WHAT'S NEW IN iTOUGH2?

Stefan Finsterle

Lawrence Berkeley National Laboratory
Earth Sciences Division
One Cyclotron Road, MS-wherever
Berkeley, CA 94720
e-mail: SAFinsterle@lbl.gov

ABSTRACT

iTOUGH2 supports the TOUGH suite of nonisothermal multiphase flow simulators by providing capabilities for sensitivity analyses, automatic parameter estimation, and uncertainty quantification. iTOUGH2 is continuously updated in response to scientific challenges and user needs, with new capabilities added to both the forward simulator and the optimization framework. This article summarizes some of these new iTOUGH2 features.

INTRODUCTION

iTOUGH2 (Finsterle 2007abc) provides inverse modeling capabilities for the TOUGH suite of nonisothermal multiphase flow simulators (Pruess et al., 1999). 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. iTOUGH2 updates are driven by scientific challenges and user needs, with new capabilities added to both the forward simulator and the optimization framework.

Recent advances related to the forward simulator include: overland flow and coupling to subsurface flow; semianalytical solution for radial heat exchange between wells and the formation; addition of gravitational potential to enthalpy; and additional time-stepping options.

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; inclusion of global sensitivity analysis methods; calculation of parameter identifiability; model reduction through automatic selection and estimation of superparameters; measuring the relative impact of omitting individual data points; evaluation of the Nash-Sutcliffe and Kling-Gupta efficiency criteria; assigning properties and sinks/sources to regions and estimation of their geometric parameters; reading spatial observation data; tying of parameters; and joint hydrogeophysical inversions.

CODE ENHANCEMENTS

The following subsections describe some of the features recently incorporated into iTOUGH2, starting with additions to the forward operator (i.e., TOUGH2), followed by enhancements of the inverse operator.

Enhancements of TOUGH2 Forward Model

iTOUGH2 is wrapped around standard TOUGH2 (Pruess et al., 1999), calling it to obtain select output evaluated for a given parameter set. However, many modifications to the TOUGH2 simulator have been made. Some of these features are motivated by the fact that—if used within the iTOUGH2 optimization framework—the simulation problem has to be solved in a single run, i.e., it cannot be interrupted, for example, to edit the mesh, or to change boundary conditions. This requirement has led to a number of useful features, such as the ability to connect steady-state and transient simulations; to change geometric mesh information after internal mesh generation; to change element volumes, primary variables, and certain material properties and flags at specified times; and to select additional convergence criteria.

Other enhancements were driven by specific user needs, such as the incorporation of non-Darcy flow based on the Forchheimer equation and choked flow in gas wells; internal generation of spatially correlated, random property fields using geostatistics (Finsterle and Kowalsky, 2007); time-dependent Dirichlet and free-drainage boundary conditions; more flexible formulations of the van Genuchten and Brooks-Corey relative permeability and capillary pressure functions; Leverett scaling of capillary strength parameter; inclusion of the active fracture concept of Liu et al. (1998); material-related sinks and sources; vapor-pressure reduction to prevent disappearance of the liquid phase; and five- to nine-character element names.

A third group of enhancements includes features that simply increase user convenience, such as the signal handler, which allows a user to request printout or to gently terminate a TOUGH2 run at any point during the simulation; free-format and tabular reading of GENER and TIMES blocks; improved time-stepping and printout control; and intermediate saving of restart files.

Most of these options are described in Finsterle (2007b; Appendix A) or in separate reports. They are useful even if iTOUGH2 is only used to perform forward simulations. The following paragraphs describe capabilities and features that were recently added to the simulator in iTOUGH2.

