Title 40 CFR Part 191
Compliance Certification Application
for the
Waste Isolation Pilot Plant

Appendix CODELINK

United States Department of Energy
Waste Isolation Pilot Plant

Carlsbad Area Office
Carlsbad, New Mexico

The WIPP 1996 Performance Assessment Codes and Their Linkages

CONTENTS

FIGURES

TABLE

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ACRONYMS

CCDF	*complementary cumulative distribution function*
LHS	Latin hypercube sampling
NON-PA SES	nonperformance assessment scientific and engineering software
PA NON-SES	performance assessment nonscientific and engineering software
PA SES	performance assessment scientific and engineering software
QA	quality assurance
SWCF	Sandia WIPP Central Files
t-field	transmissivity field
WIPP	Waste Isolation Pilot Plant

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APPENDIX CODELINK

Presented are overviews of and background for (1) the principal codes used in the analysis following Latin hypercube sampling, and (2) the principal code-linkage sequences that support the Waste Isolation Pilot Plant (WIPP) performance assessment in support of this application. Operational details and supporting references are not included nor are discussions of codes that provide input to the performance assessment. However, detailed user's manuals, one for each compliance software code, have been compiled and archived as part of the quality assurance (QA) procedure for this application. Functional descriptions of each performance assessment scientific and engineering software (PA SES) code are included as appendices. Attachment 1 to this appendix lists the compliance software and the Sandia WIPP Central Files (SWCF) records package identifiers for each code. Codes are categorized as PA SES, PA NON-SES (performance assessment nonscientific and engineering software), and NON-PA SES (nonperformance assessment scientific and engineering software) (see also Table 5-1 in Chapter 5.0 of this application).

CODELINK.1 Introduction

As discussed in Chapter 6.0 of this application, long-term performance assessments of the WIPP disposal system are carried out by applying, in sequence, a number of computer codes designed to model processes that may significantly affect transport of radionuclides from the repository via various routes through the surrounding geological units to the accessible environment. As code development has been an on-going process in WIPP performance assessment research, the codes as well as the code sequences applied to WIPP performance assessments have evolved in time. This discussion focuses on the codes and code sequences that support this compliance application. Table CODELINK-1 lists codes used in the Monte Carlo analysis for this performance assessment, their function and type, and their category with regard to supporting this application, that is, PA SES, PA NON-SES, or NON-PA SES.

Sampling methods used in the Monte Carlo analysis for the performance assessment are described in Section CODELINK.2 below. In Section CODELINK.3, the PA NON-SES utility codes that prepare the way for and support the various PA SES codes are discussed individually. The seven PA SES codes and their functions are introduced in Sections CODELINK.4 through CODELINK.7. The PA SES codes themselves, the repository, and the principal features of the repository are depicted in Figure CODELINK-1. The overall code-linkage sequence for the performance assessment is shown in Figure CODELINK-2. It serves as a guide to and connection diagram for the individual code-linkage sequences, which are shown in Figures CODELINK-3 through CODELINK-9.

CODELINK.2 Sampling Uncertain Parameters—LHS

Sampling is carried out by a code called LHS, which stands for Latin hypercube sampling. Application of LHS includes a preprocessor code PRELHS and a postprocessor code

1 **Table CODELINK-1. Codes Used in the Monte Carlo Analysis**

Code Name	Function	Category of Code[a]
ALGEBRA	Performs algebraic and other manipulations, for units conversions, calculation of derived parameters, etc.	PA NON-SES
BRAGFLO	Computes brine and gas flows throughout the controlled area.	PA SES
BRAGFLO_DBR	Calculates brine volume removed from repository due to drilling intrusion.	PA SES
CCDFGF	Combines consequence results from PA SES codes for individual events to estimate releases for scenarios, and constructs CCDFs.	PA SES
CUTTINGS_S	Calculates direct releases of radionuclides due to cuttings, cavings, and spallings.	PA SES
GENMESH	Establishes the computational grid for a given model.	PA NON-SES
GRASP-INV	Generates calibrated transmissivity fields for use in SECOFL2D.	NON-PA SES
ICSET	Establishes initial conditions for a given model.	PA NON-SES
LHS	Performs Latin-hypercube sampling of all uncertain parameters.	PA NON-SES
MATSET	Assigns material names, properties, and attribute values to specific blocks of a grid defined by GENMESH.	PA NON-SES
NUTS	Calculates types and amounts of radionuclides transported in BRAGFLO-generated flow fields.	PA SES
PANEL	Calculates radionuclide concentrations in brine as volumes calculated by BRAGFLO.	PA SES
POSTBRAG	Postprocessor for BRAGFLO; converts output to CDB format.	PA NON-SES

Table CODELINK-1. Codes Used in the Monte Carlo Analysis (continued)

Code Name	Function	Category of Code[a]
POSTLHS	Postprocessor to LHS; creates sampled vectors from LHS output for input to modeling codes.	PA NON-SES
POSTSECOFL2D	Postprocessor for SECOFL2D; converts output to CDB format.	PA NON-SES
POSTSECOTP2D	Postprocessor for SECOTP2D; converts output to CDB format.	PA NON-SES
PREBRAG	Preprocessor for BRAGFLO; constructs necessary input file for BRAGFLO.	PA NON-SES
PRELHS	Preprocessor for LHS; interprets user-specified input controls for operation of LHS.	PA NON-SES
PRESECOFL2D	Preprocessor for SECOFL2D; constructs necessary input files for SECOFL2D.	PA NON-SES
PRESECOTP2D	Preprocessor for SECOTP2D; constructs necessary input files for SECOTP2D.	PA NON-SES
RELATE	Interpolates data from one grid to another; combines two sets of data defined on same grid.	PA NON-SES
SANTOS	Used to calculate effective repository porosity for BRAGFLO, due to creep closure of halite and gas pressure.	NON-PA SES
SECOFL2D	Calculates groundwater flow in Culebra.	PA SES
SECOTP2D	Calculates radionuclide transport through Culebra to accessible environment.	PA SES
SUMMARIZE	Used for extraction of data across multiple vectors.	PA NON-SES

[a] Codes are grouped into three categories: PA SES, PA NON-SES, and NON-PA SES. PA SES and NON-PA SES codes model physical or chemical processes. PA NON-SES codes include statistical codes, which perform sampling or provide some type of statistical analysis, and utility codes, which permit user control of the other codes or provide an interface between codes. PA SES and PA NON-SES codes listed are run repeatedly in a performance assessment calculation, using the Latin hypercube sample values drawn from distribution functions for uncertain parameters. NON-PA SES codes—for example, SANTOS and GRASP-INV—are run outside of a given performance assessment calculation for a set of Latin hypercube samples as subsidiary calculations to provide input.

POSTLHS. LHS requires that each uncertain parameter be specified in terms of a probability distribution.

LHS is a stratified Monte Carlo sampling code designed to sample the entire range of variability of all uncertain WIPP parameters. For each of *m* uncertain parameters, LHS divides the likelihood-of-occurrence axis (of the cumulative distribution) into *n* equal-length segments, where *n* is the sample size, and then draws one parameter value randomly from each segment. It then combines, by random pairing, the results to form *n* input vectors, each vector containing a unique ordered set of all *m* of the required uncertain input parameters.

Thus, the outcome of LHS's sampling may be represented as an *m*-row, *n*-column matrix in which every value in a given row is different from every other value in that row. For the analysis described in Chapter 6.0 of this application, the *m*-row, *n*-column table with m=57 and n=100 is presented in Appendix IRES (Tables IRES-2, IRES-3, and IRES-4) for each of the three independent replicates. Once the matrix of actual values has been formed, a second matrix with the identical parameter ordering but listing the ranks of the sampled values is also created and reported. The code user may specify correlations *a priori*, and LHS will then combine the selected parameters in such a way as to assure that the sampled values remain correlated at the correct level.

When a performance assessment code requires sampled input parameters, it exercises POSTLHS (discussed in Section CODELINK.3.3, below). POSTLHS generates a set of *n* output files that are identical except for the values of sampled parameters associated with the code requiring them. LHS results for this performance assessment are presented in Appendix IRES (Tables IRES-2, IRES-3, and IRES-4).

CODELINK.3 PA NON-SES Utility Codes

In this section, only PA NON-SES utility codes are discussed, including all the ones that will be encountered in a performance assessment. They are discussed in roughly the order in which they are used in an actual run sequence; however, no actual performance assessment code sequences will be discussed in this section. Each PA SES code requires its own *individual* utility-code sequence before it can be exercised. Performance assessment code sequences for PA SES codes are shown in Figures CODELINK-3 through CODELINK-9, and the individual PA SES codes themselves are discussed in Sections CODELINK.4 through CODELINK.7.

