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THERMO-HYDRO-MECHANICAL MODELING OF WORKING FLUID INJECTION AND THERMAL ENERGY EXTRACTION IN EGS FRACTURES AND ROCK MATRIX

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ABSTRACT

Development of enhanced geothermal systems (EGS) will require creation of a reservoir of sufficient volume to enable commercial-scale heat transfer from the reservoir rocks to the working fluid. A key assumption associated with reservoir creation/stimulation is that sufficient rock volumes can be hydraulically fractured via both tensile and shear failure, and more importantly by reactivation of naturally existing fractures (by shearing), to create the reservoir. The advancement of EGS greatly depends on our understanding of the dynamics of the intimately coupled rock-fracture-fluid-heat system and our ability to reliably predict how reservoirs behave under stimulation and production.

Reliable performance predictions of EGS reservoirs require accurate and robust modeling for strongly coupled thermal-hydrological-mechanical (THM) processes. Conventionally, these types of problems have been solved using operator-splitting methods, usually by coupling a subsurface flow and heat transport simulators with a solid mechanics simulator via input files. An alternative approach is to solve the system of nonlinear partial differential equations that govern multiphase fluid flow, heat transport, and rock mechanics simultaneously, using a fully coupled, fully implicit solution procedure, in which all solution variables (pressure, enthalpy, and rock displacement fields) are solved simultaneously.

This paper describes numerical simulations used to investigate the poro- and thermal-elastic effects of working fluid injection and thermal energy extraction on the properties of the fractures and rock matrix of a hypothetical EGS reservoir, using a novel simulation software FALCON (*Podgorney et al.*, 2011), a finite element based simulator solving fully coupled multiphase fluid flow, heat transport, rock deformation, and fracturing using a global implicit approach. Investigations are also conducted on how these poro- and thermal- elastic effects are related to fracture permeability evolution.

INTRODUCTION

Numerical modeling has played an important role in understanding the behavior of geothermal systems for nearly half a century. While the ability to rigorously describe key controlling physics remains imperfect, there have been significant advances in recent decades. These advances are related to the exponential growth of computational power and the development of more accurate equations of state (*Wagner et al.*, 1997; *Croucher and O'Sullivan*, 2008;

IAPWS, 2008), improvements in the ability to represent heterogeneity and reservoir geometry (*Chacon and Lapenta*, 2006; *Kirk et al.*, 2006), and more robust computational schemes (*Heroux et al.*, 2008; *Knoll and Keyes*, 2004; *McHugh and Knoll*, 1994). In recent years, engineered (or enhanced) geothermal systems (EGS) have been proposed as a way to bring additional geothermal resources online; however, simulating EGS reservoir creation and operation poses additional, and very significant, computational challenges, as EGS is based on dynamic changes in fracture permeability that the current generation of continuum or dual-continuum hydrothermal models are ill-equipped to describe.

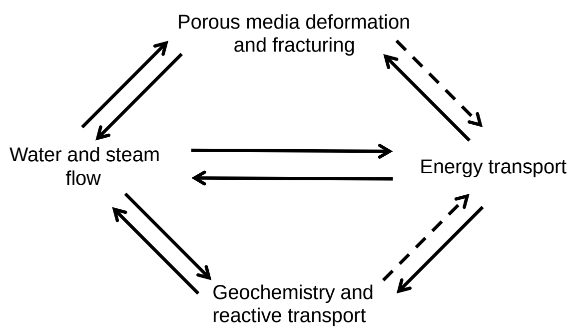


Figure 1. Strong nonlinear couplings related to geothermal systems, after Ingebritsen et al. (2008).

Multiphase fluid flow, energy transport, geomechanical deformation (and potential fracturing), and geochemically reactive transport in geothermal reservoirs are indeed a multiphysics problem in which controlling physics are all tightly coupled together (Figure 1). The feedbacks between flow-transport, equations of state, and changes of permeability and porosity due to geomechanical deformation and geochemical reactions render the system of governing partial differential equations strongly nonlinear. The ability to accurately model these tightly-coupled physics that control geothermal reservoir creation and operation are paramount for large scale implementation of EGS.

