


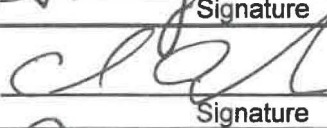
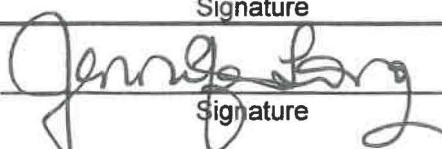


Appendix E

<p style="text-align: center;">NUCLEAR WASTE MANAGEMENT PROCEDURE</p> <p><small>Sandia National Laboratories</small></p>	<h2 style="margin: 0;">Design Document Criteria</h2>	<p>Form Number: NP 19-1-4</p> <p>Page 1 of 1</p>
<p>1. Software Name: <u>BRAGFLO</u></p> <p>2. Software Version: <u>7.00</u></p> <p>3. Document Version: <u>7.00</u></p> <p>4. ERMS #: <u>570273</u></p> <p style="font-size: small;">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.</p>		
<p>Are the following appropriately defined and documented in the DD?</p> <p>5. Major Software Components <input checked="" type="checkbox"/> Yes</p> <p>6. Technical description of the software with respect to: theoretical basis, embodied mathematical model, major control flow, control logic, and data structures <input checked="" type="checkbox"/> Yes</p> <p>7. Functionalities and interfaces of object components, functions, and subroutines. <input checked="" type="checkbox"/> Yes</p> <p>8. Allowable or prescribed ranges for inputs and outputs <input checked="" type="checkbox"/> Yes</p> <p>9. Verifiability: Is the design verifiable through testing or other means? <input checked="" type="checkbox"/> Yes</p> <p>10. Consistency and Traceability: Is the design consistent with and traceable to the software's requirements? <input checked="" type="checkbox"/> Yes</p> <p>11. Technical Feasibility: Is the design technically feasible? <input checked="" type="checkbox"/> Yes</p> <p>12. Implementation: Is the design presented in sufficient detail to allow for implementation as computer software? <input checked="" type="checkbox"/> Yes</p>		
<p>13. <u>Brad Day</u> Code Team/Sponsor <i>(print)</i></p>	<p><u></u> Signature</p>	<p><u>12/19/18</u> Date</p>
<p>14. <u>Todd R. Zeittler</u> Technical Reviewer <i>(print)</i></p>	<p><u></u> Signature</p>	<p><u>12/13/2018</u> Date</p>
<p>15. <u>Shelly Nielsen</u> QA Reviewer <i>(print)</i></p>	<p><u></u> Signature</p>	<p><u>12-19-18</u> Date</p>
<p>16. <u>Chris Camphouse</u> Responsible Manager <i>(print)</i></p>	<p><u></u> Signature</p>	<p><u>1/14/19</u> Date</p>
<p>17. <u>Jennifer Long</u> SCM Coordinator <i>(print)</i></p>	<p><u></u> Signature</p>	<p><u>1/15/19</u> Date</p>

Design Document

for

BRAGFLO Version 7.00

Document Version 7.00

ERMS# 570273

January 2019

Information Only

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1.0 INTRODUCTION

This document serves as a Design Document for BRAGFLO Version 7.00. As such, this document 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. The *BRAGFLO User's Manual* (Day 2019a) describes in detail the allowed or prescribed ranges for input data. Because BRAGFLO was acquired as developed software and has been extensively modified for performing WIPP PA calculations, this document provides an 'as built' design rather than prescribing how the code is to be developed.

1.1 Software Identifier

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

1.2 Points of Contact

Code Sponsor:	Brad Day	baday@sandia.gov	(575) 234-0178
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2.0 FUNCTIONAL REQUIREMENTS

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

- R.1 Input defining the problem to be run is read in, including mesh size, simulation time specifications, and output files to be used.
- R.2 The time and/or frequency of output to each output file and the variables whose values will be output are specified in the input.
- R.3 The code reads input defining the finite difference grid for the problem to be run, including values of Δx , Δy , and Δz , and elevations of grid block centers, or input parameters that allow BRAGFLO to calculate the elevations. These input parameters may also specify how the mesh is rotated or dipped relative to a reference right hand coordinate system.
- R.4 The default boundary conditions are no-flow conditions. BRAGFLO also allows constant pressure (Dirichlet) boundary conditions to be applied at specified grid blocks. The Dirichlet conditions fix the brine pressure and gas saturation at their initial values.
- R.5 The following initial conditions are specified on input at each grid block: brine pressure, brine saturation, iron concentration, the concentration of biodegradables and the MgO concentration.
- R.6 Parameters are inputs that control the numerical behavior of BRAGFLO. These include specifications of convergence tolerances, iteration limits, upstream weighting control parameters, dependent variable increments used to calculate Jacobian element derivatives numerically, and the solver to be used. Two solvers are currently available, the original LU decomposition solver and the point successive over-relaxation (SOR) solver, and only the original LU decomposition solver will be used in WIPP compliance calculations.
- R.7 Material maps at specified times are input. For each material, material properties are input, including two-phase flow parameters, intrinsic permeabilities, reference condition porosities, and compressibilities. Also specified are the relative permeability and capillary pressure model to be used for each material. Furthermore, BRAGFLO allows for the change of pressure and saturation values, as well as the capability to turn off the chemistry reactions when materials change.
- R.8 Relative permeabilities and capillary pressure are calculated for each material using one of several available models including original and modified versions of the Brooks-Corey and van Genuchten-Parker empirical relations, linear models, an open cavity model, and a waste area-specific model. Also, some of the QA tests use relative permeability models that are included in BRAGFLO specifically for those tests.

- R.9 A simplified rock fracture model allows the porosity and permeability to increase as pore pressure increases above a threshold value, simulating a fracture network. In the absence of fracturing, the porosity may vary slightly with pressure due to rock compressibility effects.
- R.10 The Klinkenberg effect is included, allowing the gas-phase permeability to become elevated over the intrinsic brine-phase permeability at low pressures in low-permeability materials.
- R.11 Brine salinity, density at reference conditions, and compressibility are specified by input values, and the density of brine varies as a function of pressure.
- R.12 Gas properties are given by the Redlich-Kwong-Soave (RKS) equation of state. The WIPP compliance calculations will use a single pure gas, H₂.
- R.13 Two primary chemical reactions are modeled in BRAGFLO: anoxic corrosion of iron and microbial degradation of cellulose. Both of these reactions produce gas (H₂) and consume brine according to specified stoichiometry. Reaction rates and stoichiometry are specified for brine-inundated conditions and for humid conditions.
- R.14 The effects of salt creep, whereby the surrounding halite closes in on the waste or other excavated regions, compressing them, may be simulated in BRAGFLO through the use of a closure surface input data file.
- R.15 BRAGFLO numerically calculates the flow of two phases, brine and gas, in porous media as a function of time and space, using an implicit finite difference method with variable time step control.
- R.16 Well models in BRAGFLO allow simulation of wells that are completed within the formations or porous media being modeled. The types of wells that can be specified/ modeled are constant injection or production rate wells and constant down-hole pressure wells.
- R.17 BRAGFLO simulates flow through heterogeneous as well as homogeneous porous media.
- R.18 BRAGFLO writes binary and ASCII output files. These files echo much of the input file information as well as primary and secondary dependent variables at user specified frequencies or at specific times. Many output variables are user selected and defined.
- R.19 BRAGFLO provides the user with an error check on the consistency with how waste regions are specified.
- R.20 Six additional chemical reactions are modeled in BRAGFLO: sulfidation of iron hydroxide; sulfidation of iron; hydration of MgO; carbonation of MgO; carbonation of Mg(OH)₂; and conversion of hydromagnesite. Stoichiometry is specified for each reaction with all necessary parameters specified in the input.
- R.21 Chemical rates of all reactions are zero below a specified cutoff value in saturation which is specified in the input.
- R.22 Chemical rates of all reactions are multiplied by their respective initial concentrations if specified by a flag in the input.

- R.23 BRAGFLO calculates the change in solid volume from the chemical reactions.
- R.24 BRAGFLO allows for the smooth change in permeability of materials in time as specified in the input.
- R.25 BRAGFLO allows for the calculation of mass for up to five radionuclides in up to two waste areas by accounting for radioactive decay.
- R.26 BRAGFLO allows for the calculation of radiolysis (the radiolytic breakdown of water/brine into hydrogen and oxygen) resulting from up to five inventory radionuclides. Radiolysis can result from radionuclides dissolved in brine and, optionally, from the remaining inventory of solid (precipitated) radionuclides that are in contact with brine (wetted). The fraction of disintegration energy from the solid radionuclides that contributes to radiolysis can be specified.

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3.0 MAJOR SOFTWARE COMPONENTS

There are basically three processing phases within the BRAGFLO software: problem specification, solution, and output of results. The modules that make up each of these phases can be found in the flow charts and subroutine descriptions in Section 5.0. The problem specification phase consists of reading user specified input data, defining the computation grid, mapping material parameters to the grid, defining boundary and initial conditions, and setting up the matrices and arrays that form the system of equations to be solved. Excluding the restart capability, which is not qualified for WIPP compliance calculations, there are up to two BRAGFLO input files and three output files. The general BRAGFLO input control file (.inp) and the optional salt creep closure data input file (.csd) are described in detail in the *BRAGFLO User's Manual* (Day 2019a). The solution phase consists of a time loop. Within the time loop is an iteration loop for the solution of the nonlinear mass balance equations. Within the iteration loop is an update of system matrices and arrays to reflect current conditions, a choice of solvers (detailed below), and application of solution convergence criteria. The details of the mathematical model and solution algorithm are provided in Section 4.0. The output phase consists of writing user specified variables at specified times and spatial locations to specified binary, (.xbin), and ASCII, (.xout, .sum) files. The format of these files is described in Section 6.0.

The BRAGFLO code has been maintained as a standalone code – all input comes from two-formatted text files and output is written to both binary and formatted text files for subsequent post processing. The code is interfaced to the WIPP PA ‘system’ through the pre- and post-processing tools PREBRAG (Day 2019b) and POSTBRAG (Camphouse 2012). PREBRAG reads the problem specification data and material parameters from an input CAMDAT Database file (.CDB) (Gilkey, 2006b) and creates one of the input text files. The other input text file must be built by the user and contains the salt creep closure data. Both are described in the *BRAGFLO User's Manual* (Day 2019a). POSTBRAG reads the files output by BRAGFLO and creates a computational database (.cdb) file containing the input grid and some material parameters as well as time dependent results.

