Code Selection for General Separations Area Flow Simulation and Model Calibration

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EXECUTIVE SUMMARY

Savannah River Site Performance Assessments involve solute transport simulations for the groundwater pathway based on a groundwater flow model of the General Separations Area (GSA) referred to as GSA/PORFLOW, where PORFLOW is the simulation code. The GSA/PORFLOW model is based on an earlier flow model constructed using the FACT code, now referred to as GSA/FACT. The transition from GSA/FACT to GSA/PORFLOW was primarily an effort to port the GSA flow model from the FACT code to the PORFLOW code; characterization and monitoring data, circa early 1990's, were not updated. The GSA/PORFLOW model and ancestors were calibrated using manual techniques, typical practice in that era.

Since development of the original GSA model in the early 1990s, semi-automated model calibration using optimization software has been become routine in groundwater modeling practice. Calibration using optimization algorithms is desirable because it can improve the model fit to data, reduce the calibration effort, and provide statistical information about model uncertainty. Re-calibration of the GSA/PORFLOW model, used in the 2008 E-Area PA, was recommended by the Low-Level Waste Disposal Facility Federal Review Group in their review of that PA document. Also since the early 1990's, significantly more characterization and monitoring data are now available for model development, calibration, and validation. In preparation for an upcoming E-Area PA revision, GSA/PORFLOW will be replaced with a new groundwater flow model developed from updated data and calibrated using optimization software.

Continued use of the PORFLOW is not required and a different code could be chosen for flow simulation. An optimization code for model calibration must also be selected. This report documents the pros and cons of various flow simulation and model calibration codes, and provides the rationale for choosing PORFLOW and PEST for an updated GSA flow model. Selection of PORFLOW provides a combined recharge-drain boundary condition for simulating variable seepline locations, leverages more than 20 years of experience with PORFLOW at SRNL, and provides continuity with previous PA modeling. License restrictions with PORFLOW are a drawback but not expected to significantly hinder timely progress. PEST was selected for model calibration based on its dominant market share in environmental applications. UCODE has been identified as a fallback option if warranted.

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LIST OF ABBREVIATIONS

2D	Two-Dimensional
3D	Three-Dimensional
ACRi	Analytic & Computational Research, Inc.
BC	Boundary Condition
CPU	Central Processing Unit
DOE	Department of Energy
GSA	General Separations Area
LFRG	Low-Level Waste Disposal Facility Federal Review Group
PA	Performance Assessment
QA	Quality Assurance
SRNL	Savannah River National Laboratory
WSRC	Westinghouse Savannah River Company

1.0 Introduction

DOE Order 435.1 Performance Assessments (PAs) are performed at the Savannah River Site for low-level radioactive solid waste disposal in E-Area, liquid waste disposal in the Z-Area Saltstone facility, and waste tank closures in F-Area and H-Area. Radiological dose to human receptors is considered in an all-pathways analysis, with the performance measure being a 25-mrem/yr effective dose equivalent (EDE) to representative members of the public, excluding dose from radon and its progeny in air. The groundwater pathway is the primary contributor to all-pathways dose at the Savannah River Site. Protection of groundwater resources is also considered, with the performance measures being Safe Drinking Water Act maximum contaminant levels (MCLs) for beta-gamma and alpha-emitting radionuclides.

Solute transport simulations performed for these groundwater pathway assessments are advection-dominated and rely on a numerical flow simulation to define the groundwater velocity and saturation fields. The E-, F-, H- and Z-Areas all reside within the General Separations Area (GSA, Figure 1-1). The PAs associated with facilities in these areas (e.g. WSRC 2008) are based on a groundwater flow model (Flach 2004) called GSA/PORFLOW, a reference to the geographic domain and simulation code for the model. The GSA/PORFLOW model is based on an earlier flow model (Flach and Harris 1999) constructed using the FACT code (Hamm and Aleman 2000), now referred to as GSA/FACT. The transition from GSA/FACT to GSA/PORFLOW was primarily an effort to port the GSA flow model from the FACT code to the PORFLOW code; characterization and monitoring data, circa early 1990's, were not updated. The GSA/PORFLOW model and ancestors were calibrated using manual techniques, typical practice in that era.

