and mathematical forms exist and can vary when evaluated by as much as an order of magnitude from Equation 5.30. This form was chosen for mathematical simplicity, because it represents neither the high nor the low end of the range, and because it is one of the studies that specifically looked at gas flow in highly porous materials with a large number of measurements. Within DRSPALL, the solution including the Forchheimer effect requires expressing Equation 5.28 in radial coordinates and solving the new repository flow equation.

The equation is derived by using Equation 5.28, the ideal gas equation of state:

$$p = p_0 \frac{\rho}{\rho_0} \tag{5.31}$$

and the conservation of mass:

$$\varphi \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) = 0, \tag{5.32}$$

which gives:

$$\frac{\partial p}{\partial t} = \frac{k'}{2\varphi\eta} \nabla^2 p^2 + \frac{1}{2\varphi\eta} \left(\nabla p^2\right) \nabla (k') \tag{5.33}$$

where the operator is given by

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$$\nabla^2 = \frac{1}{r^{m-1}} \frac{\partial}{\partial r}\left(r^{m-1} \frac{\partial}{\partial r} \right). \tag{5.34}$$

For an isothermal ideal gas, the pseudopressure is defined as

$$\psi = \frac{p^2}{\eta} \quad \text{or} \quad p = \sqrt{\eta \psi}\,. \tag{5.35}$$

Combining Equations 5.33, 5.34, and 5.35 leads to

$$\frac{\partial \psi}{\partial t} = \frac{D(\psi)}{r^{m-1}} \frac{\partial}{\partial r}\left(r^{m-1} \frac{\partial \psi}{\partial r} \right) + \frac{D(\psi)}{k'} \frac{\partial k'}{\partial r} \frac{\partial \psi}{\partial r} \tag{5.36}$$

where

$$D(\psi) = \frac{k'}{\phi} \sqrt{\frac{\psi}{\eta}} = \frac{k' p}{\phi \eta} \tag{5.37}$$

Since the equation of state is embedded in the pseudopressure definition as used here, no additional equation relating gas pressure and density is needed.

The singularity as r approaches zero in Equation 5.36 is not a concern since the cavity/repository boundary always occurs at finite r and the repository equation never has to be solved for r approaching zero. The boundary conditions at the inner radius of the repository are discussed in Sections 5.2 and 5.4. The condition at the outer boundary is based on no flow with an initial pressure equal to the repository pressure.

5.3.2 Elastic Response and Failure

To determine failure and fluidization, solid elastic effective stresses are required. While the fluid calculations using Equation 5.36 are fully transient, the solid stress calculations are assumed to be quasi-static. (That is, we ignore sound-speed phenomena in the solid.) The stress equations are thus found as follows.

Elastic effective stresses are (Jaeger and Cook, 1969):

$$\sigma_r'(r) = \sigma_{sr}(r) + \sigma_{ff}\left[1 - \left(\frac{r_c}{r} \right)^m \right] + p_c \left(\frac{r_c}{r} \right)^m - \beta p(r) \tag{5.38}$$

$$\sigma_\theta'(r) = \sigma_{s\theta}(r) + \sigma_{ff}\left[1 + \frac{1}{(m-1)} \left(\frac{r_c}{r} \right)^m \right] - \frac{p_c}{(m-1)} \left(\frac{r_c}{r} \right)^m - \beta p(r) \tag{5.39}$$

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where the flow-related stresses are given by (in analogy to differential thermal expansion, Timoshenko and Goodier, 1970):

$$\sigma_{sr}(r) = (m-1)\beta\left(\frac{1-2\upsilon}{1-\upsilon}\right)\frac{1}{r^m}\int_{r_c}^{r}\left[p(r)-p_{ff}\right]r^{m-1}dr \tag{5.40}$$

$$\sigma_{s\theta}(r) = -\beta\left(\frac{1-2\upsilon}{1-\upsilon}\right)\left(\frac{1}{r^m}\int_{r_c}^{r}\left[p(r)-p_{ff}\right]r^{m-1}dr - \left[p(r)-p_{ff}\right]\right) \tag{5.41}$$

Since stresses are calculated as quasi-static, an initial stress reduction caused by an instantaneous pressure drop at the cavity face propagates instantaneously through the waste. The result of calculating Equation 5.38 can be an instantaneous early-time tensile failure of the entire repository if the boundary pressure is allowed to change suddenly. This is non-physical and merely a result of the quasi-static stress assumption combined with the true transient pore pressure and flow-related stress equations. To prevent this behavior, tensile failure is not allowed until the propagation distance determined by a tensile propagation limit ("tensile failure velocity", Hansen et al., 1997), beginning at the cavity face, occurs. This should have no quantitative effect on results other than to prevent a non-physical tensile failure occurring at initial wellbore penetration. It is possible that allowing pre-penetration flow through the DDZ as described in Section 5.2 renders the introduction of this procedure unnecessary.

For tensile failure, the radial effective stress is averaged from the cavity boundary into the waste over a characteristic length L_t. If this average stress is tensile and exceeds the material tensile strength, T_0, the waste is assumed to be no longer capable of supporting radial stress, and the material from the cavity out to the characteristic length L_t is marked as failed. After failure, fluidization is allowed in the failed material. The cavity boundary does not move outward until after the failed material fluidizes, as discussed in Sections 5.3.3 and 5.3.5.

Potential shear failure locations are determined (flagged), but no relaxation associated with shear failure is used. For shear failure, the maximum shear stress

$$\tau(r) = \frac{1}{2}\left|\left(\sigma_r'(r) - \sigma_\theta'(r)\right)\right| \tag{5.42}$$

and mean normal effective stress

$$p_m'(r) = \frac{\left[\sigma_r'(r) + (m-1)\sigma_\theta'(r)\right]}{m} \tag{5.43}$$

are used to determine if maximum shear stress exceeds the linear Mohr-Coulomb shear strength

$$\tau(r) > S_0 + \mu p_m'(r) \tag{5.44}$$

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where

$$S_0 = \frac{C_0}{2}\left[\mu + \left(\mu^2 + 1\right)^{\frac{1}{2}}\right] \tag{5.45}$$

$$\mu = \tan(\theta) \tag{5.46}$$

and θ is the angle of internal friction. Again, singularities as r approaches zero are avoided because of the always-finite cavity. The solid stress boundary conditions are, for the inner boundary, no shear stress and radial stress equal to cavity pressure. For the outer boundary, the far field confining (radial) stress is set as an input parameter. There is no far-field shear stress.

5.3.3 Fluidization

In a region where tensile failure has occurred, the waste material is first assumed to be disaggregated, but not in motion. It remains as porous, bedded material lining the cavity face, and is treated as a continuous part of the repository from the perspective of the porous flow calculations. The bedded material is subject to mobilization and removal to the flow stream in the cavity by fluidized bed theory. As such, solids are allowed to flow into the cavity if the superficial gas velocity, U_s, at the cavity face exceeds a minimum fluidization velocity, U_f. Superficial gas velocity is defined as the average velocity across the entire surface area of the cavity (U_s = pore velocity × ϕ. The cavity radius will increase corresponding to the volume of solid material removed by fluidization. The minimum fluidization velocity is determined by solving the following quadratic equation (Cherimisinoff and Cherimisinoff, 1984; Ergun, 1952):

$$\frac{1.75}{a\phi^3}\left(\frac{d_p U_f \rho}{\eta}\right)^2 + 150\left(\frac{1-\phi}{a^2\phi^3}\right)\left(\frac{d_p U_f \rho}{\eta}\right) = \frac{{d_p}^3 \rho(\rho_w - \rho)g}{\eta^2}. \tag{5.47}$$

If fluidization occurs, the cavity is allowed to grow until the cavity radius equals the depth of the first intact (non tensile-failed) material. New tensile failure is allowed from the boundary into the intact repository material. Once the entire region of length L_t nearest boundary fluidizes, a new region of length L_t is defined and evaluated for failure as discussed above. With cavity growth, the gas and waste particles in the newly fluidized region must mix into the cavity in such a way as to conserve mass. To account for the fact that this mixing cannot be instantaneous, which would be non-physical and lead to numerical instability later (much as allowing instantaneous tensile failure propagation), a small artificial relaxation time, equal to the cavity radius divided by the superficial gas velocity, is imposed upon the mixing phenomenon. As fluidization occurs, the permeability of the failed waste in that region is allowed to grow according to

$$k'_f = k'(1 + 4F_f) \tag{5.48}$$

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where F_f is the fraction fluidized and is based on the fluidization relaxation time. This approximately accounts for the bulking of material as it fluidizes. It is interesting to note that the Ergun equation, which leads to Equation 5.47, can also be used to derive a non-Darcy coefficient for particulate beds (Narayanaswamy et al., 1999). This takes a similar form to Equation 5.30 (but not the same value). This suggests, as would be expected, that there is continuous transition from intact to failed to fluidized material. However, the level of accuracy inherent in the present work would not benefit from further investigation of this transition.

5.3.4 Repository Boundary Conditions

The porous flow equations are solved with a pressure (flow) boundary condition at the inner (cavity) wall and a zero pressure gradient (no-flow) condition at the outer wall. For the inner wall, the cavity pressure (either pseudo or real) sets a pressure outside the porous solid. The inner cavity wall propagates radially outward as material is drilled or failed and fluidized and moved from the repository to the cavity. Thus, the boundary condition is subsequently applied to the adjacent non-fluidized but possibly failed material. The pressure inside the porous solid then develops a gradient, based on the pressure difference, which is used to calculate a pore velocity at the boundary using Darcy's Law:

$$u_{repos} = \frac{k'}{\eta\phi}\frac{\partial p}{\partial r}\bigg|_{r=r_c} . \tag{5.49}$$

Material (gas) loss across the boundary as a function of time can then be calculated using Equation 5.26.

5.3.5 Implementation of Conceptual Submodels in DRSPALL

Some of the features of the conceptual and mathematical model discussed earlier require special implementation procedures in a finite difference code. The purpose of this section is to elucidate the implementation steps that are not necessarily clear in a discussion of the conceptual model alone.

5.3.5.1 Characteristic Length and Tensile Failure

A review of the effective stress formulation (Equation 5.38) reveals several issues that require careful consideration when applying this model to a repository domain divided into discrete computational zones. A typical radial effective stress curve is drawn in Figure 7. The tensile strength of the waste is shown in the figure as well. Effective radial tensile stresses (negative values on the stress axis) are shown to develop near to, but not exactly at the cavity wall. In fact, the effective stress exactly at the cavity wall is always $\sigma_r'(r_c) = 0$. As such, a region of tension develops that may exceed the tensile strength at radii greater than, but not at, the cavity wall. The region of material subject to tensile failure, without consideration of the characteristic length concept, is circled in Figure 7. Note that material between the failed region and the cavity wall is still intact according to the current stress model.

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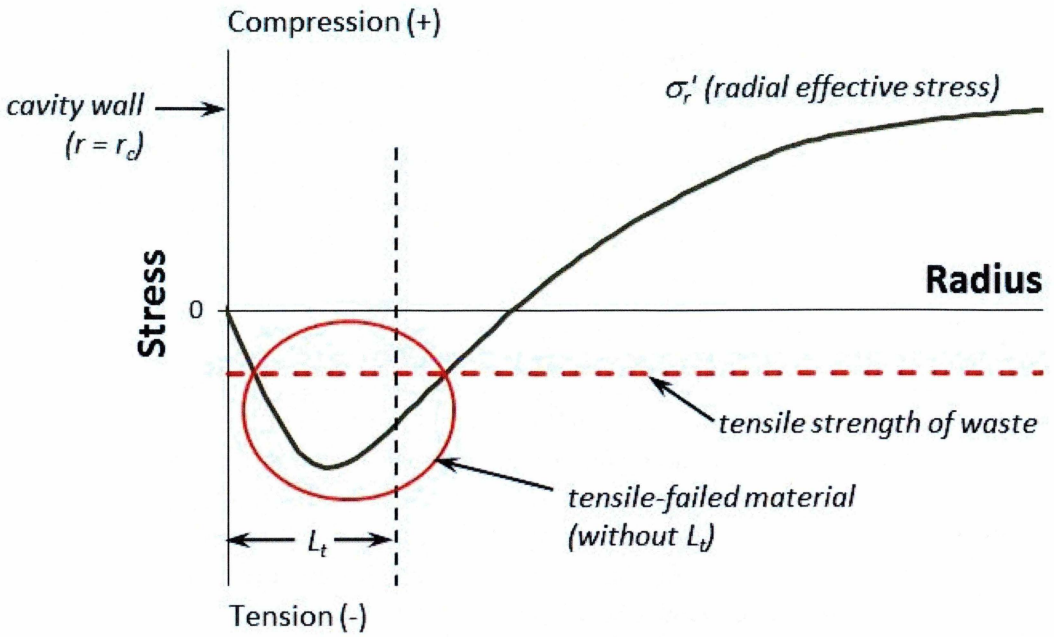


Figure 7 Drawing of typical radial effective stress curve in DRSPALL repository domain at some time during drill penetration.

Failed regions trapped between intact shells cannot, by themselves, be removed from the repository domain without first removing the intact cavity wall. It is proposed here that once a tensile-failed region exists, the cavity wall is likely to eventually succumb to buckling failure. A simple approach to this is implemented in DRSPALL by introducing a characteristic failure length L_t in which the mean tensile stress is evaluated over a region that extends from the cavity wall ($r = r_c$) to a depth of one characteristic length ($r = r_c + L_t$) into the domain. This characteristic length must be large enough to encompass several computational zones, but not so large that it masks the tensile region. If the mean tensile stress over L_t exceeds the tensile strength, all the zones in L_t fail, and they are flagged as "failed" in DRSPALL. Zones outside of L_t are not allowed to fail until all the disaggregated, bedded waste is fluidized.

5.3.5.2 Cavity Growth by Drilling

During normal drilling, when the bit penetration depth passes the outer edge of a computational zone, that zone (gas and solids) is removed from the repository domain and put into "store." From store, the drilled mass is then released to the cavity over a mixing time $t_m = (r_{c1}/U_s)$ where r_{c1} is the center of the cell that forms the cavity wall ($r_{c1} = r_c + 1/2\Delta r$). This is done because instantaneously adding the entire contents of one computational zone to the cavity introduces high frequency spikes that can lead to an increase in numerical error. The controlled release from store dampens the numerical shock to the system.

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5.3.5.3 Cavity Growth by Fluidization

In the event that a group of zones comprising L_t fails, the zones are all tested for fluidization potential using the Ergun (1952) model given in Equation 5.47. If the superficial gas velocity exceeds the minimum fluidization velocity ($U_s > U_f$), all failed zones are flagged for fluidization. The fluidization process requires a finite fluidization time $t_f = r_{cl}/U_s$. Zones must begin fluidization sequentially so that the zone comprising the cavity wall starts first, after which the next zone can start fluidization on the very next timestep. This proceeds until all zones flagged for fluidization are removed from the repository domain and thus incorporated into the wellbore domain. The cavity thus grows in zone-by-zone increments as subsequent zones complete fluidization.

5.4 Wellbore-Repository Coupling Equations Following Penetration

Upon penetration by the drillbit, the gas flow Equation 5.21 at the drillbit/cavity inner boundary is no longer used. Instead, the cavity volume is assumed to be included in the wellbore flow path as shown in Figure 6. If the cavity subsequently grows due to drilling, tensile failure and fluidization, the volume of this part of the flow path increases to be consistent with the growing cavity volume. The equivalent physical assumption is that mud flow passes through the bit nozzles, mixes fully with the gas and waste in the cavity and then the resulting mixture flows up the annulus around the drill collars. Thus no new equations are needed, other than to be sure that mass balance is maintained and that cavity volume is correct. Equation 5.26 is still used to determine gas mass flow into the cavity from the repository. Waste flows into the cavity by simply mixing in fluidized waste as discussed in Section 5.3. The mass input provided by gas and waste flowing into the cavity replace the gas mass source provided by the DDZ prior to penetration, thus mathematical consistency and continuity are maintained throughout the drilling and gas/waste flow process.