Examining coupled physics for fluid flow, energy transport, and geomechanical deformation is a relatively new area for the geothermal community; however, simulating coupled problems has been an important topic of study in the reactive transport community for decades. Yeh and Tripathi (1989) and Steefel and MacQuarrie (1996), cite three major approaches that differ in the way coupling transport and reaction have been considered for reactive transport modeling: (1) Globally Implicit Approach (GIA) that solves all governing nonlinear equations simultaneously at each time step using various forms of Newton's method, (2) sequential iteration approach (SIA) that subdivides the reactive transport problem into transport and reaction sub-problems, solves them sequentially, and then iterates, and (3) sequential non-iteration approach (SNIA) that solves the transport and reaction problems sequentially without iteration, which is often referred as operator-splitting. The operator-splitting approach is perhaps the simplest to implement and requires the least computational resources in terms of the memory and CPU time; thus, it became the method of choice for subsurface reactive transport modeling during the past three decades. Examples of reactive transport simulators that utilize the operator-splitting approach include the widely used STOMP (*White and McGrail*, 2005) and TOUGHREACT (*Xu et al.*, 2004) codes. One recent geothermal example of the SNIA approach is presented by Rutquist et al. (2002), in which the widely used flow and heat transport simulator TOUGH2 (*Pruess et al.*, 1999) is coupled to the commercial rock mechanics simulator FLAC (*Itasca*, 1997) via input files.

One potential drawback of operator-splitting approaches is the splitting error, when the physics (either reactions-transport or flow-mechanics) are tightly coupled, the solution can become inaccurate and require very small time steps (*Valocchi et al.,* 1981). For most potential EGS reservoirs, fluid flow, heat transport, and rock deformation will be strongly nonlinearly coupled. The changes in flow and energy transport properties due to fracturing and/or dissolution add further complexity and nonlinearity to the problem. For such situations, the global implicit approach (GIA) solves all solution variables simultaneously during each time step by seeking the solution of a large system of nonlinear equations via some form of Newton's method and is a more robust solution than the other two approaches (*Chacon and Lapenta*, 2006; *Hammond et al.,* 2002; *Molins et al.,* 2004).

One potential limitation of the GIA approach is the need to compute, store and invert the Jacobian matrix. This could become problematic for large systems that would be expected for reservoir-scale geothermal problems. As the number of solution variables grows, the matrix holding the Jacobian entries also grows. The increased size of the Jacobian matrix results in greater memory usage and more CPU time to solve the resulting system of linear equations within the Newton iterations. For highly nonlinear processes involving strong fluid-reservoir interactions and significant changes of flow and transport properties due to fracturing, the true Jacobian is often difficult to describe in analytical formulas. For reasons such as these, during the past three decades, despite its numerical merits of greater robustness and the ability to take larger time steps, the fully-coupled GIA method was considered to be too CPU-time and memory-intensive (*Yeh and Tripathi,* 1989) or to be computationally inefficient (*Steefel and MacQuarrie,* 1996). It has been used primarily only as a research tool for small one- or two-dimensional problems with a few thousands of unknowns. Since the first attempts of implementing the GIA approach in the early 1980s (*Valocchi et al.,* 1981; *Miller and Benson,* 1983), only a handful of examples based on this approach have been reported in the literature, compared with numerous examples of applications based on an operator splitting approach *(Xu et al.,* 2006; *Yeh et al.,* 2004; *Rutqvist et al.,* 2004).