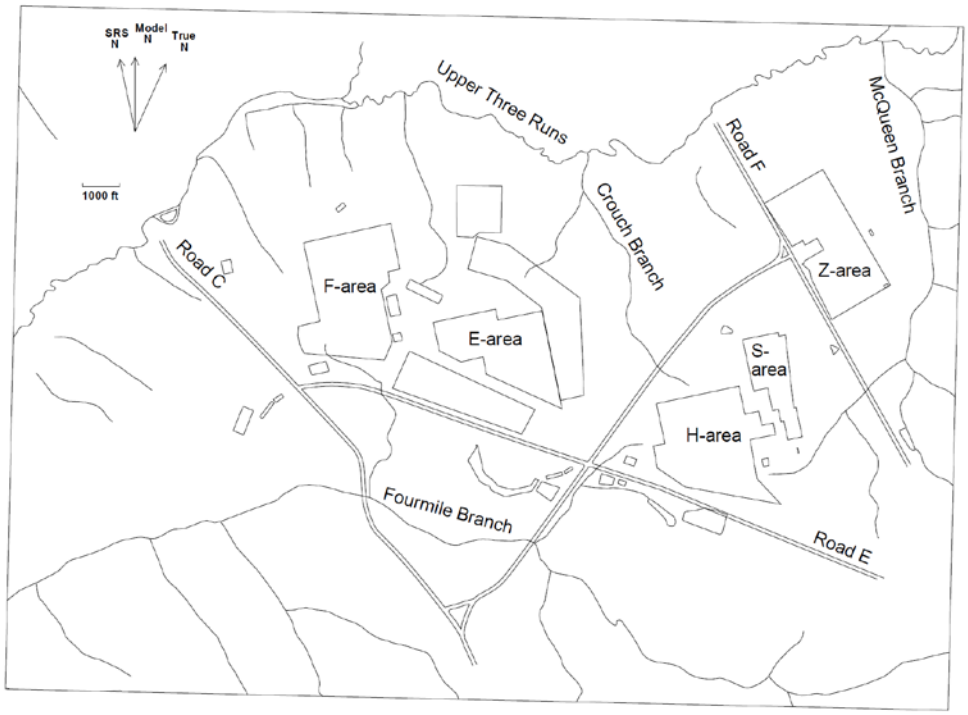


Figure 1-1. General Separations Area at the Savannah River Site (reproduced from WSRC-TR-96-0399, Rev. 1).

Since development of the original GSA model in the early 1990s, semi-automated model calibration using optimization software (e.g. PEST code) has been become routine in groundwater modeling practice. Calibration using optimization algorithms is desirable because it can improve the model fit to data, reduce the calibration effort, and provide statistical information about model uncertainty. Re-calibration of the GSA/PORFLOW model, used in the 2008 E-Area PA, was recommended by the Low-Level Waste Disposal Facility Federal Review Group in their review of that PA document (DOE LFRG 2008). Also since the early 1990's, significantly more characterization and monitoring data are now available for model development, calibration, and validation. In preparation for an upcoming E-Area PA revision, GSA/PORFLOW will be replaced with a new groundwater flow model developed from updated data and calibrated using optimization software.

Continued use of the PORFLOW is not required and a different code could be chosen for flow simulation. An optimization code for model calibration must also be selected. This report documents the pros and cons of various flow simulation and model calibration codes, and provides the rationale for choosing PORFLOW and PEST for an updated GSA flow model.

2.0 Code Selection for Groundwater Flow Simulation

Many public-domain and commercial codes are available for groundwater flow simulation (e.g. http://igwmc.mines.edu/software/category_list.html, http://www.scisoftware.com/html/products.html, http://water.usgs.gov/software/lists/groundwater, http://www.groundwatermodels.com/ESI_Software.php), and nearly all could be successfully applied to the General Separations Area with varying degrees of analyst effort and simulation quality. Among these choices PORFLOW developed by Analytic & Computational Research, Inc. (http://www.acricfd.com/software/porflow) has been selected based on 1) a couple of relatively unique capabilities, 2) resolution of a prior particle tracking deficiency, 3) the opportunity to leverage extensive PORFLOW experience and infrastructure at SRNL, and 4) to provide continuity with previous modeling. Nonetheless certain drawbacks to selecting PORFLOW were considered. The remaining discussion in this section expands on these points.

Unique features: Groundwater flow in the surficial aquifer beneath the GSA is driven by local recharge and discharge to bounding streams, with minimal leakage to the lower aquifer unit. Seepage faces adjoining Upper Three Runs to the north, Fourmile Branch to the south, McQueen Branch to the east, and associated tributaries can be expected to vary in extent and position during steady-state model calibration, as the water table rises and falls in response to conductivity and/or boundary condition changes. Seepage faces may also vary within a transient simulation. The need to automatically switch between recharge and discharge conditions at the top boundary in response to simulated hydraulic head (possibly varying in time) was recognized by Hamm and Aleman (2000) who developed a combined recharge-drain boundary condition (BC) for the FACT code. This recharge-drain BC alleviates the need to estimate beforehand the position of seepage faces, and subsequent perturbations to synchronize BCs with the predicted water level relative to the ground surface.

The recharge-drain BC of Hamm and Aleman (2000) was recently implemented in PORFLOW version 6.42. Example syntax corresponding to PORFLOW QA test problem 4.4 (Aleman 2007, Section 4.4) is

```
BOUNdary condition for P: Y+, FLUX, SEEPage function of P, qr=
8.3507E-02 cm_per_day, discharge slope= -1.0 per_day
```

where the bold characters distinguish active content from inline comments. Figure 2-1 compares simulation results from PORFLOW v6.42 to the analytic solution derived in Aleman (2007, Section 4.4). The analytic solution presented by Aleman (2007) as Equation (4.4.1) contains a typographical error and should read

$$h^2 = h_0^2 + (h_s^2 - h_0^2)\frac{x}{L_s} + \frac{Q_{src}L_s^2}{K}\left(\frac{x}{L_s}\right)\left(1 - \frac{x}{L_s}\right) \quad (1)$$

