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SOFTWARE REQUIREMENTS DESCRIPTION FOR *xFlo*, AN EXTENSIBLE FLOW AND TRANSPORT MODEL FOR USE IN U.S. NUCLEAR REGULATORY COMMISSION PERFORMANCE CONFIRMATION OVERSIGHT

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1 INTRODUCTION

The computer code MULTIFLO (Lichtner, 1996; Painter, et al. 2001) was developed at the Center for Nuclear Waste Regulatory Analyses (CNWRA) to address drift-scale and repository-scale coupled thermal-hydrological-chemical processes that could affect the performance of the repository proposed for Yucca Mountain, Nevada. Over the past several years MULTIFLO has been used by CNWRA staff working on key technical issues. Version 2.0 of MULTIFLO, which is in the final stages of development, is anticipated to be the primary tool for independent thermal-hydrological and thermal-hydrological-chemical process modeling to support reviews of the potential repository license application.

Although the capabilities in MULTIFLO Version 2.0 are expected to be adequate for license review activities, potential future performance confirmation activities will require additional capabilities for independent process modeling. For example, simulation codes to support performance confirmation will need to be robust and efficient enough to operate in combination with inversion software to facilitate the analysis of field observations. Moreover, it is inevitable that the scientific understanding of subsurface flow and transport processes will evolve during a performance confirmation period, and capability to model additional physical and chemical processes will be required.

This software requirements description (SRD) document outlines capabilities for an extensible flow model (*xFlo*) that will satisfy the demands for U.S. Nuclear Regulatory Commission performance confirmation oversight. The *xFlo* system is envisioned as a set of reusable software components and a simulation code built from these components. This approach will produce a flexible and easy-to-maintain system that can be quickly extended or reconfigured in response to changing modeling needs.

The new *xFlo* code will have significant benefits. A new code based on an object-oriented software design and written in a modern programming language will be easier to modify and maintain, thus greatly decreasing code maintenance costs. Moreover, the adoption of a modern, flexible design will make it feasible to add new physics-based models, and thus keep pace with evolving understanding of the physical processes that may affect long-term repository performance.

The initial versions of the *xFlo* system can be applied to simulate and improve understanding of processes such as

- Isothermal and nonisothermal movement of water through unsaturated rock as liquid and vapor
- The evolution of temperatures in and near the emplacement tunnels
- The evolution of groundwater compositions near and within the engineered barrier systems

- Changes in porosity and permeability of the host rock resulting from mineral alteration and the resulting effect on fluid transport

- Transport of aqueous and gaseous radionuclides from the waste package

- Transport of radionuclides or introduced tracers in the saturated zone

2 SOFTWARE REQUIREMENTS

Decoupling of the generic numerical routines from the physics-based model is an important design consideration for *xFlo*. The *xFlo* system will be comprised of four generic classes, which will be implemented as FORTRAN modules. The four generic classes are

- GRID: data structures related to grid geometry and other model independent information

- STEPPER: advances the simulation by one time step

- SOLVER: numerical routines to solve sparse linear systems

- PHYSICS: encapsulates data and numerical routines relating to specific physical and chemical models

- Input and output routines will be implemented as subclasses of the PHYSICS class

The first three of the generic classes, representing the model-independent computational framework and numerical routines, are described. Requirements for four modules (SAT, UNSAT, TH, RT) derived from the PHYSICS class are then given.

2.1 Software Function and Technical Basis for the *xFlo* Computational Framework

Specific requirements for the model-independent computational framework are

(1) The software components will be written in FORTRAN.

(2) Encapsulation will be used where possible to facilitate component reuse.

(3) Spatial discretization will be based on the integral finite difference method (Narasimhan and Witherspoon, 1976) with arbitrary interblock connectivity to allow for structured or unstructured grids in multiple spatial dimensions.

(4) The system will support the dual continuum (Pruess and Narasimhan, 1985) and active fracture (Liu, et al., 1998) models.

(5) The system will support an arbitrary number of primary variables (degrees of freedom).

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(6) Options for time-stepping will include the fully implicit method with Newton iterations to resolve nonlinear terms in the equations and an explicit method.

(7) The Jacobian matrix required for the Newton method will be generated numerically by the perturbation method and will be stored in a sparse format.