The true cylindrical cavity of increasing height formed during the drilling process must be mapped each computational step to an equivalent cavity radius in the specified one-dimensional spherical or cylindrical geometry. This mapping assumes conservation of surface area in order to preserve the early time repository pressure gradients and thus gas flux from the repository to the wellbore. Note that the drilled volume will not be conserved.

The surface area of the true cylinder cut from the waste takes the shape of a soup can with one end removed. The surface area of this cut cylinder is therefore:

$$A_{cut} = \frac{\pi d_b^2}{4} + \pi d_b \Delta H \,. \tag{5.50}$$

In spherical geometry the equivalent radius is determined by equating A_{cut} with the surface area of a hemisphere ($A = 2\pi r_{eq}^2$). Solving for r_{eq} gives:

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$$r_{eq} = \left(\frac{A_{cut}}{2\pi} \right)^{\frac{1}{2}}. \tag{5.51}$$

In cylindrical geometry the equivalent radius is determined by equating A_{cut} with the surface of a cylinder with fixed height H and open ends ($A = \pi d_b H$). Solving for r_{eq} in this case gives:

$$r_{eq} = \left(\frac{A_{cut}}{2\pi H} \right). \tag{5.52}$$

For small penetration depths this implies a very small diameter equivalent cylinder with a height equal to the repository thickness.

Equivalent volumes are calculated from the equivalent radius using the volume equation appropriate for the assumed geometry. When the bit reaches the floor of the repository, drilling is stopped and in cylindrical geometry the actual drilled and equivalent volumes will be the same. But, in spherical geometry the equivalent volume will be greater than the drilled volume.

5.5 Numerical Method – Wellbore

Both the wellbore and the repository calculations use time-marching finite differences. These are part of a single computational loop and therefore use the same time step. The differencing schemes for the wellbore and repository calculations are similar but not identical.

The wellbore is zoned for finite differencing as shown in Figure 8. This shows zones, zone indices, grid boundaries, volumes, and interface areas. The method is Eulerian. That is, zone boundaries are fixed, and fluid moves through the interfaces by convection. Quantities are zone-centered and integration is explicit in time. In the following, detailed discussion will be specific to the mass transport given by Equation 5.1 However, the differencing method for the momentum transport given by Equation 5.2 is the same.

The equations shown below are for constant zone size. All of the materials (mud, salt, gas, and waste) are assumed to move together as a mixture. Since fluid moves through the grid boundaries, calculation requires values for the flow through these boundaries during a timestep. This is obtained from difference between the fluid velocities at the zone centers, given by

$$u_{i+1/2} = \frac{1}{2}\left(u_{i+1}^{n-1} + u_i^{n-1} \right). \tag{5.53}$$

The mass transport equation, prior to any volume change, becomes

$$V_i \, \rho_i^{*} = V_i \, \rho_i^{n-1} - \Delta t \left(A_{i+1/2} \rho_{i+1/2}^{n-1} u_{i+1/2} - A_{i-1/2} \rho_{i-1/2}^{n-1} u_{i-1/2} \right) + \Delta t S_{m,i}. \tag{5.54}$$

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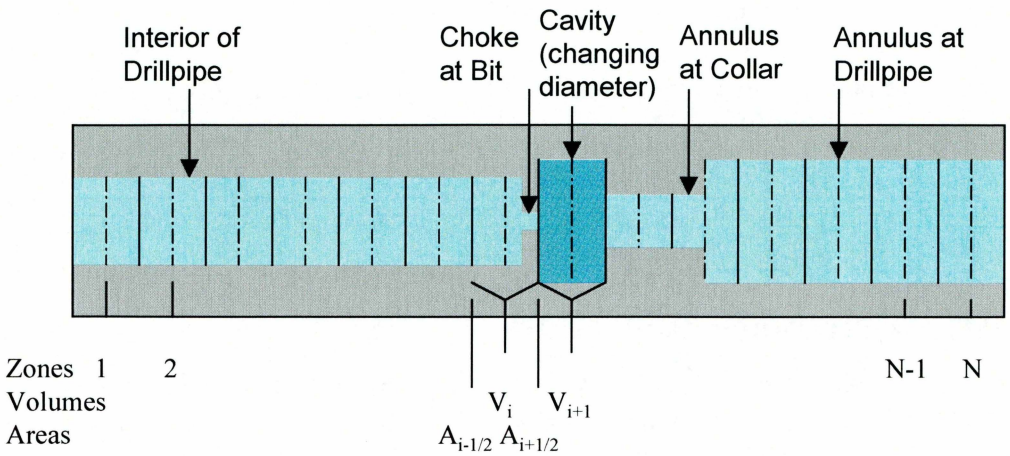


Figure 8 Finite difference zoning for wellbore.

Here the source terms ($S_{m,i}$) are set to correspond to material entering or exiting at the pump, cavity, and surface. The "upwind" zone centered densities are used for the interfaces values, $\rho_{i+1/2}^{n-1}$ and $\rho_{i-1/2}^{n-1}$. Finally we incorporate any changed volumes and add numerical mass diffusion for stability:

$$V_i\ \rho_i^n = V_i\ \rho_i^* + \Delta z_i \sum_{m=1}^{N_c} \zeta_m \left[A_{i+1/2} \left((\rho f_m)_{i+1}^{n-1} - (\rho f_m)_i^{n-1} \right) - A_{i-1/2} \left((\rho f_m)_i^{n-1} - (\rho f_m)_{i-1}^{n-1} \right) \right]. \qquad (5.55)$$

The densities, ρf_m, are for the particular constituent, m, being diffused and are calculated from the mixture density, ρ, times the mass fraction, f_m, of the constituent in the referenced cell. The numerical diffusion coefficient ζ_m is chosen empirically for stability. Separate diffusion coefficients could be used for the different materials (mud, gas, etc.). However, sufficient stability is obtained by only diffusing mud and salt using the same coefficient. This better preserves the accuracy of the location of gases and waste in the well.

Momentum is differenced as

$$\begin{aligned} V_i\ (\rho u)_i^* = V_i\ (\rho u)_i^{n-1} - \Delta t \left(A_{i+1/2} (\rho u)_{i+1/2}^{n-1} u_{i+1/2} - A_{i-1/2} (\rho u)_{i-1/2}^{n-1} u_{i-1/2} \right) \\ - V_i \left(\frac{P_{i+1}^{n-1} - P_{i-1}^{n-1}}{2\Delta z} - \rho_i^{n-1} g + F_i^{n-1} \right) + \Delta t S_{mom,i} \end{aligned} \qquad (5.56)$$

where the dissipation term F_i^{n-1} is obtained from Equation 5.8 and is constrained as follows:

$$\left| F_i^{n-1} \right| \le \left| \frac{P_{i+1}^{n-1} - P_{i-1}^{n-1}}{2\Delta z} - \rho_i^{n-1} g \right| \qquad (5.57)$$

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and the sign F_i^{n-1} is chosen such that it opposes flow.

Finally, numerical momentum diffusion is added without distinguishing between phases in the mixture (ρ is the mixture density).

$$V_i\ (\rho u)_i^n = V_i\ (\rho u)_i^* - \zeta_p \Delta z_i \left[A_{i+1/2} \left((\rho u)_{i+1}^{n-1} - (\rho u)_i^{n-1} \right) - A_{i-1/2} \left((\rho u)_i^{n-1} - (\rho u)_{i-1}^{n-1} \right) \right]. \tag{5.58}$$

5.6 Numerical Method – Repository

The time integration method for the repository flow is implicit, with spatial derivatives determined after the time increment. This method requires the inversion of a matrix for the entire repository, which is usually straightforward. The implicit scheme is unconditionally stable. However, it is still necessary to use small time steps to ensure gradient accuracy.

We start with Equation 5.36, and note that

$$\frac{\partial \ln k'}{\partial r} = \frac{1}{k'} \frac{\partial k'}{\partial r}. \tag{5.59}$$

Substituting Equation 5.59 into Equation 5.36 yields:

$$\frac{\partial \psi}{\partial t} = \frac{D(\psi)}{r^{m-1}} \frac{\partial}{\partial r} \left(r^{m-1} \frac{\partial \psi}{\partial r} \right) + D(\psi) \frac{\partial \ln(k')}{\partial r} \frac{\partial \psi}{\partial r}. \tag{5.60}$$

Expand first term on right-hand side of Equation 5.60:

$$\begin{aligned} \frac{D(\psi)}{r^{m-1}} \frac{\partial}{\partial r} \left(r^{m-1} \frac{\partial \psi}{\partial r} \right) &= D(\psi) \left[\frac{1}{r^{m-1}} \frac{\partial}{\partial r} \left(r^{m-1} \frac{\partial \psi}{\partial r} \right) \right] \\ &= D(\psi) \left[\frac{1}{r^{m-1}} r^{m-1} \frac{\partial}{\partial r} \left(\frac{\partial \psi}{\partial r} \right) + \frac{\partial \psi}{\partial r} \frac{1}{r^{m-1}} \frac{\partial \left(r^{m-1} \right)}{\partial r} \right] \\ &= D(\psi) \left[\frac{\partial^2 \psi}{\partial r^2} + \frac{\partial \psi}{\partial r} \frac{1}{r^{m-1}} (m-1) \left(r^{m-2} \right) \frac{\partial r}{\partial r} \right] \\ &= D(\psi) \left[\frac{\partial^2 \psi}{\partial r^2} + \frac{(m-1)}{r} \frac{\partial \psi}{\partial r} \right]. \end{aligned} \tag{5.61}$$

Substituting Equation 5.61 into Equation 5.60 gives:

$$\frac{\partial \psi}{\partial t} = D(\psi) \left[\frac{\partial^2 \psi}{\partial r^2} + \frac{(m-1)}{r} \frac{\partial \psi}{\partial r} + \frac{\partial \ln(k')}{\partial r} \frac{\partial \psi}{\partial r} \right]. \tag{5.62}$$

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Equation 5.62 is nonlinear due to the dependence of the parameter D on the state variable . Hence, its numerical solution requires use of an iterative scheme such as the Newton-Raphson method. However, as explained in the next section, D is treated as independent of ψ in DRSPALL calculations, so an iterative Newton-Raphson scheme is not necessary here.

5.6.1 Finite Difference Discretization

Using an implicit scheme, Equation 5.62 can be represented in finite difference form by using the central difference method to discretize the right-hand side and the forward difference method to discretize the left-hand side (Özişik, 1993, Chapter 12, "Implicit Method").

This gives:

$$\frac{\psi_j^{n+1}-\psi_j^n}{\Delta t}=D\left(\psi_j^{n+1}\right)\left[\frac{\psi_{j+1}^{n+1}-2\psi_j^{n+1}+\psi_{j-1}^{n+1}}{(\Delta r)^2}+\frac{(m-1)}{r_j}\frac{\left(\psi_{j+1}^{n+1}-\psi_{j-1}^{n+1}\right)}{2\Delta r}+\frac{\left(\ln\left(k_{j+1}^{\prime n+1}\right)-\ln\left(k_{j-1}^{\prime n+1}\right)\right)}{2\Delta r}\frac{\left(\psi_{j+1}^{n+1}-\psi_{j-1}^{n+1}\right)}{2\Delta r}\right] \tag{5.63}$$

As discussed in Lord et al. (2006), $D(\psi)$ is assumed constant over a zone, which simplifies the numerical implementation. Using its zone centered value at the current time, the linearizing approximation $D(\psi)\approx D\left(\psi_j^{n+1}\right)\approx D\left(\psi_j^n\right)\approx D_j^n$ is made. Equation 5.63 becomes:

$$\frac{\psi_j^{n+1}-\psi_j^n}{\Delta t}=D_j^n\left[\frac{\psi_{j+1}^{n+1}-2\psi_j^{n+1}+\psi_{j-1}^{n+1}}{(\Delta r)^2}+\frac{\left(\psi_{j+1}^{n+1}-\psi_{j-1}^{n+1}\right)}{2\Delta r}\left(\frac{(m-1)}{r_j}+\frac{\left(\ln\left(k_{j+1}^{\prime n+1}\right)-\ln\left(k_{j-1}^{\prime n+1}\right)\right)}{2\Delta r}\right)\right]. \tag{5.64}$$

Solve for ψ_j^n and collect similar terms:

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$$\psi_j^n = \psi_j^{n+1} - D_j^n \Delta t \left[\frac{\psi_{j+1}^{n+1} - 2\psi_j^{n+1} + \psi_{j-1}^{n+1}}{(\Delta r)^2} + \frac{\left(\psi_{j+1}^{n+1} - \psi_{j-1}^{n+1}\right)}{2\Delta r} \left(\frac{(m-1)}{r_j} + \frac{\left(\ln\left(k'^{n+1}_{j+1}\right) - \ln\left(k'^{n+1}_{j-1}\right)\right)}{2\Delta r} \right) \right]$$

$$= -D_j^n \Delta t \left[\frac{1}{(\Delta r)^2} - \frac{1}{2\Delta r} \left(\frac{(m-1)}{r_j} + \frac{\left(\ln\left(k'^{n+1}_{j+1}\right) - \ln\left(k'^{n+1}_{j-1}\right)\right)}{2\Delta r} \right) \right] \psi_{j-1}^{n+1} + \left[1 + \frac{2D_j^n \Delta t}{(\Delta r)^2} \right] \psi_j^{n+1}$$

$$- D_j^n \Delta t \left[\frac{1}{(\Delta r)^2} + \frac{1}{2\Delta r} \left(\frac{(m-1)}{r_j} + \frac{\left(\ln\left(k'^{n+1}_{j+1}\right) - \ln\left(k'^{n+1}_{j-1}\right)\right)}{2\Delta r} \right) \right] \psi_{j+1}^{n+1} \qquad (5.65)$$

$$= -\frac{D_j^n \Delta t}{\Delta r} \left[\frac{1}{\Delta r} - \frac{(m-1)}{2r_j} - \frac{\left(\ln\left(k'^{n+1}_{j+1}\right) - \ln\left(k'^{n+1}_{j-1}\right)\right)}{4\Delta r} \right] \psi_{j-1}^{n+1} + \left[1 + \frac{2D_j^n \Delta t}{(\Delta r)^2} \right] \psi_j^{n+1}$$

$$- \frac{D_j^n \Delta t}{\Delta r} \left[\frac{1}{\Delta r} + \frac{(m-1)}{2r_j} + \frac{\left(\ln\left(k'^{n+1}_{j+1}\right) - \ln\left(k'^{n+1}_{j-1}\right)\right)}{4\Delta r} \right] \psi_{j+1}^{n+1}$$

Noting that $\ln\left(k'^{n+1}_{j+1}\right) - \ln\left(k'^{n+1}_{j-1}\right) = \ln\left(k'^{n+1}_{j+1} \Big/ k'^{n+1}_{j-1} \right)$,

$$\psi_j^n = -\frac{D_j^n \Delta t}{\Delta r} \left(\frac{1}{\Delta r} - \frac{(m-1)}{2r_j} - \frac{\ln\left(k'^{n+1}_{j+1} \Big/ k'^{n+1}_{j-1} \right)}{4\Delta r} \right) \psi_{j-1}^{n+1} + \left(1 + \frac{2D_j^n \Delta t}{(\Delta r)^2} \right) \psi_j^{n+1}$$

$$- \frac{D_j^n \Delta t}{\Delta r} \left(\frac{1}{\Delta r} + \frac{(m-1)}{2r_j} + \frac{\ln\left(k'^{n+1}_{j+1} \Big/ k'^{n+1}_{j-1} \right)}{4\Delta r} \right) \psi_{j+1}^{n+1} \qquad (5.66)$$

Rewriting the equation:

$$\psi_j^n = -\alpha_1 \psi_{j-1}^{n+1} + (1 + 2\alpha) \psi_j^{n+1} - \alpha_2 \psi_{j+1}^{n+1} \qquad (5.67)$$

where

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$$\alpha = \frac{D_j^n \Delta t}{(\Delta r)^2}$$

$$\alpha_1 = \frac{D_j^n \Delta t}{\Delta r}\left(\frac{1}{\Delta r} - \frac{(m-1)}{2r_j} - \frac{\ln\left(k_{j+1}'^{n+1} / k_{j-1}'^{n+1}\right)}{4\Delta r}\right) \tag{5.68}$$

$$\alpha_2 = \frac{D_j^n \Delta t}{\Delta r}\left(\frac{1}{\Delta r} + \frac{(m-1)}{2r_j} + \frac{\ln\left(k_{j+1}'^{n+1} / k_{j-1}'^{n+1}\right)}{4\Delta r}\right)$$

and j and n are the cell and timestep indices, respectively.