Coupled overland-subsurface flow

Coupling between overland flow and subsurface flow has been added to iTOUGH2. Overland flow is solved using the non-inertial, diffusion wave form of the Saint-Venant equations, where the momentum and continuity equations are given by:

$$S_{f,i} = -\nabla(z_l + h_s) \tag{1}$$

$$\frac{\partial h_s}{\partial t} + \nabla \cdot (h_s U) = q_s \tag{2}$$

Here, $S_{f,i}$ is the friction slope [-] in the direction i, z_l is land surface elevation [L], h_s is the water depth on the surface, U is the depth-averaged flow velocity [LT^{-1}], and q_s is a source/sink term [LT^{-1}]. The Manning-Strickler formula is used for relating velocity to friction slope:

$$U_i = \frac{h_s^{2/3}}{n_{man}} \sqrt{S_{f,i}} \tag{3}$$

with n_{man} being the Manning roughness coefficient [L$^{-1/3}$T]. The diffusion wave form of the Saint-Venant equation assumes slowly varying flow.

The approach developed by Weill et al. (2009) is followed to couple the surface and subsurface flow equations. A surface layer of thickness e is expected to be present at the top of the numerical model. For liquid flow within the surface layer, Eqs. (1)–(3) are combined into a form that is similar to that describing flow in a porous medium:

$$\frac{\partial h_s}{\partial t} - \nabla \cdot \left(K_s \nabla(z_l + h_s)\right) = q_s \tag{4}$$

Here, the nondiagonal terms of the hydraulic conductivity tensor K_s are zero, and the diagonal components are

$$K_{s,xx} = \frac{h_s^{5/3}}{n_{man}\sqrt{\nabla_x (z_l + h_s)}} \tag{5}$$

$$K_{s,yy} = \frac{h_s^{5/3}}{n_{man}\sqrt{\nabla_y (z_l + h_s)}} \tag{6}$$

$$K_{s,zz} = k_{zz} \frac{k_{rl}}{\mu_l} \tag{7}$$

The horizontal hydraulic conductivities describe surface water flow, while the vertical hydraulic conductivity describes resistance to liquid flow between the surface and subsurface layer, with k_{zz} equal to the vertical permeability of the subsurface layer. The liquid pressure in the surface layer is assumed hydrostatic. Because liquid and gas pressures are continuous across the surface/subsurface boundary, negative water depths occur when there is no runoff. The volumetric liquid content in the surface layer is defined as

$$\theta_l = \begin{bmatrix} 0 & \text{for } h_s < 0 \\ h_s / e & \text{for } h_s \geq 0 \end{bmatrix} \tag{8}$$

For vertical liquid flow, the relative permeability is set to one, unless $h_s/e < 10^{-5}$, at which point it is set to zero. To capture the head due to ponding in the surface layer, a positive capillary pressure is calculated as a function of h_s.

For gas flow within the surface layer and between the surface and subsurface layers, the regular subsurface flow equations are used. If runoff occurs in the surface layer, i.e., $\theta_l > 0$, then $k_{rg} = 0$ for pressure gradients from the surface to the subsurface layers such that no gas flows into the subsurface (though it is possible for pressurized gas to escape the subsurface and flow to the surface layer), and $k_{rg} = 1$ within the surface layer such that gas flows freely into the atmosphere. If there is no runoff, $\theta_l = 0$, $k_{rg} = 1$ and the intrinsic permeability of the surface layer is assumed isotropic and equal to the vertical intrinsic permeability of the subsurface layer.

Surface water flow is solved simultaneously and fully coupled with subsurface flow using the standard TOUGH2 implicit scheme. Note that time-step size may be governed by the relatively fast flow occurring in the surface-water layer.

The implementation of each component of the coupled surface-subsurface flow model has been tested, and the new capability has been applied for the design of a rapid infiltration basin system, where the interaction of overland flow of treated wastewater and its infiltration into the unsaturated soil impacts groundwater mounding, as well as the conditions determining denitrification rates (Akhavan et al., 2012)

Semi-analytical radial heat exchange

In applications of oil, gas, and geothermal energy production, as well as geological CO_2 storage, injection and production wells serve as a conduit between the ground surface and the subsurface reservoir. The great length of these wellbores results in a very large heat exchange area between the well and the formation. If such a well is used to inject CO_2 for geological carbon sequestration, the heat transfer between the well and the surrounding formation will have a significant effect on the properties of the CO_2 as it flows down the well, and thus on the downhole conditions, potentially affecting injectivity and thereby overall storage efficiency. Similarly, the performance of an injection-production cycle in an engineered geothermal system depends on the temperature and thus phase state, density, and viscosity of the working fluid in the cool injection and hot production wells. An accurate simulation of heat-transfer processes between the formation and fluids in these wells is thus essential for performance evaluation and design of injection and production systems.