CODELINK.3.1 GENMESH and GENNET

GENMESH and GENNET are mesh-generating codes that (1) establish the computational-grid geometry of the physical domain being modeled, and (2) create the output file (known as a CDB file) that will collect sequential binary-format results and trace the path of the computational sequence throughout its entire history. Thus, in CUTTINGS_S, GENMESH grids the cylindrical borehole from the bottom of the borehole to ground level with a single grid element that is one unit wide, the width being based on the drill-bit diameter. In

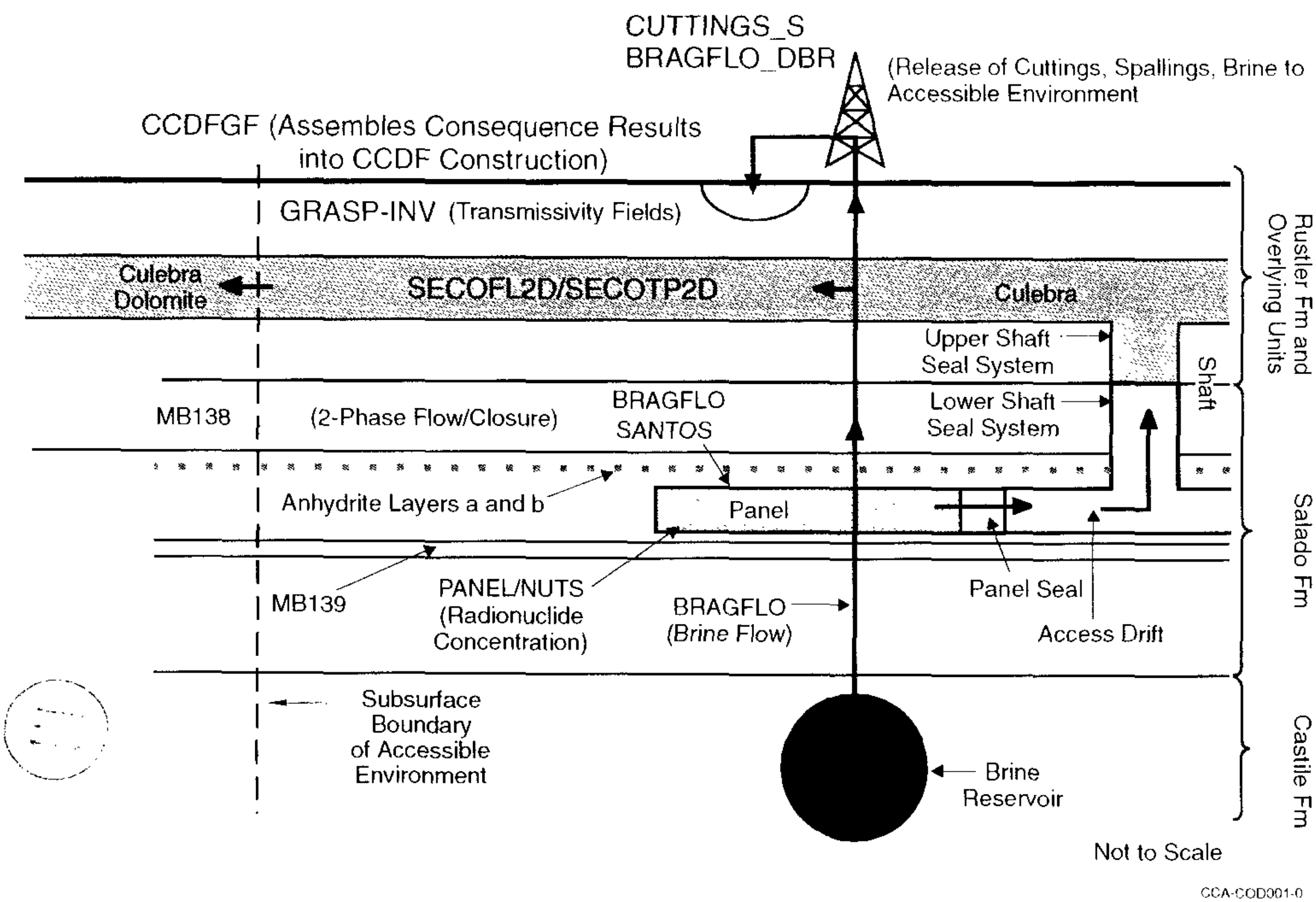

Figure CODELINK-1. Diagrammatic Representation of a Vertical Section Through the Repository, Listing the PA SES and Two NON-PA SES Codes Used in the Monte Carlo Analysis

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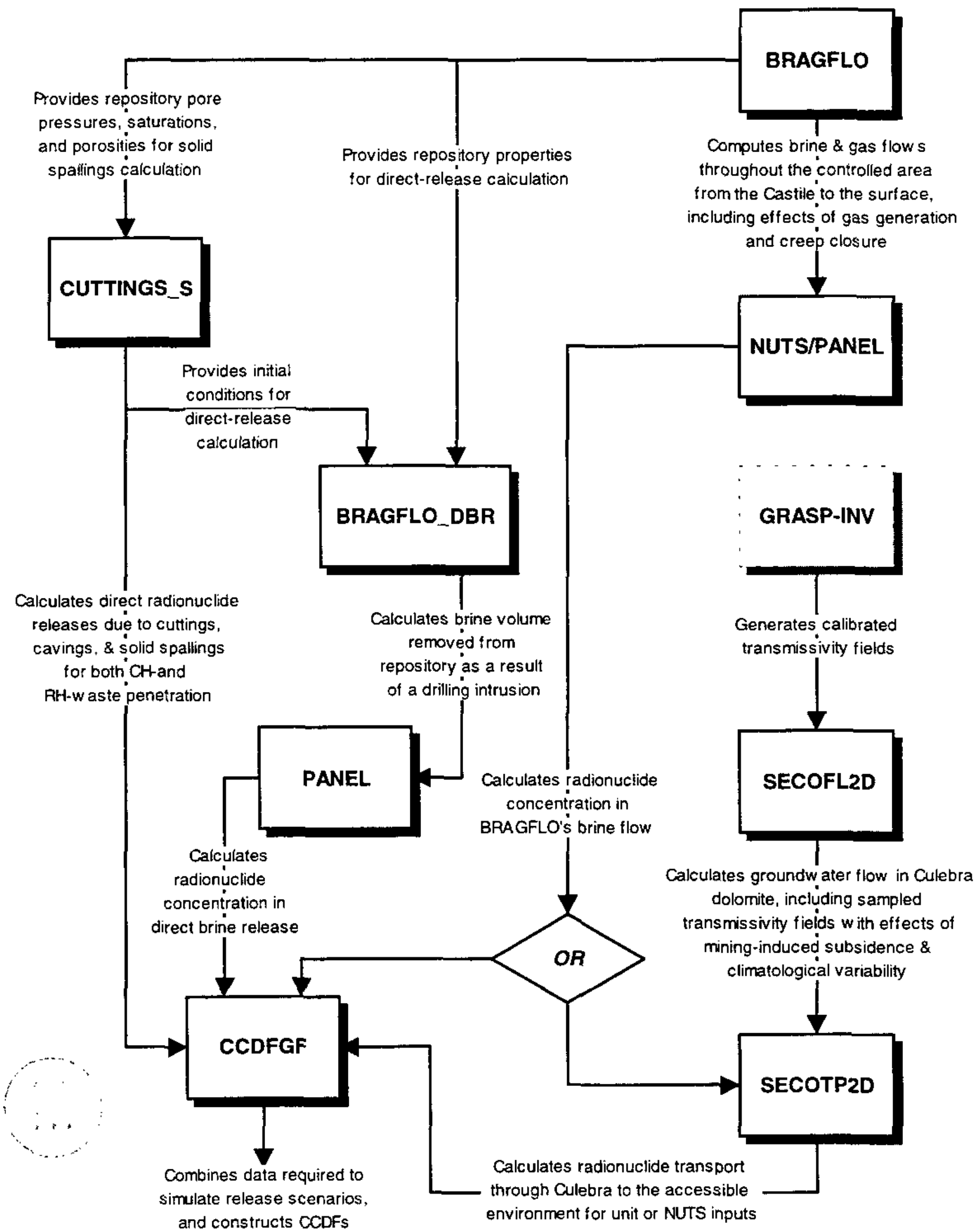

Note: PA SES codes are rectangular. The NON-PA SES code is dashed. See Figures CODELINK-3 through CODELINK-9 for more detailed representations of the individual PA SES-code sequences.

5 **Figure CODELINK-2. Overview of the Performance Assessment Code Sequence**

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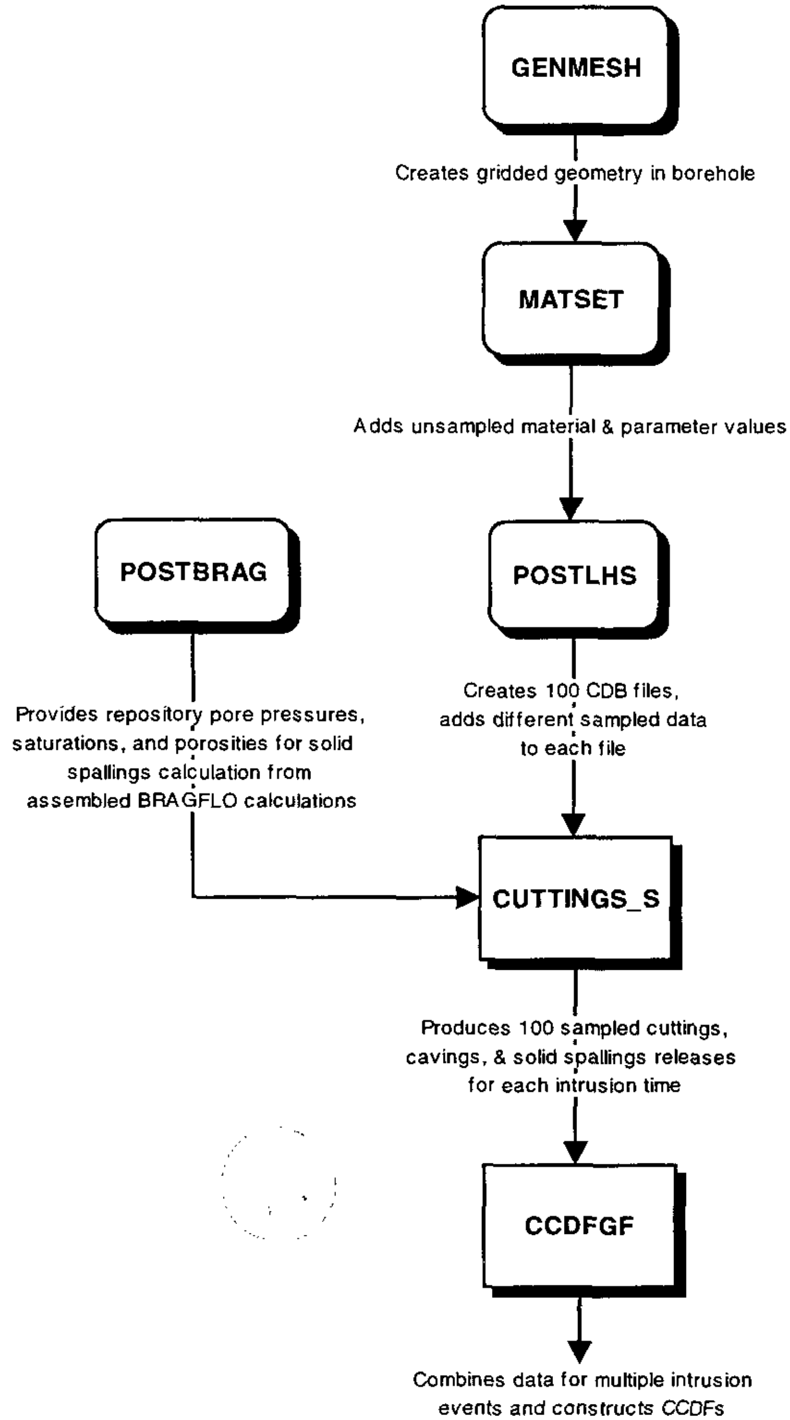

Note: PA SES codes are rectangular; PA NON-SES codes are rounded.