Reliable reservoir performance predictions of enhanced geothermal reservoir systems will require accurate and robust modeling for the coupled thermal-hydrological-mechanical processes. As stated above, these types of problems are solved using operator-splitting methods, usually by coupling a subsurface flow and heat transport simulator with a solid mechanics simulator via input files. An alternative is to solve the system of nonlinear partial differential equations that govern the system simultaneously using a fully coupled solution procedure for fluid flow, heat transport, and solid mechanics using a GIA approach. This procedure solves for all solution variables (fluid pressure, temperature/enthalpy and rock displacement fields) simultaneously, which leads to one large nonlinear algebraic system that is solved using a strongly convergent nonlinear solver. Developments over the past 10 years in the area of physics-based conditioning, strongly convergent nonlinear solvers (such as Jacobian Free Newton methods) and efficient linear solvers (such as GMRES), make this approach competitive.

In this paper, we describe the application of a globally implicit geothermal reservoir simulator, as applied to EGS reservoir simulations, using the INL code **F**racturing **A**nd **L**iquid **CON**vection, FALCON (*Podgorney et al.,* 2011).

REVIEW OF MATHEMATICAL MODELS AND GOVERNING EQUATIONS

Mathematical models describing geothermal systems and geomechanics can be found in the literature. This section will only briefly summarize the derivations described in detail in the literature for geothermal systems (e.g., *Faust and Mercer* 1979a,b; *Brownell, et al*., 1977) and geomechanics (see *Jaeger at al*, 2007). Here, we will focus our discussion on the unique aspects of coupling the governing equations for fully coupled implicit solutions. The following paragraphs briefly present conservation equations for the mass, momentum, and energy.

For water and steam to coexist system, the pressure-temperature equation is not appropriate, because there should be one independent intensive variable according to Gibbs phase law. To simulate the 2-phase water-steam system, the independent variables in the mass and energy equations are chosen as pressure (P) and mass averaged enthalpy (H), which is defined as:

$$\mathbf{H} = \rho_w s_w H_w + \rho_s s_s H_s$$

Similarly, the mass averaged density ρ is given by:

$$\rho = \rho_w s_w + \rho_s s_s$$

The mass and energy conservation equations are read as

$$\frac{\partial(n\rho)}{\partial t} + \nabla\cdot(\rho_w \mathbf{q_w} + \rho_s \mathbf{q_s}) - \acute{q} = 0$$

where q is the total source strength of water component, in unit of kg/s. The water and steam flux q_w and q_s are calculated by Darcy's law:

$$\mathbf{q_w} = -\tau_w k_{rw} \cdot (\nabla p_w - \rho_w g \nabla z)$$

$$\mathbf{q_s} = -\tau_s k_{rs} \cdot (\nabla p_s - \rho_s g \nabla z)$$

where k_{rw} and k_{rs} are the relative permeability of water and steam phase, $\tau_w = k/\mu_w$, $\tau_s = k/\mu_s$, μ_s is the steam viscosity, other notations are the same as above. The capillary pressure between water and steam phase is omitted for simplicity.

The energy balance for the pressure-enthalpy formulation is given by

$$\frac{\partial[nH + (1-n)\rho_r c_r T]}{\partial t} - \nabla\cdot(K_m \nabla T) + \nabla\cdot(\rho_w H_w \mathbf{q_w} + \rho_s H_s \mathbf{q_s}) - \acute{Q} = 0$$

with all quantities defined above.

Geomechanics of the system is described as follows

$$\rho\frac{\partial^2 \mathbf{u}}{\partial t^2} - \nabla\cdot\sigma - \rho\mathbf{g} - \alpha\nabla p - \beta K \nabla T = 0,$$

where u is the displacement vector (3 component), σ is the second-rank stress tensor (with six unknown components), g is the body force (i.e., gravity), α is the Biot effective stress coefficient and β is the thermal expansion coefficient. The preceding equation is a momentum conservation equation based on the classical linear thermoporoelasticity theory and provides stress equilibrium for a coupled thermal-hydro-mechanical (THM) problem.

The THM equation presented above is the general governing equation for thermoporoelastic problems, and needs stress-strain law for closure. In FALCON, we adopted linear elasticity and assumed infinite small strain that is often adopted in classical linear elasticity theory.

