STATE-OF-THE ART THMC COMPUTATIONAL TOOLS AND POTENTIAL APPLICATIONS

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QUALITY OF DATA, ANALYSES, AND CODE DEVELOPMENT

DATA: No CNWRA-generated data are contained in this report.

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1 INTRODUCTION

The U.S. Nuclear Regulatory Commission (NRC) has long been interested in coupled thermal-hydrologic-mechanical-chemical (THMC) processes associated with geological disposal of high-level radioactive waste. In geological disposal of spent nuclear fuels and reprocessed high-level waste (HLW), including HLW glass, THMC conditions and processes in the engineered barrier system and near-field host rock are expected to evolve over time in response to (i) rewetting of the system after construction and waste emplacement, (ii) heat generated by spent nuclear fuel, (iii) stress perturbations imposed by the openings and buffer evolution, and (iv) (biogeo)chemical processes such as corrosion, dissolution, and precipitation that affect containment integrity and release modes. Although the relative importance of particular THMC processes will depend on the host rock environment, specific disposal setting and engineered barrier system, it is likely that coupling between some subset of THMC processes will play a role in overall disposal system performance.

There are numerous simulators that consider either coupled THMC processes or various subsets of the THMC processes. The capabilities of the existing codes are expanding rapidly with respect to (i) increased coupling of physical processes and (ii) increased analysis capabilities using parallel computation.

The three-year DECOVALEX–2015 program, where DECOVALEX stands for **De**velopment of **Co**upled Models and Their **Val**idation Against **Ex**periments (https://decovalex.org/), illustrates the variety of simulation codes used for coupled modeling. The NRC and Center for Nuclear Waste Regulatory Analyses (CNWRA®) analyzed coupled thermal-hydrologic-mechanical (THM) processes associated with a heater test in a half-scale tunnel located in the Mont Terri Rock Laboratory in Task B1 of DECOVALEX–2015. Task B1 considered the response of a swelling bentonite buffer and the surrounding argillaceous host rock in three contexts: (i) a pair of borehole heaters in saturated host rock, (ii) a column heater test performed on unsaturated buffer media, and (iii) the HE-E half-scale tunnel heater experiment.

Eight different modeling teams used seven different simulation schemes for Task B1. The NRC/CNWRA modeling work (Manepally et al., 2016; Ofoegbu et al., 2015; Stothoff et al., 2015) used xFlo (Stothoff and Painter, 2016) to calculate coupled thermal-hydrologic (TH) processes, and used FLAC (Itasca Consulting Group, 2011) to calculate the mechanical responses to changes in the TH state. Other teams used OpenGeoSys (Kolditz et al., 2014), EPCA3D (Pan et al., 2009a,b; Pan and Feng, 2013), TOUGH-FLAC3D (Rutqvist et al., 2002; 2014), COMSOL (COMSOL AB, 2013); THAMES (Ohnishi et al., 1985), and FLAC3D (Itasca, 2012).

Further illustrating the variety of coupling approaches that are available, Rutqvist (2017) identified 15 models that couple the TOUGH2 simulator (Pruess et al., 2012, 1999) with some type of geomechanical model, including the TOUGH-FLAC3D code and the TOUGH-ROCMECH code (Kim and Moridis, 2013). TOUGH2 is a widely used simulator modeling coupled non-isothermal multiphase processes in porous media for a variety of fluid combinations, providing flow and transport capabilities for a variety of coupled codes. The xFlo code is restricted to an air-water system but otherwise has similar computational strategies as TOUGH2.

A new THMC simulator, TReactMech, extends the capabilities of existing TOUGH-based codes, including TOUGH-ROCMECH, to consider fully coupled reservoir-scale THMC processes in a computationally enhanced parallel processing mode. NRC and CNWRA staff attended a training short course held October 10 through 12, 2018, at Lawrence Berkeley National

Laboratories, to become familiar with the capabilities of this state-of-the-art simulator. This report summarizes knowledge gained in the training course and subsequent assessments.

2 TREACTMECH CAPABILITIES

2.1 Overview

The TReactMech simulator is a fully coupled THMC simulator, adding parallel coupled continuum geomechanics capabilities into the parallel simulator TOUGHREACT V3.X-OMP (Sonnenthal et al., 2018, 2014). The TOUGH2 multiphase flow code (Pruess et al., 2012, 1999) was updated to accommodate the coupling.

