THE TOUGH SIMULATOR: CAN IT TAKE THE HEAT?

Stefan Finsterle

Earth Sciences Division, Lawrence Berkeley National Laboratory, One Cyclotron Road. MS 74-120, Berkeley, California, USA

SAFinsterle@lbl.gov

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ABSTRACT

The TOUGH suite of nonisothermal multiphase flow and transport simulators has originally been developed in the early 1980s for applications in geothermal reservoir engineering, which required special attention to coupled fluid and heat flow, accurate description of thermophysical fluid properties, and an approach to represent fractured systems in a reasonable and computationally tractable manner. While the TOUGH simulators have evolved and are currently applied to address a wide variety of deep subsurface and near-surface problems, the highly nonlinear and coupled nature of geothermal system behavior still poses formidable challenges and provides the motivation to advance the codes. Attempts to significantly increase the worldwide production of geothermal energy led to the study and exploration of new systems for potential heat mining. Specifically, heat extraction from deeper systems with higher temperatures, the concept of enhanced geothermal system (EGS), the use of alternative working fluids (such as carbon dioxide), and the deployment of advanced drilling technologies require corresponding enhancements of simulation capabilities, including equation-of-state and reactive geochemistry modules with expanded temperature and pressure ranges, coupled thermal-hydrological-mechanical process simulations to address induced seismicity issues, and wellbore simulators linked to the reservoir model. Moreover, characterization methods need to be refined and the supporting analysis tools updated. This paper summarizes recent advances of the TOUGH suite of simulation and analysis tools, and discusses their limitations and applicability in geothermal reservoir engineering.

1. INTRODUCTION

1.1 Historical Remarks

Numerical modeling is a powerful means to understand and predict the response of geothermal systems and to design and optimize their exploitation. The strong coupling of heat and fluid flow, and the fractured nature of most hydrothermal and all enhanced geothermal systems (EGS) pose significant challenges to an accurate and efficient simulation of complex geothermal processes. Nonetheless, numerical modeling has been used to study geothermal systems since the 1970s, and has become standard practice in geothermal reservoir engineering during the last 25 years, for both generic investigations and site-specific applications (see O'Sullivan et al., 2001, for an overview).

There exist a number of computer codes for simulating non-isothermal multiphase flow, transport, and other, more complex processes in the subsurface. They differ in the features and processes being modeled and the method used to couple them, in the numerical approach, and in the support provided for setting up models and for post-processing the results. This article focuses on the TOUGH codes (Pruess et al., 1999; http://esd.lbl.gov/TOUGH), which was originally developed at the Lawrence Berkeley National Laboratory in the early 1980s for geothermal reservoir engineering, but is now widely used in universities, government organizations, and private industry for applications related to geological carbon sequestration, nuclear waste disposal, energy production from geothermal, oil and gas reservoirs as well as methane hydrate deposits, environmental remediation, vadose zone hydrology, and other uses that involve coupled thermal, hydrological, geochemical, and geomechanical processes in permeable media. Code developments and applications of the TOUGH suite of simulators are described in numerous conference papers and journal articles, a list of which can be found at http://esd.lbl.gov/research/projects/tough/documentation/.

1.2 Basic Simulation Approach

In this section, we describe the basic mass- and energy-balance equations solved by all variants of the TOUGH codes. For the governing equations of specialized modules (e.g., those including reactive transport, rock mechanics, and wellbore flow), the reader is referred to the respective manuals. The equations for nonisothermal, multiphase, multicomponent flows in fractured porous media can be written in the following general form:

$$\frac{d}{dt}\int_{V_n} M^{\kappa}\, dV_n \;=\; \int_{\Gamma_n} \mathbf{F}^{\kappa} \bullet \mathbf{n}\, d\Gamma_n + \int_{V_n} q^{\kappa}\, dV_n \qquad (1)$$

The integration is over an arbitrary subdomain V_n of the flow system, which is bounded by the closed surface Γ_n. The quantity M appearing in the accumulation term represents the mass of component κ (e.g., water, brine, CO_2, tracer, radionuclide) or energy ($\kappa = h$) per volume. **F** denotes mass or heat flux, and q denotes sinks and sources; **n** is a normal vector on the surface element $d\Gamma_n$, pointing inward into V_n. The general form of the mass accumulation term is

$$M^{\kappa} \;=\; \phi \sum_{\beta} S_{\beta}\rho_{\beta}X_{\beta}^{\kappa} + (1-\phi)\rho_R \rho_{aq} X_{aq}^{\kappa} K_d \qquad (2)$$

where ϕ is porosity, S_{β} is saturation of phase β, ρ_{β} is phase density, X_{β}^{κ} is the mass fraction of component κ in phase β, ρ_R is the rock grain density, and K_d is the aqueous phase distribution coefficient. Similarly, the heat accumulation term in a multiphase system is

$$M^{h} \;=\; (1-\phi)\rho_R C_R T + \phi \sum_{\beta} S_{\beta}\rho_{\beta}u_{\beta} \qquad (3)$$

where C_R is the specific heat of the rock, T is temperature, and u_{β} is specific internal energy of phase β. Advective mass flux is a sum over phase fluxes,

$$\mathbf{F}^{\kappa}\Big|_{adv} = \sum_{\beta} X_{\beta}^{\kappa}\mathbf{F}_{\beta} \qquad (4)$$

and individual phase fluxes $\mathbf{F}_\beta$ are given by a multiphase extension of Darcy's law:

$$\mathbf{F}_\beta = -k \frac{k_{r\beta}\rho_\beta}{\mu_\beta}(\nabla P_\beta - \rho_\beta \mathbf{g}) \quad (5)$$

Here k is absolute permeability, $k_{r\beta}$ is relative permeability to phase β, μ_β is viscosity, and $P_\beta = P + P_{c\beta}$ is the fluid pressure in phase β, which is the sum of the reference (gas) pressure and the capillary pressure $P_{c\beta}$ (≤ 0), and $\mathbf{g}$ is the vector of gravitational acceleration. The mass flux term in the TOUGH codes include multiphase and Knudsen diffusion. Moreover, vapor pressure lowering due to capillary and phase adsorption effects can be considered.