Also:

$$\alpha_1 + \alpha_2 = \frac{D_j^n \Delta t}{\Delta r}\left(\frac{1}{\Delta r} - \frac{(m-1)}{2r_j} - \frac{\ln\left(k_{j+1}'^{n+1} / k_{j-1}'^{n+1}\right)}{4\Delta r}\right) + \frac{D_j^n \Delta t}{\Delta r}\left(\frac{1}{\Delta r} + \frac{(m-1)}{2r_j} + \frac{\ln\left(k_{j+1}'^{n+1} / k_{j-1}'^{n+1}\right)}{4\Delta r}\right)$$

$$= \frac{D_j^n \Delta t}{\Delta r}\left(\frac{1}{\Delta r} + \frac{1}{\Delta r}\right) \tag{5.69}$$

$$= 2\frac{D_j^n \Delta t}{(\Delta r)^2}$$

$$\alpha_1 + \alpha_2 = 2\alpha$$

5.6.2 Boundary Conditions

For the boundary condition at the inner radius we use the method given in Thomas (1995, Section 1.6.3, "Cell Centered Grids") for cell centered grids. Using this method the difference equation is derived on the second cell in the usual, here central difference, manner. The first intact zone is the zone closest to the borehole and is indexed as 1. The boundary condition is implemented by noting that for the first intact cell ($j - 1 = 1$), ψ_1^{n+1} is the cavity psuedo pressure, ψ_{cav}^{n+1}, which is known. Therefore, $\psi_1^{n+1} = \psi_{cav}^{n+1}$ can be moved to the left-hand side of Equation 5.67.

Using $j = 2$, the second cell, Equation 5.67 gives:

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$$\psi_2^n + \alpha_1 \psi_{cav}^{n+1} = (1+2\alpha)\psi_2^{n+1} - \alpha_2 \psi_3^{n+1}. \tag{5.70}$$

The far field boundary condition is a zero gradient condition. Mathematically this is:

$$\left.\frac{\partial \psi}{\partial r}\right|_{r=\infty} = 0. \tag{5.71}$$

Discretizing using a second-order central difference formulation:

$$\begin{aligned} &\frac{\psi_{N+1}^{n+1} - \psi_{N-1}^{n+1}}{2\Delta r} = 0 \\ &\psi_{N+1}^{n+1} = \psi_{N-1}^{n+1} \end{aligned} \tag{5.72}$$

Using this to eliminate the fictitious point in the domain discretization of Equation 5.67, at node point $j = N$ (i.e., the final cell):

$$\begin{aligned} \psi_N^n &= -\alpha_1 \psi_{N-1}^{n+1} + (1+2\alpha)\psi_N^{n+1} - \alpha_2 \psi_{N+1}^{n+1} \\ &= -\alpha_1 \psi_{N-1}^{n+1} + (1+2\alpha)\psi_N^{n+1} - \alpha_2 \psi_{N-1}^{n+1} \\ &= -(\alpha_1 + \alpha_2)\psi_{N-1}^{n+1} + (1+2\alpha)\psi_N^{n+1} \end{aligned} \tag{5.73}$$

Using $\alpha_1 + \alpha_2 = 2\alpha$ (Equation 5.69), the final condition can be simplified to:

$$\psi_N^n = -(2\alpha)\psi_{N-1}^{n+1} + (1+2\alpha)\psi_N^{n+1}. \tag{5.74}$$

In a previous version of the DRSPALL design document (which was prepared for DRSPALL Version 1.10), a forward difference formulation was applied to the boundary condition Equation 5.71. Özişik (1993) shows that the error involved with the central difference representation is second-order accurate, i.e., $O\left((\Delta r)^2\right)$; whereas the error involved with the forward difference representation is first-order accurate, i.e., $O(\Delta r)$. Therefore, the central difference formulation, Equation 5.74, is used because it decreases numerical discretization errors and provides a more accurate numerical approximation to the exact solution.

5.6.3 Summary of Recommended Finite Difference Equations

The recommended tri-diagonal linear system of equations is:

$$\begin{aligned} \psi_j^n &= -\alpha_1 \psi_{cav}^{n+1} + (1+2\alpha)\psi_j^{n+1} - \alpha_2 \psi_{j+1}^{n+1} && \text{for } j = 2 \\ \psi_j^n &= -\alpha_1 \psi_{j-1}^{n+1} + (1+2\alpha)\psi_j^{n+1} - \alpha_2 \psi_{j+1}^{n+1} && \text{for } j = 3,\ldots, N-1 \\ \psi_j^n &= -(2\alpha)\psi_{j-1}^{n+1} + (1+2\alpha)\psi_j^{n+1} && \text{for } j = N \end{aligned} \tag{5.75}$$

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where

$$\alpha = \frac{D_j^n \Delta t}{(\Delta r)^2}$$

$$\alpha_1 = \frac{D_j^n \Delta t}{\Delta r}\left(\frac{1}{\Delta r} - \frac{(m-1)}{2r_j} - \frac{\ln\left(k'^{n+1}_{j+1} \Big/ k'^{n+1}_{j-1}\right)}{4\Delta r}\right) \tag{5.76}$$

$$\alpha_2 = \frac{D_j^n \Delta t}{\Delta r}\left(\frac{1}{\Delta r} + \frac{(m-1)}{2r_j} + \frac{\ln\left(k'^{n+1}_{j+1} \Big/ k'^{n+1}_{j-1}\right)}{4\Delta r}\right)$$

Figure 9 illustrates the expansion point (j, n+1) and the surrounding finite-difference molecules.

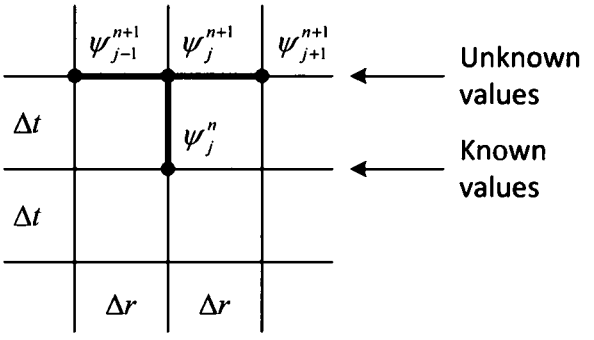


Figure 9 Finite difference molecules for the implicit scheme using constant zones sizes.

5.6.4 Repository Stress State

Once pore pressure is known, evaluation of the repository stress state, Equations 5.38 and 5.39, is algebraic except for the integral in the seepage stress calculations in Equations 5.40 and 5.41. The integrals are evaluated using trapezoidal integration with trapezoids formed between the cell centers where pore pressure and stress components are evaluated. The first increment is over the half-cell between the cavity wall and the center of the first non-fluidized cell. Radii are evaluated at cell centers, except for the left side in the first increment, which is the cavity wall radius:

$$\int_{r_c}^{r_j}\left[p(r_j) - p_{ff}\right] r_j^{m-1} dr = \left(1 - F_f(j)\right)\sum_{i=0}^{j} 0.5\left((p_{i-1} - p_n) r_{i-1}^{m-1} + (p_i - p_n) r_i^{m-1}\right)(r_i - r_{i-1}) \tag{5.77}$$

where i=1 is the first intact cell (non-fluidized); j is index of the cell for which stress components are being evaluated; r_j is radius to the center of cell j; p_0 is the cavity pressure; r_0 is the radius of

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cavity cell next to the interface; $F_f(j)$ is the fraction of cell j that has fluidized and is based on the fluidization relaxation time; and n is the index of the last computational cell. The fraction fluidized term is used to relax the seepage stresses in cells that have failed and are in the process of fluidizing.

5.7 Numerical Method – Coupling

The calculation of gas flux from the repository to the wellbore (Equation 5.26) requires the gas velocity at the cavity interface, u_{repos} (Equation 5.49). The velocity is evaluated numerically as follows:

$$u_{repos} = \frac{k_1'}{\eta\phi}\left(\frac{p_1 - p_{cav}}{\Delta r_1}\right). \tag{5.78}$$

The mass of gas flowing form the repository to the cavity at the bottom of the wellbore is then evaluated from:

$$\Delta m_{cav} = \rho_{g(repos)} u_{repos} \phi A_{cav} \Delta t\ . \tag{5.79}$$

5.8 Time Step Determination

For the wellbore, which uses a conditionally stable explicit method, the Courant condition

$$ss_m \frac{\Delta t}{\Delta z} < constant \tag{5.80}$$

is the basis of time step determination, where Δz is the zone size and ss_m is the sound speed in the mud and ρ_m is the mud density:

$$ss_m = \sqrt{\frac{1}{c_m \rho_m}}\ . \tag{5.81}$$

The wellbore timestep is calculated by replacing the inequality in Equation 5.80 with equality, solving for Δt using a user specified constant and finding the minimum over all computational cells

$$\Delta t = \min\left(constant \frac{\Delta z_i}{ss_{m_i}}\right). \tag{5.82}$$

Normally, the value of the constant is taken as 1.0 for the "standard" Courant condition. However, due to the addition of the numerical diffusion terms and the extreme conditions in the present problem, especially where mass feeds from the repository into the wellbore, *constant*

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might be much be less than 1 for a stable solution and is found by trial and error. A value that produces stable results (free of cell-to-cell oscillations) will typically work across a range of model parameter values.

For the repository, which uses an unconditionally stable implicit method, a constant timestep would typically be specified by the user. DRSPALL actually implements the timestep selection as a user specified factor, F_{rep}, that is multiplied by the Courant criteria that would normally be used by an explicit algorithm.

$$\Delta t = \min\left(F_{rep} \frac{\Delta r_i^2}{\frac{k_i'}{\varphi}\left(\frac{\psi_i}{\mu_i}\right)^{1/2}} \right) \tag{5.83}$$

where Δt is the minimum over all cells in the repository domain. Trial and error or convergence testing can be used to find a timestep factor (usually greater than 1) that gives suitable results and gradient definitions.

The final timestep used is the lesser of the wellbore-determined and repository-determined timestep.

6.0 CONTROL FLOW AND LOGIC

The major flow and control logic for DRSPALL is presented in Figure 10 in the form of a flow chart. In the flow chart subroutine names are underlined and descriptive information is in 'Sentence case'. Also shown in the figure is a mapping of Functional Requirements. The requirement numbers (i.e., R.1) corresponds to those presented in the *Requirements Document, Verification and Validation Plan, and Validation Document for DRSPALL Version 1.24* (Kicker, 2021a) and summarized in Section 2.0. Figure 10 shows the overall flow logic of DRSPALL and roughly corresponds to the DRSPALL main routine. Subsequent figures show details of modules that are first introduced in pentagonal elements in earlier figures. The modules (groups of subroutines) detailed in Figure 11 through Figure 13 are:

- DRSPALL – main program , input and initialization
- RunLoop – main calulational control including time-stepping loop
- CalculateWellBoreFlow – controls and calculates multi-component fluid flow in the wellbore and fluidization of failed waste.
- CalculateWasteFlow – controls and calculates gas flow through the waste in the repository and fluidization of the failed waste
- CalculateWasteStress – controls and calculates the effective stresses and spalling (tensile) failure in the waste.

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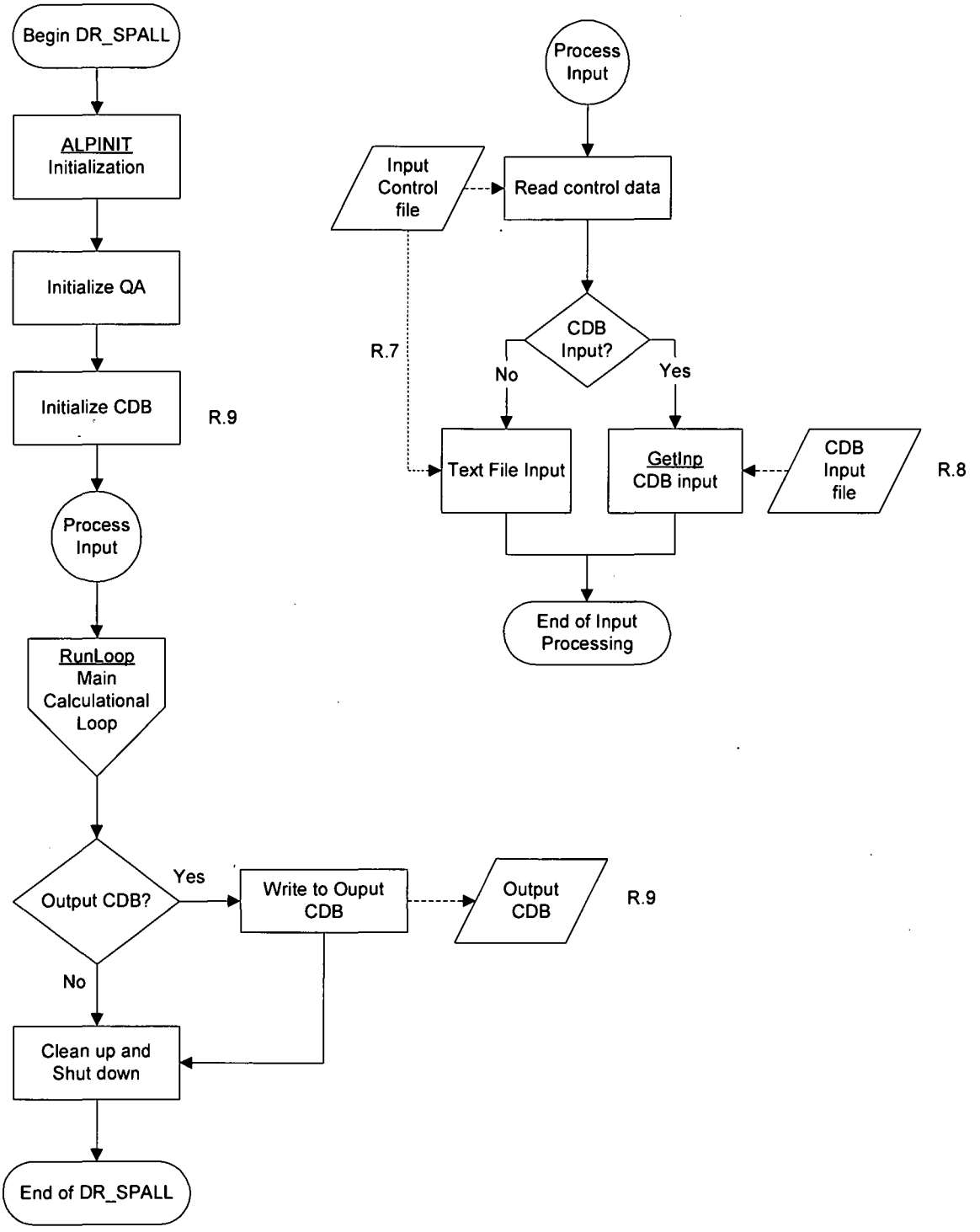


Figure 10 Flow chart for program DRSPALL.