The TReactMech simulator merges two independent simulators built upon TOUGH2 capabilities: TOUGHREACT and TOUGH-ROCMECH. TOUGHREACT (Xu et al., 2011, 2006) added process-level reactive transport modeling capabilities to TOUGH2, using TOUGH2 to handle the TH processes and a separate reactive transport module to handle the chemical (C) transport components (transport and reaction processes), including some biological processes. TOUGH-ROCMECH adds geomechanical modeling capabilities to TOUGH2, using TOUGH2 to handle the TH processes and a separate module (ROCMECH) to handle the mechanical (M) processes.

TOUGHREACT can simulate the TH processes and C processes independently, or can consider both together as a coupled problem. Like TOUGHREACT, TOUGH-ROCMECH can simulate the TH processes and M processes independently or as a coupled problem. These capabilities are combined to form the TReactMech simulator, which allows the equivalent of the TOUGHREACT and TOUGH-ROCMECH codes to be run separately or as a fully coupled simulation. This approach gives the flexibility of coupling with any combination of TH, M, and C processes.

The TReactMech code uses the sequential non-iterative (SNI) approach (Figure 1) to step through time, with a hybrid parallel computation approach. The SNI approach comprises the following calculation steps

- The TH module solves for fluid flow and heat transport over the time step
- The M module updates the stresses and strains to reach a new equilibrium condition using the updated fluid pressures and temperatures
- Aqueous and gaseous species are transported with the updated flows
- Mineral-water-gas reactions are calculated
- The porosity, permeability, and capillary pressure relationships are updated
- The next TH step begins

In practice, only a user-selected fraction (normally 0.5 to 0.25) of the cumulative incremental changes to the rock hydraulic properties are applied during the next time step; therefore, several time steps are needed to fully accommodate incremental changes. A sudden change in porosity or permeability may create a rapid, large fluid pressure change in a system saturated with a nearly incompressible fluid. Spreading the incremental changes in hydraulic