Heat flux includes conductive, convective, and radiative components

$$\mathbf{F}^h = -\lambda \nabla T + \sum_\beta h_\beta \mathbf{F}_\beta + f_\sigma \sigma_0 \nabla T^4 \quad (6)$$

where λ is effective thermal conductivity, and h_β is specific enthalpy in phase β, f_σ is the radiant emittance factor, and σ_0 is the Stefan-Boltzmann constant. All water properties (density, specific enthalpy, viscosity, saturated vapor pressure) are calculated from steam table equations.

For numerical simulation the continuous space and time variables must be discretized. Space discretization is made directly from the integral form of the conservation equations (1), without converting them into partial differential equations. This integral finite difference method avoids any reference to a global coordinate system, and thus offers the advantage of being applicable to regular or irregular discretizations in one, two, and three dimensions. Time is discretized fully implicitly as a first-order backward finite difference.

Discretization results in a set of strongly coupled nonlinear algebraic equations, with the time-dependent primary thermodynamic variables of all grid blocks as unknowns. These equations are cast in residual form and solved simultaneously using Newton-Raphson iterations. Different methods are available to solve the linear equations arising at each iteration step, including preconditioned conjugate gradient solvers, as well as sparse direct matrix methods. Parallel solvers based on domain decomposition are available as well (Zhang et al., 2008).

Dual-continua approaches can be used to model media in which a network of interconnected fractures is embedded in matrix blocks of low permeability, as is typically the case in geothermal reservoirs. Global flow in the reservoir occurs mainly through the fracture system, which is described as an effective porous continuum. Rock matrix and fractures may exchange fluid or heat locally, driven by the difference in pressures, mass fractions, or temperatures between matrix and fractures, which is assumed as being quasi-steady, with the rate of matrix-fracture interflow proportional to the gradient in (local) average state variables. In the method of multiple interacting continua (MINC), a more accurate resolution of these gradients is achieved by subgridding of the matrix blocks. Generation of the fracture and matrix continua and their interconnection is a geometrical pre-processing step that operates on the element and connection data of a porous medium mesh to calculate—for given data on volume fractions—the volumes, interface areas, and nodal distances for a secondary fractured medium mesh. The information on fracturing (spacing, number and orientation of sets, shape of matrix blocks) is provided by a proximity function, which expresses, for a given reservoir domain V_o, the total fraction of matrix material within a distance from the fractures. Note that all the necessary information about the fractures and matrix is encapsulated in the geometrical parameters of the discretized equations, i.e., there is no need to reformulate the governing equations to implement different representations of fractured-porous media (i.e., discrete fracture networks, equivalent continuum, double porosity, dual-permeability, and MINC approaches). Details about the dual-continuum approaches as well as their applicability and limitations can be found in Doughty (1999).

1.3 Simulation Needs

As numerical modeling became a more common tool in geothermal reservoir engineering, the range of science and management questions to be addressed by the model increased, so did the variety of hydrothermal systems and conditions to be analyzed. For example, the renewed interest in EGS, the potential use of alternative working fluids (Pruess, 2006; Randolph and Saar, 2011), and the assessment of very deep or very hot, magmatic geothermal systems (Friðleifsson et al., 2013) call for an expansion of the processes and thermophysical states that can be considered in the simulations. Of particular interest are the geochemical and rockmechanical effects caused by perturbations in the pressure and temperature fields as induced during the stimulation and operation of a geothermal reservoir. Accurately accounting for these coupled processes allows for improved reservoir characterization as well as more efficient and safer development and exploitation of the field. Moreover, linkages to wellbore simulators and surface installations are attempted with the ultimate goal to perform a more complete system-level analysis.

The increase in the number of features, processes, and subsystems and their coupling comes at the expense of increased model complexity, data needs, and computational demands. The following subsections describe some recent developments and enhancements of the TOUGH suite of simulators that attempt to address some of these challenges. Many of these advances have recently been presented at the TOUGH Symposium 2012 (Finsterle et al., 2012).

2. RECENT TOUGH DEVELOPMENTS

2.1 Thermophysical Properties

Simulation studies of extensional magmatic systems and assessments of the sustainability of geothermal exploitation in general require that both the more shallow cooler regions and the deep heating zones be modeled, where thermodynamic conditions are encountered that exceed the pressure and temperature range of standard TOUGH2. Attempts to extend this range and to include the supercritical region of the phase diagram date back to the 1990s, but renewed efforts have been made more recently to arrive at an accurate, robust, and efficient equation-of-state (EOS) module for such conditions. In particular, Croucher and O'Sullivan (2008) replaced the standard thermodynamic formulation with the newer IAPWS-97 (1997) formulation. By choosing density and temperature as the primary variables in the supercritical region (i.e., variables identical to those in IAPWS-97), they arrive at a mathematically robust formulation near the critical point, and they avoid the use of an iterative procedure to evaluate fluid properties. They developed a scheme to robustly perform phase transitions near the critical point, and demonstrated the accuracy and efficiency of the enhanced TOUGH2 simulator by comparing it to alternative approaches (e.g., that of Brikowski, 2001).