where $0 \leq x \leq L_s$. The missing subscript on L in the $Q_{src}L_s^2/K$ term created errors in Table 4.4.1 and Figure 4.4.5 of Aleman (2007). The correct values, those corresponding to Equation (1), are reflected in Figure 2-1. The agreement between the analytic solution and PORFLOW version 6.42 is excellent. The recharge-drain BC has been implemented in a numerically implicit manner, and the resulting convergence rate is fast as indicated by the convergence INDEX parameter in this snippet of code output:

```
*****************************************************************************
 TITLE: 4.4 Unconfined Aquifer Subject to combined recharge/drain BC
 *****************************************************************************

    STEP    INDEX  ITi ITo    HDP     PRP
 0 5.1E+07   1   1  2.12E+003  0.00E+000  0.00E+000  0.00E+000
 1 1.4E+05   1  10  2.12E+003 -1.85E-001 -1.85E-001  4.55E-014
 2   784.8   1  10  2.10E+003 -1.74E+001 -1.76E+001  6.17E-016
 33.5   1  10  2.10E+003 -1.24E-002 -1.76E+001  3.48E-018
 40.7   1   3  2.10E+003 -5.24E-005 -1.76E+001  7.04E-019
 50.4   1   1  2.10E+003 -5.57E-006 -1.76E+001  4.07E-019
 60.2   1   1  2.10E+003 -3.29E-006 -1.76E+001  2.26E-019
 70.1   1   1  2.10E+003 -1.94E-006 -1.76E+001  1.27E-019
 80.1   1   1  2.10E+003 -1.15E-006 -1.76E+001  6.72E-020
 90.0   1   1  2.10E+003 -6.76E-007 -1.76E+001  4.72E-020
100.0   1   1  2.10E+003 -3.99E-007 -1.76E+001  2.80E-020

 ============================================================================
```

A combined-drain BC has been implemented in the FACT and PORFLOW codes, and possibly the Amanzi code under development, but is not available in other groundwater flow simulation to the author's knowledge.

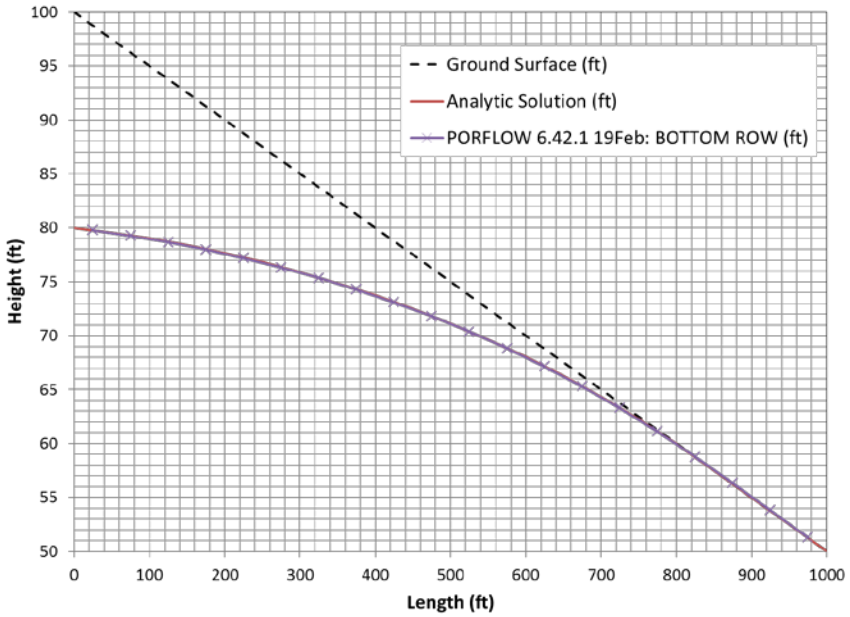
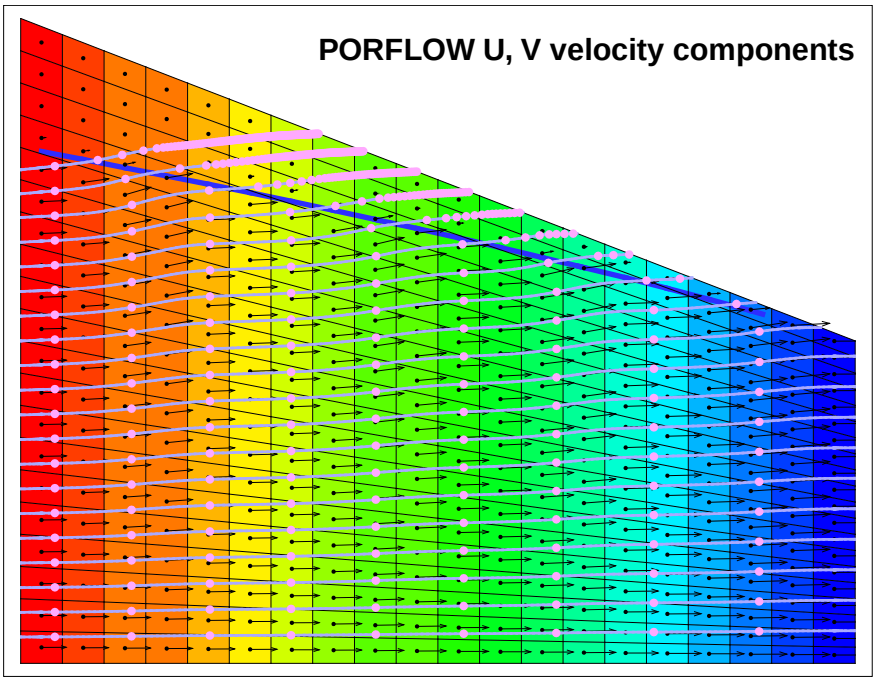


Figure 2-1. Comparison of hydraulic head from analytic solution and PORFLOW v6.42 for QA test problem 4.4 (Aleman 2007).