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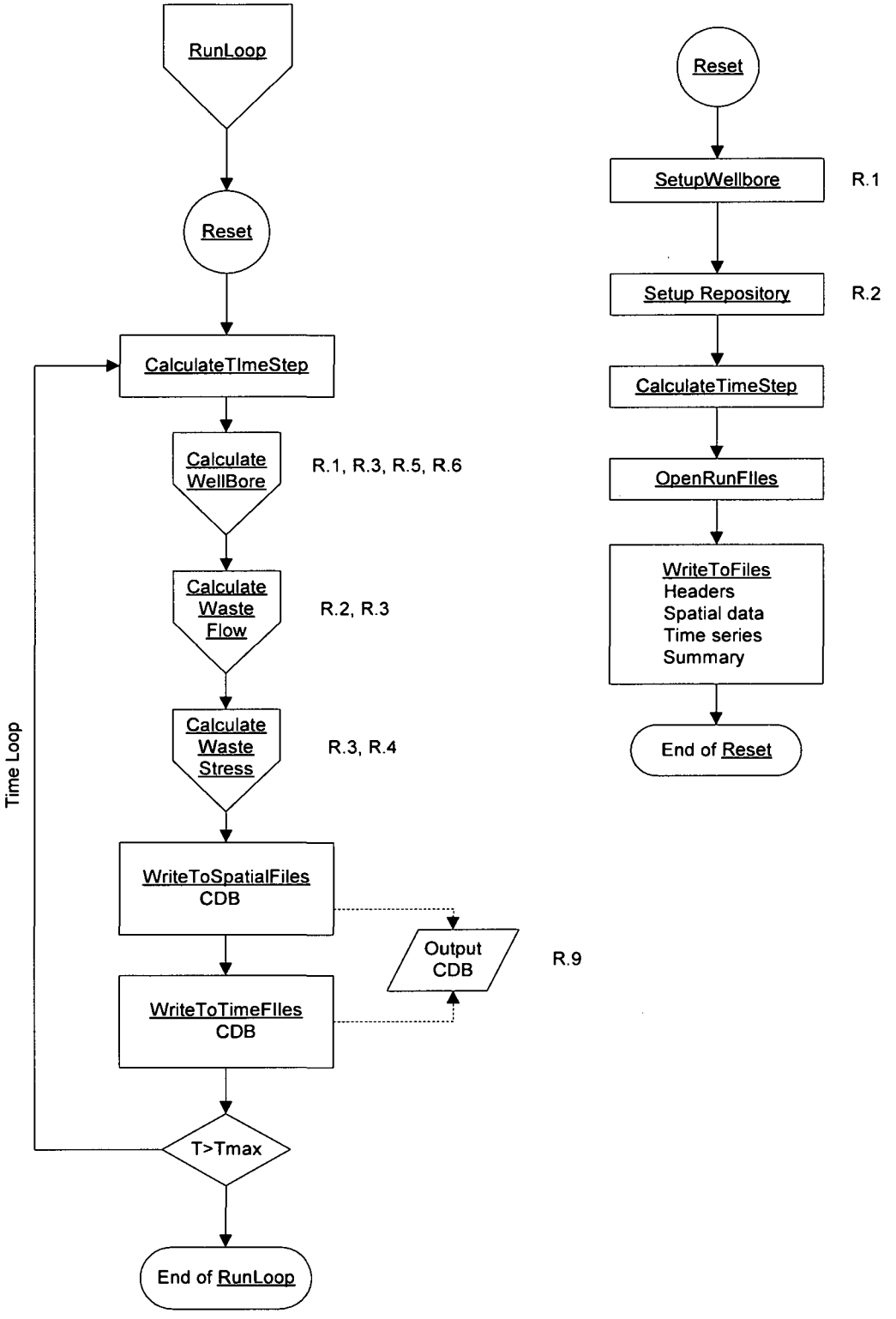


Figure 11 Flow chart for subroutine RunLoop.

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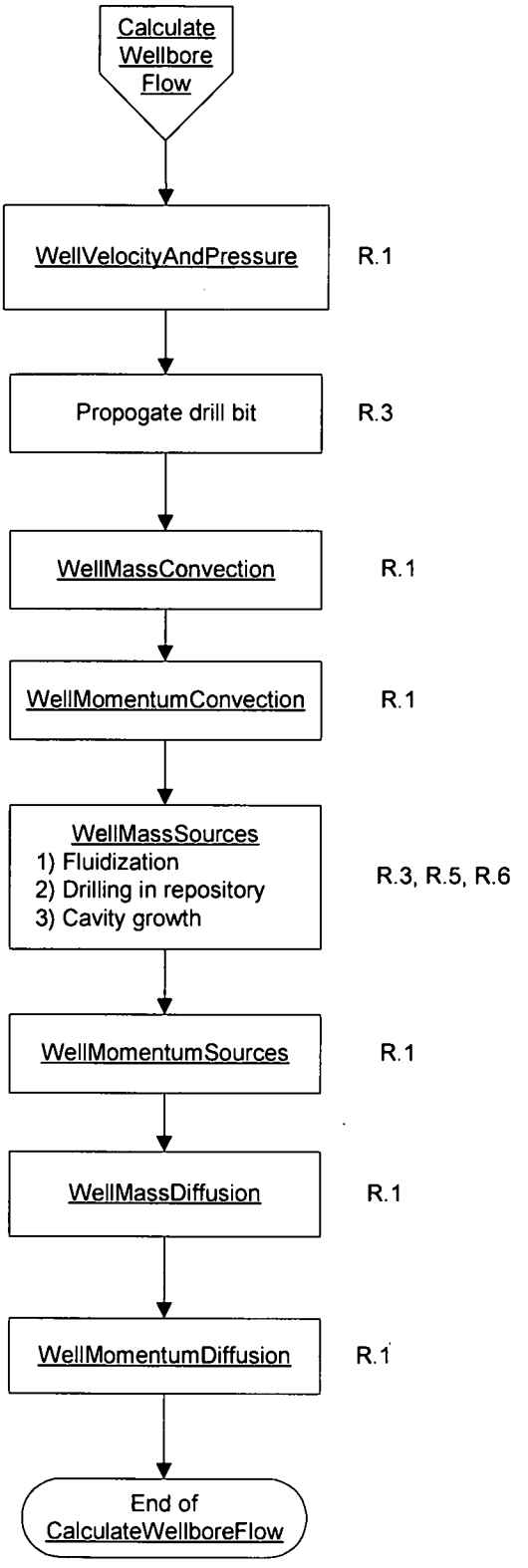


Figure 12 Flow chart for subroutine CalculateWellBoreFlow.

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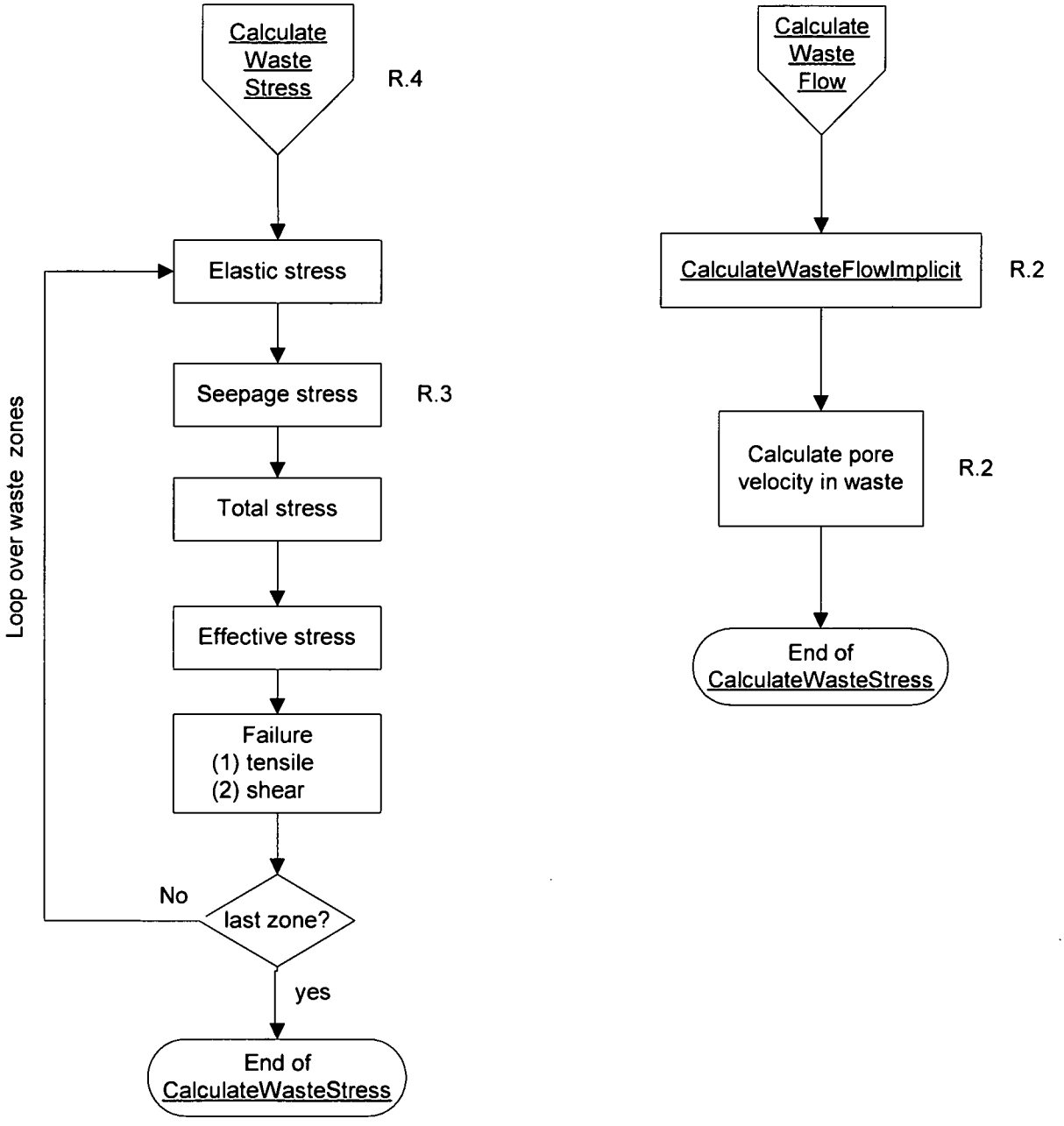


Figure 13 Flow chart for subroutines CalculateWasteStress and CalculateWasteFlow.

The following is the DRSPALL call tree that includes a brief routine (subroutine or function) description. An indentation indicates a call to the named routine. The combination of the flow charts (Figure 10 through Figure 13) and the following call tree provides a complete description of the DRSPALL flow logic:

DRSPALL	Main program
. ALPINIT	Initialization

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. . ReadControlFile	Read input control parameters, properties from control file or input CAMDAT file
. . CheckParameterBounds	Checks that input parameters are within valid range
. . InitializeTextOutput	Opens output files and writes headers
. . Reset	Problem setup control
. . . SetupWellbore	Setup wellbore flow model
. . . . ZoneWellbore	Setup grid in wellbore
. . . SetupRepository	Setup Repository waste model
. . . . CalculateWasteStresses	Initialize stress in repository
. . . CalculateTimestep	Calculate initial time step
. . . SetSpatialSaveTimes	Setup times for saving spatial variables
. . . SetTimeSaveTimes	Setup times for saving time series data
. . . OpenRunFiles	Open output text files
. . . WriteFileHeaders	Write header record to output files
. . . CloseRunFiles	If calculation finished, close files
. . CreateCDBHeader	Initializes and output CAMDAT file
. . CreateCDBVariables	Defines output variables for output CAMDAT file
. RunLoop	Calculation control

Begin Time Loop

. . CalculateTimestep	Calculate time increment for current step
. . CalculateWellboreFlow	Wellbore flow model control
. . . WellVelocityAndPressure	Fluid velocity and pressure in wellbore
. . . WellMassConvection	Mass flow (balance) in wellbore
. . . WellMomentumConvection	Momentum balance in wellbore
. . . WellMassSources	Determine mass sources (mud, gas, waste…)
. . . WellMomentumSources	Determine momentum sources
. . . WellMassDiffusion	Mass diffusion
. . . WellMomentumDiffusion	Momentum diffusion
. . CalculateWasteFlow	Gas flow in repository control
. . . CalculateWasteFlowImplicit	Implicit solver for gas flow in repository
. . CalculateWasteStresses	Effective stress model with seepage forces
. . OutputControl	Controls output to text and CAMDAT files

End of time loop

. . RunShutDown	Clean up for termination

DRSPALL is written in FORTRAN 90 for compilation under the Linux cluster, but is designed to be relatively portable. The subroutines and functions that make up DRSPALL have been logically grouped by functionality into the compilable FORTRAN 90 (*.f90*) source files that follows:

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cdbcontrol.f90	Collection of routines that read from and write to CAMDAT files.
cdbglobals.F90	Global variables related to CAMDAT files are declared here.
A1main_drspall.f90	This is the main program source file, which includes input control and initialization, QA functions and CAMDAT file initialization.
vmsfilewrite.f90; vmsoutputcontrol.f90	Collection of subroutines that write data to the output text file.
globals.F90	Global variables are declared here.
maincalc.f90	Collection of subroutines that include the main run loop and timestep calculations.
parameters.f90	Collection of subroutines that control parameter initialization and writes to the input parameter data echo.
setupcalc.f90	Collection of subroutines that initialize the wellbore, repository and other values required to start a run.
wasteflowcalc.f90	Collection of subroutines that calculate pressure and fluid flow in the repository.
wastestresscalc.f90	Subroutine that calculates solid stresses and failure in the repository.
wellborecalc.f90	Collection of subroutines that calculate fluid flow in the well, including pumping, expulsion and the coupling to the repository via the DDZ or cavity.

6.1 Data Structures

The primary data structures used by DRSPALL are the input files, output files and two FORTRAN 90 modules that contain most of the problem variables and parameters that must be shared between subroutines. Each of these structures is detailed in the following subsections.

Files are named with the prefix of the run name provided by the user and are suffixed according to the data contained in the file. The suffix and the corresponding data file description are summarized in Table 6-1.

Table 6-1– Summary of DRSPALL Input and Output Files.

Suffix	File contents
DRS	Input control and problem specification parameters
CDB	Input and output CAMDAT Database files
DBG	Input data echo and runtime diagnostics

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6.1.1 Input Files

The files associated with running DRSPALL are listed below. Additional details on input files are provided in Section 10.0. Addition details on output files are provided in Section 12.0.

6.1.1.1 Input Control and Parameter File

The input control and parameter file, prefixed 'drs' (suffixed 'inp'), lists input control and problem specification parameters. The following problem specification parameters may be specified in this file:

Land Elevation
Repository Top
Total Thickness
DRZ Thickness
DRZ Permeability
Outer Radius
Initial Gas Pressure
Far-Field In-Situ Stress
Waste Porosity
Waste Permeability
Forchheimer Beta
Biot Beta
Waste Poisson's Ratio
Waste Cohesion
Waste Friction Angle
Waste Tensile Strength
Characteristic Length (L_t)
Particle Diameter
Max Pump Pressure
DDZ Thickness
DDZ Permeability
Stop Drilling Exit Vol. Rate
Stop Pumping Exit Vol. Rate
Stop Drilling Time
Spherical/Cylindrical Geometry Flag
Fluidization Flag
Maximum Run Time
Repository Cell Length
Gas Viscosity
Mud Density
Mud Viscosity
Wall Roughness, Pipe
Wall Roughness, Annulus
Max. Solids Vol. Fraction
Solids Viscosity Exponent
Choke Efficiency
Bit Diameter
Pipe Diameter
Collar Diameter
Pipe Inside Diameter
Collar Length
Exit Pipe Length
Exit Pipe Diameter
Drilling Rate
Bit Above Repository (Initial)
Mud Pump Rate
Radius, Growth Rate
Wellbore Cell Length
Wellbore Zone Growth Rate
First Wellbore Zone
Well Stability Factor
Repository Stability Factor
Mass Diffusion Factor
Momentum Diffusion Factor
Validation Test Case
Initial Cavity Radius

6.1.1.2 Input CDB File

The user will be able to optionally read the problem specification data listed in Section 6.1.1.1 from an input CDB file. The details of the self-describing file structure can be found in Rechard et al. (1993) and in the WIPP PA *User's Manual for CAMDAT_LIB Version 1.22* (Gilkey,

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1995b). CAMDAT_LIB provides a simplified programmers interface for accessing the data contained in a CDB file through subroutine calls.