Figure CODELINK-3. The Code Sequence for CUTTINGS_S in the Performance Assessment for One Replicate with 57 Sampled Parameters and Sample Size Equal to 100

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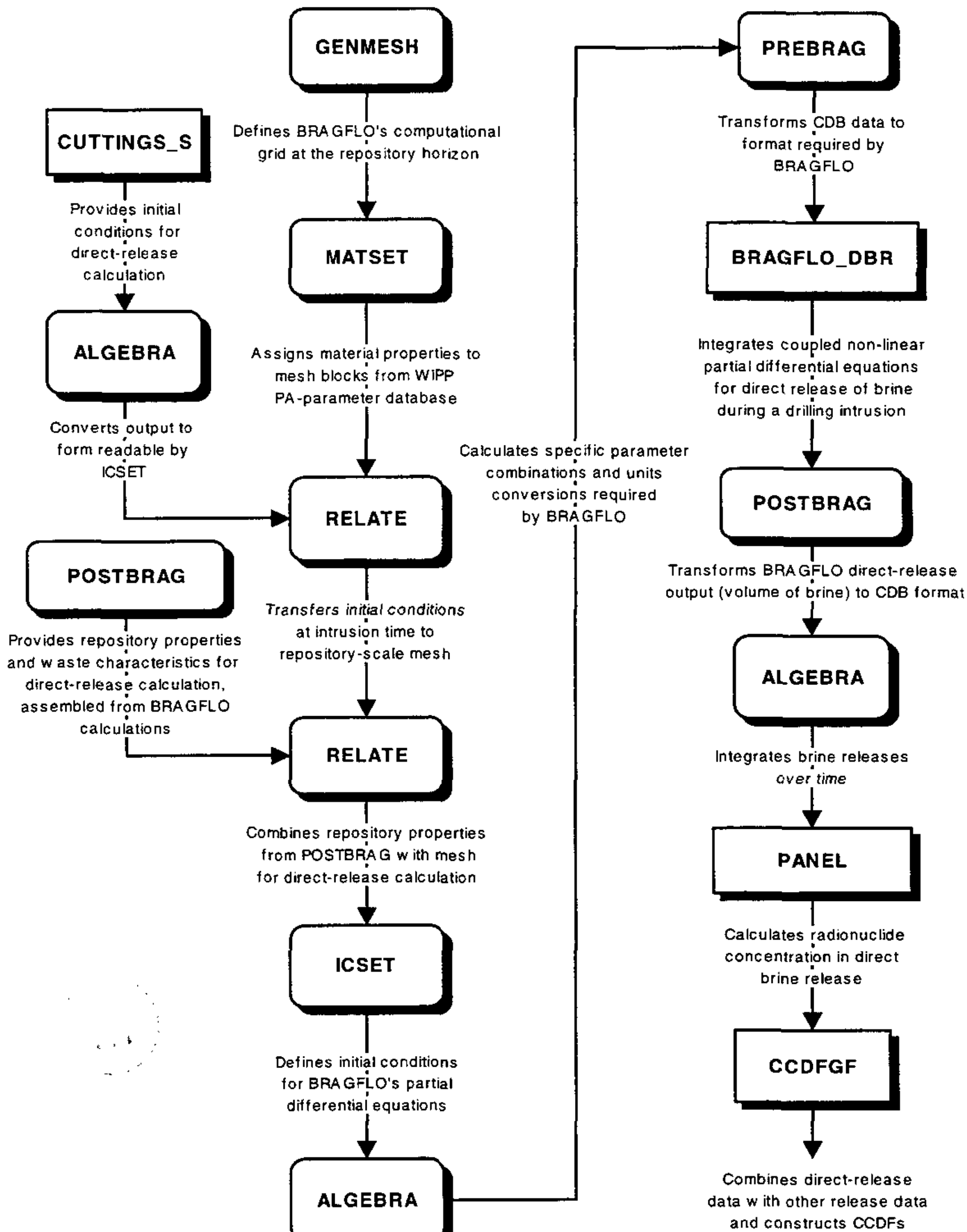

Note: PA SES codes are rectangular; PA NON-SES codes are rounded.

Figure CODELINK-4. The Code Sequence for BRAGFLO_DBR in the Performance Assessment for One Replicate with 57 Sampled Parameters and Sample Size Equal to 100

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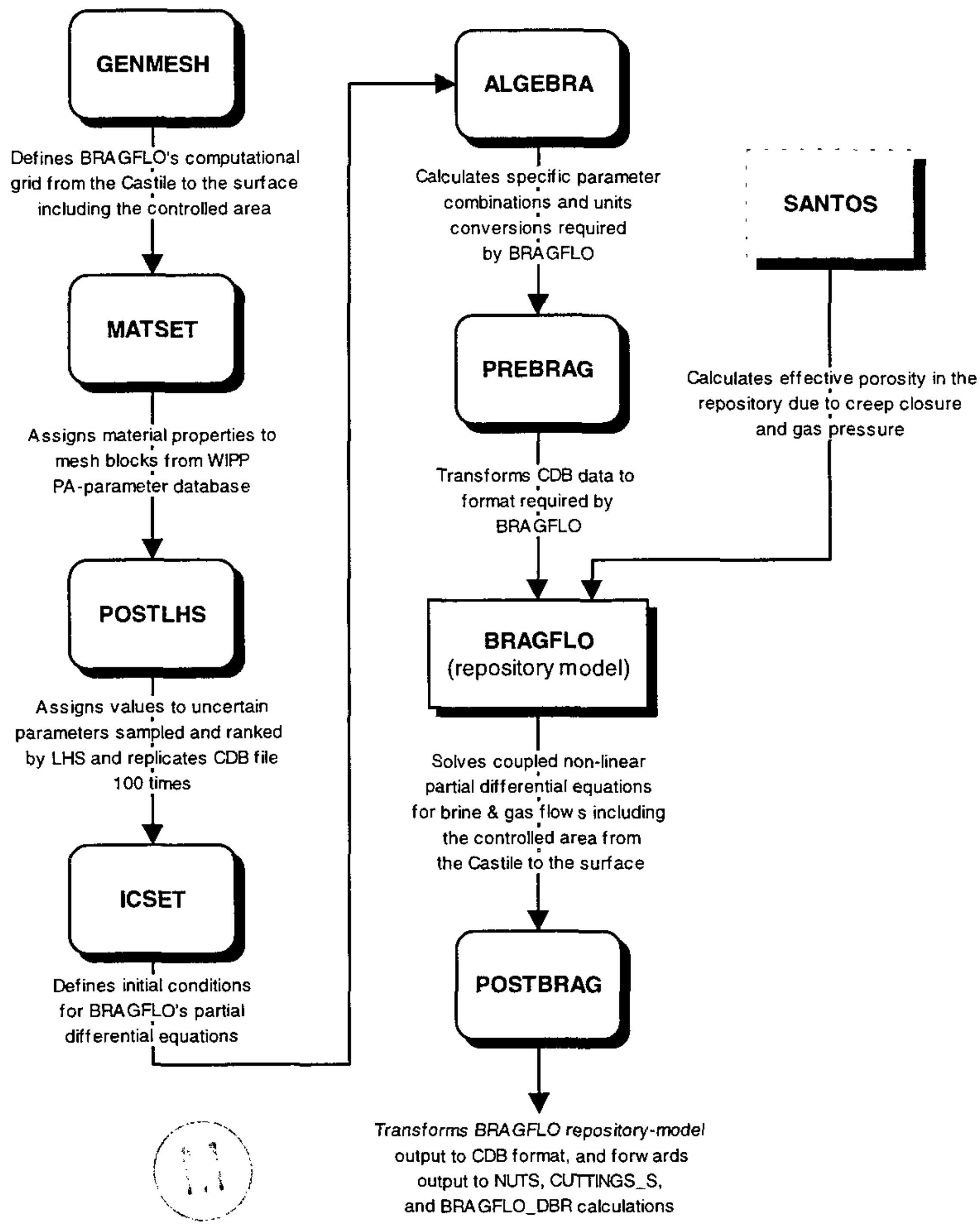

Note: PA SES codes are rectangular; PA NON-SES codes are rounded. The NON-PA SES code is dashed.