The solution phase of BRAGFLO over a time step requires the solution of a nonlinear system of mass balance equations. The nonlinear system uses a Newton-Raphson iteration, which solves successive linear approximations to the nonlinear system. At each Newton-Raphson iteration, there is an update of the matrices and arrays that form the linear approximation. A linear equation solver then provides a solution of the approximating linear system. Linear equation solvers fall into two general categories - direct or elimination type solvers and iterative solvers. Four solver packages are implemented in BRAGFLO - two direct solvers and two iterative solvers, however, only the LU decomposition direct solver is qualified for WIPP compliance calculations.

Finally, BRAGFLO makes use of the WIPP PA libraries CAMCON_LIB and CAMSUPES_LIB to standardize common user interface and I/O functions (Gilkey, 2006a; Gilkey, 2006c). These libraries are linked to the BRAGFLO executable during the build process as documented in the *BRAGFLO Implementation Document* (Day 2019c).

The CAMCON_LIB library provides a library of standardized QA and user interface routines, which provide a code banner with credits (authors), software ID, revision date, and current date

and time. File processing routines read and parse the command line, and 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, dynamic memory allocation has not been implemented in BRAGFLO.

4.0 DESCRIPTION OF THE MODELS AND METHODS

Refer to the *BRAGFLO User's Manual* (Day 2019a), Section 4.0, for a detailed description of the models and methods implemented in BRAGFLO.

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5.0 MAJOR CONTROL FLOW AND CONTROL LOGIC

The BRAGFLO control flow and logic discussed in subsequent sections provides the following: an overview of BRAGFLO using flow charts at the module and subroutine level; a hierarchical call tree that includes a brief description of all subroutines contained in BRAGFLO; and finally, data flow is presented as a common block 'include' table, common block descriptions and a description of subroutine arguments. The hierarchical structure of the call tree provides the details of which and where subroutines are called.

5.1 Flow Chart

The major control flow and control logic for BRAGFLO is presented in Figure 1 in the form of a flow chart. In the flow chart, subroutine names are shown in UPPER CASE, and descriptive information in 'Sentence case with underlined font'. Figure 1 shows the overall flow logic of BRAGFLO and that corresponds to the BRAGFLO main routine. This main routine contains the time loop. Subsequent figures show details of modules that are introduced in earlier figures and are color-indexed for reference to routine calls across the figures. The modules (groups of subroutines) detailed in Figure 1- Figure 7 are:

- BRAGFLO – Overall control of main program.
- INITAL (Initialization) – Reads input data and sets up the problem to be solved.
- SOLVER – Controls the solution for the current time step and handles solver/iteration errors.
- MATERIALS – Initializes and loads the material properties arrays, such as, relative permeability, threshold capillary pressure, creep closure, gas and brine density, consolidation and dissolved gas parameters.
- PROPS (Properties) – Calculates the above material properties and adds rock compressibility, H₂ production due to radiolysis, corrosion rates, other chemical rates, and modifies gas permeability for the Klinkenberg effect.
- RAPHSON (Newton-Raphson) – Performs Newton-Raphson iteration by updating material properties and the Jacobian, applying boundary conditions, choosing the solver, incorporating wells, and checking for convergence.
- GETJAC (Jacobian) – Controls the calculation of the Jacobian by incorporating materials properties, wells and setting boundary conditions.

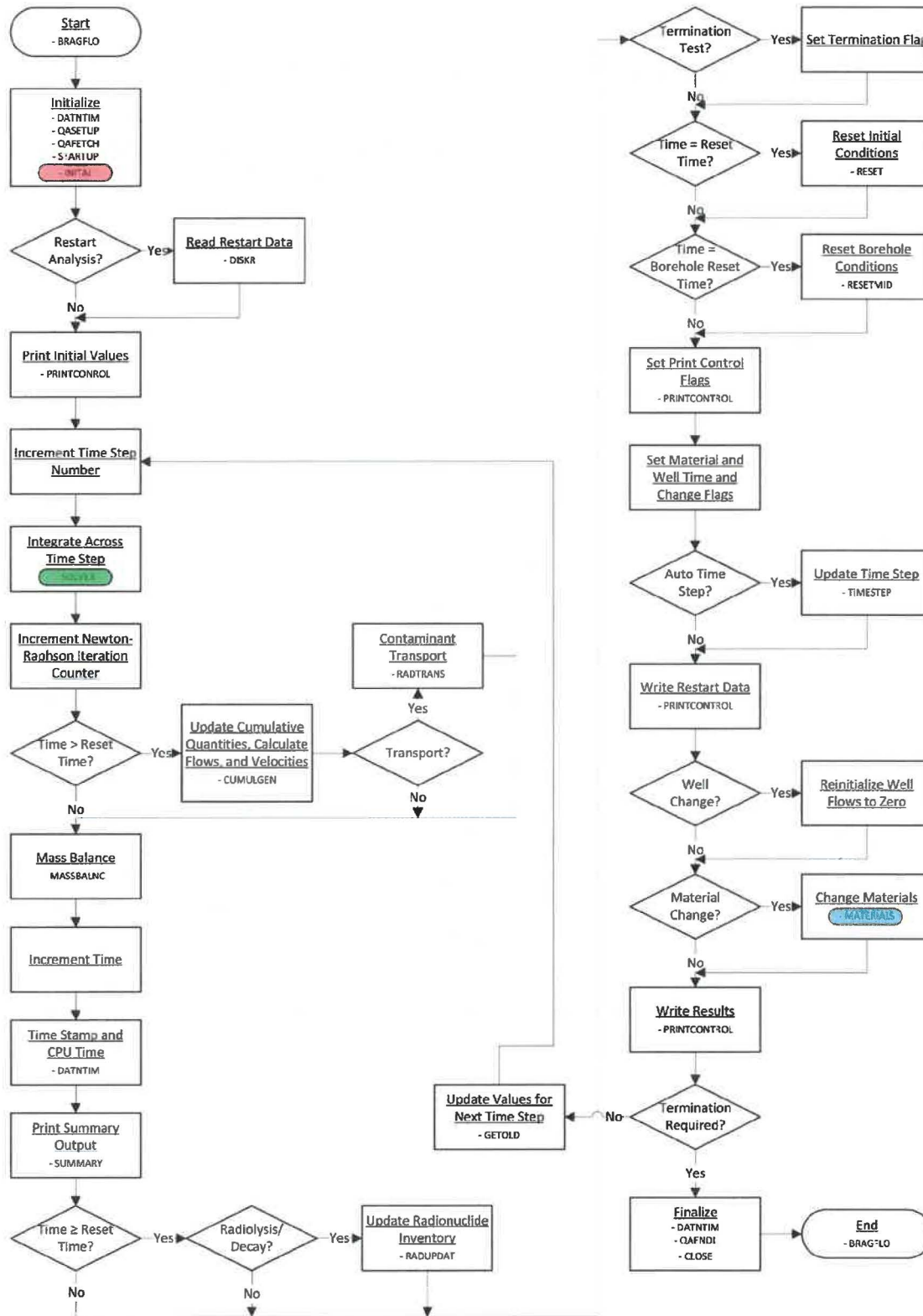


Figure 1. BRAGFLO flow chart – overall flow.

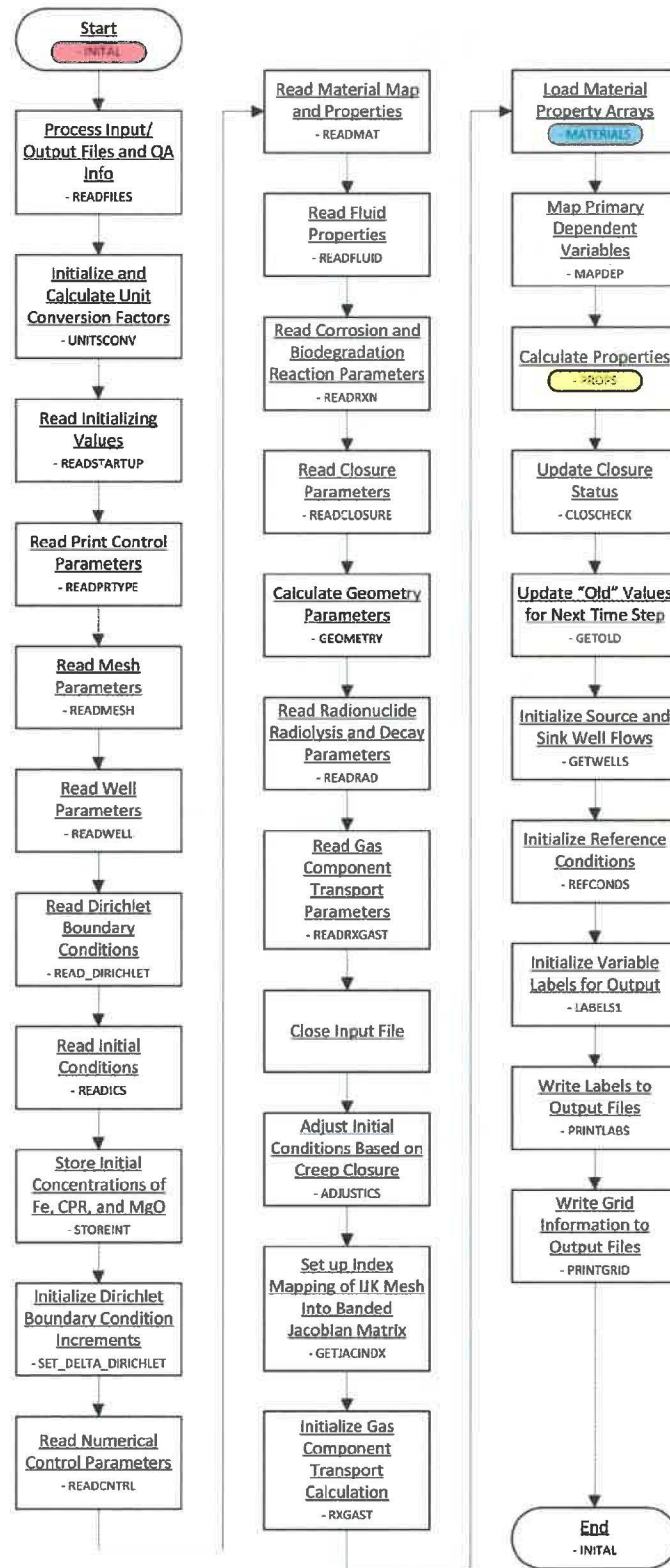


Figure 2. BRAGFLO flow chart – initialization phase.