Using linear elasticity theory, it can be then written in the following displacement form

$$\rho \frac{\partial^2 \mathbf{u}}{\partial t^2} - B^T D B \mathbf{u} - \rho \mathbf{g} - \alpha \nabla p - \beta K \nabla T = 0,$$

with

$$B = \begin{pmatrix} \partial_x & 0 & 0 \\ 0 & \partial_y & 0 \\ 0 & 0 & \partial_z \\ \partial_y & \partial_x & 0 \\ 0 & \partial_z & \partial_y \\ \partial_z & 0 & \partial_x \end{pmatrix}$$

$$D = c_1 \begin{pmatrix} 1 & c_2 & c_2 & 0 & 0 & 0 \\ c_2 & 1 & c_2 & 0 & 0 & 0 \\ c_2 & c_2 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & c_3 & 0 & 0 \\ 0 & 0 & 0 & 0 & c_3 & 0 \\ 0 & 0 & 0 & 0 & 0 & c_3 \end{pmatrix}$$

and

$$c_1 = \frac{E(1-\nu)}{(1+\nu)(1-\nu)}, c_2 = \frac{\nu}{(1-\nu)}, c_3 = \frac{1-2\nu}{2(1-\nu)},$$

here E and ν are Young's modulus and Poisson's ratio of the rock. It is worth noting that FALCON code has an option to use deformable mesh and large strain formulations.

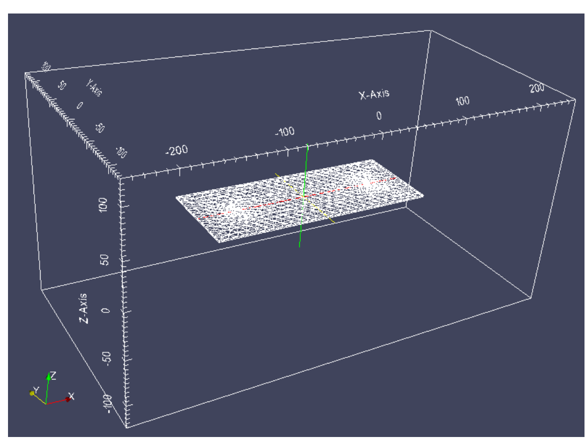
PROBLEM DESCRIPTION AND SETUP

To examine the effects of coupled THM processes on working fluid injection and thermal energy extraction in EGS reservoirs, we have created a hypothetical EGS reservoir with several fracture densities and fracture orientations, and have simulated fluid flow, energy transport, and thermal-poroelastic evolution in the reservoir using the FALCON code. The numerical results are compared the numerical solution with the Gringarten solution for the simplest case.

For this example, the level of coupling and controlling physics included in the simulations were increased incrementally; beginning with fluid flow and enthalpy transport only, and culminating with fully coupled THM simulation with stress-dependent permeability and porosity. In all cases we included pressure and temperature dependent fluid density and viscosity. Figure 2 below shows the simplest problem geometries, a single horizontal fracture zone (top) and a small fracture network consisting of two horizontal and one vertical fracture. For these simulation cases, the fracture zones are implemented at discrete areas with the finite element mesh with strong contracts in permeability, while still being considered as a porous media.

The simulated fracture zones are embedded in a low permeability porous matrix. Figure 2 also shows the mesh used to discretize the fracture zones within the porous matrix and the overall dimensionality of the problem, with is 500m X 250m X 250m. The total number of finite elements used for the simulations varied from approximately 80,000 to in excess of 200,000, with nearly 5 million degrees of freedom for the most complex simulations.

At the time of writing the paper, several additional fracture networks/meshes were under construction and will be presented in detail at the Workshop.