Figure CODELINK-5. The Code Sequence for BRAGFLO in the Performance Assessment for One Replicate with 57 Sampled Parameters and Sample Size Equal to 100

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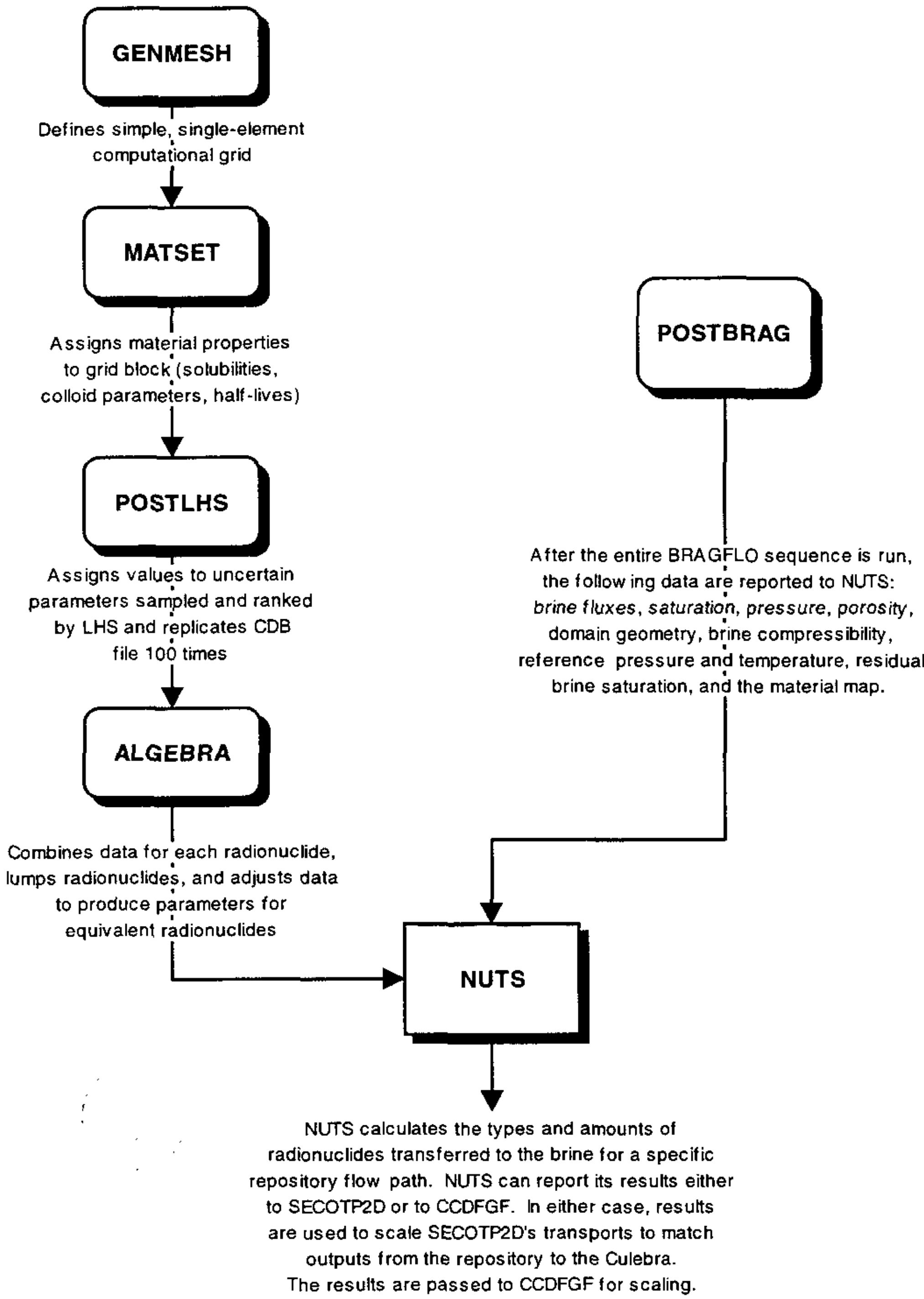

Note: PA SES codes are rectangular; PA NON-SES codes are rounded.

Figure CODELINK-6. The Code Sequence for NUTS in the Performance Assessment for One Replicate with 57 Sampled Parameters and Sample Size Equal to 100

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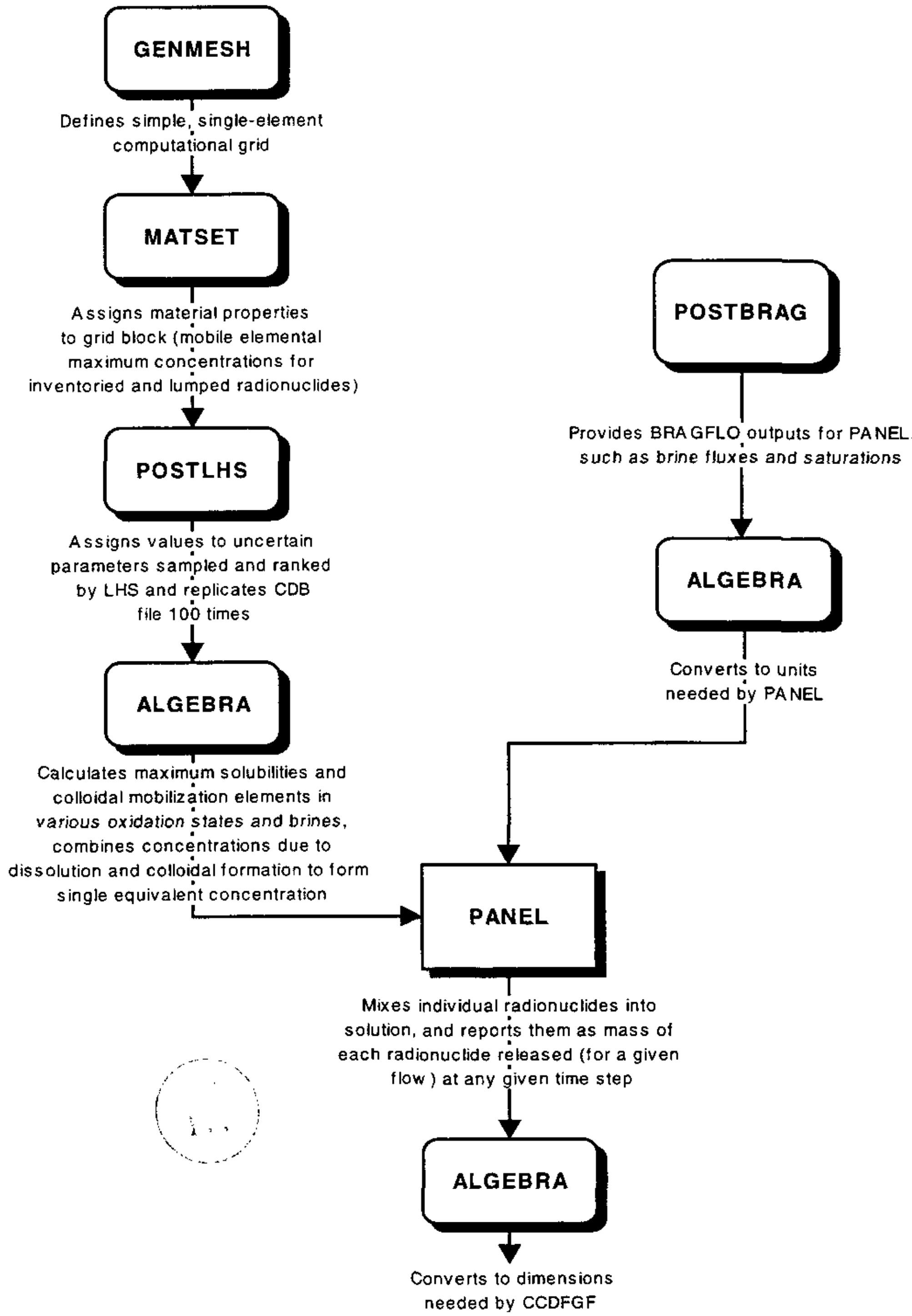

Note: PA SES codes are rectangular; PA NON-SES codes are rounded.

Figure CODELINK-7. The Code Sequence for PANEL in the Performance Assessment for One Replicate with 57 Sampled Parameters and Sample Size Equal to 100

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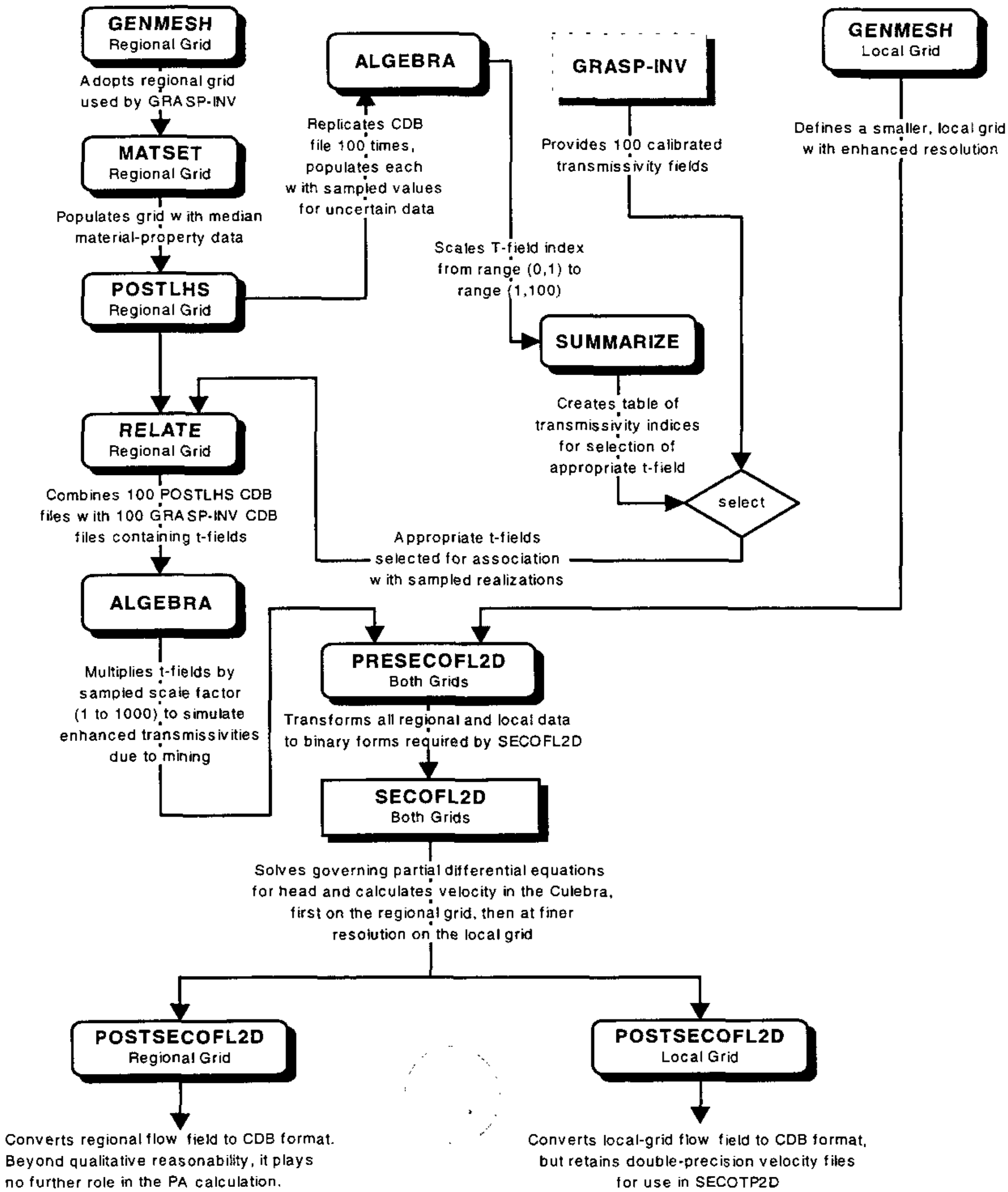

Note: PA SES codes are rectangular; PA NON-SES codes are rounded. The NON-PA SES code is dashed.