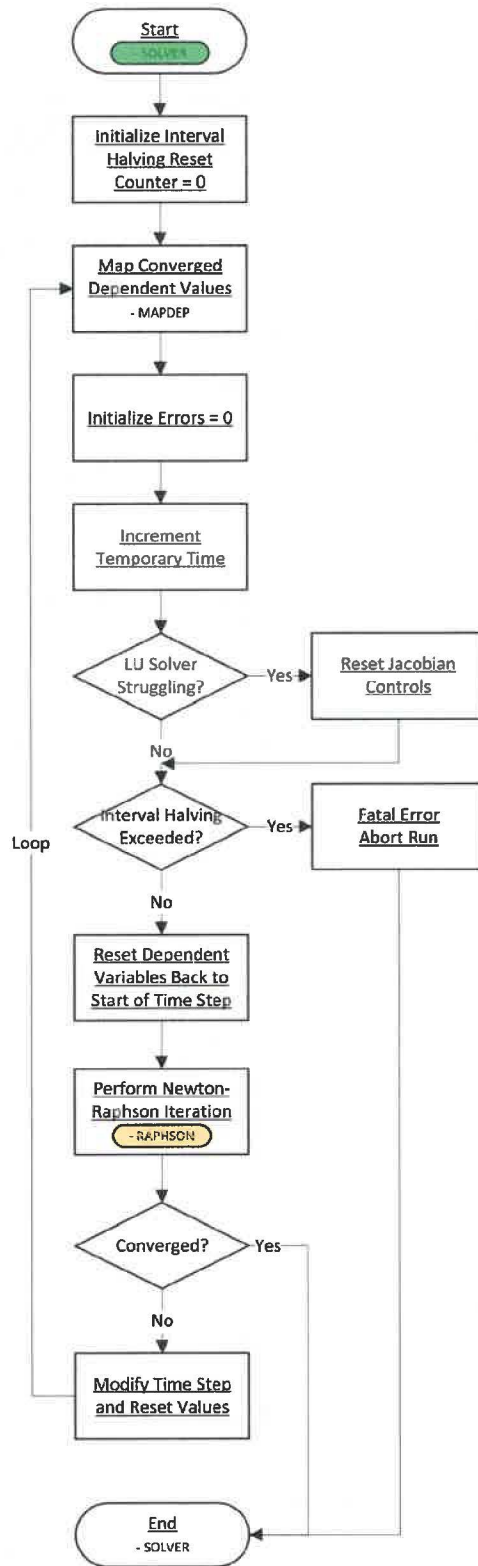
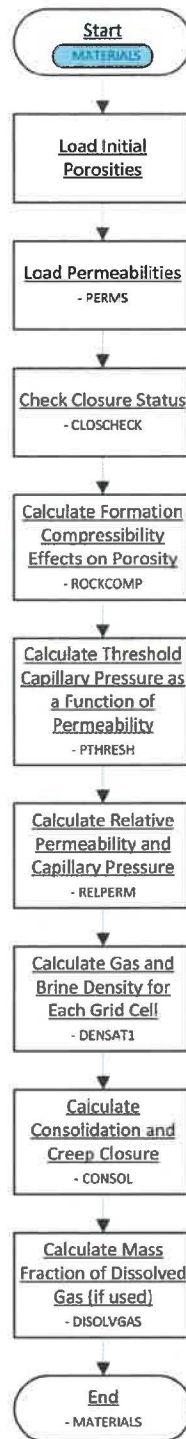


Figure 3. BRAGFLO flow chart – solver phase.



NOTE:
Conditionals that control subroutine calls are omitted for clarity.
Reference source code for details.

Figure 4. BRAGFLO flow chart – materials phase.

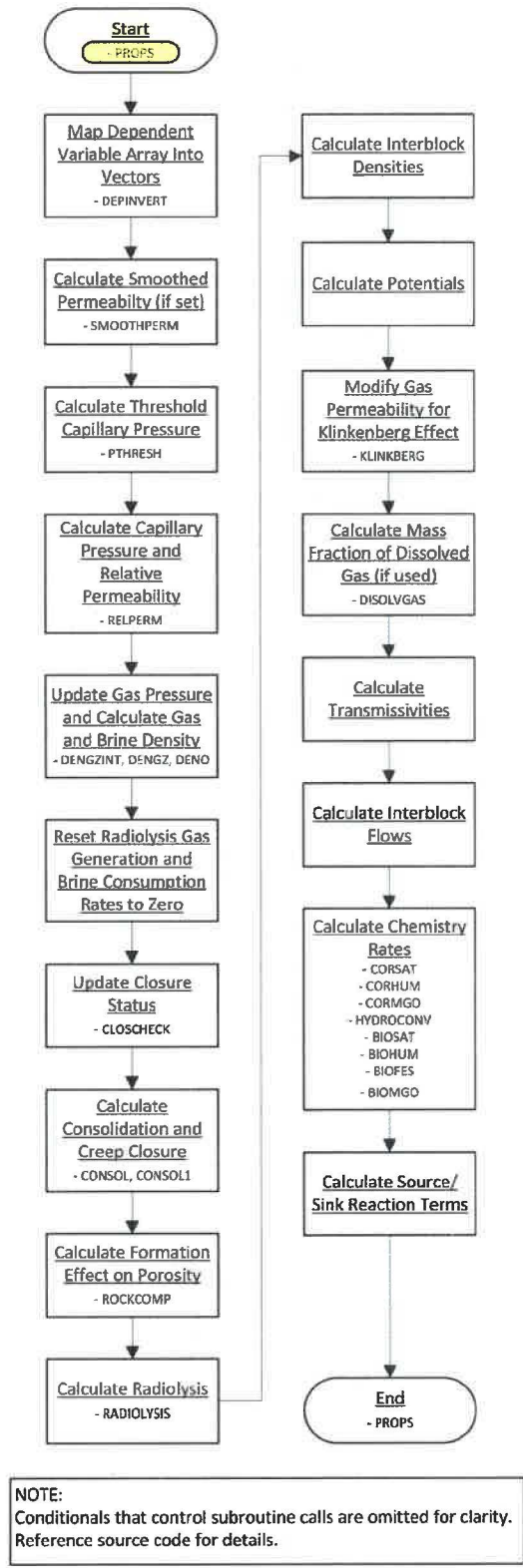


Figure 5. BRAGFLO flow chart – properties phase.

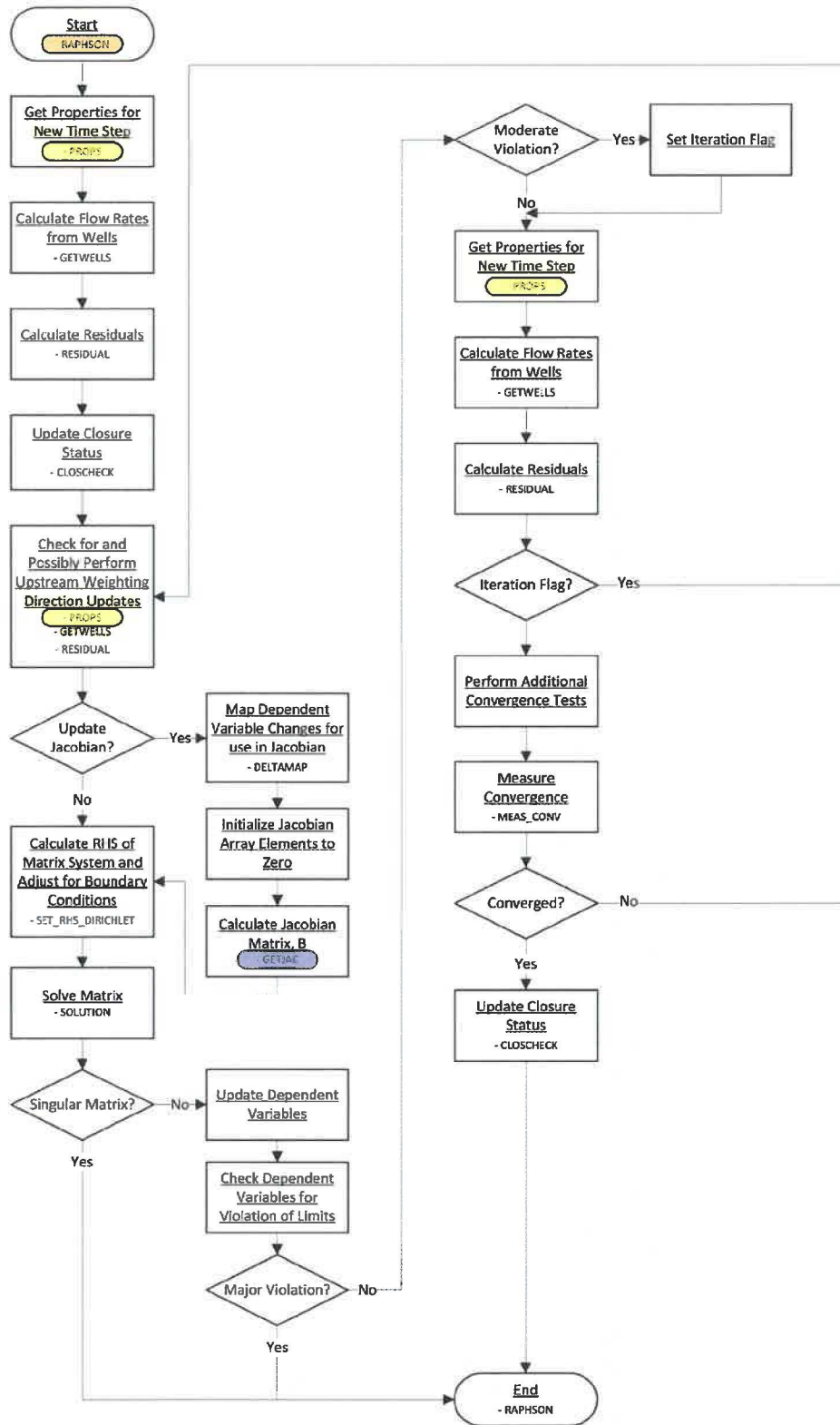


Figure 6. BRAGFLO flow chart – Newton-Raphson phase.