6.1.2 Output Files

6.1.2.1 Output Text Files

A single output text file is created (suffix .DBG) which contains

- An echo of the input .DRS file.
- A listing of the input parameters, after processing, that reflects the actual parameters used in the current analysis. This includes values of parameters that were retrieved from the input CAMDAT file.
- A several line summary of results and timing information for each timestep that data is written to the output CAMDAT file.
- Run time diagnostic messages.
- A results summary at the end of the calculation.

6.1.2.2 CDB Output File

The optional CDB output file will contain, at a minimum, all input problem specification parameters listed in Section 6.1.1.1 and all the output data listed in Section 6.1.2.1. The CDB file is flexible enough to handle both spatial and temporal variables. The self-describing file structure is documented Rechard et al. (1993) and the WIPP PA *User's Manual for CAMDAT_LIB Version 1.22* (Gilkey, 1995b). CAMDAT_LIB provides a simplified programmers interface for creating the CDB file through subroutine calls.

6.1.3 FORTRAN 90 Global Variables Modules

Two FORTRAN 90 modules (*globals.F90*, *cdbglobals.F90*) have been defined for specifying all global variables. The module *cdbglobals.F90* contains shared variables related to reading and writing CAMDAT files. The module *globals.F90* contains all other shared variables. The modules include variable type declarations (integer, real, character, logical), precision (double, single), array dimensioning, records, structures definitions and parameter value setting. All the information contained in the module is made accessible to a routine by including a "USE globals" or "USE cdbglobals" statements in the declaration section of the routine. This is typically the first executable statement in the routine. DRSPALL uses variable names that are self-descriptive and therefore, the *globals.F90* and *cdbglobals.F90* listing shown below are, essentially, self-documenting. Note that some of the lines maybe wrapped.

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```
Module Globals
!-----------------------------------------------------------------------
!
! File Globals.f90 -- contains global parameters, variables, and constants
!
!-----------------------------------------------------------------------

!Use DFWin
!Use DFLib
!Use GraphicsRecords
Implicit NONE

! Input Parameters
! ----------------

! Repository
Real(8) surfaceElevation, repositoryTop, repositoryThickness, dRZThickness, &
  dRZPerm, uncompactedWastePorosity, repositoryHeight, repositoryThickness0, &
  repositoryOuterRadius, repositoryInitialPressure, farFieldPorePressure, &
  farfieldStress, reposRadius1, growthRate

! Waste
Real(8) repositoryInitialPorosity, repositoryInitialPerm, forchBeta
Real(8) biotBeta, poissonsRatio, cohesion, frictionAngle, tensileStrength, &
        particleDiameter, fluidizationVelocity, Lt

! Gas
Real(8) gasBaseDensity, gasViscosity

! Mud
Real(8) initialMudDensity, mudViscosity, wallRoughness(2), mudSolidsMax,  &
        mudSolidsViscosityExponent

! Wellbore/Drilling
Real(8) bitDiameter, pipeDiameter, collarDiameter, pipeInsideDiameter, collarLength, &
  drillingRate, initialBitAboveRepository, mudPumpRate, dDZThickness, dDZPerm, &
  stopDrillingExitVolRate, stopPumpingExitVolRate, stopDrillingTime, timeToFloor, &
  maxPumpPressure, initialPumpRate, pitGain

! Computational
Character(1) geometry, allowFluidization
Real(8) maxTime, initialReposZoneSize, initialWellZoneSize, &
  wellStabilityFactor, reposStabilityFactor

! APG Plot axes minimums / maximums (left here for compatibility with PC version)
Real(8) minPlotRadius, maxPlotRadius, minPlotWellPos, maxPlotWellPos, &
  minPlotPressure, maxPlotPressure, minPlotStress, maxPlotStress, &
  minPlotVelocity, maxPlotVelocity, &
  minPlotWellPressure, maxPlotWellPressure, &
  minPlotWellVelocity, maxPlotWellVelocity, &
  minPlotWellRho, maxPlotWellRho, &
  minPlotWellFraction, maxPlotWellFraction
Logical newPlotRadius, newPlotWellPos, &
  newPlotPressure, newPlotStress, newPlotVelocity, &
  newPlotWellPressure, newPlotWellVelocity, newPlotWellRho, newPlotWellFraction

! Internal Parameters and Variables
! ---------------------------------

! Repository array
!dkr Logical(1)
```

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```
Logical , DIMENSION(:), ALLOCATABLE :: &
  tensileFailureStarted, tensileFailureCompleted, shearFailed, &
  fluidizationStarted, fluidizationCompleted
REAL(8), DIMENSION(:), ALLOCATABLE :: &
  reposRadius, reposRadiusH, reposPres, porosity, permeability, forchratio, &
  poreVelocity, superficialVelocity, reposFactor, pL, &
  psi, dCoeff, radEffStress, tanEffStress, shearStress, &
  fractionTensileFailed, tensileFailureTime, meanEffStress, shearStrength, &
  fractionFluidized, fluidizationTime, FluidStartTime, FluidStopTime, FailStartTime, &
  radElasticStress, tanElasticStress, radSeepageStress, tanSeepageStress, &
  reposDR, reposDRH, reposVol, reposGasMass, drillingFailure
Real(8) , DIMENSION(:), ALLOCATABLE :: aa, bb, cc, rr, gam

! Repository non-array
!dkr Integer(2)
Integer geomExponent
!dkr Integer(4)
Integer numReposZones, maxTensileFailedIndex, maxShearFailedIndex, firstIntactZone, &
           interface1, interface2, lastFailedZone, firstInternalFailedZone, &
           minNumLt
Real(8) reposZoneSize, wasteBoundaryPoreVelocity, sumReposGasMass, &
        totalGasFromWaste, totalWasteFromRepos, maxForchRatio

!JFS3
!dkr Integer(4), Logical(1)
Integer fluidizationWaitZone
Logical surfaceFailureAllowed

! Cavity
Real(8) cavityPres, initialCavityRadius, initialCavityArea, initialCavityVol,
initialCavityGasVol, &
  cavityGasMass, cavityWasteVol, cavityWasteMass, deltaGasIntoWell, deltaWasteIntoWell, &
  deltaSaltIntoWell, deltaGasFromWaste, exitPoreVelocity, exitPoreArea, &
  inputCavityRadius, cutMass, splMass, totMass, splvoleq, cutvoleq, totvoleq, &
  cutVol, splVol, splvol2, TotVol, cutTrueVol, splmass2, beddepth, minCharVel

! Wellbore array
REAL(8), DIMENSION(:), ALLOCATABLE :: &
  wellPos, wellPres, wellRhoV, wellVol, WellArea, wellZoneSize, &
  wellV, wellRho, wellAreaInt, wellDeltaVInt, wellFactor, &
  wellMudMass, wellGasMass, wellWasteMass, wellSaltMass, &
  wellMudVol, wellGasVol, wellWasteVol, wellSaltVol, hydraulicDia
REAL(8), DIMENSION(:), ALLOCATABLE :: &
  wellMassOrig, wellPresOrig, wellMudMassOrig, &
  wellGasMassOrig, wellWasteMassOrig, wellSaltMassOrig
REAL(8), DIMENSION(:), ALLOCATABLE :: &
  wellGRhoStar, wellGRhoVStar, wellGRhoT, wellGRhoVT, &
  wellVolInt, momDiff, massDiff

! Wellbore non-array
!dkr Logical(1), Integer(4)
Logical repositoryPenetrated, firstPenetration, drilling, pumping, exitPipe, &
           internalfailure

Integer numWellZones, wellBottomIndex, numExitZones, firstWellZone, &
   numWellZones1, numWellZones2, numWellZones3, numWellZones4

Real(8) wellLength, bitAboveRepository, dRZDiameter, dRZArea, wellGrowthRate,  &
  bitArea, bitFlowArea, pipeArea, collarAnnulusArea, pipeAnnulusArea, &
  exitPipeLength, exitPipeDiameter, exitPipeArea, wellDepth, &
  mudMassEjected, gasMassEjected, wasteMassEjected, saltMassEjected, &
```

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```
  totalMudInWell, totalGasInjected, totalGasInWell, totalWasteInWell, totalSaltInWell, &
  cuttingsMassMax, cuttingsRadiusMax, equivDrilledCavityRadius, &
  volStore, wasteStore, gasStore, wasteInjected,originalBitDiameter, &
  sumWellGasMass,   sumWellWasteMass, Z1, Z2, Z3, Z4

! General array
REAL(8), DIMENSION(:), ALLOCATABLE :: invPorosity

! General non-array
Real(8) invGasViscosity, invWellZoneSize, invWasteDensity, invSaltDensity,
invWaterCompressibility, &
  invInitialMudDensity, invGasBaseDensity, invInitialCavityGasVol, invPi,
invAtmosphericPressure, &
  invReposZoneSize, timeOfPenetration

! Computational Parameters and Constants
!---------------------------------------

! Run management
Real(8) runTime, deltaTime
Double Precision cpuTime, cpuBegin,cpuEnd, &  !apg REAL
        cpuT0, cpuT1, cpuT2, cpuT3, cpuWBF, cpuWSF, cpuWSS

!dkr Integer(4), Logical(1)
Integer runIndex
Logical stopRun, isRunning, pauseRun, CDBoutput, textOutput
Character*3 platform, machine
Character*132 root

! Window unit constants
!dkr Integer(4)
Integer ParameterUnit, TimeUnit, RepositorySpatialPressureUnit,
RepositorySpatialStressUnit, &
  RepositorySpatialVelocityUnit, WellboreSpatialPressureUnit, WellboreSpatialMassUnit, &
  ResultsSummaryUnit

! File logic
!Type(T_OpenFilename) fName
!Logical(1) fileLoaded, fileSaved, fileNamed
Character(255) fullParameterFilename, pressureFileName, radEffStressFileName, &
  tanEffStressFileName, poreVelocityFileName, timeFileName, summaryFileName,
outParamsFileName,&
   diagnosticFileName, validationFilePrefix
!apg Added validationFilePrefix for files below
Character(255) TC1chanFileName, TC4couplefilename, TC4stressfilename, &
   TC4Fluidfilename, TC4Ejectfilename, TC4FluidTimefilename, TC5Wellfilename

!dkr Integer(4)
Integer parameterFileID, pressureFileID, radEffStressFileID, tanEffStressFileID, &
  poreVelocityFileID, timeFileID, summaryFileID, outParamsFileID, diagnosticFileID, &
  chanValidationFileID, &
  !test case #4
  couplingValidationFileID, stressValidationFileID, fluidizationvalidationFileID, &
  expulsionValidationFileID, fluidizationTimeValidationFileID, &
  !test case #5
  wellboreValidationFileID

! Character-based user input parameter values
Character(30) gridItems(2,44)
Character(10) gridUnits(2,44)
Character(14) gridValues(2,44)
```

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```
! Parameter input grids
!dkr Integer(2)
Integer numGridRows, numGridCols, rowHeight, margin
Integer gridWidth, colWidth(3)

! DKR Graphics records moved to seperate module for portatibility with VMS

! Plot and save times
!dkr Real(4), Integer(4)
Real(8) spatialPlotTime(1000), spatialSaveTime(0:1000), &  !apg Real
   timeSaveTime(0:2000), chanSaveTime (10)
Integer spatialPlotIndex, spatialSaveIndex, timeSaveIndex, &
   chanSaveIndex

! APG for time plots
Integer ixtplt
!dkr Real(4) times 3
Real(8) finaltplt  !apg Real
Integer, Parameter :: maxtplt = 1000
Real(8) tpltTime(0:maxtplt)  !apg Real
Real(8) tpltPumpPressure(0:maxtplt), tpltWellBottomPressure(0:maxtplt),
tpltCavityPressure(0:maxtplt), &  !apg Real
  tpltDrilledRadius(0:maxtplt), tpltCavityRadius(0:maxtplt), tpltTensileRadius(0:maxtplt),
&
  tpltWasteBoundaryPoreVelocity(0:maxtplt), tpltFluidizationVelocity(0:maxtplt),
tpltMudEjectionVelocity(0:maxtplt), &
  tpltWasteInWell(0:maxtplt), tpltWasteEjected(0:maxtplt), &
  tpltGasInjected(0:maxtplt), tpltGasInWell(0:maxtplt), tpltGasEjected(0:maxtplt), &
  tpltGasPosInWell(0:maxtplt), tpltWastePosInWell(0:maxtplt)

! for plotting and saving
! time plots
!dkr Real(4)
Real(8) curTime, &  !apg Real
  curPumpPressure, curWellBottomPressure, curCavityPressure, &
  curDrilledRadius, curCavityRadius, curTensileRadius, &
  curWasteBoundaryPoreVelocity, curFluidizationVelocity, curMudEjectionVelocity, &
  curWasteInWell, curWasteEjected, &
  curGasInjected, curGasInWell, curGasEjected, &
  curGasPosInWell, curWastePosInWell

!dkr Real(4) times 2
Real(8) prevTime  !apg Real
Real(8) prevPumpPressure, prevWellBottomPressure, prevCavityPressure, &  !apg Real
  prevDrilledRadius, prevCavityRadius, prevTensileRadius, &
  prevWasteBoundaryPoreVelocity, prevFluidizationVelocity, prevMudEjectionVelocity, &
  prevWasteInWell, prevWasteEjected, &
  prevGasInjected, prevgasInWell, prevGasEjected, &
  prevGasPosInWell, prevWastePosInWell

! summary display
!dkr Real(4)
Real(8) displayedTime, &  !apg Real
  displayedPumpPressure, displayedBitAbove, &
  displayedWellBottomPressure, displayedCavityPressure, displayedWasteBoundaryPoreVelocity,
&
  displayedFluidizationVelocity, displayedEquivDrilledCavityRadius, displayedCavityRadius,
&
  displayedTensileFailedRadius, displayedShearFailedRadius, displayedGasInjected, &
  displayedMudInWell, displayedGasInWell, displayedWasteInWell,displayedSaltInWell, &
```

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```
  displayedMudVelocity, displayedMudVolRate, displayedMudEjected, displayedGasEjected,
displayedWasteEjected, displayedSaltEjected, &
  displayedMudExitFraction, displayedGasExitFraction, displayedWasteExitFraction,
displayedSaltExitFraction, &
  displayedGasPosInWell, displayedWastePosInWell, displayedradEffStress,
displayedFirstIntactZone

Integer cellControl(5), oldCellControl,stepControl, oldStepControl
Integer DisplayedCell
Character*8 stepControlName(5),displayedControl

! Validation Test Case specific parameters
!dkr Integer(2)
Integer validationTestCase, validationSubcase
Real(8)    characteristicTime

!test case #4
Real(8) stressSaveTime, stressSaveDelta, fluidizationSaveTime, fluidizationSaveDelta,&
       initialGasInRepository

!DKR - parameters switched to variables. set in reset
REAL(8) gravity, MassDiffusionFactor, MomentumDiffusionFactor, chokeEfficiency, &
        WaterCompressibility, GasConstant, ReposTemp, WasteDensity, saltDensity, &
        BitNozzleNumber,BitNozzleDiameter, Pi, AtmosphericPressure, shapeFactor, &
        TensileVelocity
!dkr Integer(2)
Integer FIX, ENG

! Constants
!dkr Interger(2) times 3
Integer, Parameter :: FULL_RESET = 1
Integer, Parameter :: RUNNING    = 2
Integer, Parameter :: REOPENING  = 3

end

!-------------------------------------------------------------------------------------------

MODULE CDBGlobals
!-----------------------------------------------------------------------
! This module conatins variables required to read or write a CDB
!
! By:   David Rudeen
!       GRAM, Inc.
!
! Modification History
! 12/19/02 - DKR: Original version
!-----------------------------------------------------------------------
IMPLICIT NONE
INTEGER, PARAMETER :: nev=26, nhv=47
CHARACTER*8   HisName(nhv), NAMXYZ(3), EleName(nev), blockName
CHARACTER*80  HEAD
CHARACTER*255 outCDBFilename, inCDBFilename
INTEGER       IDBout, NOUT, NumHisVar, LDUM, IERRDB, NDIM, NUMNP, &
              NELBLK, NELX, NELY, NELZ, MAXLNK, NEB, NUMPRP, NUMATR, &
             NUMEL, NumEleVar, outCDBFileID, inCDBFileID, &
             NINFO, numCDBsteps, numParam
INTEGER       IDBin, NQAREC, NELBLKin, NUMATRin, NUMPRPin, NUMNPS, LNPSNL, &
              NUMESS, LGELEL, LGNODL, DRSblock, reposBlock, wellBLock1, wellBlock2
LOGICAL,     DIMENSION(:,:), ALLOCATABLE :: ISEVOK, ISPROK
LOGICAL,     DIMENSION(:),   ALLOCATABLE :: ISATOK
```

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```
INTEGER,      DIMENSION(:,:), ALLOCATABLE :: Link
INTEGER,      DIMENSION(:),   ALLOCATABLE :: EleMap, IDELB, NUMLNK, NUMELB
REAL(4),      DIMENSION(:),   ALLOCATABLE :: Xn, Yn, ELEVAT, THICK, DEL_Y, DEL_X
REAL(4),      DIMENSION(:,:), ALLOCATABLE :: EleVal, PROP
CHARACTER*80,DIMENSION(:),    ALLOCATABLE :: INFO
CHARACTER*8 ,DIMENSION(:),    ALLOCATABLE :: NAMELB, PRPname, ParamName, NAMATR
CHARACTER*8 ,DIMENSION(:,:), ALLOCATABLE :: QAREC

REAL(4)      RMEM(1), HisVal(nhv), ZN(1)
CHARACTER*1 CMEM(1)
LOGICAL      WHOLE, CDBinput

END
```

6.2 Allowable/Prescribed Ranges for Input and Output

Many of the parameters must be within certain acceptable ranges to represent physical reality or true repository and/or wellbore conditions or for compatibility with other input parameters. Where possible, a limitation scheme involving parameter range checking at the time parameters are read in will flag unacceptable parameter values and stop execution. But, because DRSPALL has been designed for any self-consistent set of input parameters and any single parameter value can vary significantly depending on the system of units, it is not possible to provide upper bounds for many of the input parameters. Table 6-2 lists all input variables and provides parameter bounds when they can be reasonably defined.