The use of CO_2 as an alternative working fluid in EGS has been originally proposed by Brown (2000) as a means to combine effective geothermal energy capture with geologic carbon storage. The concept was explored in more detail by Pruess (2006) and adapted by Randolph and Saar (2011). Under geothermal conditions, CO_2 is a supercritical fluid with liquid-like density and gas-like viscosity, which (along with its much larger compressibility and thermal expansivity) leads to favorable flow and wellbore hydraulics conditions and thus an overall higher heat mining efficiency compared to that of water, despite its lower heat capacity. Other factors (specifically related to geochemistry and economic viability) need to be further assessed.

The TOUGH codes are extensively used to study large-scale storage of greenhouse gases in deep geologic formations (saline aquifers, depleted oil and gas reservoirs, and coalbeds). The TOUGH2 EOS modules ECO2N and ECO2M were specifically developed for such applications. ECO2N (Pruess, 2005) considers all sub- and supercritical CO_2 as a single non-wetting phase, a concept that can successfully capture the conditions in the storage formation as well as certain paths within the phase diagram. However, it is limited to systems in which there is no change of phase between liquid and gaseous CO_2, and in which liquid and gaseous CO_2 do not co-exist. To overcome this limitation, ECO2M (Pruess, 2011) was developed, a module that describes the pure-component and mixture properties of water, NaCl, and CO_2 in the full range of phase conditions, including those on the liquid-gas saturation line with the potential for three-phase conditions. Both of these modules work up to temperatures of about 110°C, which make them unsuitable for applications in deep geothermal reservoirs. The challenge of extending the temperature range lies in the correlations needed to compute the mutual solubilities of CO_2 and chloride brines. Such correlations have been presented by Spycher and Pruess (2009) and are implemented in a new, high-temperature version of ECO2N (dubbed ECO2H), which is currently being tested for public release.

Battistelli (2012) updated the treatment of saline solutions in EWASG (Battistelli et al., 1997) for more accurate calculations of brine density, enthalpy and vapor pressure, halite density, enthalpy and solubility, as well as vapor adsorption and capillary condensation effects at high temperatures.

2.2 Wells

Injection and production wells are key elements of a geothermal system. It is therefore essential that the well hydraulics and interactions between the well and the reservoir are properly captured. This is especially important for multiphase flow systems, where gas compression and exsolution greatly affect the flow resistance and thus pressure and temperature distribution along the well, with related impacts on the reservoir behavior, injectivities, and production rates and enthalpies. Standard TOUGH2 provides a number of options to represent wells. New options have been added by various research groups to simulate more complex real-world scenarios (e.g., Yeh et al., 2012).

The coupling between the wellbore and reservoir has been addressed multiple times, with various approaches and degrees of sophistication. Recently, Pan et al. (2011) presented T2Well, a coupled wellbore-reservoir simulator, which uses the drift-flux model and related conservation equations for describing transient two-phase nonisothermal wellbore flow. The mass and thermal energy balance equations are solved numerically by a finite difference scheme with wellbore heat transmission to the surrounding rock handled either semi-analytically or numerically. The momentum balance equation for the flow in the wellbore is solved numerically with a semi-explicit scheme.

Any coupled wellbore-reservoir simulator requires that the well be explicitly discretized to get the correct well volumes and exchange areas with the formation. Such discretization can be simplified. For example, following the trajectory of the well, cylindrical grid blocks can be inserted into the existing elements of a basic grid. These well elements are connected to each other in the axial direction and to the elements in which they are embedded. This approach is implemented in WinGridder and was used to insert three conventional wells and 40 microholes into a three-dimensional, unstructured-grid reservoir model (see red lines in Figure 1).

For the wellbore sections above the model domain, i.e., from the land surface to a depth of 3.8 km, where the surrounding rock is not included in the reservoir model, a semi-analytical solution for radial heat exchange with the formation is used (Zhang et al., 2011) to efficiently calculate heating of the injected water and heat losses from the produced water as it flows along the wells through rocks that exhibit a geothermal gradient. Given the relatively long vertical flow distance in these wellbore sections, the gravitational potential is added to the energy balance equation (Stauffer et al., 2003). This effect, which is similar in magnitude to the temperature changes caused by the negative Joule-Thomson coefficient of water, is added to avoid an overprediction of the temperature and heat content of the produced fluid.

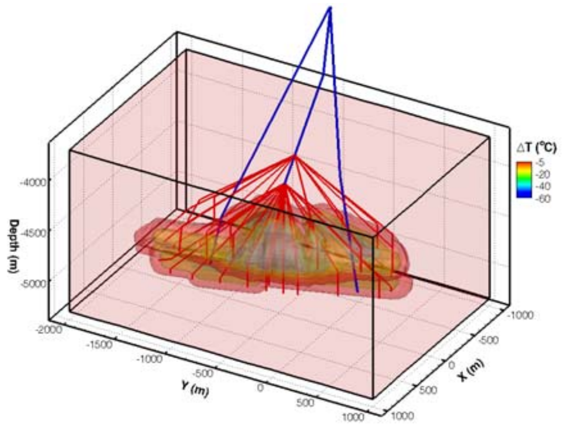

Figure 1: Simulated temperature-change distribution after 30 years of exploitation using a microhole array (Finsterle et al., 2013).