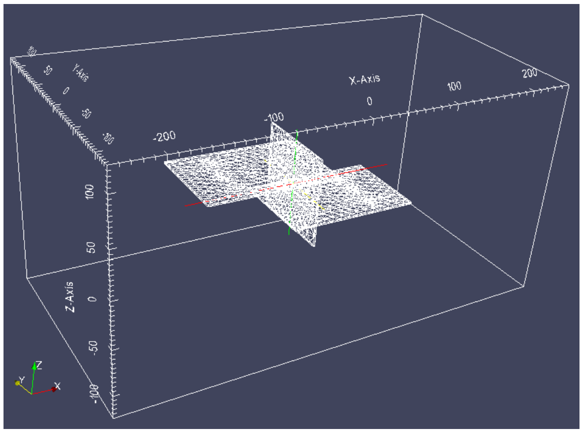


Figure 2. Three-dimensional mesh for the simplest fracture flow problems under consideration.

Table 1 below lists the property set values used in the simulations. Simulation run times were set between 1 and 10 years, injecting 100 ^{o}C water into an initially 200 ^{o}C reservoir. Initial pressure in the reservoir was set to 18.5 MPa, with an overburden stress of 25 MPa and lateral confinement of 12.5 MPa. Temperature and enthalpy are fixed at all outer surfaces of the model domain, and the effects of gravity have been neglected.

Table 1: Selected material property values used in the simulations.

Property	Matrix Domain	Fracture Domain	Units
Permeability	1e-16	1e-12	m^2
Porosity	0.1	0.1	--
Thermal Conductivity	2.5	25	W/m K
Young's Modulus	1.5e10	1.5e10	Pa
Thernmal Expansion Coef.	2.0e-6	2.0e-6	1/K
Poissons Ratio	0.3	0.3	--

PRELIMINARY RESULTS

At the time of Workshop submission deadline, most of the simulation cases were incomplete, therefore this section will only present a brief highlight of the preliminary results to date, with the detailed results being presented at the Workshop.

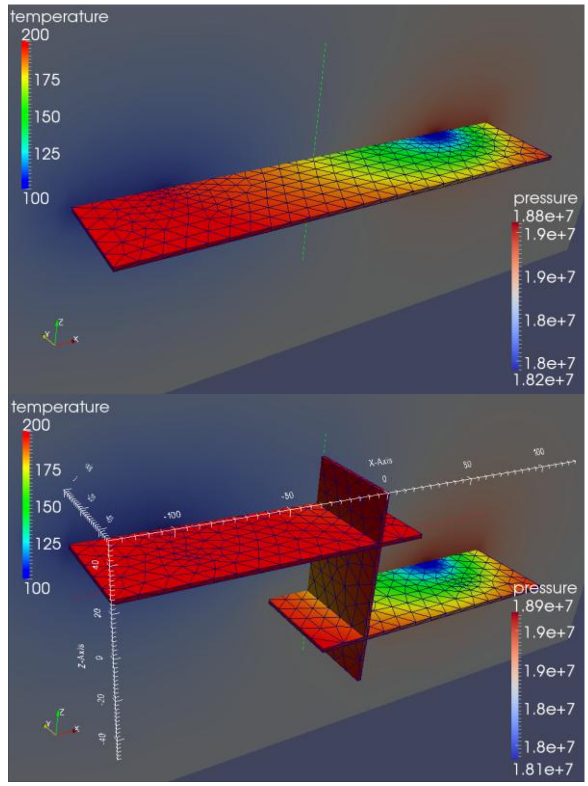


Figure 3. Temperature (in fracture domain) and pressure along the center of the reservoir matrix domain for tow simulation cases.

Figure 3 shows the simulated temperature and pressure for two examples after several years of injection and production. As can be seen on the figure, cold fluid is injected into the right hand side of the fracture domain, while production occurs from a symmetrical location on the left. At this early time, little changes are observed in the temperature field in the vicinity of the production location. The "hot" color scheme on Figure 3 illustrates the temperature in the fracture domain, while the reservoir matrix has been but away along the centerline of the Y-axis to allow for visualization of the pressure distribution with the reservoir.