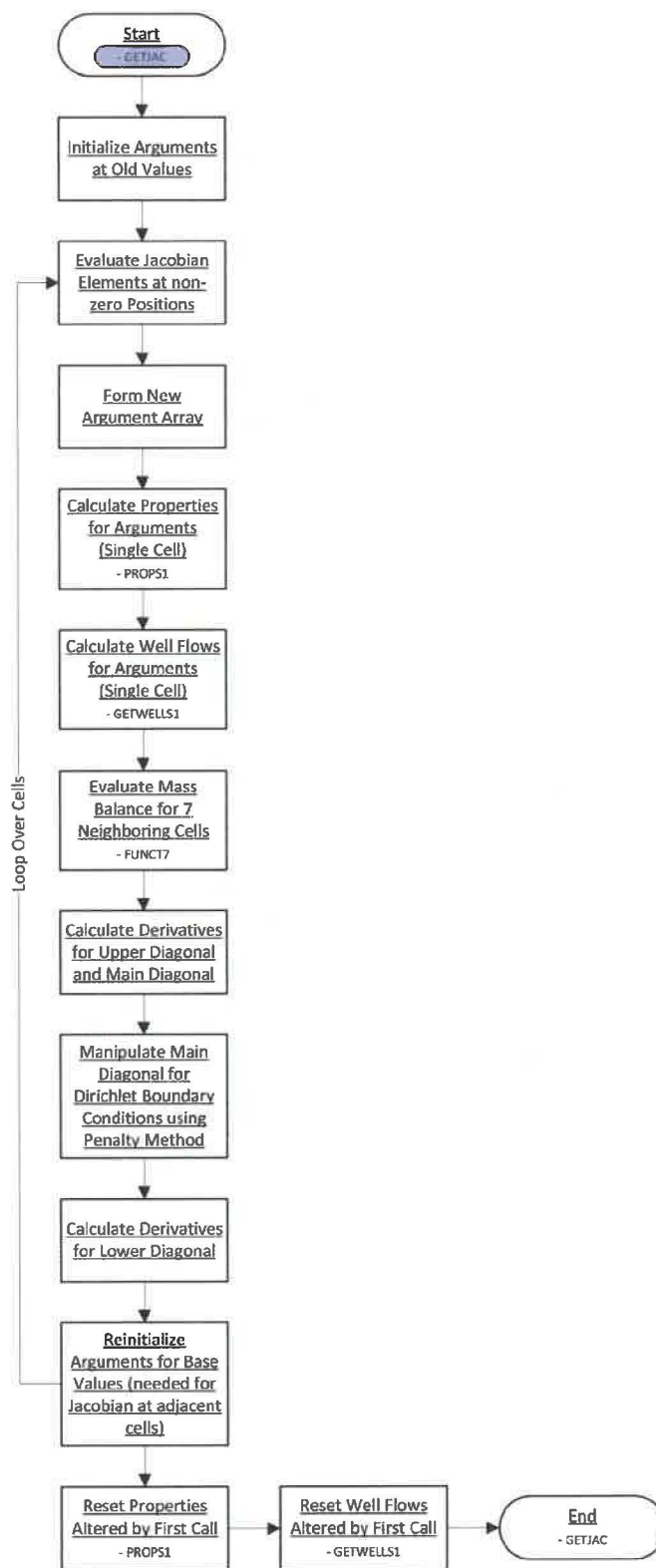
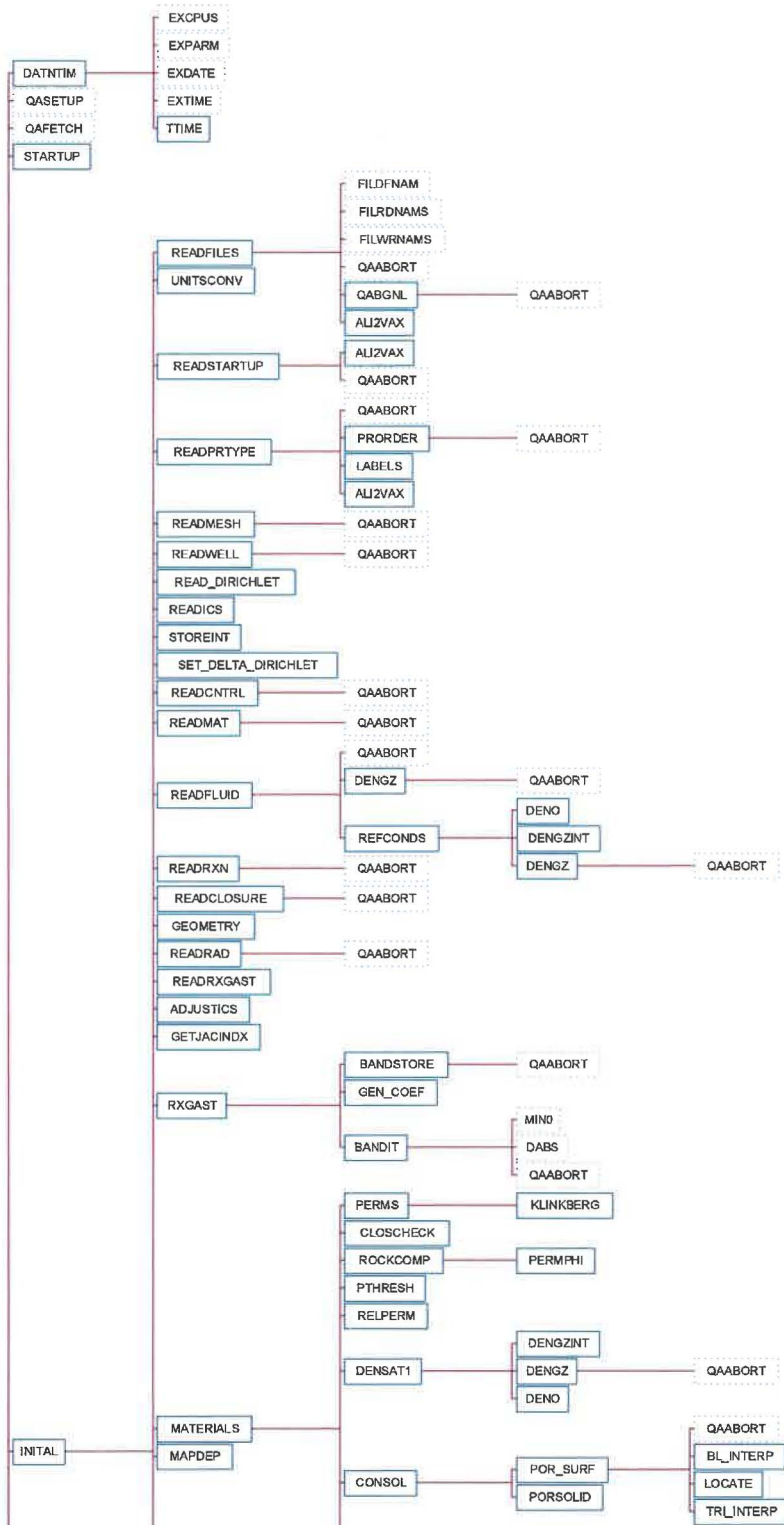
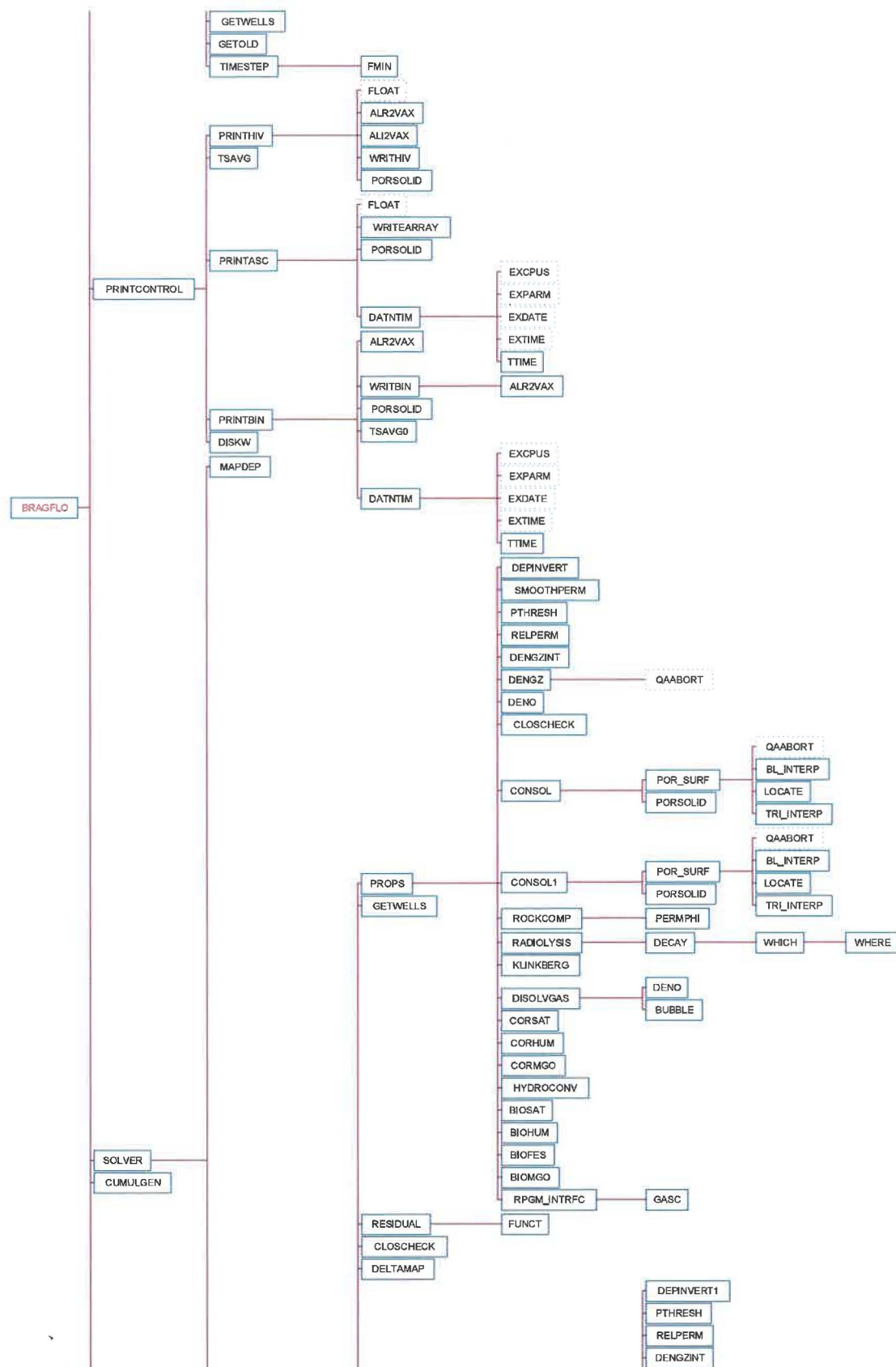


Figure 7. BRAGFLO flow chart – Jacobian phase.