Figure CODELINK-8. The Code Sequence for SECOFL2D in the Performance Assessment for One Replicate with 57 Sampled Parameters and Sample Size Equal to 100

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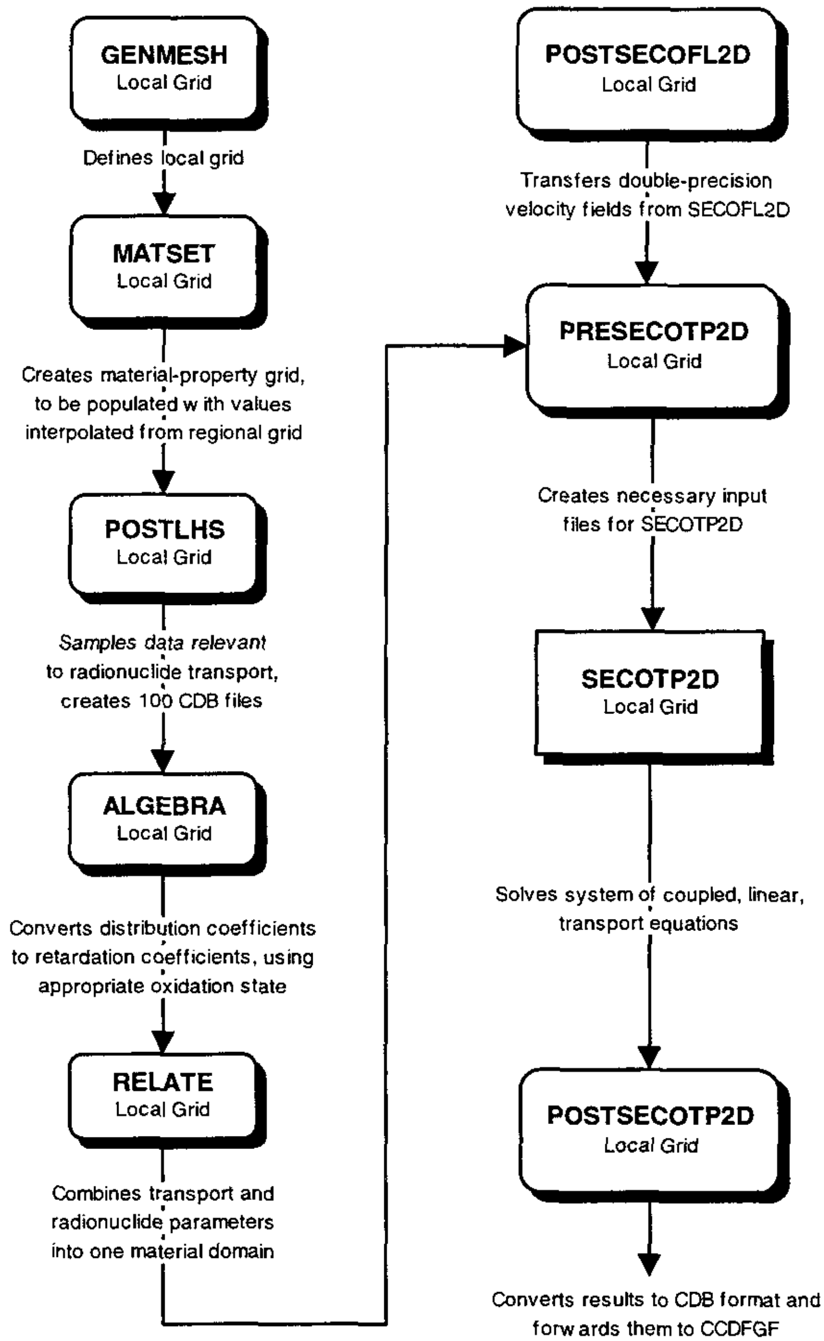

Note: PA SES codes are rectangular; PA NON-SES codes are rounded.

Figure CODELINK-9. The Code Sequence for SECOTP2D in the Performance Assessment for One Replicate with 57 Sampled Parameters and Sample Size Equal to 100

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BRAGFLO, GENMESH grids the entire repository region and surrounding formation from the Castile to the ground surface. In the vertical, it extends from the hypothesized underlying brine reservoir, throughout the Salado, to the overlying Culebra, and on upward to the ground-surface level, which is a boundary of the accessible environment. In the SECO codes, GENMESH grids the Culebra in a horizontally nonuniform regional grid that provides higher resolution in the vicinity of boreholes. It also grids the Culebra in a nonuniform, higher-resolution, local grid centered over the repository.

GENNET is a simplified mesh-generating code that is used for simple code geometries (for example, PANEL).

CODELINK.3.2 MATSET

MATSET's function is to assign material names, associated property values, and attribute values to specific blocks of grid elements identified by material region and defined by GENMESH. It creates its output file by adding its information to the input file it receives from GENMESH (or GENNET), the source of the new data being the performance assessment parameter data base. If used in default mode, MATSET chooses median values for all uncertain parameters. The user may, however, instruct MATSET to choose mean values. Neither alternative is used in probabilistic performance assessment calculations for uncertain parameters, which are sampled, but may be used for fixing values for nonsampled parameters. In performance assessments, the very next code in the utility run sequence is POSTLHS, which replaces MATSET's data choices with sampled values for all uncertain parameters. Thus, MATSET's choices of numerical values for uncertain parameters serve strictly as placeholders.

CODELINK.3.3 POSTLHS

As discussed in Section CODELINK.2 above, POSTLHS is LHS's postprocessor, LHS being the principal Latin-hypercube sampling code and the code whose output file contains the entire suite of *n* sampled values and rank orderings for all *m* uncertain parameters. POSTLHS's principal functions are: (1) to replicate the input file it receives from MATSET *n* times, (2) to assign to each such replicated MATSET file a different numerically-sequential name, and (3) to overwrite on each such file a different sampled value for each parameter from the suite of uncertain parameters that arise for that PA SES code. Except for sampled data, POSTLHS's *n* output CDB files are identical to one another and to the MATSET CDB file from which they came.

CODELINK.3.4 ICSET

All PA SES codes deal with systems of differential equations that are written as boundary-value problems. For transient problems, all unknown dependent variables must be specified over the entire computational domain, including all interior and boundary-value nodes, at the initial instant from which the computation begins. In physical terms, initial conditions describe the initial configuration of the physical system, which may or may not have a significant impact on the long-term behavior of the system.

ICSET's principal task is to assign user-specified initial numerical values to all unknown dependent parameters at every point in the computational grid (specified by GENMESH or GENNET). In time-stepping methods, the initial values are the original known quantities from which numerical approximations of the dependent variables and their derivatives are calculated and from which they evolve in time.

ICSET does not appear in the utility code sequence of every PA SES code because some of the codes (SECOFL2D, for example) set initial conditions internally, and others (CUTTINGS_S, for example) use analytically-integrated results that have already incorporated their initial conditions.

CODELINK.3.5 ALGEBRACDB

Occasionally, a parameter, attribute, or value may be listed or output from a code in a form that is unsuitable for direct use in a subsequent code. Typically, parameter units (that is, dimensions) may be inconsistent, a vector magnitude may be required rather than coordinate components of the vector, or the components of a tensor may be decomposed in a different coordinate system. ALGEBRACDB (often called simply ALGEBRA) is designed to make the appropriate changes. ALGEBRA is capable of performing most common algebraic manipulations and/or evaluating most common transcendental functions (trigonometric, logarithmic, exponential, etc.). It reads its instructions from a user-specified ASCII input control file that employs, for user convenience, an algebraic syntax that is similar in appearance to normal FORTRAN syntax.

ALGEBRA does not occur in the preparatory run stream for every PA SES code.

CODELINK.3.6 RELATE

RELATE serves two principal purposes. First, it is capable of interpolating data from one coordinate grid to a different coordinate grid that overlies it. Second, it is capable of combining two data files that are defined over the same grid. For example, SECOFL2D uses RELATE to add to its data files the sampled transmissivity values.

RELATE is not used by every PA SES code.

CODELINK.3.7 SUMMARIZE

SUMMARIZE can produce a single output file that contains similar data collected from across all the sampled CDB data files, thus allowing analysts to choose specific values from different modeling-code runs, at identical intermediate times, from each of the n sampled data files. If data-recording times are not identical on the various sampled files, SUMMARIZE can interpolate data on subsequent files to match the times used on the first file, or it can choose nearest values, as directed by the user. Thus, it facilitates comparisons as may be required by system analysts. Secondly, although it is able to read CDB format, SUMMARIZE outputs data to other common file formats, such as ASCII text, database, and spreadsheet formats.