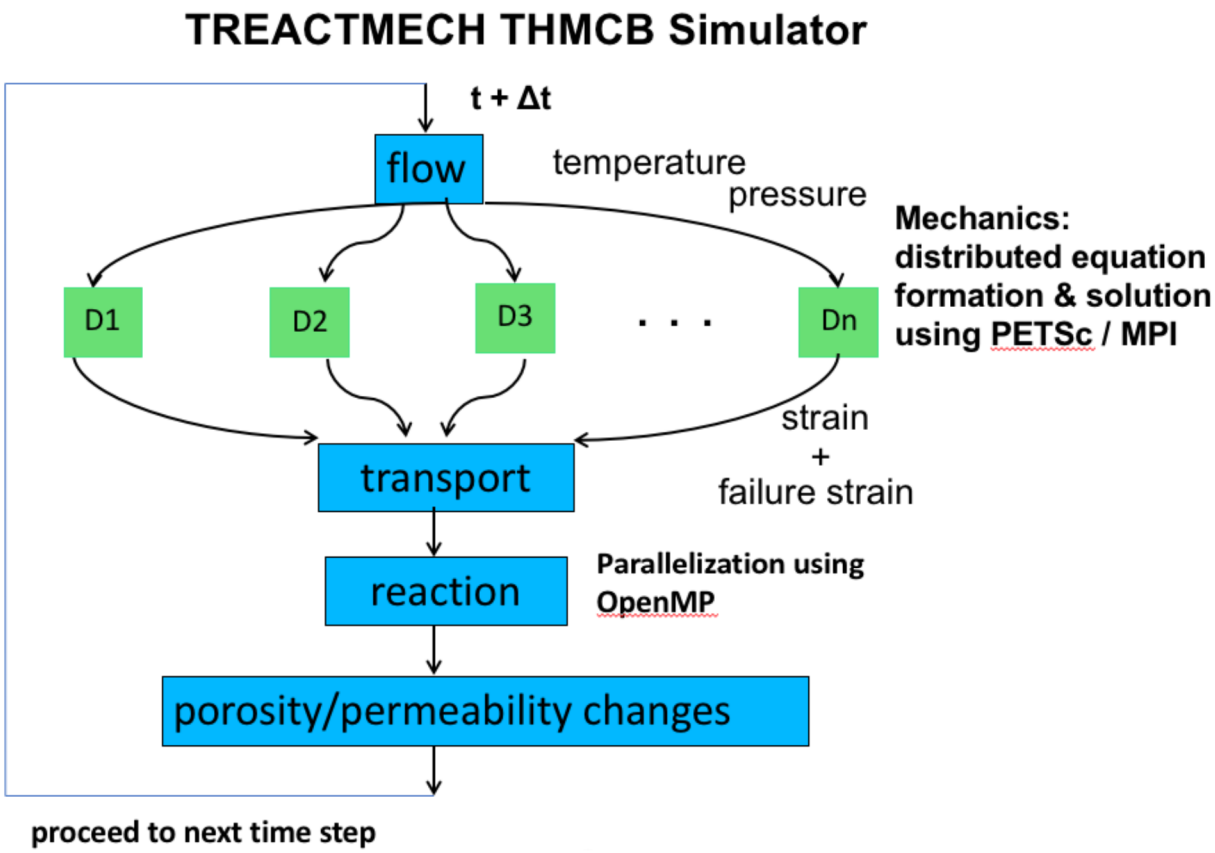

Figure 1. TReactMech flowchart (reproduced from Figure 1 of Smith and Sonnenthal, 2018).

properties over a number of time steps improves TH convergence rates by reducing the size of transient pressure fluctuations, at the cost of smearing coupled responses out over time. Both the TH and transport calculations are currently performed using an approach with a sequential solver on a single processor. The stress/strain equations are solved in parallel using functionality provided by the Portable, Extensible Toolkit for Scientific Computation (PETSc) with the Message Passing Interface (MPI). The reactive chemistry calculations are performed in parallel using OpenMPI. PETSc (https://www.mcs.anl.gov/petsc/index.html) and OpenMPI (https://www.open-mpi.org/) are both open source. The current code version uses PETSc V3.9 and OpenMPI V3.0.1.

The PETSc package is popular for providing scalable parallel computational capabilities for a wide variety of numerical simulators. Examples of codes for geoscience applications include PFLOTRAN (Lichtner et al., 2017; Hammond et al., 2012), MIN3P-THCm (Su et al., 2017), and OpenGeoSys (Wang et al., 2014).

2.2 Code Structure

The input files for TReactMech follow the modular structure of the code. A separate control file is provided for the TOUGH, React, and ROCMECH modules, as well as input files describing module-specific parameters, initial conditions, and boundary conditions.

The gridding files are common to all modules. When TOUGHREACT thermal-hydrologic-chemical (THC) simulations are run, the gridding is based on the requirements for TOUGH2, which is an integrated finite volume model based on grid cells and one-dimensional links between cells. The shape of the grid cells is not considered in the finite volume formulation, providing considerable flexibility in gridding. The TOUGHREACT model handles anisotropic permeability by providing three permeability values per grid cell, with the user specifying the permeability that is used for each connection between grid cells, updating the original TOUGH2 approach of using a single permeability value per grid cell. This approach for representing anisotropy is most accurate when the grid and flow are aligned with the principal directions of anisotropy. Thermal conductivity and diffusion of transported constituents are represented with a single conductivity/diffusion coefficient per grid cell, thus these parameters are not represented as anisotropic.

The ROCMECH module solves the stress equations using a finite-element model. The current implementation is based on quadrature of the governing equations at six points inside three-dimensional (3-D) topologically cubic elements (eight corner nodes), with the stresses converted to equivalent forces at the nodes in order to calculate displacement. The current mesh is restricted to 3-D right-rectangular prism elements for all geomechanics calculations. This approach leads to a grid that is in essence a finite difference grid; all grid cells can be represented with an index for the row, column, and layer. Corner nodes for the elements are used to define displacements and stresses in geomechanical calculations, and are not used in TOUGHREACT calculations. The code is designed for large field-scale geothermal problems, with the grid aligned roughly with the principal stress directions, and the boundary conditions assume that the normal to the grid is an axis of principal stress. In order to maintain compatibility during geomechanical coupling, the TOUGHREACT modules are also restricted to topologically cubic grid cells, which may place limits on flexibility for representing interfaces.