Figure 4 shows the increase is the stress magnitude in the vicinity of the injection point for the simple fracture network case. As is expected, the poroelastic dilation and thermoelastic contraction resulting from cold-water injection into the reservoir is at it maximum near the injection point. Resulting changes in porosity and permeability are also observed in response to the injection, which is consistent with field observations.

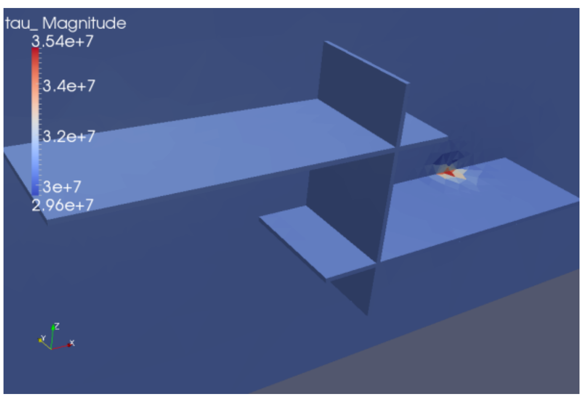


Figure 4. Early-time stress magnitude change in the vicinity of the injection horizon within the simulation domain.

Time series plots of the temperature of the produced water and the reservoir pressure in the vicinity of the extraction well are shown in Figure 5. As can be seen on the Figure, the thermal drawdown is delayed in the simulation case containing the fracture network, due in large part to the larger amount of surface area available to the fluid between the injection and extraction points.

The pressure drop at the simulated production well or the fracture network case is considerably larger than that predicted for the single fracture case.

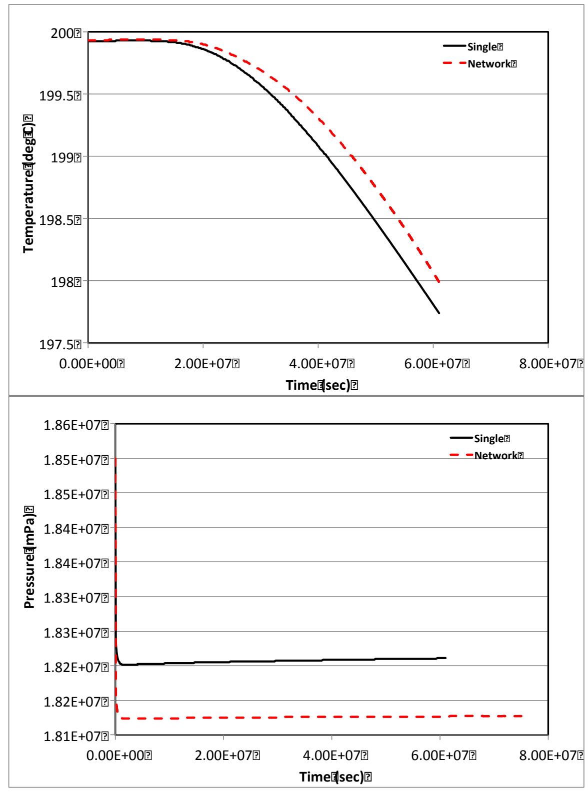


Figure 5. Comparison of produced fluid temperature and pressure for the simulation cases shown on Figure 3.

DISCUSSION AND CONCLUSIONS

Commercial scale deployment of EGS greatly depends on our understanding of the dynamics of the coupled rock-fracture-fluid-heat system and our ability to reliably predict how reservoirs behave under stimulation and production, to include an understanding of the thermal drawdown behavior of EGS reservoirs.

The work described in this paper presents a preliminary evaluation of the thermo-mechanical effects and their influence reservoir production. The work described here is quite preliminary and further, detailed studies will be required for a through understanding of reservoir behavior. Several areas that deserve considerable attention include

- An evaluation of confining /overburden stress and working pressures with the reservoir
- An evaluation of the fracture orientation in relation to regional confining stress magnitude and orientation and it's affect on the evolution of permeability
- A detailed evaluation of localized thermo-mechanic effects in the vicinity of the injection well

While not discussed in this paper, the additional complication of reactive geochemistry is of considerable importance for long-term EGS reservoir operation.