CODELINK.3.8 Actual Utility Code Usage

The performance assessment code run sequences for the principal PA SES codes differ somewhat from one another, although all use PA NON-SES utility codes from the set of codes discussed in this section. The specific performance assessment code sequences are not discussed here; however, they are shown in correct order in Figures CODELINK-3 through CODELINK-9.

CODELINK.4 PA SES Codes and Performance Assessment Code Sequence

The PA SES codes are exercised together to produce a complete suite of radionuclide-release results, depending on the scenario under consideration. These PA SES codes are discussed briefly below, and each is treated in detail in its own appendix.

One principal performance assessment code sequence calculates long-term releases following drilling that occur through subsurface transport to the accessible environment (see Section 6.4.7.2 in Chapter 6.0 of this application). The performance assessment code sequence involves five PA SES codes: BRAGFLO, NUTS, PANEL, SECOFL2D, and SECOTP2D. Of these, all but NUTS and PANEL are exercised as a triad of codes that include pre- and postprocessor codes.

Another performance assessment code sequence calculates direct releases during drilling to the accessible environment, at ground-surface level immediately above the repository (see Section 6.4.7.1 in Chapter 6.0). The relevant performance assessment code sequences here involve the two PA SES codes CUTTINGS_S and BRAGFLO_DBR.

Each PA SES code is exercised near the end of a sequence of PA NON-SES utility codes that is designed to fit that particular code and interface it to its controlled database. The individual sequences are shown in Figures CODELINK-3 through CODELINK-9. Section CODELINK.5, below, treats only the PA SES codes that arise in direct-release calculations. Section CODELINK.6 treats only the PA SES codes that arise in the code sequence for long-term releases following drilling. The net release for each of the n input vectors is the sum of its direct and long-term releases, both for undisturbed conditions and following drilling. The total release for each sampled future is given by Equation 4.1 in Appendix CCDFGF.

CODELINK.5 PA SES Codes for Calculating Direct Releases

Two codes called CUTTINGS_S and BRAGFLO_DBR model the outcomes associated with direct transport to the surface during the drilling of a borehole that is hypothesized to penetrate the repository. There are four principal categories of phenomena, namely material removal (1) by cuttings, (2) by cavings, (3) by solid spallings, and (4) by direct brine release. CUTTINGS_S treats the first three items. BRAGFLO_DBR treats the fourth.

CODELINK.5.1 CUTTINGS_S

CUTTINGS_S estimates the direct removal of solid wastes from the repository as the result of inadvertent penetration by a borehole drilled at some time in the future. The word "direct" refers to the fact that CUTTINGS_S releases occur directly to the surface *at the time* of drilling.

Cuttings are those portions of the waste that are directly removed by the drill string and the drilling fluid. The volume of repository material removed as cuttings is the portion of the repository cut by the drill bit. Solids that originally bordered the borehole on its exterior and erode into the drilling fluid as a result of the fluid's frictional effects on the outer cylindrical surface of the borehole are called cavings. Because of that action, the volume of wastes removed from the repository can be larger than the volume of the borehole originally cut through the wastes. CUTTINGS_S allows for both laminar and turbulent shear flow in the circulating fluids, which, in turn, leads to two different models to estimate material removal due to erosion. CUTTINGS_S also calculates spall releases. Appendix CUTTINGS contains a detailed discussion of CUTTINGS_S, and the conceptual models for direct release as discussed in Chapter 6.0 (Section 6.4.7). The total volume of direct-released solids is the sum of these three releases, that is, cuttings, cavings, and spallings.

CUTTINGS_S acquires its parameter data from (i) the input CDB files provided by the codes MATSET and BRAGFLO, (ii) a user-supplied input text file, and (iii) the performance assessment parameter database. Discrete values of sampled data are provided by the code POSTLHS. CUTTINGS_S input includes the rotational speed of the drill string, cutting-bit diameter, the shear-rate-dependent viscosity and density parameters for the drilling mud, borehole roughness, the compacted repository thickness and porosity, the drilling mud flow rate, the drill collar diameter, and the effective failure shear strength of the compacted repository material.

CODELINK.5.2 BRAGFLO_DBR

BRAGFLO_DBR (also referred to as DBR_BRAGFLO) models the brine released to the surface as a direct result of a drilling intrusion into the repository (Appendix MASS, Attachment 16-2). It is in fact a different application (that is, a different grid, a different material map, and a different time scale) of the code BRAGFLO (see Section CODELINK.6.1 herein). The Poettmann-Carpenter wellbore model is implemented to calculate the flowing bottom-hole pressure that is needed to determine the volume of brine released to the surface.

Only the repository horizon is modeled. Local scale features (for example, salt pillars, panel seals, rooms, and passageways) are modeled. Initial brine saturation and pressure, porosity, and panel height within the waste are determined from the 10,000-year BRAGFLO results, using interpolation over intrusion times in the CUTTINGS_S code (Section CODELINK.5.1

above and Appendix MASS, Attachment 16-2). Unsampled parameter values are obtained directly from the performance assessment parameter database, and sampled parameters are incorporated from BRAGFLO results through a RELATE step.

CODELINK.6 PA SES Codes for Calculating Long-Term Releases

In the performance assessment code sequence, BRAGFLO simulates flow of brine and gas within and through the repository and surrounding formation from the Castile to the surface. NUTS and PANEL calculate the amount of radionuclides mobilized by fractions of the repository brine flows estimated by BRAGFLO. Together, they estimate the mass of radioactive material transported to the Culebra or above and through the anhydrite layers, MB138, a & b, and MB139. SECOFL2D simulates the natural groundwater flow in the Culebra on a regional scale (tens of kilometers) centered approximately over the repository's location, and uses it for a recalculation of the flow on a smaller local scale (a few kilometers) in the Culebra immediately above the controlled area. SECOTP2D estimates the amounts of radionuclides that would be transported by SECOFL2D's Culebra flow field given (1) the inputs from NUTS or PANEL, (2) the radioactive decay, and (3) the retarding properties of the Culebra matrix materials. The five PA SES codes are exercised in that order. They are discussed in the same order in the five subsections that follow. Because SECOTP2D is linear in the source term, it is exercised for unit inputs of each radionuclide and its results scaled to NUTS's or PANEL's estimates for each release pathway.

CODELINK.6.1 BRAGFLO

BRAGFLO calculates brine and gas flow everywhere within the controlled area and beyond from the Castile to the ground surface. As discussed in Chapter 6.0 (Section 6.4.2), regions of note include (1) the Culebra, (2) the repository, which is comprised primarily of (3) a thick relatively-impermeable crystalline halite with (4) thin interspersed interbeds of anhydrite materials, (5) disturbed rock zones in the immediate vicinity of the repository and (6) the shaft-seal systems. If exploratory drilling is hypothesized, the above regions are permitted to become interconnected by boreholes that (a) may or may not penetrate the hypothesized brine reservoir, and (b) are assumed to be plugged (prior to abandonment) in ways that reflect present-day practice. BRAGFLO couples the flow of brine and gas to other important repository processes such as creep closure and gas generation. The resulting brine-phase, transient-flow fields are used by NUTS to simulate radionuclide transport in these flow fields.

BRAGFLO is discussed in detail in Appendix BRAGFLO. The conceptual model implemented by BRAGFLO for the performance assessment is described in Chapter 6.0 (Section 6.4).

CODELINK.6.2 NUTS

NUTS is a radionuclide transport code. Its principal capabilities are (1) to decay the inventory, using Bateman's equations, and (2) to transport radionuclides through porous or fractured media considering advection, diffusion, dispersion, and sorption processes. The latter three processes are not included in the NUTS code for the performance assessment. The largest such path, in terms of volume rate of flow, leads to the Culebra, whose flow field is resolved by SECOFL2D (see Section CODELINK.6.4). NUTS's estimates of the amounts are forwarded as multipliers for the results of SECOTP2D (see Section CODELINK.6.5), the transport code that transports unit inputs of mobilized radionuclides through the Culebra to the edge of the controlled area. NUTS serves that role for most of the consequence analyses for this performance assessment. Some analyses are made with PANEL and these are discussed in Section CODELINK.6.3. NUTS is discussed in detail in Appendix NUTS. The conceptual model implemented by NUTS for the performance assessment is discussed in Chapter 6.0 (Section 6.4.5.4).

NUTS requires the following input parameters: (1) fluxes of brine, saturation, pressure, porosity, and computational-domain geometry from BRAGFLO's binary-output CDB file; (2) brine compressibility, reference pressure and temperature, residual brine saturation, and the material map from BRAGFLO's ASCII input-file, and (3) solubilities, inventories, half-lives and atomic weights of all the inventoried radioisotopes, free-water molecular diffusivity, dispersivities, tortuosity, rock density, and standard-condition density of the brine.

CODELINK.6.3 PANEL

PANEL is a radionuclide mobilization and decay code. Its principal functions are (1) to decay the inventory, which it does using Bateman's equations, and (2) to use the decayed inventory together with the repository brine volume and outflow rate, and the dissolved and colloidal actinide source terms, to estimate the quantity of all modeled radionuclides that are transported up the borehole.

PANEL treats each repository panel as a single isolated mixing cell, and so is not a transport model. In consequence analyses that approximate those conditions, PANEL is applied. PANEL also provides radioisotope concentrations for BRAGFLO_DBR applications.

PANEL is discussed in detail in Appendix PANEL. The conceptual model implemented for PANEL for the performance assessment is described in Chapter 6.0 (Section 6.4.7). PANEL's output is delivered as moles of each radioisotope that is released from the repository (for the assumed flow rate). These are inconvenient units, so the outputs are run through a postprocessing ALGEBRA step. This is a different application of ALGEBRA than the one that precedes PANEL. For BRAGFLO runs, it converts releases in moles to releases in mass (kilograms) for the outflow rates provided it. For BRAGFLO_DBR applications, it converts PANEL's outputs at any given time to units of concentration by dividing them by the mass of brine that flowed through the repository during that time. The mass-per-unit-mass concentration units are then converted to normalized EPA units per cubic meter of brine. These data are then directly usable by BRAGFLO_DBR, whose output is in cubic meters of brine. The product of the two is the direct release to the surface in normalized EPA units.