Table 6-2– Input Parameters and Ranges.

Parameter Description	**Range**
Land Elevation	> Repository Top
Repository Top	Any real
Total Thickness	≥ 0
DRZ Thickness	> 0
DRZ Permeability	> 0
Outer Radius	> 0.5 * Bit Diameter
Initial Gas Pressure	> 0, < Overburden ($\rho_s gh$); h = Land Elevation – Repository Top
Far-Field In-Situ Stress	> 0, < Overburden
Waste Porosity	0 < Porosity < 1.0
Waste Permeability	> 0
Forchheimer Beta	> 0
Biot Beta	$\geq 0, \leq 1$
Waste Poisson's Ratio	0 < Poisson's Ratio < 0.5
Waste Cohesion	> 0
Waste Friction Angle	0 < Friction Angle < 90°
Waste Tensile Strength	< 0
Failure Characteristic Length (Lt)	> 0
Waste Particle Diameter	< Bit Diameter

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Parameter Description	Range
Gas Density at STP	> 0
Gas Viscosity	> 0
Mud Density	> 0
Mud Viscosity	> 0
Wall Roughness Pipe	> 0
Wall Roughness Annulus	> 0
Max. Solids Vol. Fraction	> 0, < 1
Solids Viscosity Exponent	< 0
Bit Diameter	> 0
Pipe Diameter	>0, < Bit Diameter
Collar Diameter	> Pipe Diameter, < Bit Diameter
Pipe Inside Diameter	> 0, < Pipe Diameter
Collar Length	> 0, < h
Exit Pipe Length	> 0
Exit Pipe Diameter	> 0
Drilling Rate	> 0
Bit Above Repository (Initial)	> 0, < h
Mud Pump Rate	> 0
Max Pump Pressure	> 0
DDZ Thickness	> 0
DDZ Permeability	> 0
Stop Drilling Exit Vol. Rate	> 0
Stop Pumping Exit Vol. Rate	> 0
Stop Drilling Time	> 0
Spherical/Cylindrical Geometry Flag	S or C
Fluidization Flag	Y or N
Maximum Run Time	> 0
Repository Cell Length	> 0
Radius, Growth Rate	> 0, 1.0
Wellbore Cell Length	> 0
Wellbore Cell Growth Rate	1.0
First Wellbore Zone	> 0
Well Stability Factor	> 0
Repository Stability Factor	> 0
Mass Diffusion Factor	> 0
Momentum Diffusion Factor	> 0
Initial Cavity Radius	> 0
Minimum Characteristic Velocity	> 0
Minimum Number Zones/L_t	≥ 1
Pi	3.141592653589793d0
Atmospheric Pressure	> 0
Gravity	9.8067d0

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Parameter Description	Range
Gas Constant	4124.0d0
Repository Temperature	> 0
Water Compressibility	> 0
Waste Density	> 0
Salt Density	> 0
Shape Factor	> 0, ≤ 1
Tensile Velocity	> 0
Bit Nozzle Number	> 0
Bit Nozzle Diameter	> 0
Choke Efficiency	> 0, < 1

6.3 Test Case Control Logic

Each of the validation test cases described in the *Requirements Document, Verification and Validation Plan, and Validation Document for DRSPALL Version 1.24* (RD/VVP/VD, Kicker, 2021a), requires some code control logic specific to the test case. This involves either turning off functionality not required in the test case, setting special boundary conditions, or creating formatted ASCII output files that are analyzed and evaluated against the acceptance criteria outlined in the RD/VVP/VD. The input control file to DRPSPALL contains a parameter that identifies the specific test case running, i.e., "1.2." The subsequent discussion identifies the code logic specific to these test cases, and includes rationale for why the logic is used.

The nomenclature used in this section is shown in Table 6-3.

Table 6-3– Nomenclature for Test Case Control Logic.

Symbol	Definition	Units
a	Cavity radius	m
A	Surface area of cavity forming interface between repository domain and wellbore domain	m^2
D_b	True diameter of drill bit	m
D_E	Effective diameter of drill bit required to simulate full penetration at early time for the porous flow test problem	m
η	Gas viscosity	Pa·sec
H	Height of repository at time of penetration	m
k	Repository permeability	m^2
ϕ	Repository porosity	--
$P(r)$	Gas pressure as a function of radius at a given time	Pa
P_I	Initial repository pressure	Pa
τ	Dimensionless time	--
t_o	Characteristic time	sec
t	Time	sec

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Symbol	Definition	Units
Ψ	Dimensionless pseudopressure	--
z	Dimensionless radius	--
ζ	Dimensionless plotting parameter	--

6.3.1 Porous Flow Test Problem

The purpose of the gas flow test problem is to determine whether DRSPALL can accurately calculate transient gas pressures in the repository during the first few seconds after a borehole intrusion. The problem is designed to simulate the repository domain only. As such, the wellbore domain is decoupled from the repository and inactive during execution of the test problem. Input parameters pertaining to the wellbore are therefore irrelevant in this test case, as are any code output describing wellbore conditions.

6.3.1.1 Constant Pressure Inner Boundary

The test problem calls for a constant pressure inner boundary. While normal execution of DRSPALL couples the repository and wellbore with a common pressure boundary, this test case circumvents the coupling by assigning an inner boundary gas pressure of $P = 0$ MPa.

6.3.1.2 Effective Bit Diameter

Drilling does not actually progress in this test case. Rather, the problem starts with a "cavity" cut out of the repository that has a surface area equivalent to the area of the cavity face that would result from the penetration of the true bit diameter Db through a repository of height H. The surface area A of this cylinder representing the borehole wall is evaluated as:

$$A = \pi D_b H \tag{6.1}$$

where the flat ends of the cylinder are not considered because these do not transfer gas between the repository and the wellbore at full penetration. For the purpose of this test case, an effective bit diameter D_E must be defined that represents a hypothetical bit that creates a cavity of area A the instant it touches the repository. The initial contact geometry of the bit with the repository is a circle, with diameter D_E. The effective diameter is therefore related to the cavity area by the formula for the area of a circle:

$$A = \frac{\pi D_E^2}{4}. \tag{6.2}$$

Setting the surface areas in Equations 6.1 and 6.2 equal to one another yields:

$$A = \frac{\pi D_E^2}{4} = \pi D_b H \tag{6.3}$$

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and rearranging to solve for D_E yields:

$$D_E = 2\sqrt{D_b H}\,. \tag{6.4}$$

The effective diameter is calculated by the code only if this test case flag is turned on. While the actual bit diameter D_b is read as an input variable for this test case, D_E is calculated according to Equation 6.4 and used in the porous flow calculations.

The cavity radius, a, used for the characteristic time shown in Table 8-2, is defined depending on the problem geometry. For the cylindrical case, a is equal to the true bit radius:

$$a = D_E/2 \tag{6.5}$$

and for the spherical case, a is defined as the radius of a hemisphere with area A:

$$a = \sqrt{\frac{A}{2\pi}} \tag{6.6}$$

6.3.1.3 Special Output and Dimensionless Variables

The methodology outlined in Chan et al. (1993) calls for the definition of several special variables defined in Table 6-4.

Table 6-4– Special variables defined for Porous Flow Test Problem.

Variable name	Definition	Equation number
Dimensionless pseudopressure	$\Psi = \frac{P(r)^2}{P_1^2}$	6.7
Dimensionless time	$\tau = \frac{t}{t_0}$	6.8
Characteristic time (sec)	$t_0 = \frac{\phi\eta a^2}{kP_1}$	6.9
Dimensionless radius	$z = ln(r/a)$ cylindrical $z = a/r$ spherical	6.10
Dimensionless plotting parameter	$\zeta = \frac{(e^z - 1)}{\tau^{1/2}}$ cylindrical $\zeta = \frac{(1/z - 1)}{\tau^{1/2}}$ spherical	6.11

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Relevant variables are defined in the nomenclature table for test case control logic (Table 6-3). The scaling of output to dimensionless space allows us to compare DRSPALL results to different solutions without matching specific input conditions (i.e., values for variables in Table 6-3). As such, selection of input parameter values is not instrumental to proper solution of this test case. Logic is built into the code such that upon activating this test case, the code will:

- calculate the characteristic time to for the particular set of input variables
- calculate dimensional times $t = t_o\tau$ corresponding to dimensionless times $\tau = 0.01$, 0.1. 1.0, and 10. 0
- write to an output ASCII file the following data at $\tau = 0.01$, 0.1. 1.0, and 10. 0
  - t
  - τ
  - r, $P(r,t)$, ζ, ψ ....for ~25 computational cells in the domain starting at the cavity wall.

6.3.2 Coalbed Methane Field Scale Test Case

This test case is designed to validate the total spallings solids release model against field observations of coalbed methane cavity completion ("cavitation") operations. The problem does not include drilling or mud. Only gas plus coal solids flow in the well. Therefore, some special logic is included in the problem setup modules to properly define the problem. The time step algorithm is modified to use the sound speed in gas rather than mud. The wellbore pressure logic uses the mixture equation-of-state, but without the presence of mud and salt.

6.3.3 Internal Logic Checks Test Problem

This test case demonstrates that DRSPALL accurately calculates:

1. Coupling of flows in the wellbore and the repository
2. Tensile failure of homogenous waste material using effective stress and seepage laws
3. Fluidized bed transport of disaggregated waste material
4. Expulsion of disaggregated waste material at the land surface.

There is no special code logic for this test case that affects the calculations. There is coding that creates and formats four ASCII output files that are used in the post-processing of the test case data. The format and content of these files are discussed in RD/VVP/VD for DRSPALL (Kicker, 2021a).

6.3.4 Wellbore Hydraulics Model Test Case

The objective of wellbore hydraulics test case is to validate the DRSPALL wellbore calculations against an independent computational fluid dynamics model FLUENT. This problem is designed to study the wellbore only. As such, the repository domain is decoupled from the

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wellbore and inactive during execution of the test problem. Input parameters pertaining to the repository are therefore irrelevant in this test case, as are any code output describing repository conditions.

The lower boundary to the wellbore domain corresponds to the very bottom of the borehole where repository gases and solids may enter the mud flow stream. In normal DRSPALL execution, the bottomhole pressure acts as a common boundary condition for the inner boundary of the repository and the bottom of the wellbore. Gas and potentially solids are transferred from the repository domain to the wellbore domain at this boundary. For this test case, the lower boundary requires specific control over the mass loading rate of gas and/or solids in order to set up analogous runs with the computational tool FLUENT. These mass loading rates are pre-determined and described in the RD/VVP/VD for DRSPALL (Kicker, 2021a). They are implemented in DRSPALL by circumventing the normal coupling function with the repository and building the mass loading directly into the wellbore mass transfer algorithm.

7.0 REQUIRED USER TRAINING AND/OR BACKGROUND

To exercise DRSPALL, users should have basic knowledge of the Linux operating system, and access to the WIPP computing cluster.

Because DRSPALL manipulates a CAMDAT database, users should have an understanding of the CAMDAT terminology and contents. For a detailed description of the CAMDAT database, refer to Chapter 7 of the WIPP PA *User's Manual for CAMDAT_LIB Version 1.22* (Gilkey, 1995b).

It is highly recommended that the new user read the DRSPALL theoretical basis (Section 4.0) and models and methods (Section 5.0) before setting up and executing DRSPALL. DRSPALL's conceptual and mathematical models rely on the conservation of wellbore surface area to equivalence the two-dimensional real-world problem to the 1-dimensional cylindrical or spherical model geometry. Understanding these concepts as well as the WIPP PA specific application is essential for proper execution of the code.

8.0 CAPABILITIES AND LIMITATIONS

DRSPALL (from Direct Release Spall) is written to calculate the volume of WIPP solid waste subject to material failure and transport to the surface as a result of an inadvertent drilling intrusion. The code calculates coupled repository and wellbore transient mixed-phase compressible fluid flow before, during, and after the drilling intrusion process. Mathematical models are included of bit penetration, mixed-phase (mud, salt, waste, and gas) fluid flow in the well, fluid expulsion at the surface, coupling of the well and the drilled repository, repository spalling (tensile) failure, fluidized bed transport of failed waste, and repository internal gas flow. The wellbore model is one-dimensional with linear flow, while the repository model is one-dimensional with either spherical or cylindrical radial flow. Flow in the well is treated as a

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compressible, viscous, multi-phase mixture of mud, gas, salt, and possibly waste solids. Flow in the repository is treated as viscous, compressible single-phase gas flow in a porous solid

DRSPALL was developed specifically for calculating the volume of WIPP solid waste subject to material failure and transport to the surface as a result of an inadvertent drilling intrusion. Therefore, many input parameters have been bounded to ranges established for WIPP specific materials, WIPP repository geometry and standard drilling practices in the Delaware basin and are documented in the *Parameter Justification Report for DRSPALL* (Hansen et al., 2003). Specific parameters and ranges are tabulated in Section 10.0, Table 10-1.

9.0 USER INTERACTIONS WITH THE SOFTWARE

DRSPALL executes on a CentOS platform. To execute DRSPALL, the program executable name (drspall) must be in the user's current PATH or referenced by its path name.

DRSPALL expects four 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.

DRSPALL expects the following command line arguments:

1. –user The input control file. This required file sets the values for the problem specification parameters. If an input CAMDAT file is specified, the parameters may be read from CAMDAT properties specified in the input control file. The input control file is described in Section 10.1.

2. –debug The output diagnostics file. This file contains a listing of the input control file and the input problem specification parameters. The output diagnostics file is described in Section 12.1.

3. –input An optional input CAMDAT file. This file contains certain problem specification parameters, defined as properties and referenced by the input control file. If the user enters "CANCEL", all input must come from the input control file. The input CAMDAT file is described in Section 10.2.

4. –output An output CAMDAT file. This file contains the results of the DRSPALL execution. The output CAMDAT file is described in Section 12.2.

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10.0 DESCRIPTION OF INPUT FILES

DRSPALL inputs a set of problem specification parameters from the input control file. The format of the input control file is described in Section 10.1. If an input CAMDAT file is specified as described in Section 9.0, the input control file may reference values from the input CAMDAT file. The format of the input CAMDAT file is described in Section 10.2.