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REFERENCES

Brown, P. N. and Y. Saad (1990). Hybrid Krylov methods for nonlinear systems of equations. SIAM J. Sci. Statist. Comput. 11(3), 450–481.

Brownell, D., S. Garg, and J. Pritchett (1977). Governing equations for geothermal reservoirs. Water Resources Research 13(6), 929–934.

Chacon, L. and G. Lapenta. (2006) A fully implicit, nonlinear adaptive grid strategy. J. Comput. Phys., 212(2):703–717

Croucher, A.E. and M.J. O'Sullivan. (2008). Application of the computer code TOUGH2 to the sim- ulation of supercritical conditions in geothermal systems. Geothermics, 37:622–634

Faust, C. and J. Mercer (1979a). Geothermal reservoir simulation .1. Mathematical-models for liquid- dominated and vapor-dominated hydrothermal systems. Water Resources Research, 15(1), 23–30.

Faust, C. and J. Mercer (1979b). Geothermal reservoir simulation .2. Numerical-solution techniques for liquid-dominated and vapor-dominated hydrothermal systems. Water Resources Research, 15(1), 31–46.

Garg S. and D. Kassoy (1981). Convective heat and mass transfer in hydrothermal systems, *in* L. Rybach and L. Muffler, eds. Geothermal Systems: Principles and Case Histories. Wiley.

Gaston, D., C. Newman, G. Hansen, and D. Lebrun-Grandi ́e (2009). MOOSE: A parallel computational framework for coupled systems of nonlinear equations. Nucl. Engrg. Design 239, 1768–1778.

Hammond, G.E., A.J. Valocchi, and P.C. Lichtner (2005). Application of jacobian-free newton-krylov with physics-based preconditioning to biogeochemical transport. Advances in Water Resources, 28(4):359–376.

Henson, V. E. and U. M. Yang (2002) BoomerAMG: A parallel algebraic multigrid solver and preconditioner. Appl. Numer. Math. 41:155–177.

Heroux, M, et al. (2008) Trilinos: an object-oriented software framework for the solution of large- scale, complex multi-physics engineering and scientific problems. http://trilinos.sandia.gov

IAPWS. Release on the iapwsf ormulation 2008 for the viscosity of ordinary water substance. Technical report, International Association Properties of Water and Steam, 2008.

Ingebritsen, S., W. Sanford, and C. Neuzil (2008). Groundwater in geolofic processes, 2nd ed., Cambridge University Press, Cambridge, UK. 536 p.

Itasca Consulting Group. (1997). *FLAC 3D, Fast Lagrangian Analysis of Continua in 3 Dimensions. Version 2.0.* Five volumes. Minneapolis, Minnesota, Itasca Consulting Group.

Jaeger, J.C., N.G.W. Cook, and R.W. Zimmerman. (2007). Fundamentals of rock mechanics, 4th ed., Blackwell.

Knoll, D. A. and D. E. Keyes (2004). Jacobian-free Newton- Krylov methods: a survey of approaches and applications. J. Comput. Phys. 193(2), 357–397.

Kirk, B.S., J. W. Peterson, R. H. Stogner, and G. F. Carey (2006). . libMesh: a C++ library for parallel adaptive mesh refinement/coarsening simulations. Eng Comput-Germany, 22(3-4):237–254

McHugh, P.R. and D. A. Knoll (1994). Inexact Newton's method solutions to the incompressible Navier-Stokes and energy equations using standard and matrix-free implementations. AIAA J., 32:2394

Mercer, J. and C. Faust (1979). Geothermal reservoir simulation .3. Application of liquid-dominated and vapor-dominated hydrothermal modeling techniques to Wairakei, New Zealand. Water Resources Research ,15(3), 653–671.