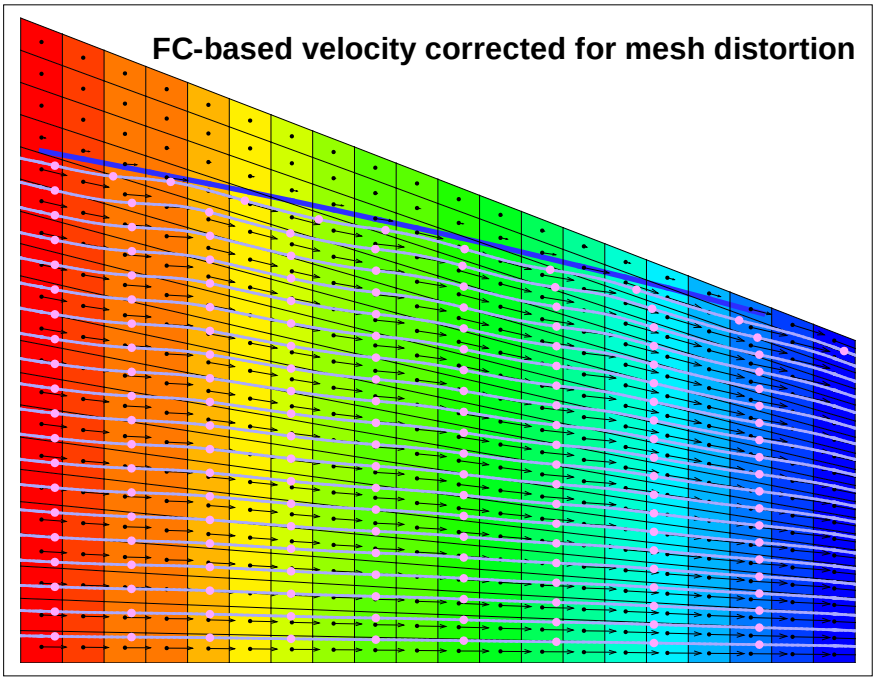
Although not directly pertaining to groundwater flow, a second relatively unique and desirable feature of PORFLOW is the ability to simulate radioactive decay chains, specifically progeny ingrowth in addition to first-order decay. For radiological Performance Assessments the ability to simulate radionuclide decay chains is required. Selecting PORFLOW as the groundwater flow simulator facilitates follow-on radionuclide transport simulations at the GSA scale. Such simulations can be anticipated to simulate seepline concentrations or define surface water source terms for a Composite Analysis. Selection of an alternative groundwater flow simulation code would require development of a translator to provide flow field information in a PORFLOW transport compatible format.

Resolved particle tracking deficiency: Particle tracking is routinely performed after a groundwater flow numerical simulation to better understand the dynamics of the flow field and/or as an indication of the trajectory and timing of advective solute transport. Particle tracks are computed by integrating the velocity field from cell to cell starting from designated seed (starting) positions. An accurate velocity field is required to attain accurate particle tracks. However, the PORFLOW (U, V, W) velocity components do not account for mesh distortion if present, or stated more precisely, grid cell faces that may lie outside an x, y or z plane in a Cartesian coordinate system. For such non-orthogonal grids, particle tracks deviate from true paths in proportion to mesh distortion.

Figure 2-2(a) illustrates this behavior for a 2D example involving a sloped ground surface and gridlines interpolated to conform to a flat bottom and the sloped upper boundary. The grid and problem statement are taken from PORFLOW test problem 4.4 (Aleman 2007) mentioned earlier, except that recharge is set to zero. In Figure 2-2(a) particle tracks generated by Tecplot (http://www.tecplot.com/) based on PORFLOW (U, V) are observed to angle upward and cross the water table, indicated by the heavy blue concave down line, whereas upper streamlines should instead follow the water table. Flach (2015) developed a means to rigorously compute velocity from the PORFLOW FC variable, defined as the volumetric flowrate crossing a cell face. The calculation method accounts for the orientation of grid faces to a Cartesian coordinate system, and thus produces accurate velocity vectors and particle tracks on both orthogonal and distorted meshes. Figure 2-2(b) illustrates particle tracking based on Flach (2015). The streamtraces are observed to conform to the water table as expected.



(a)



(b)

Figure 2-2. Particle tracking based on Darcy velocity (a) approximated by PORFLOW (*U*, *V*) and (b) rigorously defined from PORFLOW *FC* following SRNL-STI-2015-00115 (Flach 2015).