The DRSPALL input parameters are listed in Table 10-1, along with their default values, units, and range. The input parameters should be self-explanatory. More information is available in Sections 3.0 through 6.0. The parameters are grouped into categories (e.g., Repository, Waste). All numeric parameters are double-precision real numbers, unless otherwise noted. The parameter ranges identified in Table 10-1 represent the ranges of validity in the judgment of the code designers. The code will abort if the user attempts to operate outside these specified ranges. The ranges in Table 10-1 should not be confused with the parameter ranges defined in the WIPP PA database, which represent the justified ranges for the materials and properties directly relevant to WIPP. The ranges in Table 10-1 will necessarily be the same or larger than the WIPP PA database parameter ranges.

The input parameters are listed twice in the output diagnostics file, described in Section 12.1. The first listing is a direct echo of the input control file. The second listing writes the values that are being used by DRSPALL. If there is an error in the input parameters, it will be reflected in the second listing.

10.1 The Input Control File

The input control file is an ASCII text file that defines the problem specification parameters. An example of an input control file is shown in Figure 14.

The parameters are grouped in categories in Table 10-1 and in the input control file. In Table 10-1, the category name appears as a shaded row, with the parameters listed under the category. In the input control file, the category name must be followed by a record for each parameter within the category, in order. The categories themselves may appear in the input control file in any order, but the parameters within the category must appear in the order listed in Table 10-1. Optional categories are noted in the table; all other categories are required. Comment records may appear outside of the category definitions.

The start of the category is recognized by the first few letters of the category name. The bold letters of the category name in Table 10-1 are enough to identify the category. All letters are converted to uppercase before any parsing is done, and leading blanks are ignored.

A record for each parameter within the category must follow, in the order listed in Table 10-1, directly after the category name. The parameter records are in free-format, as follows:

text : *value*.

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Table 10-1– DRSPALL Input Parameters.

Category and Parameters	Units	CAMDAT*	Default	Range
REPOSITORY				
Land elevation	m	YES	1037.3	900.0 – 1100.0
Repository top	m	YES	385.31	300.0 – 500.0
Repository thickness	m	YES	0.0	0.0 – calculated internally 1.0 – 2.0 use specified value
DRZ# thickness	m	YES	0.85	0.1 – 1.0
DRZ permeability	m^2	YES	1.0e-15	1.0e-21 – 1.0e-11; < DDZ Permeability
Outer radius	m	YES	19.2	10.0 – 50.0; > 0.5 * Bit Diameter
Initial gas pressure	Pa	YES	14.5e6	6.0e6 – 18.0e6; ≤ far-field in-situ stress
Far-field In-Situ Stress	Pa	YES	14.8e6	14.0e6 – 18.0e6
WASTE				
Repository initial porosity	–	YES	0.575	0.20 – 0.85
Repository initial permeability	m^2	YES	1.7e-13	1.0e-17 – 1.0e-12
Forchheimer beta	–	YES	1.15e-6	1.0e-12 – 1.0e-4
Biot beta	–	YES	1.0	0.5 – 1.0
Poisson's ratio	–	YES	0.35	0.2 – 0.45
Cohesion	Pa	YES	1.23e5	1.0e4 – 1.0e7
Friction angle	deg	YES	45.0	30.0 – 60.0
Tensile strength	Pa	YES	6895.0	6.89e3 – 6.91e6
Characteristic failure length	–	YES	0.02	0.0 – 0.1
Particle diameter	m	YES	0.001	0.001 – 1.0;
Gas viscosity	Pa-s	YES	10.0e-6	1.0e-6 – 1.0e-4
MUD				
Initial mud density	kg/m^3	YES	1210.0	1000.0 – 1500.0
Mud viscosity	Pa-s	YES	0.01	1.0e-4 – 1.0e-1
Wall roughness pipe	m	YES	0.5e-5	1.0e-14 – 1.0e-2
Wall roughness annulus	m	YES	0.5e-5	1.0e-14 – 1.0e-2
Max mud solids vol. Fraction	–	YES	0.6	0.5 – 0.8
Mud solids viscosity exponent	–	YES	-1.8	-2.0 – -1.2
WELLBORE/DRILLING				
Bit diameter	m	YES	0.3112	0.25 – 1.32
Pipe diameter	m	YES	0.1143	0.1 – 0.15; < Bit Diameter
Collar diameter	m	YES	0.2032	0.15 – 0.25; > Pipe Diameter, < Bit Diameter
Pipe inside diameter	m	YES	0.1005	0.08 – 0.13; < Pipe Diameter
Collar length	m	YES	182.9	0.0 – 250.0
Exit pipe length	m	YES	15.24	0 – 25.0
Exit pipe diameter	m	YES	0.0508	0.0254 – 0.3048
Drilling rate	m/s	YES	0.005	0.0 – 0.01

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Category and Parameters	Units	CAMDAT*	Default	Range
Initial bit height above repository	m	YES	0.15	0.01 – 1.0
Mud pumping rate	m^3/s	YES	0.021443	0.001 – 0.1
Maximum pump pressure	Pa	YES	27.5e6	1.0e5 – 100.0e6
DDZ# thickness	m	YES	0.15	0.1 – 0.3
DDZ permeability	m^2	YES	1.0e-14	1.0e-21 – 1.0e-12; > DRZ Permeability
Stop drilling exit volume rate	m^3/s	YES	1000.0	0.05 – 2000.0
Stop pumping exit volume rate	m^3/s	YES	1000.0	1.0 – 2000.0
Stop drilling time	s	YES	1000.0	≥0
COMPUTATIONAL				
Spherical / Cylindrical	–	NO	S	S or C (Spherical or Cylindrical)
Allow fluidization	–	NO	Y	Y or N or A (Yes, No or Always)
Maximum run time	s	NR	900.0	> 0
Repository zone size	m	NR	0.002	>0
Region of constant zone size, zone Growth Rate	m, –	NO	0.5, 1.00	>0.0, =1.00
Wellbore zone size	m	NR	2.0	>0
Wellbore zone growth rate	–	NR	1.00	=1.00
First wellbore zone	–	NR	2	1 – model inside pipe >1 – model annulus only
Well stability factor	–	NR	0.1	<1.0
Repository stability factor	–	NR	5.0	>0.0
Mass diffusion factor	–	NR	0.02	0 – 0.05 (0.002 recommended)
Momentum diffusion factor	–	NR	0.002	0 – 0.05
VALIDATION	Optional Category to run validation tests described in the RD/VVP/VD (Kicker, 2021a)			
Validation Test Case	–	NR	0.0	*testcase. subcase* (see RD/VVP/VD)
PARAMETERS AND CONSTANTS	Optional Category			
Pi	–	YES	3.14159263589793	–
Atmospheric Pressure	Pa	YES	101300.0	–
Gravity	m/s^2	YES	9.8067	–
Gas Constant	J/kg K	YES	4124.0	–
Repository Temperature	K	YES	300.0	–
Water Compressibility	1/Pa	YES	3.1e-10	–
Waste Density	kg/m^3	YES	2650.0	–
Salt Density	kg/m^3	YES	2201.0	–
Shape Factor	–	YES	1.0	-0 < x ≤1.0
Tensile Velocity	m/s	YES	1000.0	–
Bit Nozzle Number	–	YES	3.0	–
Bit Nozzle Diameter	m	YES	0.011112	–
Choke Efficiency	–	YES	0.9	-.0 < x ≤ 1.0
	Optional Parameters – highlighted characters must be specified in text field			
INITIAL CAVITY RADIUS	m	YES	0.0	=0 – calculated internally >0.0 – use specified value

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Category and Parameters	Units	CAMDAT*	Default	Range
MINIMUM CHARacteristic Velocity for Fluidization	m/s	YES	1.0e-6	>0
MINIMUM NUMBer of zones per Characteristic Length	–	YES	5	1≤ n ≤10

DRZ – Disturbed Rock Zone; DDZ – Drill Damage Zone

* NO – cannot be read from CAMDAT file; NR – not recommended to read from CAMDAT file; YES – can be read from CAMDAT file

```
REPOSITORY
Land Elevation                    (m):  DRSPALL SURFELEV
Repository top                    (m):  DRSPALL REPOSTOP
Total Thickness                   (m):  0.0
DRZ Thickness                     (m):  DRSPALL DRZTCK
DRZ Permeability                (m^2):  DRSPALL DRZPERM
Outer Radius                      (m):  1.9200E+01
Initial Gas Pressure              (m):  DRSPALL REPIPRES
Far-Field In-Situ Stress          (m):  DRSPALL FFSTRESS

WASTE
Porosity                          (-):  DRSPALL REPIPOR
Permeability                    (m^2):  DRSPALL REPIPERM
Forch Beta                        (-):  DRSPALL FRCHBETA
Biot Beta                         (-):  DRSPALL BIOTBETA
Poisoson   Ratio                  (-):  DRSPALL POISRAT
Cohesion                         (Pa):  DRSPALL COHESION
Friction Angle                  (deg):  DRSPALL FRICTANG
Tensile Strength                 (Pa):  DRSPALL TENSLSTR
Lt                                (m):  0.02
Particle Diameter                 (m):  DRSPALL PARTDIAM
Gas Viscosity                  (Pa-s):  DRSPALL GASVISCO

MUD
Density                      (kg/m^3):  DRSPALL INITMDEN
Viscosity                      (Pa-s):  DRSPALL MUDVISCO
Wall Roughness Pipe               (m):  DRSPALL PIPEROUG
Wall Roughness Annulus            (m):  DRSPALL ANNUROUG
Max Solids Vol. Frac.          (Pa-s):  DRSPALL MUDSOLMX
Solids Viscosity Exp.          (Pa-s):  DRSPALL MUDSOLVE

WELLBORE/DRILLING
Bit Diameter                      (m):  DRSPALL BITDIAM
Pipe Diameter                     (m):  DRSPALL PIPEDIAM
Collar Diameter                   (m):  DRSPALL COLRDIAM
Pipe Inside Diameter              (m):  DRSPALL PIPEID
Collar Length                     (m):  DRSPALL COLRLNGT
Exit pipe Length                  (m):  DRSPALL EXITPLEN
Exit Pipe Diameter                (m):  DRSPALL EXITPDIA
```

Figure 14 Example DRSPALL Input Control File.

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```
Drilling Rate                    (m/s):  DRSPALL DRILRATE
Bit Above Repository (init.)       (m):  DRSPALL INITBAR
Mud Pump Rate                  (m^3/s):  DRSPALL MUDPRATE
Max Pump Pressure                (Pa):  27.5d6
DDZ Thickness                      (m):  DRSPALL DDZTHICK
DDZ Permeability                 (m^2):  DRSPALL DDZPERM
Stop Drill Exit Vol Rate       (m^3/s):  DRSPALL STPDVOLR
Stop Pump Exit Vol Rate        (m^3/s):  DRSPALL STPPVOLR
Stop Drilling Time                 (s):  DRSPALL STPDTIME

COMPUTATIONAL
Spherical/Cylindrical            (S/C): S
Allow Fluidization               (Y/N): Y
Max Run Time                       (s):  1.0
Respository Cell Length            (m):  0.002
Radius, Growth rate              (m,-):  0.5, 1.00
Wellbore Cell Length               (m):  1.0
wellbore Zone Growth Rate          (-):  1.00
First wellbore Zone                (-):  10
Well Stability factor              (-):  0.02
Repository Stability factor        (-):  5.0
Mass Diffusion factor              (-):  0.002
Momentum Diffusion factor          (-):  0.002

VALIDATION
Validation Test Case               (-): 4.2

PARAMETERS
Pi                                 (-):  REFCON   PI
Atmospheric Pressure              (Pa):  1.0170E+05
Gravity                        (m/s^2):  REFCON   GRAVACC
Gas Constant                  (J/kg K):  BLOWOUT  RGAS
Repository Temperature             (K):  BLOWOUT  TREPO
Water Compressibility           (1/Pa):  12.4e-10
Waste Density                  (kg/m^3):  BLOWOUT  RHOS
Salt Density                   (kg/m^3):  2.1800E+3
Shape Factor                       (-):  DRSPALL SHAPEFAC
Tensile Velocity                 (m/s):  DEFAULT
Bit Nozzle Number                  (-):  DEFAULT
Bit Nozzle Diameter                (m):  DEFAULT
Choke Efficiency                   (-):  DEFAULT