2.3 Rock Mechanics

2.3.1 Overview

Reservoir creation through hydraulic or thermal stimulation, as well as pressure and temperature changes induced by fluid circulation in an EGS or conventional hydrothermal reservoir lead to stress changes and associated elastic-plastic deformations or even rock failure that induces seismic events. Having the capabilities to simulate these coupled thermal-hydrologic-mechanical (THM) processes is essential, as they help to design reservoir stimulation activities, to examine and mitigate risks, and to assess the success of the stimulation. The coupling of TOUGH's non-isothermal multiphase flow and transport processes with rock mechanics is an active area of research and code development.

A number of alternative and complementary approaches have been developed to account for the coupling between pressure and temperature changes and induced stress changes with associated thermo-poro-elastic and plastic deformations. Fracture propagation and the coupling to geochemical processes pose additional, unique challenges. These approaches differ in the assumptions about the mechanical behavior of porous and fractured geologic media, the numerical method used to perform the stress-strain calculation, the discretization scheme and how state variables and parameters calculated for potentially different meshes are mapped to each other, and the way to couple flow and geomechanics. The approaches integrated into the TOUGH framework range from simple models that only account for uniaxial poro-elastic deformations due to external load changes, to more general formulations that relax these assumptions, to complex models that capture fracture initiation and propagation mechanisms in multi-porosity systems. The following is a short description of some of these coupled models.

2.3.2 TOUGH-FLAC enhancements

The TOUGH-FLAC simulator has been the first TOUGH-related simulator capable of modeling coupled THM processes. It employs a sequential coupling whereby pore pressure and temperature calculated by TOUGH2 are transferred to a compatible numerical grid for FLAC3D, which then calculates effective stresses and associated deformations, returning updated values for porosity, permeability, and capillary strength parameter back to the flow simulator. Details about this approach can be found in Rutqvist et al. (2002).

To better represent the mechanical behavior of highly fractured formations, TOUGH-FLAC was enhanced to include a modified version of the crack tensor model of Oda (1986), which calculates a discrete summation of contributions from each fracture that intersects an element volume to arrive at upscaled, stress-dependent, anisotropic permeability and compliance tensors. This approach transforms a discrete fracture network model into a grid-based continuum model. More details can be found in Wang et al. (2012).

2.3.3 Implicit volumetric strain approach

Hu et al. (2012) added a mean stress equation for thermo-poro-elastic multiporosity media to the standard set of governing multiphase flow equations of TOUGH2-MP. In this formulation, the mean total stress is included as an additional primary variable, and the coupled THM system is solved fully implicitly, obtaining volumetric strain and associated changes in porosity and permeability. Geochemical reactions based on the TOUGHREACT code have also been included in this formulation.

2.3.4 Rock Discontinuous Cellular Automaton

Pan et al. (in press) coupled TOUGH2 to RDCA (Rock Discontinuous Cellular Automaton), a code capable of simulating nonlinear and discontinuous deformation behavior, such as plastic yielding and the initiation, propagation and coalescence of cracks induced by changes of fluid pressure and temperature. RDCA uses a special displacement function to represent internal discontinuities. A level set method tracks the fracturing path, and a partition-of-unity method is used to improve the integral precision of fracture surface and fracture tip calculations. The mechanical state is evaluated by a cellular automaton updating rule, whereby a mixed-mode fracture criterion determines the fracturing behavior. In this approach, the discontinuity of a crack is incorporated independently of the mesh, such that the crack can be arbitrarily located within an element, i.e., the method does not require any re-meshing for crack growth, which greatly simplifies the modeling procedure and its sequential integration with TOUGH2 through external coupling modules.

2.3.5 Multi-continua approach for fracture propagation

Kim et al. (2012) developed a simulator for vertical hydraulic fracturing that involves continuous updating of the boundary conditions and connectivity data. As a result of fracturing, the domain description changes from a single continuum to double or multiple continua. The algorithm allows for an explicit description of nonlinear permeability and geomechanical moduli, provides two-way coupling between fluid and heat flow and geomechanics, continuously tracks changes in the fractures and in the pore volume, and fully accounts for leak-off in all directions during hydraulic fracturing. The approach also accounts for geochemical reactions with associated changes in pore volume from dissolution and precipitation.

2.3.6 Rigid-body-spring-network approach

Asahina et al. (in press) used a Voronoi-based discretization technique for coupled thermo-hydrologic-mechanical modeling that includes the formation and propagation of discrete fractures embedded in a three-dimensional rock matrix. Elastic response and fracture development is modeled by a mechanical damage model that is based on the rigid-body-spring network, where spring constants are related to elastic rock mechanical properties, and fracture initiation is determined using a classical brittle approach. Fracture configurations are mapped onto an unstructured Voronoi grid, which is based on a deterministic or random set of spatial points. The resulting discrete fracture network is represented by the connections of the edge of a Voronoi cell, avoiding numerical gridding issues and allowing for flow and transport through a network that also interacts with the permeable matrix.