CODELINK.6.4 GRASP-INV and SECOFL2D (Regional and Local)

GRASP-INV is used outside the performance assessment code runstream. It generates a calibrated field of transmissivities in the Culebra on a regional scale for each of the *n* input vectors. SECOFL2D calculates a groundwater flow field for each of the *n* transmissivity fields. The two-dimensional, single-phase groundwater flow is governed by Darcy's law. Direct measurements of Culebra transmissivities exist at a number of locations throughout the WIPP region. GRASP-INV uses those measurements, their statistical properties, and other related information to solve the inverse groundwater-flow problem, and thereby generate an ensemble of fields that define transmissivity values at *each* node in the computational domain. The transmissivity fields produced have the same statistical properties (means, variances, covariances) as the measured data set, and they agree with measured transmissivities at all points where data exist. GRASP_INV and SECOFL2D are described in Appendices TFIELD and SECOFL2D, respectively. The conceptual model implemented by these codes for the performance assessment is described in Chapter 6.0 (Section 6.4.6.2). After each new transmissivity-field realization has been completed, GRASP-INV writes a new CDB file that contains (1) defining information specifying the computational grid, (2) head values that will be used by SECOFL2D as boundary conditions, and (3) the sampled transmissivity field, which is reported numerically as hydraulic conductivities at each grid block.

Before GRASP-INV's transmissivity fields are reported to SECOFL2D, they are modified by ALGEBRA to simulate the effects of potash mining that may take place in the future (see Section 6.4.6.2.3 of Chapter 6.0).

The SECOFL2D flow calculation is carried out sequentially over two different, overlying meshes for regional and local domains. Boundary conditions for the local domain, which is nested within the regional domain, are interpolated from the regional flow solution, and material properties for the local grid are interpolated from the material properties of the regional grid.

SECOFL2D (i) solves Darcy's system of differential equations for the nonhydrostatic component of the pressure field on the regional grid, (ii) interpolates calculated regional heads to the local grid boundary, and (iii) solves the same system of differential equations a second time on the finer-scale local grid. It produces four output files. Two are results files and contain the calculated heads, Darcy velocities (x and y components), volumetric fluxes (x and y components), and salt concentrations if the working fluid is brine. One is for the regional flow-field calculation and the other is for the local flow-field calculation. A third output file contains all the information derived from the regional flow that is necessary to initialize and run a local-flow calculation. It is useful if several local calculations are to be run from a single regional calculation, which is the case if parametric effects are being studied. However, in normal performance assessment runs, this file may be regarded as a temporary file and discarded. The fourth output file is an ASCII text file that lists summary information about the run and serves as a debug file.

CODELINK.6.5 SECOTP2D

The transport of radionuclides in the Culebra is calculated by SECOTP2D using the flow field generated by SECOFL2D for the local grid. Advection is the main transport process in SECOTP2D, but it is modified by (i) diffusion into the matrix, (ii) chemical retardation, and (iii) natural radioactive decay. For each flow field, SECOTP2D (1) combines the flow results with material and transport parameters that affect radionuclide transport in the Culebra, (2) calculates the concentration of radionuclide everywhere in the local domain as a function of time, and (3) calculates the integrated discharge across user-defined boundaries. SECOTP2D is described in Appendix SECOTP2D. The conceptual model implemented by SECOTP2D for the performance assessment is discussed in Chapter 6.0 (Section 6.4.6.2).

To prepare for the SECOTP2D calculation, it is necessary to create data files that contain the flow fields from SECOFL2D, all the necessary material parameters, and all the required sampled parameters that affect transport. These data files will serve as the input data files for the SECOTP2D code.

The *n* sampled data files needed by SECOTP2D must contain SECOFL2D's *n* flow fields as well as POSTLHS's *n* sampled material parameters. Each of the *n* transmissivity fields is associated with one of the *n* data files.

The inputs to SECOTP2D are the three output files from PRESECOTP2D. The outputs of SECOTP2D are a binary transfer file that gives the spatial distribution of radioisotopes throughout the local grid as a function of time, and a debug file. If it is specified in the PRESECOTP2D text input file, the SECOTP2D output can also include, as a function of time, the amount of each radioisotope transported across a prespecified rectangular box surrounding the source (the user-specified discharge boundary). The latter result is included in the CCDF plots that are used to summarize performance assessment results (see Figure CODELINK-9).

CODELINK.7 CCDF Construction and Statistical Analyses

CCDFGF assembles results obtained from calculations using the described sequences of PA SES codes into the CCDFs. CCDFGF scales BRAGFLO_DBR's and SECOTP2D's results to match radionuclide outputs calculated by NUTS and PANEL. CCDFGF combines all the calculated release data to simulate many different repository histories, generating random sequences of future events, calculating the probabilities associated with those random sequences and, preparing in numerical format, all the data required to produce the CCDF plots that summarize the WIPP's predicted performance. Only a plotting code is required after CCDFGF to represent the entire summary results of the release calculation graphically as CCDFs. The code CCDFGF is treated independently in Appendix CCDFGF.

STEPWISE and PCCSRC are PA NON-SES statistical-analysis codes used in parameter-sensitivity studies. STEPWISE is a stepwise-regression code designed to treat multiple-parameter systems, and PCCSRC is a partial-correlation-coefficient/standardized-regressioncoefficient code. Utility codes like CCD2STEP and LHS2STEP are used to interface with STEPWISE and PCCSRC.

ATTACHMENTS

Attachment 1: Requirements of 40 CFR §194.23(c) and Records Package Identifiers for Software Quality Assurance Documentation in which Requirements are Addressed

Attachment 2: Analysis Packages

Title 40 CFR Part 191 Compliance Certification Application for the Waste Isolation Pilot Plant

CODELINK Attachment 1

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ATTACHMENT 1

Table CODELINK-A1. Requirements of 40 CFR §194.23(c) and Records Package Identifiers for Software Quality Assurance Documentation in which Requirements Are Addressed.

Requirements:

(1) Descriptions of the theoretical backgrounds of each model and the method of analysis or assessment;

(2) General descriptions of the models; discussions of the limits of applicability of each model; detailed instructions for executing the computer codes, including hardware and software requirements, input and output formats with explanations of each input and output variable and parameter (e.g., parameter name and units); listings of input and output files from a sample computer run; and reports on code verification, benchmarking, validation, and quality assurance procedures;

(3) Detailed descriptions of the structure of computer codes and complete listings of the source codes;

(4) Detailed descriptions of data collection procedures, sources of data, data reduction and analysis, and code input parameter development;

(5) Any necessary licenses; and

(6) An explanation of the manner in which models and computer codes incorporate the effects of parameter correlation.

Notes:

(1) These requirements are generally addressed in the User's Manual (UM), although in some instances a Theory Manual may exist. Some codes will be described and validated in an Analysis Plan (AP) or similar documentation. See also the applicable appendices.

(2) Most of these requirements are addressed in the User's Manual (UM); however, the code-verification and quality-assurance items will be found elsewhere, usually in the Requirements Document / Verification and Validation Plan (RD/VVP) and the Validation Document (VD). Some codes will be described and validated in an Analysis Plan (AP) or similar documentation. See also the applicable appendices.

(3) These are generally provided in the Implementation Document (ID). Some codes will be described and validated in an Analysis Plan (AP) or similar documentation.

(4) Except as described in Requirement (2), these issues are not addressed in any of the code documentation, and thus *will not be treated in this table.* See Appendix PAR for the discussion of parameters.

(5) This requirement *will not be treated in this table.*

(6) This requirement is addressed in Appendix PAR, and *will not be addressed in this table.*

Table CODELINK-A1. Requirements of 40 CFR §194.23(c) and Records Package Identifiers for Software Quality Assurance Documentation in which Requirements Are Addressed. (continued)

CODE	Requirement 1	Requirement 2	Requirement 3
ALGEBRACDB	UM - WPO# 28110	UM - WPO# 28110 RD/VVP - WPO# 28109 VD - WPO# 28112	ID - WPO# 28111
BLOTCDB	UM - WPO# 37501	UM - WPO# 37501 RD/VVP - WPO# 37499 VD - WPO# 37502	ID - WPO# 37500
BRAGFLO	UM - WPO# 30703	UM - WPO# 30703 RD/VVP - WPO# 30702 VD - WPO# 30705	ID - WPO# 30704
CAMCON_LIB	UM - WPO# 27738	UM - WPO# 27738 RD/VVP - WPO# 27736 VD - WPO# 27741	ID - WPO# 27740
CAMDAT_LIB	UM - WPO# 27727	UM - WPO# 27727 RD/VVP - WPO# 27726 VD - WPO# 27730	ID - WPO# 27728
CAMSUPES_LIB	UM - WPO# 27745	UM - WPO# 27745 RD/VVP - WPO# 27744 VD - WPO# 27747	ID - WPO# 27746
CCD2STEP	UM - WPO# 36246	UM - WPO# 36246 RD/VVP - WPO# 36244 VD - WPO# 36247	ID - WPO# 36245
CCDFGF	Design Document - WPO# 31235	UM - WPO# 31236 RD - WPO# 31233 VVP - WPO# 31234 VD - WPO# 31238	ID - WPO# 31237
CCDFSUM	AP for Task 7 - WPO # 36336	AP for Task 7 - WPO # 36336	AP for Task 7 - WPO # 36336
COLUMN	COLUMN: A Computer Program for Fitting Model Parameters to Column Flow Breakthrough Curves (V. 1.3), 4/27/96 - WPO# 37867	COLUMN: A Computer Program for Fitting Model Parameters to Column Flow Breakthrough Curves (V. 1.3), 4/27/96 - WPO# 37867	COLUMN: A Computer Program for Fitting Model Parameters to Column Flow Breakthrough Curves (V. 1.3), 4/27/96 - WPO# 37867
CUTTINGS_S	UM - WPO# 37765	UM - WPO# 37765 RD/VVP - WPO# 37763 VD - WPO# 37768	ID - WPO# 37764
BRAGFLO_DBR	UM - WPO# 30703 SNL Memo - WPO# 38134	UM - WPO# 30703 RD/VVP - WPO# 38122 VD - WPO# 38135	ID - WPO# 38133
EPAUNI	AP#017 - WPO# 39259	AP#017 - WPO# 39259	AP#017 - WPO# 39259
EQ3/EQ6	AP# 32 - Primitive Baseline WPO# 37423	AP# 32 - Primitive Baseline WPO# 37423	AP# 32 - Primitive Baseline WPO# 37423