(8) Iterative solution methods will be used to solve the sparse linear systems generated at each iteration in the Newton method.

(9) Time-dependent boundary conditions and sources will be accommodated.

(10) Output will be written at a set of user nominated target times.

(11) Dynamic memory allocation will be used throughout.

2.2 Software Function and Technical Basis for SAT Module

SAT will encapsulate physics models for saturated flow and heat transport. Specific requirements for the SAT module are

(1) It will be based on standard conservation equations for water in fully saturated media coupled with conductive and convective heat transport.

(2) Mass fluxes will be described by Darcy's law.

(3) The thermophysical properties of water will be based on tabulated values or accurate empirical fits.

(4) Full (cell-by-cell) heterogeneity for major physical properties will be supported.

2.3 Software Function and Technical Basis for UNSAT Module

UNSAT will encapsulate physics models for unsaturated flow in isothermal conditions. Specific requirements for the UNSAT module are

(1) It will be based on conservation equations for air and water as described in the MULTIFLO User Guide (Painter, et al., 2001).

(2) Mass fluxes will be described by the multiphase extension of Darcy's law combined with binary diffusion in the gas phase. Diffusion of dissolved air will also be included.

(3) The van Genuchten (1980) model and the Brooks and Corey (1964) model will be used to relate saturation, capillary pressure, and relative permeability.

(4) The equation-of-state for water will be based on tabulated values or accurate empirical fits.

(5) Full (cell-by-cell) heterogeneity for major physical properties will be supported.

2.4 Software Function and Technical Basis for TH Module

TH is the thermal-hydrological module which solves for two-phase nonisothermal flow. Specific requirements for the TH module are

(1) It will be based on conservation equations for air, water, and energy as described in the MULTIFLO User Guide (Painter, et al., 2001).

(2) The module will accommodate fully saturated, fully dry, and partially saturated conditions.

(3) Mass fluxes will be described by the multiphase extension of Darcy's law with binary diffusion in the gas phase. Diffusion of dissolved air will also be included.

(4) The van Genuchten (1980) model and the Brooks and Corey (1964) model will be used to relate saturation, capillary pressure, and relative permeability.

(5) The equation-of-state for water and the thermophysical properties of water will be based on tabulated values or accurate empirical fits.

(6) Full (cell-by-cell) heterogeneity for major physical properties will be supported.

2.5 Software Function and Technical Basis for the RT Module

RT is the multiphase, multicomponent reactive transport module.

(1) The governing equations for the RT physics module will be those developed by Lichtner (1996) and will include conservation equations for mass in aqueous, gaseous, mineral, and sorbed phases.

(2) The module will accommodate an arbitrary number of chemical species.

(3) The processes modeled will include advection, dispersion, diffusion, aqueous speciation, kinetic aqueous reactions, kinetic mineral forming/dissolving reactions, and nonequilibrium sorption processes.

(4) RT will accept temperature, liquid saturation, and flow velocity fields as calculated by the TH, SAT, or UNSAT modules.

(5) Changes in porosity and permeability associated with mineral precipitation or dissolution will be passed back to the TH, SAT, or UNSAT modules.

(6) Updating between the RT and Flow modules will be via the sequential noniterative method.

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3 TECHNICAL APPROACH

The project will be completed in seven phases:

(1) Detailed design of the system
(2) Implementation and testing of the model-independent part of the *xFlo* system
(3) Implementation and testing of the SAT module
(4) Implementation and testing of the UNSAT module
(5) Implementation and testing of the TH module
(6) Implementation and testing of the RT module
(7) Implementation and testing of the fully coupled *xFlo* with the TH and RT modules

3.1 Data Flow and User Interface

Data input and output will be through a series of ASCII files. Input will be in a keyword-driven format. Output shall be written in a format compatible with the Tecplot (Amtec Engineering, Inc., 2000) visualization code.

Any graphical user interfaces, preprocessing, postprocessing, or visualization functions will be handled in separate applications and are not covered by this SRD.

3.2 Hardware and Software Requirements

The programming language will be FORTRAN.

The target platforms are SUN and PC. The target operating systems are UNIX and Windows NT/95/98/2000.

3.3 Graphics Requirements

There are no special graphics requirements.

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