2.4 Reactive Transport

Reactive transport modeling was first coupled to TOUGH2 by White (1995), who used an implicit scheme in which batch reactions are separated from the transport terms. This code, named ChemTOUGH, was mainly applied to geothermal reservoir problems (e.g., Kissling et al., 1996). Essentially the same concept of separating reactions from flow and transport (but using a sequential iterative approach) was later used for the development of TOUGHREACT (Xu et al., 2001). It considers thermo-hydrological-chemical (THC) processes under various conditions, including concentrated aqueous solutions. The code can accommodate an arbitrary number of chemical species that can be present in liquid, gas and solid phases in media with physical and chemical heterogeneity. Thermophysical and geochemical properties are calculated as a function of pressure and temperature as well as of thermodynamic and kinetic data for mineral-water-gas reactions. Multiphase transport of aqueous and gaseous species occurs by advection and molecular diffusion. Aqueous and surface complexation, acid-base, redox, gas dissolution and exsolution, and multi-site cation exchange are considered under the local equilibrium assumption. Mineral dissolution and precipitation proceed under either equilibrium or kinetic constraints, leading to changes in porosity, permeability, and capillary strength. Intra-aqueous kinetics and biodegradation and surface complexation using non-electrostatic, constant capacity and double layer electrostatic models have been incorporated into Version 2 of TOUGHREACT (Xu et al., 2011). Linear adsorption and decay can be also included.

TOUGHREACT has been applied to a wide variety of problems, including the simulation of mineral alteration in hydrothermal and geothermal systems.

2.5 Inverse Modeling

2.5.1 Overview

iTOUGH2 provides inverse modeling capabilities for most modules of the TOUGH suite of simulators. By running TOUGH simulations multiple times for different input parameter sets, iTOUGH2 can be used for parameter estimation through automatic model calibration, for formalized sensitivity analyses, and for assessing the uncertainty of model predictions. In geothermal applications, matching past production data to determine reservoir properties is appropriate, as the data contain information about the relevant properties and on right scale. This means that for the subsequent predictive simulations, only limited extrapolations to conditions different from those encountered during calibration need to be made.

Recent advances within the inversion framework include a link from iTOUGH2's optimization and analysis routines to any simulation software that uses text files for input and output (Finsterle and Zhang, 2011a), inclusion of global sensitivity analysis methods (Wainwright et al., 2013), joint multi-physics inversion, improved statistical measures of model fit, data contribution, and parameter identifiability, and other features making input to the forward and inverse part of the simulation-optimization code more convenient. The following subsections summarize some of the features added to the iTOUGH2 optimization framework.

2.5.2 Link to external models through PEST protocol

While the original iTOUGH2 code is tightly linked to the TOUGH2 simulator, its optimization routines are general enough to also be applicable to other forward models. The forward model can be separated from the inversion framework through an interface such as the PEST protocol (Banta et al., 2008), provided that the application model (1) submits input through one or more ASCII input files, (2) returns output to one or more ASCII output files, (3) runs the model or multiple models using a system command, and (4) runs the models to completion without user intervention. iTOUGH2's core, its optimization routines and related analysis tools, remains unchanged; only the communication format between input parameters, the application model, and output variables are borrowed from PEST.

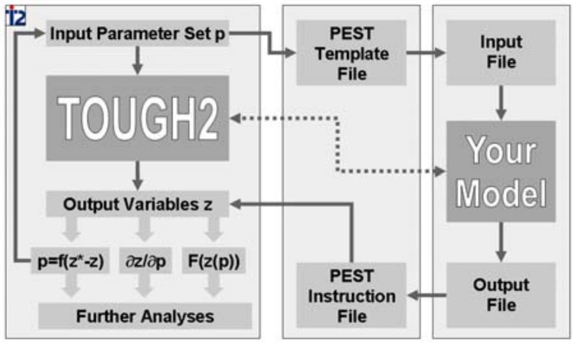

Figure 2: Optimization and analysis tools evaluate the system response z as a function of adjustable input parameters p, where the relation between z and p is either given by the fully integrated TOUGH2 simulator or by an external model through the PEST protocol, which uses text-based template and instruction files for communication with the external model's input and output files.

The extended code (Figure 2; Finsterle and Zhang, 2011b) allows the user to invoke optimization of TOUGH2 models, which are fully integrated within iTOUGH2, or any external models, which are loosely linked by the PEST protocol, or a combination thereof. The latter is especially powerful, since it allows the user to include TOUGH2 pre- or postprocessors within the iTOUGH2 optimization framework. Wellmann et al. (in press) demonstrate a use case in which an entire model set-up and analysis workflow (from the development of a geologic framework model to the analysis of TOUGH simulation results) is automated and thus accessible for parameter estimation and uncertainty quantification using iTOUGH2. Finally, this new capability allows users to perform inverse analyses of TOUGH-related models that are not tightly integrated into iTOUGH2, such as TOUGHREACT, TOUGH2-MP, and TOUGH+.

2.5.3 Global sensitivity analysis

The derivative-based minimization algorithms implemented in iTOUGH2 require the calculation of a Jacobian matrix, whose elements are the partial derivatives of each observable variable z_i with respect to each parameter p_j. This Jacobian matrix provides information for a local sensitivity analysis based on individual and composite measures.