5.2 Call Tree

The following is the BRAGFLO call tree. Descriptions of the routines can be found in Section 5.3. The call tree is represented in a multi-page schematic that illustrates the subroutine calls (Figure 8). The combination of the flow charts in Section 5.1 and the following call tree provides a primary description of the BRAGFLO flow logic. Conditional elements that influence control are detailed in the source code. Routines that are either not used or qualified for WIPP compliance are included in the table for completeness.





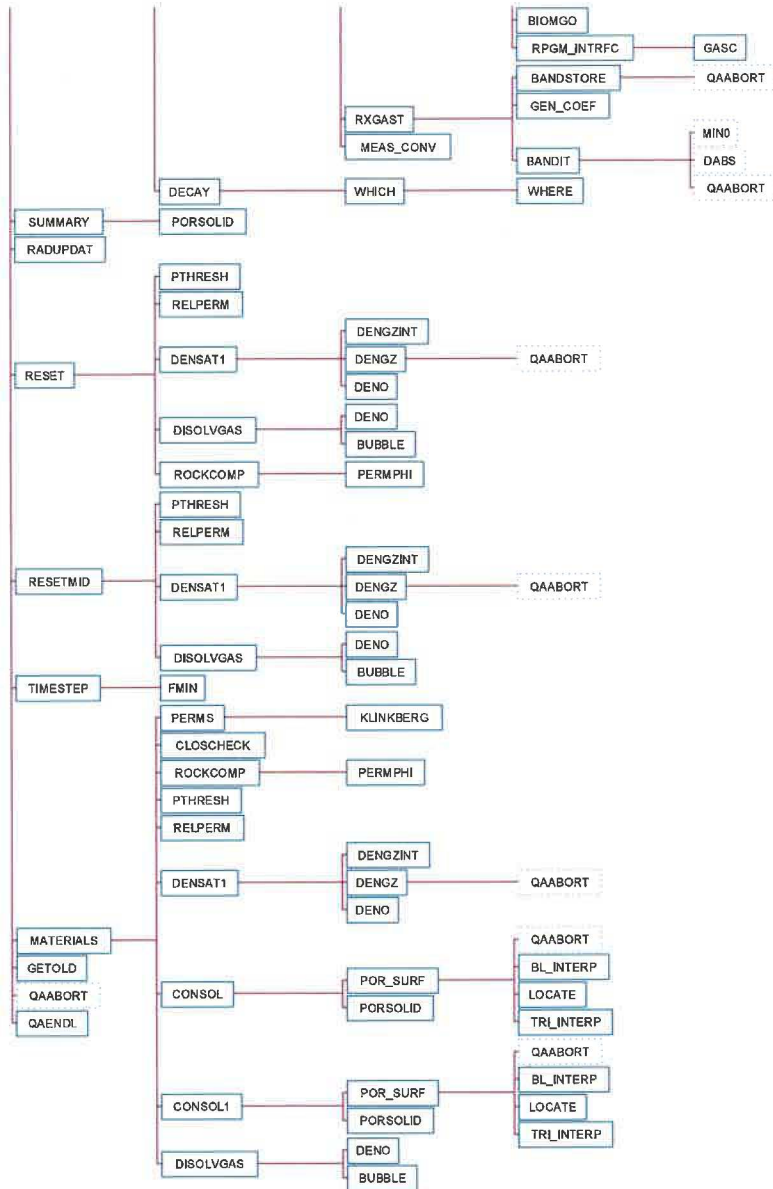


Figure 8. BRAGFLO call tree.

5.3 Subroutine Descriptions

Including the main program BRAGFLO, there are 125 subroutines and functions that comprise the BRAGFLO code. The following table provides a brief description of each of these code entities.

Table 1. Subroutine Descriptions

Entity	Description
ADJUSTICS	Adjusts initial conditions, depending on whether or not closure is to be used.
ALI2VAX	Swaps bytes to convert Alliant INTEGER*4 word into VAX INTEGER*4.
ALR2VAX	Swaps bytes to convert Alliant (IEEE) REAL*4 word to VAX REAL*4.
BANDIT	Band solver with row interchange.
BANDSTORE	Assign locations to pointer array. This directs the storage of the coefficients in the banded matrix structure.
BIOFES	Calculates the iron and iron hydroxide sulfidation rates.
BIOHUM	Calculates the biodegradation reaction rate for cellulose under humic conditions.
BIOMGO	Calculates the rate of carbonation of MgO and magnesium hydroxide.
BIOSAT	Calculates the biodegradation reaction rate for cellulose under inundated conditions.
BL_INTERP	Performs bilinear interpolation over four points.
BRAGFLO	Main program.
BUBBLE	Calculates bubble pressure point.
CLOSCHECK	Checks whether closure gets turned off, either temporarily or permanently.
CONSOL	Determines waste porosity for the entire waste region as a function of time and pressure from "porosity surface" data.
CONSOL1	Determines waste porosity for individual grid blocks as a function of time and pressure from "porosity surface" data.
CORHUM	Calculates the corrosion reaction rate for iron under humic conditions.
CORMGO	Calculates the MgO hydration rates.
CORSAT	Calculates the corrosion reaction rate for iron under inundated conditions.

Entity	Description
CUMULGEN	Updates concentrations, calculates cumulative quantities, and calculates flows and Darcy velocities.
DASUM	Calculates the sum of absolute values.
DATNTIM	Gets Date & Time from machine-dependent system subroutines.
DAXPY	Calculates the result of a constant times a vector plus another vector.
DDOT	Forms the dot product of two vectors.
DECAY	Calculates radioactive decay.
DECBR	Constructs the LU decomposition of a band matrix A in the form $L*U = P*A$, where P is a permutation matrix, L is a unit lower triangular matrix, and U is an upper triangular matrix. The matrix A is assumed here to be stored by rows in the array B.
DELTAMAP	Convert variable changes to correspond to mapping used in MAPDEP.
DENGZ	Computes density and compressibility factor for gases using either 1) Redlich-Kwong-Soave Equation of State or 2) Ideal gas law.
DENGZINT	Calculates gas density by interpolating linearly in a table of gas density computed using Redlich-Kwong-Soave EOS at fixed temperature.
DENO	Calculates brine density at pressure P at fixed temperature, using compressible liquid equation of state.
DENSAT1	Calculates gas and brine density for a single grid block.
DEPINVERT	Convert array into individual dependent variable arrays according to the same mapping as in MAPDEP.
DEPINVERT1	Single grid block version of DEPINVERT.
DGBCO	Factors a double precision band matrix by Gaussian elimination and estimates the condition of the matrix.
DGBFA	Factors a double precision band matrix by elimination.
DGBSL	Back solves a band system $A*X=B$ using factors computed by DGBCO or DGBFA.
DISKR	Reads a restart file.
DISKW	Writes a restart file.
DISOLVGAS	Calculates gas and brine mass fractions using one of the following to account for dissolved gas: 1) Bubble point, 2) Henry's Law, or 3) No dissolved gas.
DSCAL	Scales a vector by a constant.
FMAX	Finds the maximum value of a one-dimensional array.

Entity	Description
FMIN	Finds the minimum value of a one-dimensional array.
FUNCT	Evaluates PDE's for system to be solved.
FUNCT7	Evaluates PDE's for system to be solved. Does 7 evaluations for the 7-spot in a single call, saving results in F7 array.
GASC	Temporary placeholder, not used.
GEN_COEF	Generates coefficients for component gas transport.
GEOMETRY	Calculates various geometric factors (wells, average transmissibilities, alpha, etc.)
GETJAC	Forms banded Jacobian.
GETJACINDX	Sets up indices for mapping I-J-K mesh into banded Jacobian matrix.
GETOLD	Update old values for next time step with current converged values
GETWELLS	Calculate flow rates from production and injection wells.
GETWELLS1	Calculate flow rates from production and injection wells. Used only in evaluating the Jacobian; applied to a single grid block.
HYDROCONV	Calculates the hydromagnesite conversion rates.
IDAMAX	Finds the index of element having the maximum absolute value.
INITAL	Makes calls to read input file and do initial processing of input data.
KLINKBERG	Modify gas permeabilities for Klinkenberg effect.
LABELS	Initializes ASCII printout titles & units labels, and values of units conversions, depending on output units system specified. Prepares variable names that POSTBRAG can use and computes units conversion factors from UNITSO to SI units for use by POSTBRAG.
LOCATE	Determines if test point is to the left of line connecting two nodes.
MAPDEP	Map dependent variables into a single array.
MASSBALNC	Calculates mass balances.
MATERIALS	Loads material property arrays.
MEAS_CONV	Evaluates the iteration change in the variable value relative to the corresponding convergence criteria and the value of the balance equation relative to the corresponding convergence criteria.
MULTIGRID	Temporary placeholder, not used.
PERMPHI	Calculates formation permeabilities in fractured material.

Entity	Description
PERMS	Loads permeabilities from arrays XKX, YKY, and ZKZ into arrays PERMBX, PERMGX, etc. Includes Klinkenberg effect.
PORSOLID	Determines the modifier to porosity due to solids in a particular cell.
POR_SURF	Determines porosity from time and pressure table data.
PRINTASC	Writes results to ASCII output file.
PRINTBIN	Writes results to binary output file.
PRINTCONTROL	Checks to see if printing is required and calls appropriate printing routine.
PRINTGRID	Prints grid block information.
PRINTHIV	Prints history variables to binary output file.
PRINTLABS	Prints out labels for used variables.
PROPS	Calculates reservoir and material properties over the entire mesh.
PROPS1	Calculates reservoir and material properties for a single grid block when evaluating the Jacobian.
PRORDER	Arranges times in ascending order and eliminates duplicate times.
PTHRESH	Calculates threshold capillary pressure as a function of permeability.
QABGNL	Produces QA info at the beginning of a program run.
QAENDL	Produces a QA line at the end of a program run.
RADIOLYSIS	Calculates amount of H ₂ produced by radiolysis, with decay of radionuclide inventory.
RADTRANS	Performs rudimentary transport/particle tracking.
RADUPDAT	Updates the radionuclide inventory in waste cells at the start of a new timestep to be equal to that calculated due to decay from the previous successful timestep.
RAPHSON	Formulates and controls the Newton-Raphson solution method.
READCLOSURE	Reads input data for creep-closure-related parameters.
READCNTRL	Reads input data for numerical control.
READFILES	Processes files for I/O: names and opens files, does inquiries, and writes names to output files.
READFLUID	Reads input data for fluid properties.
READICS	Reads input data for initial conditions.
READMAT	Reads input data for material map and properties.
READMESH	Reads input data for mesh setup.