Table CODELINK-A1. Requirements of 40 CFR §194.23(c) and Records Package Identifiers for Software Quality Assurance Documentation in which Requirements Are Addressed. (continued)

CODE	Requirement 1	Requirement 2	Requirement 3
FMT	UM - WPO# 28119	UM - WPO# 28119 RD/VVP - WPO# 28118 VD - WPO# 28121	ID - WPO# 28120
GENII-A	UM - WPO# 27751	UM - WPO# 27751 RD/VVP - WPO# 27750 VD - WPO# 27753	ID - WPO# 27752
GENMESH	UM - WPO# 30698	UM - WPO# 30698 RD/VVP - WPO# 30697 VD - WPO# 30700	ID - WPO# 30699
GRASP-INV	UM - WPO# 30636	UM - WPO# 30636 RD/VVP - WPO# 30634 VD - WPO# 30637	ID - WPO# 30635
GROPECDB	UM - WPO# 37496	UM - WPO# 37496 RD/VVP - WPO# 37494 VD - WPO# 37497	ID - WPO# 37495
GTFM-PC	UM - WPO# 40244	UM - WPO# 40244 RD/VVP - WP 40245; VD - WPO# 40246	*
ICSET	UM - WPO# 30693	UM - WPO# 30693 RD/VVP - WPO# 30692 VD - WPO# 30695	ID - WPO# 30694
LHS	UM - WPO# 30732	UM - WPO# 30732 RD/VVP - WPO# 30731 VD - WPO# 30734	ID - WPO# 30733
LHS2STEP	UM - WPO# 36916	UM - WPO# 36916 RD/VVP - WPO# 36913 VD - WPO# 36918	ID - WPO# 36915
MATSET	UM - WPO# 30688	UM - WPO# 30688 RD/VVP - WPO# 30687 VD - WPO# 30690	ID - WPO# 30689
NONLIN	UM - WPO# 30740	UM - WPO# 30740 RD/VVP - WPO# 30738 VD - WPO# 30743	ID - WPO# 30742
NUCPLOT	UM - WPO# 37506	UM - WPO# 37506 RD/VVP - WPO# 37504 VD - WPO# 37507	ID - WPO# 37505
NUTS	UM - WPO# 37927	UM - WPO# 37927 RD/VVP - WPO# 37924 VD - WPO# 37929	ID - WPO# 37926
ORIGEN2	Analysis Report - WPO# 36974	Analysis Report - WPO# 36974	Analysis Report - WPO# 36974
PANEL	UM - WPO# 37361	UM - WPO# 37361 RD/VVP - WPO# 37358 VD - WPO# 37362	ID - WPO# 37360

Table CODELINK-A1. Requirements of 40 CFR §194.23(c) and Records Package Identifiers for Software Quality Assurance Documentation in which Requirements Are Addressed. (continued)

CODE	Requirement 1	Requirement 2	Requirement 3
PCCSRC	UM - WPO# 27773	UM - WPO# 27773 RD/VVP - WPO# 27772 VD - WPO# 27775	ID - WPO# 27774
PLT_LIB	UM - WPO# 37491	UM - WPO# 37491 RD/VVP - WPO# 37489 VD - WPO# 37492	ID - WPO# 37490
POSTBRAG	UM - WPO# 30683	UM - WPO# 30683 RD/VVP - WPO# 30681 VD - WPO# 30685	ID - WPO# 30684
POSTGENII	UM - WPO# 27756	UM - WPO# 27756 RD/VVP - WPO# 27755 VD - WPO# 27758	ID - WPO# 27757
POSTLHS	UM - WPO# 30722	UM - WPO# 30722 RD/VVP - WPO# 30719 VD - WPO# 30724	ID - WPO# 30723
POSTSECOFL2D	UM - WPO# 35721	UM - WPO# 35721 RD/VVP - WPO# 35717 VD - WPO# 35722	ID - WPO# 35718
POSTSECOTP2D	UM - WPO# 37306	UM - WPO# 37306 RD/VVP - WPO# 37304 VD - WPO# 37307	ID - WPO# 37305
PREBRAG	UM - WPO# 30677	UM - WPO# 30677 RD/VVP - WPO# 30676 VD - WPO# 30679	ID - WPO# 30678
PREGENII	UM - WPO# 27763	UM - WPO# 27763 RD/VVP - WPO# 27762 VD - WPO# 27765	ID - WPO# 27764
PRELHS	UM - WPO# 30714	UM - WPO# 30714 RD/VVP - WPO# 30712 VD - WPO# 30716	ID - WPO# 30715
PRESECOFL2D	UM - WPO# 35711	UM - WPO# 35711 RD/VVP - WPO# 35709 VD - WPO# 35713	ID - WPO#35710
PRESECOTP2D	UM - WPO# 37297	UM - WPO# 37297 RD/VVP - WPO# 37295 VD - WPO# 37299	ID - WPO# 37296
RELATE	UM - WPO# 24186	UM - WPO# 24186 RD/VVP - WPO# 24184 VD - WPO# 24183	ID - WPO# 34413
SANTOS	Santos User's Manual - WPO# 35674	Santos User's Manual - WPO# 35674 Santos Validation Dcmt - WPO# 35675 QA Dcmt for Santos - WPO# 35673	*

Table CODELINK-A1. Requirements of 40 CFR §194.23(c) and Records Package Identifiers for Software Quality Assurance Documentation in which Requirements Are Addressed. (continued)

CODE	Requirement 1	Requirement 2	Requirement 3
SDBREAD_LIB	UM - WPO# 30629	UM - WPO# 30629 RD/VVP - WPO# 30627 VD - WPO# 30630	ID - WPO# 30628
SECOFL2D	UM - WPO# 37271	UM - WPO# 37271 RD/VVP - WPO# 37269 VD - WPO# 37272	ID - WPO# 37270
SECOTP2D	UM - WPO# 36695	UM - WPO# 36695 RD/VVP - WPO# 36693 VD - WPO# 36696	ID - WPO# 36694
SPECTROM-32	SPECTROM-32 User's Manual - WPO# 20149	SPECTROM-32 User's Manual - WPO# 20149 SPECTROM-32 Code Verification - WPO# 20155 WPO# 20157 WPO# 20159	SPECTROM-32 Source Code Listing - WPO# 20167 WPO# 20155
SPECTROM-41	SPECTROM-41 User's Manual - RE/SPEC internal number RSI-0266, Vol 2-User's Manual	SPECTROM-41 User's Manual - RE/SPEC internal number RSI-0266, Vol 2-User's Manual SPECTROM-41 Code Verification - RE/SPEC internal number RSI-0266, Vol 3-Code Verification	SPECTROM-41 Source Code Listing - RE/SPEC internal number RSI-0266, Vol 4-Source Code listing
SPLAT	UM - WPO# 37484	UM - WPO# 37484 RD/VVP - WPO# 37482 VD - WPO# 37485	ID - WPO# 37483
STEPWISE	UM - WPO# 27768	UM - WPO# 27768 RD/VVP - WPO# 27767 VD - WPO# 27770	ID - WPO# 27769
SUMMARIZE	UM - WPO# 37460	UM - WPO# 37460 RD/VVP - WPO# 37458 VD - WPO# 37461	ID - WPO# 37459
SWIFTII	"Primitive Baseline Software Documentation Package for SWIFT-II, Sandia Waste Isolation Flow and Transport Code (SWIFT II, Version 2F, Primitive Baseline, Volume I & II" - WPO # 38219	"Primitive Baseline Software Documentation Package for SWIFT-II, Sandia Waste Isolation Flow and Transport Code (SWIFT II, Version 2F, Primitive Baseline, Volume I & II" - WPO # 38219	*

Table CODELINK-A1. Requirements of 40 CFR §194.23(c) and Records Package Identifiers for Software Quality Assurance Documentation in which Requirements Are Addressed. (continued)

CODE	Requirement 1	Requirement 2	Requirement 3
THEMM	UM - WPO# 35261	UM - WPO# 35261 RD/VVP - WPO# 35263 VD - WPO# 35259	ID - WPO# 35260
TOUGH28W	UM - WPO# 36535	UM - WPO# 36535 RD/VVP - WPO# 36532 VD - WPO# 36536	ID - WPO# 36537

* *These are virtually commercial codes and source code is proprietary. However, the executables used for the performance assessment are archived and available.*

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CODELINK Attachment 2

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Table CODELINK-A2. Analysis Packages

Package Name	WPO
Analysis Package for the Salado Flow Calculations (Task 1) of the Performance Assessment Analyses Supporting the Compliance Certification Application	40514
Analysis Package for the Salado Transport Calculations (Task 2) of the Performance Assessment Analysis Supporting the Compliance Certification Application	40515
Analysis Package for the Culebra Flow and Transport Calculations (Task 3) of the Performance Assessment Analyses Supporting the Compliance Certification Application	40516
Analysis of the Generation of Transmissivity Fields for the Culebra Dolomite	40517
Analysis Package for the BRAGFLO Direct Release Calculations (Task 4) of the Performance Assessment Analyses Supporting the Compliance Certification Application	40520
Analysis Package for the Cuttings and Spalling Calculations (Tasks 5 and 6) of the Performance Assessment Analyses Supporting the Compliance Certification Application	40521
Analysis Package for the CCDF Construction (Task 7) of the Performance Assessment Analyses Supporting the Compliance Certification Application	40524

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