Such a sensitivity analysis is local in the sense that it is valid for a specific point in the parameter space. If the model is nonlinear, however, sensitivity coefficients are different for each parameter combination. Global sensitivity-analysis methods address this issue by examining many combinations within the range of acceptable parameter values. Two global sensitivity-analysis methods have been implemented into iTOUGH2 (Wainwright et al., 2013). In the Morris one-at-a-time elementary-effects method (Morris, 1991), each axis of the parameter hypercube is subdivided, and a perturbation is then calculated for each parameter. Next, a random grid point in the parameter space is selected, the model is run, and the performance measure is evaluated. Then—one at a time and in random order—each parameter is perturbed, the model is rerun to recalculate the performance measure, and the corresponding impact (or elementary effect) on the output is computed from the relative difference between the model output. The procedure is repeated for multiple, randomly selected starting points of a path in the parameter space. After completion of a number of such paths, the mean and standard deviation of the absolute elementary effects is calculated. The mean assesses the overall influence of the respective parameter on the output; the standard deviation indicates whether the effects are linear and additive or nonlinear, or whether interactions among the parameters are involved. As a second approach, the method of Saltelli et al. (2008) provides the variance-based sensitivity index for parameter importance (which is equivalent to the Sobol' index). Conceptually, this measure quantifies the percentage contribution of each parameter to the uncertainty of the output. In addition, the total sensitivity index is evaluated, which can be used to identify parameters with negligible effects. An application of global sensitivity analysis for the determination influential parameters of a geothermal reservoir model can be found in Finsterle et al. (2013a).

2.5.4 Statistical analyses

iTOUGH2 performs a rather extensive residual and uncertainty analysis (Finsterle and Zhang, 2011b), helping the user to decide whether the model is a likely representation of the real system, and to examine the reliability and usefulness of certain observations. This analysis has been expanded to include the Nash-Sutcliffe (NS) and Kling-Gupta (KG) efficiency criteria. The NS index can be interpreted as the relative ability of a model to predict the data, where NS = 0 indicates that the model is not a better predictor than simply obtaining the mean of the observed values. The KG index allows a breakdown of the misfit in contributions from correlation errors, variability, and bias (Gupta et al., 2009). These indices are goodness-of-fit criteria that can be used for model comparison studies, or directly as objective functions to be minimized by iTOUGH2. An application is described in Kowalsky et al. (2012).

As part of the residual analysis, iTOUGH2 now also calculates the relative impact of omitting an individual observation. This measure is useful during the design stage of a project to evaluate "data worth," i.e., the potential benefit of taking a certain measurement for parameter estimation. The measure is calculated based on the D-optimality criterion. If omitting a certain data point from a synthetic inversion leads to a significant increase in the determinant of the covariance matrix of the estimated parameters, then this data point should be collected, because it contributes substantially to obtaining a more accurate solution of the inverse problem. Note that the inverse problem needs to be solved only once to obtain the data-worth measure for all observations.

2.5.5 Multi-physics joint inversion

The ultimate success of an inverse analysis depends on the availability of data that contain sufficient information about the relevant parameters. The coupling of THMC processes as discussed above provides an opportunity to considerably increase the amount and types of data that can be included in an inversion. Specifically, geophysical data (such as seismic and electro-magnetic data) may help identify the geologic structure and the extent and migration of phase boundaries. Combining geophysical imaging with estimation of hydrogeologic, thermal, geochemical, and mechanical parameters within a multi-physics joint inversion framework has the potential to significantly improve reservoir characterization. The basic concept is described in Finsterle and Kowalsky (2008). Considerable advances have been made to implement multi-physics joint inversion into the iTOUGH2 framework (Commer et al., 2013).

2.6 Reduced order modeling

The TOUGH codes provide high-fidelity multi-physics simulation capabilities. As more features and processes are added to the codes, and larger, three-dimensional problems are tackled within a many-query context (such as Monte Carlo simulations for uncertainty quantification, sampling-based global sensitivity analyses, and high-dimensional joint inversions), the computational demands become prohibitive. In addition to reducing computational time through parallelization, we consider various model reduction methods, in which either the forward model itself or select model outputs or a response surface are approximated by a low-order surrogate model, and the approximation error is quantified and accounted for in the respective many-query application. The strong nonlinearities inherent in geothermal reservoir modeling make it difficult to find accurate, robust, and efficient reduced order models. Nevertheless, the initial efforts by Cui et al. (2011) and Pau et al. (2013) are promising.

3. OUTLOOK AND CONCLUDING REMAKRS

The TOUGH codes have been originally developed for geothermal applications, and the codes have demonstrated their usefulness for both fundamental studies of the complex coupled processes occurring in geothermal reservoirs, as well as applied simulations for resource assessment, optimization of field operations, and sustainability evaluations. The codes have been continually updated, driven by application needs. In recent years, the renewed efforts to make enhanced geothermal systems a viable alternative energy resource triggered many research projects and code developments to address challenging issues such as reservoir stimulation and induced seismicity.

For the TOUGH suite of simulators to be able to make substantial contributions to address these challenges in geothermal reservoir engineering, it is essential that key capabilities be developed not only for the simulator but also its supporting infrastructure. The latter includes improved model setup and post-processing tools, data assimilation and multi-physics joint inversion capabilities, uncertainty quantification, optimization, risk assessment and decision support tools, and reduced order modeling. While the TOUGH codes have stood the test of time, continual updating and enhancement of process descriptions is needed in addition to improvements of its data structure, flow logic, and computational performance.

The developer team at LBNL and other organizations worldwide strives to keep the TOUGH simulators at the forefront of scientific research, and at the same time improve the maintainability of the codes and their applicability to problems of practical relevance.

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REFERENCES

Asahina, D., Houseworth, J.E., Birkholzer, J.T., and Bolander, J.E.: Hydro-mechanical model for fracture development and fluid transport in geomaterials. *Computers & Geosciences*. (in press).

Banta, E.R., Hill, M.C., Poeter, E., Doherty, J.E. and Babendreier, J.: Building model analysis applications with the Joint Universal Parameter IdenTification and Evaluation of Reliability (JUPITER) API. *Computers & Geosciences*, *34*, pp. 310 – 319. (2008).