Entity	Description
READPRTYPE	Reads input data for printout control.
READRAD	Reads radionuclide radiolysis and decay parameters.
READRXGAST	Reads input data for gas component transport.
READRXN	Reads input data for corrosion and biodegradation reaction parameters.
READSTARTUP	Reads input data for starting up a run.
READWELL	Reads input data for wells.
READ_DIRICHLET	Initializes and reads blocks that have constant Dirichlet boundary conditions.
REFCONDS	Calculates reference conditions.
RELPERM	Calculates relative permeability and capillary pressure.
RESET	Resets pressures and saturations at the end of the startup procedure.
RESETMID	Resets saturations for borehole materials.
RESIDUAL	Calculates residual arrays.
ROCKCOMP	Calculates formation compressibility effects on porosity.
RPGM_INTRFC	Interface between the Reaction Path Gas generation Model (GASC) and BRAGFLO.
RXGAST	Driver for computing the transport of the reaction gases.
SET_DELTA_DIRICHLET	Sets the delta pressure and saturation required to keep constant boundaries.
SET_MAIN_DIRICHLET	Manipulates the main diagonal submatrix to set constant pressure or saturation, or both, Dirichlet boundary conditions.
SET_RHS_DIRICHLET	Manipulates the right hand side to set constant pressure or saturation, or both, Dirichlet boundary conditions using the Penalty method.
SMOOTHPERM	Smooths permeability as a function of time with up to a 7 th order polynomial.
SOLBR	Computes the solution of the banded linear system $A \cdot X = C$.
SOLUTION	Driver for calling the various solvers.
SOLVER	Driver for the Newton-Raphson iteration solution technique.
SOR	Solves a block matrix equation by a point successive-over-relaxation technique.
STARTUP	Initializes variables in labeled COMMON blocks.
STOREINT	Stores the initial concentrations of iron, CPR, and MgO.
SUMMARY	Prints out 1-line summary at each time step along with certain results at the monitor blocks.

Entity	Description
TIMESTEP	Determines the time step size to be used for next time step.
TRI_INTERP	Performs interpolation of a function over three points.
TSAVG	Computes time-step averages for velocities and interblock flows.
TTIME	Calls Alliant subroutine TIME.
UNITSCONV	Initializes and calculates units conversion factors for converting between SI & English units.
WHERE	Determines the identifier of the stable isotope that terminates a decay chain.
WHICH	Determines which isotopes to include in a decay chain.
WRITBIN	Writes output to the binary file.
WRITEARRAY	Prints array values to the ASCII output file.
WRITHIV	Puts history variables into single vector for simpler printout.

5.4 Data Flow

The flow of data through BRAGFLO occurs in two ways, either through FORTRAN common blocks that are included in the routines where the data is needed, or the data is passed as arguments in the routines call list. Routines use one or both of the data flow methods. Both methods are utilized and discussed below.

5.4.1 Common Blocks

Data within BRAGFLO common blocks are closely related to specific physical process models or component areas and are grouped for convenience in handling. Table 2 provides an alphabetical list of all 75 common blocks along with a brief description of the type of data stored.

Table 2. Common Block Descriptions

Common Block	Description
(Unnamed Common)	Miscellaneous
BAND	Band storage pointer array and equation index pointer array.
BASE	For Gas Generation Reaction Path Model.
BF	Brine flow, production/consumption rates.
BRATE	Reaction path gas generation model parameters.
BRINETERMS	Brine properties and parameters.
CCONVR	Control and monitoring parameters for used by subroutine SOLUTION.
CLOSURE	Creep closure data.
CMULTG	Conjugate gradient solver flags.
CONC	Dissolved gas terms.
CONPRE	Dirichlet boundary condition parameters.
CPRINT	CPU time parameters.
CPUNTC	Iteration counters for Multigrid solver.
CRESTART	Restart control parameters.
CRESTARTc	Restart control file parameters.
CUM	Cumulative component quantities.
DIR_MULTIPLIERS	Dirichlet boundary condition multipliers.
FLAWS	Phase component flows.
FRACTURE	Fracture model parameters.
FUN	Coefficients for PDEs to be solved.
GASINTERMS	RKS Gas EOS interpolation table parameters.
GASTERMS	Gas parameters.
GEOTRANS	Geometric parameters at cell block interfaces used for harmonic averaging.
ICRESET	Parameters used for resetting initial conditions.
INITL	Initial saturation and pressure.
IO	I/O control parameters.
IOc	I/O file name.
JACOBIAN	Parameters used to define Jacobian.
LU	LU decomposition solver parameters.
MACHINE	Flags for writing output on an Alliant computer.
MASSBAL	Brine and gas mass balance arrays and parameters.
MATTERMS	Material Properties arrays.

Common Block	Description
MODELTYPE	Geometry model flag.
MONITOR	Solution monitoring parameters.
MXTDIM	Bandwidth parameters.
NEWTON	Newton-Raphson control parameters.
NUCLIDE	Radionuclide tracking parameters and arrays.
OLD	Parameter values at previous step.
PHYSCON	Physical constants.
PERMPARM	Parameters for permeability characteristic curves.
PRNTC	Character arrays used as printed labels.
PRNTI	Integer variables used to control printing.
PRNTR	Real arrays and parameter storage for printed output.
PROGRAM	Program QA parameters – name, version, revision data, etc.
PROP	Arrays for reservoir material properties.
PT	Potential and density arrays.
RADACT	For Gas Generation Reaction Path Model.
RADCHAIN	Radionuclide properties.
RATES	For Gas Generation Reaction Path Model.
REF	Reference temperatures and densities.
REU	Initial concentrations of CPR, iron, and MgO
RELPERMS	Relative permeability parameters.
RKSEOS	RKS EOS parameters.
RPGM	Reaction path gas generation model parameters.
RPGMCONC	Reaction path gas generation model - gas concentrations.
RPGMGR	Reaction path gas generation model- gas generation rates.
RPGMR	Reaction path gas generation model parameters.
RSIZE	Grid description variables.
RSTBR	Parameters for the resetting of borehole pressure, saturation, and concentration.
RXN	Average Stoichiometry Gas Generation model parameters.
SATN	Saturation arrays and corrosion product concentrations.
SIZES	Array sizing parameters.
SMPRM	Parameters for the smooth change in permeability.
SUBS	Reaction path model parameters.
SWITCH	Variable switching maps.

Common Block	Description
T	Various time related variables.
TERMS	Harmonically averaged transmissibility arrays.
TSOLVER	Coefficient matrix, C for gas component transport.
UNITCNV	Unit conversion factors.
UNITCNVc	Units.
UPSTREAM	Arrays used for upstream weighting direction.
VEL	Inter-block fluxes and velocities.
VELAVE	Time averaged inter-block fluxes and velocities.
WELLS	Well parameters.
WELLSc	Well type.

The flow of the common block data through BRAGFLO is represented in Table 3 - **Error! Reference source not found.** All routines that include common block are listed in the first column. All common blocks (with names starting with name ranges identified table caption) are listed in the first row. A check mark indicates that the common block is used in the corresponding routine. Looking down a column one can determine where a common block is used. Looking along a row (over all four tables), one can determine which common blocks are used by a given routine.

Table 3. Common Block Usage (A thru F)

Routine / Block Names	(Unnamed Common)	BAND	BASE	BF	BRATE	BRINETERMS	CCONVR	CLOSURE	CMULTG	CONC	CONPRE	CPRINT	CPUNTC	CRESTART	CRESTARTc	CUM	DIR MULTIPLIERS	FLAWS	FRACTURE	FUN
ADJUSTICS						✓														
ALI2VAX																				
ALR2VAX																				
BANDIT																				
BANDSTORE		✓																		
BIOFES																				
BIOHUM																				
BIOMGO																				
BIOSAT																				
BL INTERP																				
BRAGFLO												✓		✓	✓				✓	
BUBBLE						✓														
CLOSCHECK								✓												
CONSOL								✓									✓			
CONSOLI								✓												
CORHUM																				
CORMGO																				
CORSAT																				
CUMULGEN						✓		✓			✓					✓		✓		✓
DASUM																				
DATNTIM																				
DAXPY																				
DDOT																				
DECAY																				
DECBR																				
DELTAMAP																				
DENGZ																				
DENGZINT																				

Routine / Block Names	(Unnamed Common)	BAND	BASE	BF	BRATE	BRINETERMS	CCONVR	CLOSURE	CMULTG	CONC	CONPRE	CPRINT	CPUNTC	CRESTART	CRESTARTc	CUM	DIR MULTIPLIERS	FLAWS	FRACTURE	FUN
DENO						✓														
DENSAT1																				
DEPINVERT																				
DEPINVERT1																				
DGBCO																				
DGBFA																				
DGBSL																				
DISKR							✓	✓	✓	✓		✓	✓	✓	✓	✓			✓	
DISKW							✓	✓	✓	✓		✓	✓	✓	✓	✓				
DISOLVGAS						✓				✓										
DSCAL																				
FMAX																				
FMIN																				
FUNCT										✓								✓		✓
FUNCT7										✓								✓		✓
GASC																				
GEN COEF		✓																✓		
GEOMETRY																				✓
GETJAC								✓										✓		
GETJACINDX																				
GETOLD								✓		✓										
GETWELLS										✓								✓		
GETWELLS1										✓								✓		
HYDROCONV																				
IDAMAX																				
INITAL																				
KLINKBERG																				
LABELS																				
LOCATE																				

Routine / Block Names	(Unnamed Common)	BAND	BASE	BF	BRATE	BRINETERMS	CCONVR	CLOSURE	CMULTG	CONC	CONPRE	CPRINT	CPUNTC	CRESTART	CRESTARTc	CUM	DIR MULTIPLIERS	FLAWS	FRACTURE	FUN
MAPDEP																				
MASSBALNC											✓									
MATERIALS						✓	✓		✓											
MEAS CONV																				
MULTIGRID																				
PERMPHI																			✓	
PERMS																			✓	
PORSOLID																				
POR SURF								✓												
PRINTASC				✓						✓		✓				✓		✓		
PRINTBIN				✓						✓						✓		✓		
PRINTCONTROL														✓	✓					
PRINTGRID																				
PRINTHIV				✓						✓		✓				✓		✓		
PRINTLABS																				
PROPS						✓	✓		✓										✓	✓
PROPS1						✓	✓		✓										✓	✓
PRORDER																				
PTHRESH																				
QABGNL																				
QAENDL																				
RADIOLYSIS																				
RADTRANS																				
RADUPDAT																				
RAPHSON								✓			✓	✓							✓	
READCLOSURE								✓												
READCNTRL									✓										✓	
READFILES														✓	✓					
READFLUID						✓														