The ROCMECH module is linked to the TOUGHREACT modules by couplings between the fluid pressure and temperature state variables and the parameters affecting fluid flow. Changes in fluid pressure and temperature affect the volumetric stress in the ROCMECH module, while changes in stress and strain are linked to changes in porosity. Reactive transport also affects porosity through mineral precipitation and dissolution. Changes in porosity are linked to changes in permeability, with both changes feeding back into flow.

2.3 Conceptual Approaches for Geomechanical Modeling

The ROCMECH module currently is based on the conceptual model of an equivalent continuum of fractures and matrix, reflecting a development background strongly affected by geothermal applications. In this conceptual model, flow is governed by an equivalent permeability and porosity representing the combination of fracture and matrix properties. The geomechanical formulation is based on a 3-D continuum finite-element model with full 3-D stress calculations and plastic deformations resulting from shear and tensile failures (Kim et al., 2012, 2015; Smith et al., 2015). The formulation maps the cells of the TOUGHREACT mesh to the interior of the ROCMECH elements, and assumes that temperature and pressure are scalar values within each element (i.e., constant within the element) while stress and strain are represented as 3 × 3 tensors.

In geothermal applications, equivalent permeability is often dominated by higher-permeability fractures embedded in a low-permeability matrix, while the porosity is often dominated by the matrix. The TReactMech code tracks changes to the fracture and matrix properties separately, then aggregates the properties when passed to other modules.

The stress/strain relationship is assumed to be elastic until failure occurs. The Mohr-Coulomb model is used to calculate shear and tensile failures. During failure, displacements are adjusted to maintain the stress state on the failure envelope. Changes in displacement result in changes in porosity. These porosity changes preferentially open and close the fractures, depending on the direction of principal stresses relative to the orientation of the fracture sets. Increased compression perpendicular to a fracture set reduces the fracture porosity, and decreased compression increases the fracture porosity. Shear along the fracture plane also is accommodated.

Several relationships are available to link the change in fracture porosity to fracture permeability. Fracture flow resistance is often described using a cubic law or similar nonlinear relationship between aperture and transmissivity (e.g., permeability multiplied by aperture). The ROCMECH module assumes that fracture aperture is proportional to fracture pore volume.

2.4 Comparison to Current xFlo-FLAC Model Approach

The current xFlo-FLAC approach is broadly similar to the THM components of TReactMech. Development of xFlo was patterned after TOUGH2, so the TH model components are inherently very similar. FLAC uses an integrated finite difference approach based on quadrilateral elements to solve geomechanics problems (FLAC3D uses hexahedral elements), while ROCMECH is based on hexahedral finite elements. Both FLAC and ROCMECH can be run using multiple processors.

The current xFlo-FLAC implementation uses FLAC to solve for an equilibrium set of strains based on changes to the applied volumetric stresses from pressure and temperature changes, similar to TReactMech. The xFlo-FLAC implementation only considers elastic deformation. The plastic behavior in the variable saturation MCUS model developed for FLAC is based on the yield function in the modified CAM-Clay model for saturated clay soils, which considers plastic behavior with the Mohr-Coulomb theory, similar to the TReactMech model.

Some aspects of the model implementations are quite different, reflecting the different emphasis during applications. The xFlo-FLAC model has an emphasis on allowing conceptual model exploration, especially with respect to the interactions between engineered components and the near field, while the TReactMech model was developed largely in the context of simulating reservoir behavior with less focus on engineered components. FLAC was developed to simulate a variety of geomechanical processes, ranging from elastic deformation to elastic-plastic deformation to viscous creep, while the ROCMECH model is more focused on representing fractured and faulted hard rock reservoirs.

The implementation of coupling between the TH and M modules is substantially different for the two codes. TReactMech couples the TH and M modules each time step, with the coupling coded in Fortran. With all coding in Fortran, data can be maintained in memory, minimizing communication (i.e., information transfer) overhead.