The current GSA/PORFLOW model exhibits mesh distortion because nominally horizontal grid surfaces are made to conform to undulating stratigraphic surfaces as illustrated in Figure 2-3. Similar grid distortion is anticipated in a new GSA groundwater flow model. The method described by Flach (2015) enables accurate particle tracking using Tecplot and PORFLOW FC output going forward, such that inaccurate particle tracking is no longer a PORFLOW related deficiency.

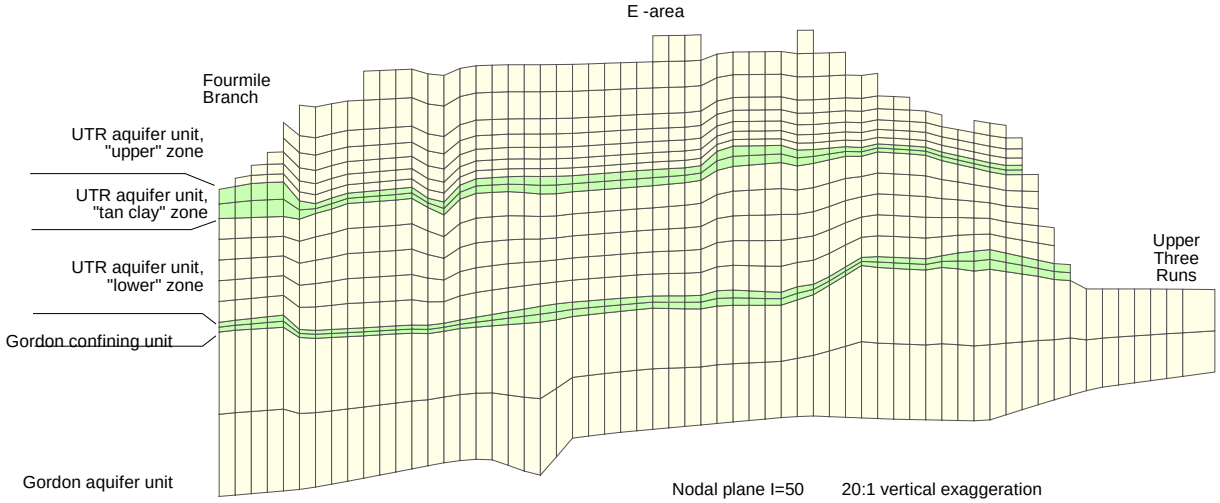


Figure 2-3. Grid cross-section through E-Area from the GSA/PORFLOW groundwater flow model (WSRC-TR-2004-00106 Figure 2-1).

PORFLOW experience and infrastructure: PORFLOW has been the software chosen for multi-dimensional solute transport numerical simulations supporting Savannah River Site Performance Assessments for over 20 years (Martin Marietta Energy Systems et al 1994, Appendix B). As a result of this experience SRNL PA analysts have gained extensive expertise with PORFLOW capabilities, nuances, and correct application to specific problems. A substantial array of supporting pre- and post-processing scripts and programs has been developed for input file creation, plotting, and diagnostics (e.g. Flach and Smith 2012). SRNL has also developed software for extracting sub-regions of a GSA/PORFLOW flow solution and refining the velocity and saturation fields for input to a local-scale, refined grid, transport simulation (Flach 2012). This approach avoids the need for an explicit local-scale flow simulation, maintains consistency with the GSA/PORFLOW model, and enables mesh refinement to avoid excessive numerical dispersion. An extensive software Quality Assurance testing (e.g. Aleman 2007) and documentation have been developed over the years, indicating satisfactory PORFLOW performance (Butcher 2011). Retaining PORFLOW as the GSA flow simulation code leverages general SRNL experience and existing infrastructure for efficiency and reduced project cost.

Continuity with previous modeling: A final benefit of retaining PORFLOW is continuity with previous GSA groundwater flow modeling. In particular, selecting PORFLOW will allow reuse of many project-specific components of GSA/PORFLOW model development for added efficiency. From a general stakeholder perspective, continuation with PORFLOW will minimize changes with respect to the current model, making the model update more evolutionary than alternative code selections.

Drawbacks of PORFLOW: While PORFLOW has strong advantages, certain drawbacks were considered prior to selecting PORFLOW. PORFLOW is commercial proprietary software and the source code is not accessible to the end-user, which can be useful to better understand code functionality or customize the software for project-specific needs. PORFLOW licensing involves an annual subscription cost and limits the number of simultaneous simulations and CPUs used. The licensing cost is somewhat mitigated by the fact that PORFLOW will continue to be used for PA transport simulations under current plans, so PORFLOW will be generally available regardless of code selection for a GSA model update. Limitations on PORFLOW instances and CPUs are an issue of more significant concern. Model calibration using an optimization algorithm is a form of inverse modeling and inherently requires many forward simulations to achieve model parameter convergence. Depending on the number of PORFLOW licenses purchased and potential demand from other projects, progress on model calibration could be significantly slowed. Should that prove to be the case, one option is to purchase additional “temporary” (using ACRi parlance; typically of 2-3 month duration) PORFLOW licenses at reduced cost to handle the peak load.