Battistelli A., Calore, C. and Pruess K.: The simulator TOUGH2/EWASG for modelling geothermal reservoirs with brines and a non-condensible gas. *Geothermics*, *26*(4), pp. 437 – 464. (1997).

Battistelli A.: Improving the treatment of saline brines in EWASG for the simulation of hydrothermal systems. *Proc. TOUGH Symposium 2012*. Report LBNL-5808E. Lawrence Berkeley National Laboratory, Berkeley, California, pp. 192 – 200. (2012).

Brikowski, T. H.: Modeling supercritical systems with TOUGH2: The EOS1sc equation of state module and a basin and range example. *Geother. Resources Council Transact*., Davis, Calif., 25, pp. 285 – 289. (2001).

Brown, D.: A Hot Dry Rock geothermal energy concept utilizing supercritical CO_2 instead of Water. *Proc., Twenty-Fifth Workshop on Geothermal Reservoir Engineering*, Stanford University, pp. 233 – 238. (2000.)

Commer, M., Kowalsky, M.B., Doetsch, J., Newman, G.A. and Finsterle, S.: MPiTOUGH2: A parallel parameter estimation framework for hydrological and hydrogeophysical applications. *Computers & Geosciences*. doi:10.1016/j.cageo.2013.06.011. (2013).

Croucher, A.E. and O'Sullivan, M.J.: Application of the computer code TOUGH2 to the simulation of supercritical conditions in geothermal systems. *Geothermics*, *37*(6), pp. 622 – 634. (2008).

Cui, T., Fox, C. and O'Sullivan, M.J.: Bayesian calibration of a large-scale geothermal reservoir model by a new adaptive delayed acceptance Metropolis Hastings algorithm. *Water Resour. Res.*, *47*, W10521. (2011).

Doughty, C.: Modeling geologic storage of carbon dioxide: comparison of non-hysteretic and hysteretic characteristic curves. *Energy Conversion and Management,* 48(6), pp. 1768 – 1781. (2007).

Finsterle, S. and Kowalsky, M.B.: Joint hydrological-geophysical inversion for soil structure identification. *Vadose Zone Journal*, *7*, pp. 287 – 293. (2008).

Finsterle, S. and Zhang. Y.: Solving iTOUGH2 simulation and optimization problems using the PEST protocol. *Environmental Modelling and Software*, *26*, pp. 959 – 968. (2011a).

Finsterle, S., and Zhang. Y.: Error handling strategies in multiphase inverse modeling. *Computers & Geosciences*, *37*, pp. 724 – 730. (2011b).

Finsterle, S., Hawkes, D., Moridis, G., Mukhopadhyay, S., Oldenburg, C., Pfeiffer, L., Rutqvist, J., Sonnenthal, E., Spycher, N., Valladao, C. and Zheng, L. (Eds.): *Proceedings of the TOUGH Symposium 2012*. Report LBNL-5808E. Lawrence Berkeley National Laboratory, Berkeley, California, 910 pp. (2012).

Finsterle, S., Zhang, Y., Pan, L., Dobson, P. and Oglesby, K.: Microhole arrays for improved heat mining from enhanced geothermal systems. *Geothermics*, *47*, pp. 104–115. (2013).

Friðleifsson, G.Ó., Elders, W.A. and Albertssson, A.: The concept of the Iceland deep drilling project. *Geothermics*, doi:10.1016/j.geothermics.2013.03.004. (2013).

Gupta, H.V., Kling, H., Yilmaz, K.K. and Martineza, G.F.: Decomposition of the mean squared error and NSE performance criteria: Implications for improving hydrological modeling. *J. Hydrol. 377*, pp. 80 – 91. (2009).

Hu, L., Winterfeld, P.H., Fakcharoenphol, P., Wu, Y.-S., Zhang, K. and Xu. T.: A novel, fully coupled flow and geomechanics model in porous and fractured geothermal reservoirs. *Proc. TOUGH Symposium 2012*. Report LBNL-5808E. Lawrence Berkeley National Laboratory, Berkeley, California, pp. 254 – 262. (2012).

IAPWS-97: Release on the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam. Erlangen, Germany. (1997).

Kim, J., Sonnenthal, E., and Rutqvist, J.: Formulation and sequential numerical algorithms of coupled fluid/heat flow and geomechanics for multiple porosity materials. *Int. J. Numer. Meth. Engng. 92*, pp. 425 – 456. (2012).

Kissling, W.M., Brown, K.L., O'Sullivan, M.J., White, S.P. and Bullivant, D.P.: Modelling chloride and CO_2 chemistry in the Wairakei geothermal reservoir. *Geothermics 25*, pp. 285 – 305. (1996).

Kissling, W.M., Weir, G.J.: The spatial distribution of the geothermal fields in the Taupo Volcanic Zone, New Zealand. *J. Volcanol. Geotherm. Res.*, *145*, pp. 136 – 150. (2005).

Kowalsky, M.B., Finsterle, S., Williams, K.H., Murray, C., Commer, M., Newcomer, D., Englert, A., Steefel, C.I. and Hubbard, S.S.: On parameterization of the inverse problem for estimating aquifer properties using tracer data. *Water Resour. Res.*, *48*, W06535. (2012).

Morris, M.D.: Factorial sampling plans for preliminary computational experiments. *Technometrics*, *33*(2), pp. 161 – 174. (1991).