Routine / Block Names	(Unnamed Common)	BAND	BASE	BF	BRATE	BRINETERMS	CCONVR	CLOSURE	CMULTG	CONC	CONPRE	CPRINT	CPUNTC	CRESTART	CRESTARTc	CUM	DIR MULTIPLIERS	FLAWS	FRACTURE	FUN
READICS																				
READMAT								✓											✓	
READMESH																				
READPRTYPE														✓	✓					
READRAD																				
READRXGAST																				
READRXN						✓														
READSTARTUP														✓	✓					
READWELL																				
READ DIRICHLET												✓								
REFCONDS						✓				✓						✓				
RELPERM													✓							
RESET						✓		✓		✓										
RESETMID						✓		✓		✓										
RESIDUAL											✓									
ROCKCOMP																			✓	
RPGM INTRFC	✓		✓	✓	✓															
RXGAST		✓																		
SET DELTA DIRICHLET												✓								
SET MAIN DIRICHLET												✓					✓			
SET RHS DIRICHLET												✓					✓			
SMOOTHERM																				
SOLBR																				
SOLUTION							✓		✓			✓	✓							
SOLVER						✓		✓	✓	✓		✓							✓	
SOR																				
STARTUP							✓	✓				✓	✓	✓	✓	✓		✓		
STOREINT																				
SUMMARY									✓			✓								

Routine / Block Names	(Unnamed Common)	BAND	BASE	BF	BRATE	BRINETERMS	CCONVR	CLOSURE	CMULTG	CONC	CONPRE	CPRINT	CPUNTC	CRESTART	CRESTARTc	CUM	DIR MULTIPLIERS	FLOWS	FRACTURE	FUN
Timestep								✓												
TRI INTERP																				
TSAVG																				
TTIME																				
UNITS CONV																				
WHERE																				
WHICH																				
WRITBIN																				
WRITEARRAY																				
WRITHIV																				

Table 4. Common Block Usage (G thru P)

Routine / Block Names	GASINTERMS	GASTERMS	GEOTRANS	ICRESET	INITL	IO	IOc	JACOBIAN	LU	MACHINE	MASSBAL	MATTERMS	MODELTYPE	MONITOR	MXDIM	NEWTON	NUCLIDE	OLD	PERMPARM	PHYSCON
ADJUSTICS				✓	✓	✓	✓					✓								
ALI2VAX																				
ALR2VAX																				
BANDIT																				
BANDSTORE															✓					
BIOFES																				
BIOHUM																				
BIOMGO																				
BIOSAT																				
BL_INTERP																				
BRAGFLO				✓		✓	✓			✓		✓					✓			
BUBBLE																				
CLOSCHECK					✓	✓	✓					✓								
CONSOL		✓		✓								✓							✓	
CONSOL1		✓		✓								✓							✓	
CORHUM																				
CORMGO																				
CORSAT																				
CUMULGEN			✓					✓				✓								
DASUM																				
DATNTIM										✓										
DAXPY																				
DDOT																				
DECAY																				✓
DECBR								✓	✓							✓				
DELTAMAP								✓												
DENGZ		✓																		✓
DENGZINT	✓																			

Routine / Block Names	GASINTERMS	GASTERMS	GEOTRANS	ICRESET	INITL	IO	IOc	JACOBIAN	LU	MACHINE	MASSBAL	MATTERMS	MODELTYPE	MONITOR	MXTDIM	NEWTON	NUCLIDE	OLD	PERMPARM	PHYSCON
DENO																				
DENSATI	✓	✓																		
DEPINVERT								✓												
DEPINVERT1								✓												
DGBCO																				
DGBFA																				
DGBSL																				
DISKR	✓	✓		✓		✓	✓					✓					✓			
DISKW				✓		✓	✓					✓					✓			
DISOLVGAS		✓																		
DSCAL																				
FMAX																				
FMIN																				
FUNCT													✓							
FUNCT7													✓							
GASC																				
GEN COEF																		✓		
GEOMETRY			✓	✓								✓	✓							
GETJAC								✓												
GETJACINDX								✓								✓				
GETOLD																		✓		
GETWELLS			✓															✓		
GETWELLS1			✓															✓		
HYDROCONV																				
IDAMAX																				
INITAL						✓	✓													
KLINKBERG																				
LABELS						✓	✓													
LOCATE																				

Routine / Block Names	GASINTERMS	GASTERMS	GEOTRANS	ICRESET	INITL	IO	IOc	JACOBIAN	LU	MACHINE	MASSBAL	MATTERMS	MODELTYPE	MONITOR	MXDIM	NEWTON	NUCLIDE	OLD	PERMPARM	PHYSCON
MAPDEP								✓												
MASSBALNC								✓			✓									
MATERIALS				✓		✓	✓					✓					✓			
MEAS CONV						✓	✓	✓	✓							✓				✓
MULTIGRID																				
PERMPHI												✓								
PERMS					✓							✓								
PORSOLID																				
POR SURF						✓	✓													
PRINTASC						✓	✓				✓						✓			
PRINTBIN						✓	✓			✓	✓						✓			
PRINTCONTROL				✓		✓	✓													
PRINTGRID						✓	✓													
PRINTHIV						✓	✓			✓	✓						✓			
PRINTLABS						✓	✓			✓										
PROPS	✓	✓	✓	✓		✓	✓					✓	✓			✓	✓		✓	✓
PROPS1	✓	✓	✓	✓		✓	✓					✓				✓	✓		✓	✓
PRORDER						✓	✓													
PTHRESH						✓	✓					✓								
QABGNL										✓										
QAENDL																				
RADIOLYSIS																				
RADTRANS			✓	✓		✓	✓					✓	✓				✓			✓
RADUPDAT				✓													✓			
RAPHSON						✓	✓	✓	✓			✓				✓				✓
READCLOSURE						✓	✓					✓								
READCNTRL						✓	✓	✓								✓				
READFILES						✓	✓			✓										
READFLUID	✓	✓				✓	✓													✓

Routine / Block Names	GASINTERMS	GASTERMS	GEOTRANS	ICRESET	INITL	IO	IOc	JACOBIAN	LU	MACHINE	MASSBAL	MATTERMS	MODELTYPE	MONITOR	MXTDIM	NEWTON	NUCLIDE	OLD	PERMPARM	PHYSCON
READICS					✓	✓	✓													
READMAT				✓		✓	✓					✓							✓	✓
READMESH						✓	✓						✓							✓
READPRTYPE						✓	✓			✓				✓						
READRAD				✓		✓	✓					✓					✓			✓
READRXGAST						✓	✓													
READRXN		✓		✓		✓	✓												✓	
READSTARTUP						✓	✓			✓			✓							
READWELL						✓	✓													
READ DIRICHLET						✓	✓													
REFCONDS	✓	✓				✓	✓													
RELPERM																				✓
RESET				✓	✓							✓								
RESETMID												✓								
RESIDUAL								✓												
ROCKCOMP												✓						✓		✓
RPGM INTRFC																				
RXGAST															✓					
SET DELTA DIRICHLET					✓															
SET MAIN DIRICHLET								✓												
SET RHS DIRICHLET								✓	✓											
SMOOTHPERM												✓								
SOLBR								✓	✓								✓			
SOLUTION						✓	✓	✓	✓								✓			
SOLVER				✓		✓	✓	✓				✓				✓		✓		
SOR																				
STARTUP		✓		✓		✓	✓	✓		✓		✓				✓	✓			✓
STOREINT																				
SUMMARY				✓		✓	✓				✓	✓		✓					✓	

Routine / Block Names	GASINTERMS	GASTERMS	GEOTRANS	ICRESET	INITL	IO	IOc	JACOBIAN	LU	MACHINE	MASSBAL	MATTERMS	MODELTYPE	MONITOR	MXTDIM	NEWTON	NUCLIDE	OLD	PERMPARM	PHYSCON
TIMESTEP				✓							✓	✓						✓		
TRI_INTERP																				
TSAVG																				
TTIME																				
UNITSCONV																				
WHERE																				
WHICH																				
WRITBIN						✓	✓			✓										
WRITEARRAY						✓	✓						✓							
WRITHIV																				

Table 5. Common Block Usage (P thru R)

Routine / Block Names	PRNTC	PRNTI	PRNTR	PROGRAM	PROP	PT	RADACT	RADCHAIN	RATES	REF	RELPERMS	REU	RKSEOS	RPGM	RPGMCONC	RPGMGR	RPGMR	RSIZE	RSTBR	RXXN
ADJUSTICS						✓								✓			✓	✓		✓
ALI2VAX																				
ALR2VAX																				
BANDIT																				
BANDSTORE																				
BIOFES																				
BIOHUM																				
BIOMGO																				
BIOSAT																				
BL_INTERP																				
BRAGFLO	✓	✓	✓	✓														✓	✓	
BUBBLE																				
CLOSCHECK					✓	✓												✓		
CONSOL					✓	✓												✓		✓
CONSOL1					✓	✓														✓
CORHUM																				
CORMGO																				
CORSAT																				
CUMULGEN				✓	✓	✓			✓									✓		✓
DASUM																				
DATNTIM				✓																
DAXPY																				
DDOT																				
DECAY								✓												
DECBR																				
DELTAMAP																				
DENGZ													✓							
DENGZINT																				

Routine / Block Names	PRNTC	PRNTI	PRNTR	PROGRAM	PROP	PT	RADACT	RADCHAIN	RATES	REF	RELPERMS	REU	RKSEOS	RPGM	RPGMCONC	RPGMGR	RPGMR	RSIZE	RSTBR	RXN
DENO																				
DENSAT1					✓	✓				✓										
DEPINVERT						✓														
DEPINVERT1						✓														
DGBCO																				
DGBFA																				
DGBSL																				
DISKR				✓	✓	✓				✓	✓			✓				✓		✓
DISKW				✓	✓	✓					✓			✓				✓		✓
DISOLVGAS					✓	✓							✓					✓		✓
DSCAL																				
FMAX																				
FMIN																				
FUNCT					✓	✓												✓		✓
FUNCT7					✓	✓												✓		✓
GASC																				
GEN COEF					✓									✓		✓		✓		
GEOMETRY																		✓		
GETJAC					✓													✓		
GETJACINDX																				
GETOLD					✓	✓								✓				✓		
GETWELLS					✓	✓												✓		
GETWELLS1					✓	✓												✓		
HYDROCONV																				
IDAMAX																				
INITAL																				
KLINKBERG																				
LABELS	✓	✓	✓					✓												
LOCATE																				