The processes to be considered in the low-permeability caprock above the target reservoir mainly include nonisothermal, multiphase fluid flow within the wellbore and conductive heat exchange between the wellbore and the geologic formation. The processes within the well can be modeled using Darcy's law with an effective permeability, or a numerical wellbore simulator, such T2Well, which uses a drift-flux model (Pan et al., 2011). However, numerical modeling of the conductive heat exchange between the cased well and the formation would be computationally costly if the region around the well affected by this heat transfer were fully discretized, especially when the target formation is very deep. Because the only process involved in this transfer is heat conduction (e.g., no fluid exchange), a viable alternative is to solve the heat conduction problem between the wellbore and formation analytically. Avoiding numerical discretization of the formation above the reservoir significantly reduces computational cost.

A semi-analytical solution using a time-convolution approach was implemented into iTOUGH2 for efficiently calculating radial conductive heat exchange between a wellbore and the surrounding formation. The details of the approach can be found in Zhang et al. (2011). The model allows for a nonconstant initial temperature profile, and heterogeneity in thermal properties along the well. The model was used to examine how radial heat exchange affects CO_2 injection into a deplete gas reservoir. The comparison included four conceptual models: (1) the numerical solution of a fully discretized model; (2) the new semi-analytical approach; (3) the analytical solution of Ramey (1962); and (4) the response of a system in which the heat transfer between the wellbore and the formation is ignored.

Figure 1 shows the simulated temperature evolution at the bottom of the wellbore for the four scenarios. Upon initial injection, the bottomhole temperature decreases sharply as the cooler CO_2 arrives at depth. However, after this initial drop, as the pressure in the well increases during this constant-rate injection period, injection temperature also increases due to the large Joule-Thomson coefficient of CO_2, which is dominant so that the temperature in the well follows the injection rate change. During high-rate periods, conductive heat exchange with the formation is negligible compared to the convective heat transport and Joule-Thomson effects; as a result, the details of the heat-exchange model are irrelevant, and all solutions coincide. However, when the injection rate is low, Joule-Thomson cooling due to decompression of the fluid and the reduced advective downflow of relatively cool CO_2 are insufficient to counter the heating of the wellbore by conduction from the formation. During these transient periods, the choice of the heat-exchange model is significant, with the numerical and proposed semi-analytical solutions yielding consistent results. Ramey's solution, which makes a steady-state heat flow assumption in the wellbore, does not properly react to these changes in wellbore conditions, and overestimates the heat uptake from the formation. Conversely, neglecting any heat exchange between the well and the formation results in a drastic underestimation of injection temperatures, since no warming of the CO_2 occurs as it flows down the well at a relatively slow velocity.

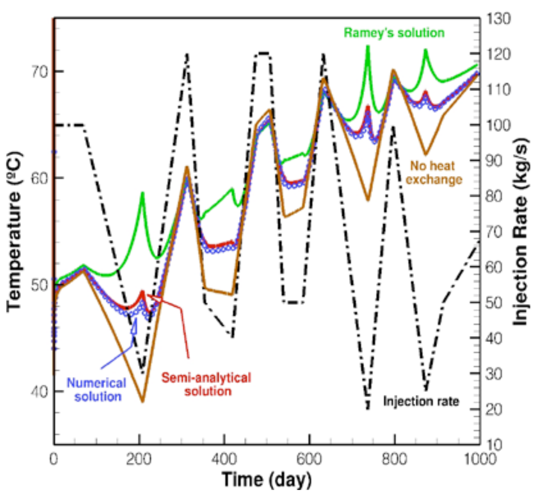

Figure 1. Injection rate and temperature change at the well obtained with four heat-exchange modeling approaches.