Other candidates: The preceding discussion focused on pros and cons of PORFLOW without explicit reference to other candidate codes. Table 2-1 compares PORFLOW to codes developed by the federal government and deemed to be competitive alternatives. All candidates except PORFLOW and possibly AMANZI lack a combined recharge-drain boundary condition. Alternatives to PORFLOW also lack existing SRNL software QA documentation and a supporting pre- and post-processing software infrastructure. STOMP version -W or –W-R and FEHM are relatively strong candidates, having no other apparent disadvantages. TOUGH codes do not appear to offer radionuclide transport beyond a simple parent-progeny pair. MODFLOW, developed by the United States Geological Survey, is the most popular groundwater flow modeling software in the United States and generally "considered to be the *de facto* standard code for aquifer simulation" (http://en.wikipedia.org/wiki/MODFLOW). The primary drawback of MODFLOW is the lack of a built-in capability for simulating solute transport with radionuclide decay. Transport codes that provide a direct linkage to MODFLOW output (e.g. MT3D and variants) do not appear to offer a general capability to simulate radionuclide chains, and a translator would be required to convert MODFLOW output to PORFLOW input. Although a "Research" version of AMANZI has been released, the code is still under active development and not sufficiently stable and documented to be considered viable at this time. The main advantages of the PORFLOW alternatives are the licensing arrangements: no-cost, no restrictions on the number of simultaneous simulations, and access to source-code in some cases.

Summary: On the balance, PORFLOW advantages were judged to significantly outweigh disadvantages. The primary advantage of PORFLOW is an existing SRNL support infrastructure, including SRNL software QA documentation, pre- and post-processing utilities, and extensive analyst expertise gained from two decades of use at SRNL. The primary disadvantage of using PORFLOW is licensing restrictions. License restrictions can be relaxed through the purchase of additional short-term licenses at reduced marginal cost. With this consideration, schedule and budget risk are deemed to be acceptable. Selection of a different flow simulation code was judged to compromise treatment of seepage faces, and involve significant effort (labor cost) to establish software QA documentation and reproduce existing pre- and post-processing tools developed for PORFLOW.

Table 2-1. Comparison of selected codes for potential GSA groundwater flow simulation.

Attribute	PORFLOW	MODFLOW	STOMP	TOUGH2	FEHM	AMANZI
Status	Released	Released	Released	Released	Released	Development
Primary/ baseline Version	Current version 6.42.x	MODFLOW-2005 v.1.11.00	STOMP-W	TOUGH2	FEHM V3	"Community" code release anticipated October 2015
Variants of interest	SRNL currently uses v6.30.2	MODFLOW-NWT MODFLOW-USG GSFLOW MODFLOW-LGR	STOMP-W-R	TOUGH+ iTOUGH	N/A	"Research" code release
Recharge-drain BC	Yes	No	No	No	No	Yes?
Radionuclide chain transport	Yes	No (flow only)	Yes	Two species (parent-progeny)	Yes	Yes?
User documentation	Yes	Yes	Yes	Yes	Yes	Yes?
Documented QA testing	Yes	Third party	Yes	Yes	Yes	Yes?
Licensing	Commercial	Open-source	No cost Gov't license	No cost Gov't license	No cost executable; source-code available	Open-source
Developer support	Included with annual license subscription	Minimal	Minimal	Minimal	Minimal	Uncertain
User community support/forum	None	Yes	No	Yes	No	No
Graphical user interface	ACRi	GMS and others	No	PetraSim	No	AKUNA (under development)
SRNL QA documentation	Yes	No	No	No	No	No
SRNL supporting software	Extensive	None	None	None	None	Limited

3.0 Code Selection for Flow Model Calibration

Several specialized inverse modeling codes exist for parameter estimation in groundwater applications, for example AQTESOLV to analyze aquifer tests (http://www.aqtesolv.com). For general parameter estimation in groundwater flow modeling, two codes appear to occupy the vast majority of the market share, PEST (http://www.pesthomepage.org) and UCODE (http://igwmc.mines.edu/freeware/ucode). Both codes are open-source, free of cost, and well documented. PEST appears to have undergone fairly continuous development with current version 13.3 being released in December 2014. UCODE releases have been much less frequent; UCODE 2005 was just superseded by UCODE 2014 released in January 2015.

Table 3-1 and Table 3-2 provide summary information for PEST and UCODE, respectively, reproduced from their websites. Both codes offer the key capabilities of interest for GSA flow modeling: parameter-estimation/calibration, prediction, and uncertainty analysis. Both codes perform non-linear regression using a weighted least-squares method, and provide methods for dealing with parameter non-uniqueness such as Singular Value Decomposition and Tikhonov regularization. Both codes interface with the flow simulation code through its existing input and output text file structures and formats. The relative technical merits of each software product have not been investigated in any depth for this study. Both codes offer the optimization capabilities needed to perform model calibration, making either code a suitable choice. However, PEST appears to have a significantly larger user base than UCODE. On this basis, PEST was chosen for initial GSA flow model calibration, with UCODE considered a fallback option if needed.

Table 3-1. Key attributes of PEST; reproduced from http://www.pesthomepage.org/Specifications.php (accessed 03Mar2015).