Oda, M.: An equivalent continuum model for coupled stress and fluid-flow analysis in jointed rock masses. *Water Resour. Res. 22*(13), pp. 1845 – 1856. (1986).

O'Sullivan, M.J., Pruess, K. and Lippmann, M.J.: State of the art of geothermal reservoir simulation. *Geothermics*, 30, pp. 395 – 429. (2001).

Pan, L., Oldenburg, C.M., Pruess, K. and Wu, Y.S.: Transient CO_2 leakage and injection in wellbore-reservoir systems for geologic carbon sequestration. *Greenhouse Gases: Science and Technology*, *1*(4), pp. 335 – 350. (2011).

Pan, P.-Z., Rutqvist, J., Yan, F., and Feng, X.-T.: Modeling of multiple fractures interaction in caprock during CO_2 injection into a deep brine aquifer using TOUGH-RDCA. *Computers & Geosciences* (in press).

Pau, G., Zhang, Y. and Finsterle, S.: Reduced order models for many-query subsurface flow applications. *Computational Geosciences*, *17*(4), pp. 705 – 721. (2013).

Pruess, K., Oldenburg, C. and Moridis, G.: *TOUGH2 User's Guide, Version 2.1*. Report LBNL-43134, Lawrence Berkeley National Laboratory, Berkeley, California, 204 pp. (1999).

Pruess, K.: *ECO2N: A TOUGH2 Fluid Property Module for Mixtures of Water, NaCl, and CO_2*. Report LBNL-57952, Lawrence Berkeley National Laboratory, Berkeley, California, 66 pp. (2005).

Pruess, K.: Enhanced geothermal systems (EGS) using CO_2 as working fluid—A novel approach for generating renewable energy with simultaneous sequestration of carbon. *Geothermics*, *35*, pp. 351 – 367. (2006).

Pruess, K.: ECO2M: A TOUGH2 Fluid Property Module for Mixtures of Water, NaCl, and CO_2, Including Super- and Sub-critical Conditions, and Phase Change Between Liquid and Gaseous CO_2. Report LBNL-4590E, Lawrence Berkeley National Laboratory, Berkeley, California, 83 pp. (2011).

Randolph, J.B. and Saar, M.O.: Combining geothermal energy capture with geologic carbon dioxide sequestration. *Geophys. Res. Lett.*, *38*, L10401, doi:10.1029/2011GL047265. (2011).

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

Saltelli, A., Ratto, M., Andres, T., Campolongo, F., Cariboni, J., Gatelli, D., Saisana, M. and Tarantola, S.: *Global Sensitivity Analysis, The Primer*. John Wiley & Sons Ltd., West Sussex, England, 292 pp. (2008).

Spycher, N. and Pruess, K.: A phase-partitioning model for CO2-brine mixtures at elevated temperatures and pressures: Application to CO2-enhanced geothermal systems. *Transport in Porous Media*, *82*(1), pp. 173 – 196. (2010).

Stauffer, P.H., Stein, J.S., Travis, B.J.: *The Correct Form of the Energy Balance for Fully Coupled Thermodynamics in Liquid Water*. Report LA-UR-03-1555, Los Alamos National Laboratory, Los Alamos, New Mexico, USA, 9 pp. (2003).

Wainwright, H., S. Finsterle, Y. Jung, Q. Zhou and J.T. Birkholzer. Making sense of global sensitivity analyses. *Computers & Geosciences*, doi:10.1016/j.cageo.2013.06.006. (2013).

Wang, Z., Rutqvist, J., Wang, Y., Leung, C., Hoch, A. and Dai, Y.: The effect of stress on flow and transport in fractured rock masses using TOUGH-FLAC and modified crack tensor theory. *Proc. TOUGH Symposium 2012*. Report LBNL-5808E. Lawrence Berkeley National Laboratory, Berkeley, California, pp. 433 – 440. (2012).

Wellmann, F., Croucher, A. and Finsterle, S.: Adding geology to the equation: towards integrating structural geological data into inverse modeling with iTOUGH2. *Computers & Geosciences*. (in press).

White, S.P.: Multiphase non-isothermal transport of systems of reacting chemicals. *Water Resour. Res. 32*(7), pp. 1761 – 1772. (1995).

Xu, T., Pruess, K.: Modeling multiphase non-isothermal fluid flow and reactive geochemical transport in variably saturate fractured rocks: 1. Methodology. *Am. J. Sci.*, *301*, pp. 16 – 33. (2001).

Xu, T., Spycher N., Sonnenthal E., Zhang G., Zheng L. and Pruess, K.: TOUGHREACT Version 2.0: A simulator for subsurface reactive transport under non-isothermal multiphase flow conditions. *Computers & Geosciences*, *37*, pp. 763 – 774. (2011).

Yeh, A., Croucher, A.E. and O'Sullivan, M.J.: Recent developments in the AUTOUGH2 simulator. *Proc. TOUGH Symposium 2012*. Report LBNL-5808E. Lawrence Berkeley National Laboratory, Berkeley, California, pp. 340 – 347. (2012).

Zhang, K., Wu, Y.-S. and Pruess, K.: *User's Guide for TOUGH2-MP—A Massively Parallel Version of the TOUGH2 Code.* Report LBNL-315E, Lawrence Berkeley National Laboratory, Berkeley, California, 108 pp. (2008).

Zhang, Y., Pan, L., Pruess, K., Finsterle, S.: A time-convolution approach for modeling heat exchange between a wellbore and surrounding formation. *Geothermics*, *40*(4), pp. 251 – 266. (2011).