Routine / Block Names	PRNTC	PRNTI	PRNTR	PROGRAM	PROP	PT	RADACT	RADCHAIN	RATES	REF	RELPERMS	REU	RKSEOS	RPGM	RPGMCONC	RPGMGR	RPGMR	RSIZE	RSTBR	RXN
MAPDEP						✓														
MASSBALNC																		✓		
MATERIALS					✓	✓					✓							✓		
MEAS CONV																				
MULTIGRID																				
PERMPHI																				
PERMS					✓	✓														
PORSOLID												✓								✓
POR_SURF																				
PRINTASC	✓	✓	✓		✓	✓								✓	✓	✓		✓		✓
PRINTBIN	✓	✓	✓		✓	✓								✓	✓	✓		✓		✓
PRINTCONTROL	✓	✓	✓																	
PRINTGRID																			✓	
PRINTHIV	✓	✓	✓		✓	✓								✓	✓	✓		✓		✓
PRINTLABS	✓	✓	✓																	
PROPS					✓	✓	✓		✓	✓	✓	✓	✓	✓	✓	✓	✓	✓		✓
PROPS1					✓	✓	✓		✓	✓	✓	✓	✓	✓	✓	✓	✓	✓		✓
PRORDER																				
PTHRESH											✓									
QABGNL				✓																
QAENDL				✓																
RADIOLYSIS								✓												
RADTRANS					✓			✓										✓		
RADUPDAT								✓												
RAPHSON						✓					✓			✓			✓	✓		
READCLOSURE																				
READCNTRL														✓			✓			
READFILES				✓																
READFLUID					✓				✓			✓								✓

Routine / Block Names	PRNTC	PRNTI	PRNTR	PROGRAM	PROP	PT	RADACT	RADCHAIN	RATES	REF	RELPERMS	REU	RKSEOS	RPGM	RPGMCONC	RPGMGR	RPGMR	RSIZE	RSTBR	RXN	
READICS																					
READMAT					✓						✓									✓	
READMESH																			✓		
READPRTYPE	✓	✓	✓																✓		
READRAD								✓											✓		
READRXGAST														✓							
READRXN																	✓				✓
READSTARTUP																			✓		
READWELL																					
READ_DIRICHLET																					
REFCONDS					✓	✓				✓									✓		
RELPERM																					
RESET					✓	✓					✓										
RESETMID					✓	✓					✓	✓								✓	
RESIDUAL																					
ROCKCOMP																					
RPGM_INTRFC								✓	✓					✓		✓	✓				
RXGAST					✓									✓	✓	✓	✓	✓			
SET_DELTA_DIRICHLET																					
SET_MAIN_DIRICHLET																					
SET_RHS_DIRICHLET																					
SMOOTHERM					✓																
SOLBR																					
SOLUTION																					
SOLVER	✓	✓	✓		✓	✓					✓								✓		✓
SOR																					
STARTUP	✓	✓	✓			✓		✓			✓		✓				✓	✓			✓
STOREINT												✓									
SUMMARY					✓	✓					✓								✓		✓

Routine / Block Names	PRNTC	PRNTI	PRNTR	PROGRAM	PROP	PT	RADACT	RADCHAIN	RATES	REF	RELPERMS	REU	RKSEOS	RPGM	RPGMCONC	RPGMGR	RPGMR	RSIZE	RSTBR	RXN
TIMESTEP	✓	✓	✓		✓	✓												✓		
TRI INTERP																				
TSAVG																				
TTIME																				
UNITS CONV																				
WHERE								✓												
WHICH								✓												
WRITBIN																				
WRITEARRAY																				
WRITHIV	✓	✓	✓																	

Table 6. Common Block Usage (R thru Z)

Routine / Block Names	SATN	SIZES	SMPRM	SUBS	SWITCH	T	TERMS	TSOLVER	UNITCNV	UNITCNVc	UPSTREAM	VEL	VELAVE	WELLS	WELLSc
ADJUSTICS	✓	✓			✓										
ALI2VAX															
ALR2VAX															
BANDIT															
BANDSTORE		✓													
BIOFES															
BIOHUM															
BIOMGO															
BIOSAT															
BL_INTERP															
BRAGFLO		✓			✓									✓	✓
BUBBLE															
CLOSCHECK	✓	✓			✓										
CONSOL	✓	✓			✓			✓	✓						
CONSOL1	✓	✓			✓			✓	✓						
CORHUM															
CORMGO															
CORSAT															
CUMULGEN	✓	✓				✓						✓	✓	✓	✓
DASUM															
DATNTIM															
DAXPY															
DDOT															
DECAY															
DECBR		✓													
DELTAMAP		✓			✓										
DENGZ															
DENGZINT															

Routine / Block Names	SATN	SIZES	SMPRM	SUBS	SWITCH	T	TERMS	TSOLVER	UNITCNV	UNITCNVc	UPSTREAM	VEL	VELAVE	WELLS	WELLSc
DENO															
DENSAT1	✓														
DEPINVERT	✓	✓			✓										
DEPINVERT1	✓				✓										
DGBCO															
DGBFA															
DGBSL															
DISKR	✓	✓			✓	✓	✓							✓	✓
DISKW	✓	✓			✓	✓	✓							✓	✓
DISOLVGAS	✓	✓			✓		✓								
DSCAL															
FMAX															
FMIN															
FUNCT		✓					✓								
FUNCT7		✓					✓								
GASC															
GEN COEF	✓	✓						✓				✓			
GEOMETRY		✓													
GETJAC		✓					✓								
GETJACINDX		✓													
GETOLD	✓	✓			✓		✓								
GETWELLS		✓												✓	✓
GETWELLS1		✓												✓	✓
HYDROCONV															
IDAMAX															
INITAL		✓													
KLINKBERG															
LABELS		✓							✓	✓					
LOCATE															

Routine / Block Names	SATN	SIZES	SMPRM	SUBS	SWITCH	T	TERMS	TSOLVER	UNITCNV	UNITCNVc	UPSTREAM	VEL	VELAVE	WELLS	WELLSc
MAPDEP	✓	✓			✓										
MASSBALNC	✓	✓					✓								
MATERIALS	✓	✓				✓	✓								
MEAS CONV	✓	✓			✓		✓								
MULTIGRID															
PERMPHI															
PERMS		✓													
PORSOLID	✓	✓													
POR SURF															
PRINTASC	✓	✓				✓			✓	✓		✓	✓		
PRINTBIN	✓	✓				✓			✓	✓		✓	✓		
PRINTCONTROL						✓									
PRINTGRID		✓							✓	✓					
PRINTHIV	✓	✓				✓			✓	✓		✓			
PRINTLABS		✓													
PROPS	✓	✓				✓	✓				✓	✓			
PROPS1	✓	✓				✓	✓				✓	✓			
PRORDER															
PTHRESH		✓													
QABGNL															
QAENDL															
RADIOLYSIS															
RADTRANS	✓	✓				✓						✓			
RADUPDAT		✓				✓									
RAPHSON	✓	✓			✓	✓	✓								
READCLOSURE		✓							✓	✓					
READCNTRL					✓	✓			✓	✓					
READFILES															
READFLUID		✓			✓				✓	✓					

Routine / Block Names	SATN	SIZES	SMPRM	SUBS	SWITCH	T	TERMS	TSOLVER	UNITCNV	UNITCNVc	UPSTREAM	VEL	VELAVE	WELLS	WELLSc
READICS	✓	✓							✓	✓					
READMAT		✓	✓			✓			✓	✓					
READMESH		✓							✓	✓					
READPRTYPE						✓			✓	✓					
READRAD		✓							✓	✓					
READRXGAST		✓													
READRXN									✓	✓					
READSTARTUP		✓				✓			✓	✓					
READWELL		✓				✓			✓	✓				✓	✓
READ DIRICHLET		✓													
REFCONDS	✓	✓							✓	✓					
RELPERM															
RESET	✓	✓			✓	✓	✓								
RESETMID	✓	✓					✓								
RESIDUAL	✓	✓					✓								
ROCKCOMP															
RPGM INTRFC				✓					✓	✓					
RXGAST	✓	✓						✓							
SET DELTA DIRICHLET		✓													
SET MAIN DIRICHLET															
SET RHS DIRICHLET		✓													
SMOOTHPERM		✓	✓												
SOLBR		✓													
SOLUTION		✓				✓									
SOLVER	✓	✓			✓	✓			✓	✓					
SOR															
STARTUP					✓	✓						✓	✓	✓	✓
STOREINT	✓	✓													
SUMMARY	✓	✓				✓			✓	✓		✓	✓		

Routine / Block Names	SATN	SIZES	SMPRM	SUBS	SWITCH	T	TERMS	TSOLVER	UNITCNV	UNITCNVc	UPSTREAM	VEL	VELAVE	WELLS	WELLSc
TIMESTEP	✓	✓			✓	✓								✓	✓
TRI INTERP															
TSAVG		✓										✓			
TTIME															
UNITSCONV								✓	✓						
WHERE															
WHICH															
WRITBIN		✓													
WRITEARRAY		✓													
WRITHIV															

5.4.2 Subroutine Arguments

The second method of data flow through BRAGFLO is by passing the required data as arguments in the routines call list. For each routine that uses arguments, the BRAGFLO source code contains a comment section that describes all variables passed as arguments. Since this design document is an 'as built' the reader is referred to the source code for a complete description of the argument lists. Shown below is an example pseudo code fragment for the subroutine ADJUSTICS that uses arguments. The code fragment contains the subroutine name, the argument list and descriptions are provided in a comment section for the routine. The following subroutine declaration and argument list comments were extracted from the BRAGFLO source code and is representative of BRAGFLO routines using an argument list.

```
      SUBROUTINE ADJUSTICS (ICWASTE, POWASTEIC, SOWASTEIC)
C
C      Input Arguments:
C      -----
C      ICWASTE   = Flag to indicate whether to reset input initial
C                  conditions in waste to uniform IC's POWASTEIC and
C                  SOWASTEIC, as when initializing waste as an empty
C                  cavity to simulate operational phase.
C      POWASTEIC = Array of initial waste brine pressure, used to
C                  simulate empty excavation during operational phase.
C      SOWASTEIC = Array of initial waste brine saturation, used to
C                  simulate empty excavation during operational phase.
C
C-----
```

6.0 DATA STRUCTURES

Refer to the *BRAGFLO User's Manual* (Day 2019a), Section 7.0, for a detailed description of parameter specifications, input, and output file descriptions.

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7.0 CAPABILITIES AND LIMITATIONS OF THE SOFTWARE FOR THE WIPP APPLICATION

Refer to the *BRAGFLO User's Manual* (Day 2019a), Section 6.0, for a detailed listing of capabilities and limitations of the software.

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8.0 REFERENCES

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- Camphouse, R.C. 2012. "*POSTBRAG, Version 4.02*" Carlsbad, NM: Sandia National Laboratories. ERMS 557827.
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