This example demonstrates the sensitivity of predicted wellbore and formation temperatures to the choice of the heat-exchange model. Accounting for heat exchange and coupled thermal-hydraulic processes is especially significant for fluids whose properties vary considerably as a function of pressure and temperature, such as CO_2. The comparison between the developed solution and fully discretized numerical solution shows that the proposed semi-analytical solution is a good approximation.

For long vertical wells, the gravitational potential needs to be 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 in iTOUGH2 to avoid an overprediction of the temperature and heat content of the produced fluid.

Regions

Sinks and sources, as well as permeabilities, can be assigned to regions (boxes, ellipsoids, cylinders) that are defined by a few geometrical parameters. These geometrical parameters can be adjusted by iTOUGH2, allowing the user to, for example, examine the impact of the location of a fault, or to estimate the location and extent of a heat upflow zone in a geothermal system.

Enhancements of iTOUGH2 Optimization Framework

The following subsections summarize some of the features added to the iTOUGH2 optimization framework.

Link to external models with 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 concept of separating the forward model and inversion framework has long been followed by general, model-independent, nonlinear parameter estimation packages, specifically Doherty (2008). The PEST protocol (Banta et al., 2008) defines the interface between the analysis tool and the input and output files of the application software. To make iTOUGH2 capabilities accessible to more application models, the subroutines comprising the PEST protocol have been implemented into iTOUGH2 (Finsterle, 2010).

PEST protocol requires the application model (1) to provide input through one or more ASCII input files (or the keyboard), (2) to return output to one or more ASCII output files (or the screen), (3) to run the model or multiple models using a system command (an executable or script/batch file), and (4) to run the models to completion without user intervention. For each forward run invoked by iTOUGH2, selected parameters in the application model input files are overwritten with values updated by iTOUGH2, and selected variables in the output files are extracted and returned to iTOUGH2. 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.

The inclusion of the PEST protocol into the iTOUGH2 architecture is shown in Figure 2. The parameter vector **p** (which is updated by iTOUGH2's minimization algorithm or by the sampling procedure used for uncertainty quantification) is transferred to the PEST protocol, which replaces generic parameter names in the so-called template file with the appropriate numerical values, and generates a valid input file. The external model is executed using a system call, which may be the name of an executable code, a command line, or a script file. After completion of the model run, the resulting output files are parsed using directives from the PEST instruction file, and the values of interest are extracted and filled into the observation vector **z**, which is then used by iTOUGH2 to evaluate the objective function or for further analysis.

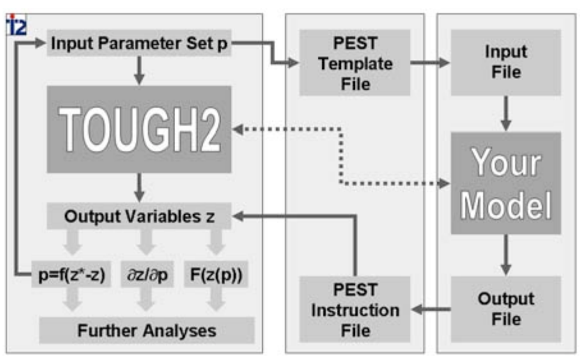

Figure 2. iTOUGH2 optimization and analysis tools evaluate the system response **z** as a function of adjustable input parameters **p**, where the relation between **z** and **p** is either given by the fully integrated TOUGH2 simulator or by an external model through the PEST protocol, which uses text-based template and instruction files for communication with the external model.

The extended code 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.

Illustrative applications of the PEST protocol as part of iTOUGH2 are discussed in Finsterle and Zhang (2011) and Wellmann et al. (2012). In particular, this new capability allows users to perform inverse analyses of TOUGH-related models that are not integrated into iTOUGH2, such as TOUGHREACT (Xu et al., 2012), TOUGH2-MP (Zhang et al., 2008), and TOUGH+Hydrate (Moridis et al., 2008).