Category	Features
Operational Modes	Parameter estimation Predictive analysis Regularization Pareto
Parameter Estimation	Gauss Marquardt Levenberg with Broyden Jacobian updating Shuffled Complex Evolution Covariance Matrix Adaptation
Parameters	No upper limit on number of parameters Log-transformed Untransformed Fixed Tied to other parameters Parameter scaling and offsetting Arbitrary parameter transformation and mathematical manipulation Self-regularizing parameter bounds enforcement through temporary, sequential fixing
Observations	Individually weighted Covariance matrix can be supplied to grouped observations Objective function contributions calculated for individual observation groups Adjustment of observation group weight factors for equalization of contribution to objective function Computation of orthogonal "super observations" No limit to number of observations
Prior Information	Applied to individual parameters or to linear relationships between parameters Individually weighted Covariance matrix can be supplied to grouped prior information equations Objective function contributions calculated for individual prior information groups No limit to number of prior information equations
Regularization	Truncated singular value decomposition Tikhonov Pareto-adjustable Tikhonov Subspace-enhanced Tikhonov LSQR "SVD-Assist" All combinations of the above "Automatic user intervention"
Model Interaction	Writes model input files using templates of those files Reads model output files using instruction sets Runs model (or sequence of models) through system call Option to receive model-computed Jacobian matrix from model Parallelization of model runs across different nodes or machines

Category	Features
Derivatives	Two, three or five point finite difference stencil Parabolic, outside-points or best-fit options for three point stencil Maximum precision or minimum error variance options for five point stencil User-selectable relative or absolute parameter increments and/or combination of these Analysis of finite-difference derivatives integrity Partial detection and elimination of numerically-corrupted derivatives Computation of composite sensitivities Display, analysis and manipulation (including singular value decomposition) of (weighted) Jacobian matrix
Uncertainty Analysis	Linear over-determined Nonlinear over-determined through calibration-constrained predictive maximization/minimization Linear highly-parameterized parameter/predictive error variance assessment Linear highly-parameterized parameter/predictive uncertainty assessment Nonlinear, regularized, calibration-constrained parameter/predictive maximization/minimization Random parameter generation Monte Carlo analysis Post-calibration null-space Monte Carlo analysis "Predictive calibration" analysis Pareto-adjustable hypothesis testing
Uncertainty-Related	Parameter identifiability Relative parameter error variance reduction and uncertainty reduction Resolution matrix Parameter (group) contributions to predictive error variance Parameter (group) contributions to predictive uncertainty Worth of different new or existing measurements in reducing parameter/predictive error variance Worth of different new or existing measurements in reducing parameter/predictive uncertainty Solution and null space contributions to parameter/predictive error variance Optimality of singular value truncation for minimization of predictive error variance Inference statistics such as observation leverage, Cook's D, DFBETAS Kullback-Leibler (K-L) Information Loss Statistics
Other	Restart without loss of data User-intervention Formulation of equivalent linear model Formulation of input dataset for scaled parameters General manipulation of matrices and vectors Global Jacobian matrix assembly from submatrices Comprehensive checking of PEST input dataset for correctness and consistency Automatic generation of PEST input dataset
Operating System	PC or UNIX (source code provided for compilation under UNIX) 32 bit and 64 bit executables available for PC

Table 3-2. Key attributes of UCODE; reproduced from http://igwmc.mines.edu/freeware/ucode/ucode_2014.txt (accessed 03Mar2015).

UCODE_2014, with New Capabilities to o Define Parameters Unique to Predictions, o Calculate Weights using Simulated Values, o Estimate Parameters with SVD, o Evaluate Uncertainty with MCMC, o and More ABSTRACT: The UCODE_2014 report documents additions to the computer program UCODE_2005 and implemented in UCODE_2014. UCODE_2005 is described below. The new capabilities include support of parameters that are required for predictions but that had not been considered previously in model development. Examples of situations with such parameters are storage parameters when calibration conditions are steady-state and prediction conditions are transient, and transport parameters when calibration conditions involve only a flow field and prediction conditions include advective, advective-dispersive, or advective-dispersive-reactive transport. Second, weighting based on user-supplied coefficients of variation are supported more thoroughly in UCODE_2014 than in previous versions of UCODE and, we believe, any other available software package. Third, the use of singular value decomposition (SVD) for parameter estimation has been integrated into UCODE_2014 and the transparency offered to SVD users by sensitivity analysis is stressed. The implementation of SVD in UCODE_2014 is useful for estimating parameters in some circumstances, and guidance is provided for migrating to PEST when its unique capabilities are of interest. Inclusion of Markov-chain Monte Carlo (MCMC) uncertainty measures means that UCODE_2014 has three methods of uncertainty evaluation that proceed from (i) linear uncertainty intervals that are very computationally frugal (commonly 10s to 100s of parallelizable model runs) and depend on the model not being too nonlinear and errors being approximately Gaussian, to (ii) nonlinear uncertainty intervals with moderate computational demands (commonly 1,000s of model runs) and depend on model smoothness and Gaussian errors, to (iii) MCMC uncertainty intervals that are computationally demanding (commonly 10,000s of model runs and more) and few restrictive assumptions. Having this range of methods in one program encourages application and exploration of the entire range of methods. Auxiliary programs introduced since UCODE_2005 are described briefly. This includes three auxiliary programs: MMA for multi-model analysis, OPR-PPR for value of information measures, and Sim-Adjust for when simulated equivalents to observations cannot be calculated. Three graphical interfaces are also described: ModelMate for constructing and running applications of UCODE_2014, GW_Chart for evaluating model fit, sensitivity analysis results, and uncertainty measures, including support for the new capabilities, and enhancements to Model Viewer for plotting objective-function surfaces using the UCODE _sos data-exchange files. Two minor auxiliary codes were added: "concatenate_intconfpred" which concatenates results from multiple nonlinear uncertainty runs to facilitate plotting of nonlinear confidence intervals that were calculated in separate runs; and "convert_pest_prior_info" which reads a pest file, finds the prior items and uses them to create a UCODE Linear_Prior_Information input block. Instructions are provided for using UCODE_2014 with programs constructed using MATLAB and models run using graphical interfaces, using HYDRUS as an example. Example and test cases include surface-water and groundwater problems. UCODE_2014 is constructed in a modular fashion using JUPITER API conventions and modules.
UCODE_2014 IS AN ADVANCEMENT OF UCODE_2005, THUS THE FOLLOWING DESCRIPTION OF UCODE_2005 IS INCLUDED IN THIS FILE: UCODE_2005 and its six post-processors can be used with existing process models to perform sensitivity analysis, data needs assessment, calibration, prediction, and uncertainty analysis. Any process model or