!Optional parameters
Initial Cavity Radius              (m):  0.0
Minimum Characteristic vel       (m/s):  1e-6
Minimum Number of zones per Lt   (-):  5
```

Figure 14 Example DRSPALL Input Control File (Continued).

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Any text before the colon is ignored. The text usually includes the parameter name for readability. (An equal sign, "=", may be substituted for the colon.)

The value field for a single numeric parameter may be one of the following:

- Blank or "DEFAULT" (case is unimportant and leading spaces are ignored) to assign the default value to the parameter. The default values are listed in Table 10-1.

- A specific value to assign to the parameter, in any valid FORTRAN format for a double-precision real number.

- The material name and property name of the CAMDAT property that contains the value of the parameter. The material name and property name may be separated by a comma, a colon, an equal sign, or blanks. See Section 10.2 for more information on the input CAMDAT file. If the property is not present on the input CAMDAT file, the parameter is assigned its default value. This option is only available if an input CAMDAT file has been specified as described in Section 9.0 and if the parameter has "Yes" in the CAMDAT column in Table 10-1.

For a text parameter (e.g., Spherical/Cylindrical), the first non-blank character (case is unimportant) after the colon must be an allowable value for the text parameter, as listed in Table 10-1.

The *value* field for a parameter that expects two values (e.g., Repository radius, Growth) should contain the two values in any valid FORTRAN format for a double-precision real number or integer, as appropriate. The two values should be separated by a comma or blank(s).

Note that although the text in a parameter record is not processed in any way, the parameter records are also read when the parser is searching for the start of a category. Thus, if the first characters of the text of a parameter record are the same as the first few letters of any category name (case is unimportant and leading blanks are ignored), that category name must appear before the parameter record. For example, in the input control file shown in Figure 14, the text "Repository" appears as the first word in several parameter records. This would conflict with the category name "REPOSITORY" if this category appeared later in the file.

Comment lines may appear outside of the category definitions. That is, a comment record may not be inserted between the start of the category and the end of the parameter records for that category. It is suggested that the comment lines begin with a special character such as "!" to avoid problems with parsing.

10.2 The Input CAMDAT File

The input CAMDAT file is a binary, sequential file used by many WIPP codes. A detailed description of the CAMDAT file format is given in Chapter 7 of the WIPP PA *User's Manual for*

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CAMDAT_LIB Version 1.22 (Gilkey, 1995b). The input CAMDAT file is optional, and is only available if it has been specified as described in Section 9.0.

The input control file may reference specific property values on the input CAMDAT file. A property is a single value that is associated with a material. ("Material" and "element block" are synonymous.) Both the material and the property are referenced by name. Properties may be assigned to the CAMDAT file with the MATSET program, described in the *Design Document and User's Manual for MATSET Version 9.25* (Feng, 2021). DRSPALL limits the number of materials on the input CAMDAT file to 200.

The value of any property referenced by the input control file is printed to the output diagnostics file. If the referenced property does not exist on the input CAMDAT file, a message to that effect is printed to the output diagnostics file and the property is assigned its default value.

11.0 ERROR MESSAGES

The error messages that DRSPALL may generate are listed below, along with the cause of the error, and suggested action. The error messages are divided into three sections based on when the error may occur: while the user is specifying the file names, while reading the input control file, and during the simulation execution.

Unless otherwise noted, error messages are written to the output diagnostics file, described in Section 12.1. The messages below are of the following type:

- Fatal errors cause the program to abort. Fatal error messages are written to the diagnostics file and to the screen, although the messages may differ slightly.
- Other errors indicate problems that should be addressed. These errors usually lead to a fatal error later in processing.
- Warnings indicate possible problems. They do not cause the program to abort.
- Information-only messages are not errors, and thus only a few of these messages are listed below. The messages listed below are those that may be confused with error messages or those that provide information that may be especially useful in detecting problems.

11.1 File Assignment Errors

The errors in this section concern the DRSPALL input/output files that the user specifies at the start of execution. See Section 9.0 for information on specifying files.

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FATAL ERROR – Incorrect file assignments

This fatal error occurs when the user does not specify the files correctly. Common causes are specifying an input file that does not exist or not specifying a required file.

ERROR: must specify CDB or test output

This fatal error occurs when the user does not specify either the output text files or the output CAMDAT file.

FATAL ERROR – PROBLEM WITH INPUT CDB

This fatal error occurs when an input CAMDAT file is specified, but it is not a valid CAMDAT file.

11.2 Input Control File Errors

The errors in this section may occur while DRSPALL is processing the input control file. See Section 10.0 for information on the input control file and the input CAMDAT file. Although DRSPALL checks for errors as the input control file is read, the user must take care to correctly define the parameters. In particular, missing or misplaced parameter records or values in an invalid FORTRAN format may cause DRSPALL to abort without an explicit error message. The output diagnostics file, described in Section 12.1, contains a listing of all the parameters that were set by the input control file, including all the parameters read from the CAMDAT file. If the user suspects that there are problems with the input parameters, this file should be examined.

FATAL ERROR – IN DBIELBK

This fatal error indicates that the input CAMDAT file is invalid. One possible cause is that a CAMDAT property is requested, but no input CAMDAT file is specified.

FATAL ERROR – OVER 200 EL BLKS IN DBVALUE

This fatal error occurs if the input CAMDAT file contains more than 200 materials (element blocks). This is a hard-coded limit in DRSPALL.

FATAL ERROR – OVER 50 PROPERTIES IN DBVALUE

This fatal error occurs if over 50 properties are requested from the input CAMDAT file. No more than 50 input parameters in the input control file may reference a CAMDAT property. This error should never occur because there are less than 50 input parameters that allow CAMDAT properties as values.

ERROR: Unable to find Keyword *category*

Screen message: **ERROR: Unable to find Keyword**

This fatal error occurs when the input control file does not contain the category name indicated by *category* (REPOSITORY, WASTE, MUD, WELL, COMPUTATIONAL).

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Default parameter values will be used

This information-only message indicates that the input control file does not contain the Parameters and Constants category, and that the default parameters will be used for this category.

ERROR: Could not find property *varname*

Screen message: **ERROR: Could not find property**

The fatal error occurs when the *varname* parameter record indicates that its value is a CAMDAT property, but the record contains a material name, but no property name. Note that the parameter name as indicated in this document may not exactly match *varname*.

ERROR: Could not find data on input record for *varname*

Screen message: **ERROR: Could not find data on input record**

The fatal error occurs when the *varname* parameter record does not contain a ":" (or "=") and a value. Note that the parameter name as indicated in this document may not exactly match *varname*.

ERROR: Could not find delimiter for variable=*varname*

Screen message: **ERROR: Could not find delimiter for variable**

This fatal error occurs when the *varname* text parameter record does not contain a ":" or "=" to delimit the expected text value. Note that the parameter name as indicated in this document may not exactly match *varname*.

FROM CDB, *material property* : *value*

This information-only message indicates that the indicated value was read from the CAMDAT property. The property was requested by listing *material* and *property* as the value on a parameter record.

PROPNAM *property* NOT FOUND!! SET TO DEFAULT: *value*

This information-only message indicates that the indicated CAMDAT property was not found on the input CAMDAT file. The property was requested by listing the *material* and *property* as the *value* on a parameter record. The *material* or *property* may not be defined on the CAMDAT file, or the *property* may not be defined in the indicated *material*. If the *property* was not found, the parameter is set to the default *value* shown. This message does not cause DRSPALL to abort, but it may indicate a problem with the input CAMDAT file or the input control file.

ERROR: *varname=value* Outside parameter bounds, (*minval*, *maxval*)

This error occurs when the *varname* input parameter is outside the prescribed range. The value for the parameter, as indicated by the input control file, is listed. The range for the input parameter is listed in Table 10-1, but the *minval* to *maxval* range is the range checked by DRSPALL. Note that the parameter name as indicated in this document may

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not exactly match *varname*. Also note that some ranges listed in the table may not be checked by DRSPALL. This error will trigger a fatal error once the ranges of all input parameters are checked.

ERROR: Parameter Bounds Exceeded

This fatal error occurs if the range of any input parameter is outside its bounds. If this occurs, an error message identifying the parameter(s) will precede this error message in the output diagnostics file.

11.3 Execution Errors

The errors in this section may occur after DRSPALL has processed the input control file. Since the simulation is controlled by the input parameters, the user should inspect the input parameters if the simulation does not proceed as expected. The output diagnostics file, described in Section 12.1, contains a listing of all the input parameters.

FATAL ERROR – PROBLEM WITH OUTPUT CDB
FATAL ERROR – PROBLEM WITH DBOQAREC
FATAL ERROR – PROBLEM WITH DBOHEAD

These fatal errors occur when the output CAMDAT file cannot be opened or written. This may occur when the user does not have write access or the disk is full.

WARN: wellgasvol=', wellgasVol(*i*)

This warning message is printed when the well gas volume is less than zero.

WARNING: Viscous choking(1 or 2) at *i*

This warning message is printed when

(1) The well solids fraction is greater than maximum allowed, or

(2) The viscous term is greater than the acceleration a term, usually due to oscillation in the velocity flow.

12.0 DESCRIPTION OF OUTPUT FILES

12.1 The Output Diagnostics File

The output diagnostics file contains a listing of the input control file, followed by a listing of the actual parameter values as they will be used by DRSPALL. It also lists the value of any CAMDAT property that was read from the input CAMDAT file. If the user suspects that there are problems with the input parameters, this file should be examined. The user should examine the listing of the actual parameter values, rather than the listing of the input control file.

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12.2 The Output CAMDAT File

The output CAMDAT file is a binary, sequential file used by many WIPP codes. A detailed description of the CAMDAT file format is given in Chapter 7 of the WIPP PA *User's Manual for CAMDAT_LIB Version 1.22* (Gilkey, 1995b). This document only mentions the CAMDAT entities that are specific to the DRSPALL program.

12.2.1 Output CAMDAT Materials and Mesh

DRSPALL defines a mesh on the output CAMDAT file. The mesh consists of a set of elements. Each element must be contained within a named material. ("Material" and "element block" are synonymous.) DRSPALL defines three materials that contain elements: the repository, the wellbore inside the drill pipe, and the wellbore outside the drill pipe. If a material does not contain any elements, that material may only be used to contain property values. The output CAMDAT file generated by DRSPALL copies zero-element materials (with their properties) from the input CAMDAT file, if one is specified. DRSPALL adds one 0-element material (DATAUSED) that contains the parameters as read by DRSPALL.

Table 12-1 describes the materials, with their elements, that DRSPALL defines on the output CAMDAT file.

Table 12-1– CAMDAT Materials and Elements.

Material Name	Description of Material and its Elements
DATAUSED	Contains properties with parameters as read by DRSPALL.
REPOS	Contains an element for each repository cell.
DOWN_WB	Contains an element for each wellbore cell inside the drill pipe.
UP_WB	Contains an element for each wellbore cell in the annulus outside the drill pipe.
xxxxxx	Contains properties copied from input CDB where the material names *xxxxxx* are defined on the input CDB

12.2.2 Output CAMDAT Properties

Table 12-2 describes the properties that DRSPALL writes to the output CAMDAT file. The properties are all contained within the DRSPALL material. The values of the properties are copied from the appropriate DRSPALL input parameter.

If an input CAMDAT file is specified (as described in Section 9.0), the properties from the input CAMDAT file will be copied to the output CAMDAT file. All input parameters used by DRSPALL are echoed to material block DATAUSED. Input properties values contained in input material blocks remain unchanged.

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Table 12-2– CAMDAT Output Properties.

Property Name	DRSPALL input parameter
SURFELEV	Land elevation
REPOSTOP	Repository top
REPOSTCK	Total thickness
DRZTCK	DRZ thickness
DRZPERM	DRZ permeability
REPOTRAD	Outer radius
REPIPRES	Initial gas pressure
FFPORPRS	Far-field Pore Pressure
FFSTRESS	Far-field In-Situ Stress
REPIPOR	Repository initial porosity
REPIPERM	Repository initial permeability
FRCHBETA	Forchheimer beta
BIOTBETA	Biot beta
POISSRAT	Poisson's ratio
COHESION	Cohesion
FRICTANG	Friction angle
TENSLSTR	Tensile strength
CHARLEN	Characteristic failure length
PARTDIAM	Particle diameter
GASBSDEN	Gas base density
GASVISCO	Gas viscosity
INITMDEN	Initial mud density
MUDVISCO	Mud viscosity
PIPEROUG	Pipe roughness
ANNUROUG	Annulus roughness
MUDSOLMX	Max mud solids vol. Fraction
MUDSOLVE	Mud solids viscosity exponent
BITDIAM	Bit diameter
PIPEDIAM	Pipe diameter
COLRDIAM	Collar diameter
PIPEID	Pipe inside diameter
COLRLNGT	Collar length
EXITPLEN	Exit pipe length
EXITPDIA	Exit pipe diameter
DRILRATE	Drilling rate
BITABOV	Initial bit above repository
MUDPRATE	Mud pump rate
MAXPPRES	Mud pump pressure
DDZTHICK	DDZ thickness
DDZPERM	DDZ permeability
STPDVOLR	Stop drilling exit volume rate

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Property Name	DRSPALL input parameter
STPPVOLR	Stop pumping exit volume rate
STPDTIME	Stop drilling time
REPODR	Initial repository cell length
REPODDR	Repository cell growth rate
WELLDZ	Initial wellbore cell length
WELLDDZ	Well cell growth Rate
GEOMEXP	Geometry exponent
ALLOWFLD	Fluidization flag
WELLSTAB	Well stability factor
REPOSTAB	Repository stability factor
MASSDIFF	Mass diffusion factor
MOMDIFF	Momentum diffusion factor
VALIDTC	Validation test case flag
PI	Pi
REFPRES	Atmospheric pressure
GRAVACC	Gravity
RGAS	Gas constant
TREPO	Repository temperature
H2OCOMP	Water compressibility
WASTDENS	Waste density
SALTDENS	Salt density
SHAPFAC	Shape factor
TENSVEL	Tensile velocity
BITNZNO	Bit nozzle number
BITNZDIA	Bit nozzle diameter
CHOKEFF	Choke efficiency
CAVRAD0	Initial cavity radius
MINCHVEL	Minimum characteristic velocity
MINNUMLT	Minimum number of zones per characteristic length

12.2.3 Output CAMDAT Time Steps and Variables

DRSPALL outputs information to the output CAMDAT file at sequential "time steps". Each time step contains the simulation time, in seconds, and the history variables defined by DRSPALL. A history variable has a single value for each time. Certain time steps may contain the element variables defined by DRSPALL, as well as the history variables. An element variable has a value for each element.

The time at which each time step is output is determined by DRSPALL. DRSPALL outputs a new time step when a certain period of time has passed, and when wellbore interface velocity changes by more than 20%.

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Table 12-3 describes the history variables that DRSPALL writes to the output CAMDAT file.

Table 12-3– CAMDAT History Variables.

History Variable Name		Description
1	PUMPRS	Pump pressure
2	BOTPRS	Well bottom pressure
3	CAVPRS	Cavity pressure
4	DRILLRAD	Equivalent Drilled radius
5	CAVRAD	Equivalent Cavity radius
6	TENSRAD	Equivalent Tensile radius
7	CUTRAD	Maximum Equivalent Cuttings radius (constant)
8	WBSUPVEL	Waste boundary pore velocity
9	FLUIDVEL	Fluidization velocity
10	MUDEJVEL	Mud ejection velocity
11	WASWELL	Waste in Well
12	WASEJCT	Waste ejected at surface
13	CUTMASMX	Maximum Cuttings mass
14	GASINJ	Gas injected into well
15	WELLGAS	Gas in Well
16	GASEJCT	Gas ejected at surface
17	GASPOSN	Gas position in well
18	WASPOSN	Waste position in well
19	CPUTIME	CPU time
20	RUNSTEP	Run step index
21	VOLSTORE	Volume failed/drilled material in storage(released from repository but not in well)
22	GASTORE	Gas mass in temporary storage
23	WASTORE	Waste mass in temporary storage
24	WASINJ	Waste injected into well
25	GASCAV	Cavity gas mass
26	SWELLGAS	Sum of well gas mass/cell
27	SREPOGAS	Sum repository gas mass/cell
28	GASTOTAL	(16)+(22)+(25)+(26)+(27)
29	GASFROMW	Total gas from waste
30	CUTMASS	Mass of cuttings
31	SPLMASS	Mass of spalled material
32	TOTMASS	Total mass of material removed
33	CUTVOLEQ	Equivalent uncompacted cuttings volume
34	SPLVOLEQ	Equivalent uncompacted spall volume
35	TOTVOLEQ	Equivalent uncompacted total volume
36	CUTRUVOL	True cuttings volume

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History Variable Name		Description
37	CUTRUMAS	True cutting mass
38	PUMPRATE	Mud pump rate
39	SHEARRAD	Maximum radius of shear failure
40	NOZLVEL	Nozzle fluid velocity
41	WBUPVEL	Fluid velocity near well bottom
42	FLUIDTIM	Characteristic fluidization time
43	SWELLWAS	Sum well waste mass /cell
44	WASFROMR	Total waste mass from repository
45	WASTOTAL	Total waste in system (removed from repository)
46	PITGAIN	Pitgain $= \Sigma (\Delta m \rho - R_p \Delta t)$, Δm = ejected mud mass; ρ mud density; R_p= mud pump rate; Δt = time increment
47	MUDEJCT	Accumulated mud mass ejected at surface
48	SPLVOL2	Incremental equivalent uncompacted spalled volume
49	SPLMAS2	Incremental equivalent spalled mass
50	BEDDEPTH	Bed depth TENSRAD-CAVRAD
51	FORCHRAT	Forchheimer test ratio

Table 12-4 describes the element variables that DRSPALL writes to the output CAMDAT file. Each element variable is only defined for certain materials, as indicated in the "Where Variable Defined" column in the table. (The materials and elements are described in 12.2.1). Variables defined for the "Repository" are only valid for the elements in the REPOS material; variables defined for the "Wellbore" are only valid for the elements in the DOWN_WP and UP_WB materials.

Table 12-4– CAMDAT Element Variables.

Element Variable Name		Where Variable Defined	Description
1	POREPRS	Repository	Repository pressure
2	RADEFSTR	Repository	Radial effective stress
3	TANEFSTR	Repository	Tangential effective stress
4	POREVEL	Repository	Pore velocity
5	RADELSTR	Repository	Radial elastic stress
6	TANELSTR	Repository	Tangential elastic stress
7	RADSPSTR	Repository	Radial seepage stress
8	TANSPSTR	Repository	Tangential seepage stress
9	FLUDSTRT	Repository	Fluidization start time
10	FLUDSTOP	Repository	Fluidization stop time
11	FAILSTRT	Repository	Failure start time
12	SUPRVEL	Repository	Superficial velocity
13	WELLPRS	Wellbore	Pressure
14	WELLVEL	Wellbore	Mixture velocity

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Element Variable Name		Where Variable Defined	Description
15	WELLGSMS	Wellbore	Gas mass
16	WELLWSMS	Wellbore	Waste mass
17	WELLRHO	Wellbore	Mixture density
18	WELLWSVF	Wellbore	Waste volume fraction
19	WELLGSVF	Wellbore	Gas volume fraction
20	WELLSAVF	Wellbore	Salt volume fraction
21	WELLWSMF	Wellbore	Waste mass fraction
22	WELLGSMF	Wellbore	Gas mass fraction
23	WELLMDMF	Wellbore	Mud mass fraction
24	WELLVOL	Wellbore	Cell volume
25	COORD	Repository, Wellbore	Repository and well coordinate positions (center of cell)

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