The analogous coupling between the TH module (xFlo) and M module (FLAC) is provided with a Matlab-based interface. Matlab (Mathworks, 2015) is a commercially available high-level language and interactive environment for numerical computation, visualization, and programming. The Matlab-based interface provides an additional time-stepping strategy, intended to reduce the frequency that the xFlo and FLAC modules exchange data, and a capability to nest xFlo grid cells inside FLAC cells. The second time-stepping strategy permits the TH and M modules to hopscotch in time and allows several xFlo time steps before

exchanging information to spread some of the communication overhead. The hopscotch approach uses data from several past TH exchange times to project the TH results forward half a time step to the end of the M time step, and uses data from several past M exchange times to project the M results forward half a time step to the end of the TH time step.

The Matlab interface coupling xFlo with FLAC uses files to transfer inputs and outputs between the interface and xFlo, and between the interface and FLAC. Transferring data to and from the Matlab interface imposes larger communication overhead than the TReactMech strategy, but the implementation allows a substantial flexibility in exchange by allowing all input parameters, sources, and boundary conditions to be manipulated based on the current set of state variables. The Matlab interface provides a programmable workspace for the user to define the input parameters for each code, using Matlab-interpreted commands to interpret commands provided in the Excel® input file. With this approach, complex constitutive relationships describing input parameters can be coded and transparently archived in the input spreadsheet without modifying the xFlo code or FLAC constitutive modules.

The xFlo-FLAC modeling approach is also conceptually similar to the TOUGH-FLAC3D coupling approach (Rutqvist, 2017), although the implementation is quite different. The TOUGH-FLAC3D implementation uses the FLAC3D interface to develop the grid and model inputs. The implementation uses code developed in the FISH language to port the model to TOUGH2 and adds geomechanical constitutive models as dynamic link library files coded in C++.

3 POTENTIAL APPLICATIONS IN HIGH-LEVEL WASTE DISPOSAL

The mechanical component of the TReactMech code currently considers elastic deformations and associated changes to matrix and fracture properties, including plastic deformation resulting from shear and tensile failure. This type of mechanical model is appropriate for hard rock reservoir applications, but may be poorly suited to materials that exhibit significant plastic deformation (e.g., clay) or creep (e.g., salt). The developers are considering adding these additional mechanical behaviors to the code in future work.

The capabilities of the code are well suited to considering near- and far-field THMC processes in a geologic system with hard or brittle rock, such as an indurated volcanic or sedimentary rock. The current code restriction of approximately orthogonal gridding constrains how a curved interface, such as the interface between the host rock and a drift or borehole, can be represented. Curved interfaces may require “stair-stepped” grids along the opening, which may influence flow across the interface and may create anomalous stress concentrations. The influence of stair-stepped gridding on flow near an opening would be more pronounced in a partially saturated environment than a saturated environment, because of potential contrasts in capillary pressure.

The TReactMech code currently may be less suited to host environments that exhibit substantial plastic deformation that is not related to opening and closing of fractures. For example, the HE-E half-scale tunnel heater test suggested that plastic deformation may be an important process affecting fluid flow near the tunnel in the Opalinus Clay, an argillaceous formation (Stothoff et al., 2016). It is not clear that the current constitutive models in the TReactMech code would represent this type of plastic deformation. However, there is no inherent limitation in the TReactMech code that would preclude adding an appropriate constitutive model.

The TReactMech code may require additional work in order to represent host environments that exhibit substantial viscoelastic deformation, because the modeling approach assumes that the geologic medium reaches an equilibrium strain during each time step. Media such as salt continue to deform over time even with a constant applied stress, and the deformation is not necessarily related to fracture characteristics. The current TReactMech code would not be capable of representing the closing of a cavern opening in salt, for example. Again, there is no inherent limitation in the TReactMech code that would preclude adding an appropriate constitutive model.

The TReactMech code would require adding a constitutive model to represent swelling buffer materials based on bentonite. However, swelling in part depends on the chemical composition of the pore waters, and the TReactMech code should be fully capable of handling the chemical component of swelling in constitutive model. Furthermore, the inherent TOUGH2 capabilities for modeling multi-porosity media should allow the TReactMech code to be fully capable of handling a constitutive model with multi-porosity media, such as granular bentonite pellets.

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