set of models can be used; the only requirements are that models have numerical (ASCII or text only) input and output files, that the numbers in these files have sufficient significant digits, that all required models can be run from a single batch file or script, and that simulated values are continuous functions of the parameter values. Process models can include pre-processors and post-processors as well as one or more models related to the processes of interest (physical, chemical, and so on), making UCODE_2005 extremely powerful. An estimated parameter can be a quantity that appears in the input files of the process model(s), or a quantity used in an equation that produces a value that appears in the input files. In the latter situation, the equation is user-defined.

UCODE_2005 can compare observations and simulated equivalents. The simulated equivalents can be any simulated value written in the process-model output files or can be calculated from simulated values with user-defined equations. The quantities can be model results, or dependent variables. For example, for ground-water models they can be heads, flows, concentrations, and so on. Prior, or direct, information on estimated parameters also can be considered. Statistics are calculated to quantify the comparison of observations and simulated equivalents, including a weighted least-squares objective function. In addition, data-exchange files are produced that facilitate graphical analysis.

UCODE_2005 can be used fruitfully in model calibration through its sensitivity analysis capabilities and its ability to estimate parameter values that result in the best possible fit to the observations. Parameters are estimated using nonlinear regression: a weighted least-squares objective function is minimized with respect to the parameter values using a modified Gauss-Newton method or a double-dogleg technique. Sensitivities needed for the method can be read from files produced by process models that can calculate sensitivities, such as MODFLOW-2000, or can be calculated by UCODE_2005 using a more general, but less accurate, forward- or central-difference perturbation technique. Problems resulting from inaccurate sensitivities and solutions related to the perturbation techniques are discussed in the report. Statistics are calculated and printed for use in (1) diagnosing inadequate data and identifying parameters that probably cannot be estimated; (2) evaluating estimated parameter values; and (3) evaluating how well the model represents the simulated processes.

Results from UCODE_2005 and codes RESIDUAL_ANALYSIS and RESIDUAL_ANALYSIS_ADV can be used to evaluate how accurately the model represents the processes it simulates. Results from LINEAR_UNCERTAINTY can be used to quantify the uncertainty of model simulated values if the model is sufficiently linear. Results from MODEL_LINEARITY and MODEL_LINEARITY_ADV can be used to evaluate model linearity and, thereby, the accuracy of the LINEAR_UNCERTAINTY results. UCODE_2005 can also be used to calculate nonlinear confidence and prediction intervals, which quantify the uncertainty of model simulated values when the model is not linear. CORFAC_PLUS can be used to produce factors that allow intervals to account for model intrinsic nonlinearity and small-scale variations in system characteristics that are not explicitly accounted for in the model or the observation weighting.

The six post-processing programs of UCODE_2005 can use the results of other programs that produce the required data-exchange files.

UCODE_2005 and the other six codes are intended for use on any computer operating system. The programs consist of algorithms programmed in Fortran 90/95, which efficiently performs numerical calculations. The model runs required to obtain perturbation sensitivities can be performed using multiple processors. The programs are constructed in a modular fashion using JUPITER API conventions and modules. For example, the data-exchange files and input blocks are JUPITER API conventions and many of those used by UCODE_2005 are read or written by JUPITER API modules. UCODE-2005 includes capabilities likely to be required by many applications (programs) constructed using the JUPITER API, and can be used as a starting point for such programs.

4.0 Conclusions

PORFLOW and PEST have been selected for groundwater flow simulation and model calibration, respectively, for updating the current GSA/PORFLOW model supporting Savannah River Site Performance Assessments. Selection of PORFLOW provides a combined recharge-drain boundary condition for simulating variable seepline locations, leverages more than 20 years of experience with PORFLOW at SRNL, and provides continuity with previous PA modeling. License restrictions with PORFLOW are a drawback but not expected to significantly hinder timely progress. PEST was selected for model calibration based on its dominant market share in environmental applications. UCODE has been identified as a fallback option if warranted.

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