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, supported by iTOUGH2.

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. In the Morris one-at-a-time (MOAT) elementary-effects method (Morris, 1991), each axis of the parameter hypercube is subdivided into k-1 intervals for a total of k^n grid points, where n is the number of parameters. A perturbation Δ is then calculated for each parameter i:

$$\Delta_i = \frac{k}{2(k-1)} \cdot (p_{i,\max} - p_{i,\min}) \qquad (9)$$

Next, a random grid point in the parameter space is selected, the model is run, and the performance measure z is evaluated. Then—one at a time and in random order—each parameter p_i is perturbed by Δ_i, the model is run to recalculate z, and the corresponding impact (or elementary effect, EE_i) on the output is computed as

$$EE_i = \frac{z(p_1,\ldots,p_i+\Delta_i,\ldots,p_n)-z(p_1,\ldots,p_n)}{\Delta_i} \quad (10)$$

The procedure is repeated for multiple, randomly selected starting points of a path in the parameter space that consists of n steps and n+1 simulation runs for the evaluation of the elementary effect in the vicinity of this point. 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. A second, variance-based method (Saltelli et al., 2008) is also implemented. However, it usually requires a large number of model evaluations and is thus less practical for computationally expensive models. Applications of iTOUGH2's global sensitivity-analysis methods are described in Wainwright et al. (2012).

Statistical analyses

iTOUGH2 performs a rather extensive residual and uncertainty analysis (Finsterle and Zhang, 2011), 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. (See Gupta et al. (2009) for a detailed interpretation.) 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 (with the estimated error variance as the third, standard alternative). An application is described in Kowalsky et al. (2012a).

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 an 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.

The sensitivity analysis is expanded to include a statistic for evaluating parameter identifiability. Introduced by Doherty and Hunt (2009), parameter identifiability indicates the degree to which a parameter lies within the calibration solution space, which is obtained by truncated singular value decomposition (SVD) of the weighted parameter sensitivity matrix. A similar concept is used to define so-called superparameters (Tonkin and Doherty, 2009), which allow parameter estimation in a subspace of the original parameter hypercube. This implementation is an extension of the approach described in Finsterle and Kowalsky (2011). Note that these approaches are based on linear theory, and additional testing is required to assess their usefulness for highly nonlinear TOUGH2 models.

Hydrogeophysics

The capabilities for jointly inverting hydrological and geophysical data for the estimation of hydrogeological, geophysical, and geostatistical parameters have been extended, as is described in Kowalsky et al. (2012b), Doetsch et al., (2012), and Commer et al. (2012).

Other user features

The following user features have been added to iTOUGH2:

(1) Parameters can be tied to a parent parameter, so that a single value is estimated and then assigned to all tied parameters (potentially with shifts and scaling factors applied). Parameters defined in an iTOUGH2 input file can also be made inactive.

(2) Observations with a relatively large support scale generally refer to lists of elements or connections. Region definitions (boxes, cylinders, and ellipsoids) can now be used to internally generate these lists. Moreover, the geometrical parameters of these regions can be updated or estimated, whereby the contribution of the output at a given location is weighted according to its distance from the center of the region, thus assuring a differentiable result (see Finsterle and Zhang (2011) for an example).

(3) iTOUGH2 mainly supports time-series data, i.e., measurements that are taken at a few points in space and many points in time. For geophysical applications, however, the reverse is often the case, i.e., data of high spatial resolution are taken at only a few points in time. The reading and processing of spatial data is now supported.

(4) iTOUGH2 now supports automatic selection of measurement times as calibration times, with the user having the flexibility to define additional points in time where the measured and calculated system response will be compared.

WHAT'S NEXT?

We will continue to update iTOUGH2 and add new features and analysis methods to both its forward model and inversion framework in response to user requests and to address scientific challenges. Emphasis will be placed on reduced-order modeling and subspace approaches (Pau et al., 2012) and hydrogeophysical applications. We will report on these enhancements in due time.

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