Miller, C.W. and L.V. Benson (1983). Simulation of solute transport in a chemically reactive hetero- geneous system - model development and application. Water Resources Research, 19(2):381– 391

Molins, S., J. Carrera, C. Ayora, and M.W. Saaltink (2004). A formulation for decoupling compo- nents in reactive transport problems. Water Resources Research, 40(10)

Oldenburg, C. and K. Pruess (1995). Dispersive transport dynamics in a strongly coupled groundwater-brine flow system. Water Resources Research, 31(2), 289–302.

Park, H., D. A. Knoll, D.R. Gaston, and R.C. Martineau (2010) Tightly coupled multiphysics al- gorithms for pebble bed reactors. Nuclear Science and Engineering, *in review*.

Podgorney, R.K., H. Huang, C. Lu, D. Gaston, C. Permann, L. Guo, and D. Andrs (2011). FALCON: A Physics-Based, Massively Parallel, Fully-Coupled, Finite Element Model for Simultaneously Solving Multiphase Fluid Flow, Heat Transport, and Rock Deformation for Geothermal Reservoir Simulation, Idaho National Laboratory Report INL/EXT-11-23351, 90 p.

Pruess, K., C. Oldenburg, G. Moridis. (1999). TOUGH2 User's Guide, Version 2.0, Report LBNL-43134. Lawrence Berkeley National Laboratory, Berkeley, CA.

Rutqvist, J., Y.-S. Wu, C.-F. Tsang and G. Bodvarsson (2002), A modeling approach for analysis of coupled multiphase fluid flow, heat transfer, and deformation in fractured porous rock. *Int. J. Rock Mech. Min. Sc.i.* 39, 429–442

Steefel, C.I. and K.T.B. MacQuarrie (1996). Approaches to modeling of reactive transport in porous media. Reviews in Mineralogy and Geochemistry, 34:83–129

Valocchi, A.J., R.L. Street, and P.V. Roberts (1981). Transport of ion-exchanging solutes in ground-water - chromatographic theory and field simulation. Water Resources Research, 17(5):1517– 1527

Wagner, W., J.R. Cooper, A. Dittman, J. Kijima, H.-J. Kretzschmar, A. Kruse, R. Mares, K. Oguchi, H. Sato, I. Stocker, O. Sifner, Y. Takaishi, I. Tanishita, J. Trubenbach, and Th. Willkommen

(1997). The IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam. Trans. ASME, 150(122):150–182

White, M.D. and B.P. McGrail (2005). Stomp (subsurface transport over multiple phase) version 1.0 addendum: Eckechem equilibrium-conservation-kinetic equation chemistry and reactive transport. Technical Report PNNL-15482, Pacific Northwest National Laboratory, Richland, WA

Xu, T., E.L. Sonnenthal, N. Spycher, and K. Pruess (2004). TOUGHREACT user's guide: A simulation program for non-isothermal multiphase reactive geochemical transport in variable saturated geologic media. Technical Report LBNL-55460, Lawrence Berkeley National Lab- oratory, Berkeley, CA

Xu, T., E. Sonnenthal, N. Spycher, and K. Pruess (2006). TOUGHREACT - A simulation program for non-isothermal multiphase reactive geochemical transport in variably saturated geologic media: Applications to geothermal injectivity and CO2 geological sequestration. Computers & Geosciences, 32(2):145–165

Yeh, G.T. and V.S. Tripathi (1989). A critical-evaluation of recent developments in hydrogeochem- ical transport models of reactive multichemical components. Water Resources Research, 25(1):93–108

Yeh, G.T., J. Sun, P.M. Jardine, W.D. Burgos, Y. Fang, M.-H. Li, and M.D. Siegel (2004). HYDROGEOCHEM 5.0: A Coupled Model of Fluid Flow, Thermal Transport, and HYDROGEO-CHEMical Transport through Saturated-Unsaturated Media: Version 5.0. Technical Report ORNL/TM-2004/107, Oak Ridge National Laboratory, Oak Ridge, TN