FUTURE DIRECTIONS IN GEOTHERMAL MODELLING

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ABSTRACT

Numerical modelling is increasingly playing a key role in the planning and management of geothermal developments, but many of the modelling tools that are used today have origins in the 1980s. This heritage poses significant challenges for developing the complex models that are required today. This paper will use the modelling of Wairakei and other geothermal systems to provide a context for considering what the next generation geothermal reservoir simulator should look like. Matters that will be discussed include:

- Modelling complex geologies and linking with tools such as MVS and Leapfrog
- Advanced treatments of wells
- Modelling the top of the system - surface features, groundwater levels and capping structures
- Modelling moving fronts, boiling zones, and chemistry
- Model calibration
- Very deep systems and supercritical fluids
- Fluid rock interactions
- Numerics
- Model management

1. HISTORY OF GEOTHERMAL MODELLING

The history of geothermal modelling goes back to the early 1970s (see O'Sullivan et al., 2001 and 2009, for more details). The starting point for the acceptance of numerical modelling by the geothermal industry was the 1980 Code Comparison Study (Stanford Geothermal Program, 1980). In that study, several geothermal simulators, including SHAFT79 (a predecessor of TOUGH2), were tested on a suite of six problems. The University of Auckland (UOA) had an entrant in the Code Comparison Study that performed quite well, but the flexible grid structure and the ability to easily add new equations of state offered by MULKOM (the replacement for SHAFT79) made it superior to our code, and we at UOA switched codes and have remained enthusiastic users of MULKOM and later TOUGH2 since the early 1980s.

Experiences with geothermal modelling at Industrial Research Limited (IRL, previously Applied Mathematics Division, DSIR) are similar. Early modelling studies of the Kawerau system were carried out with an in-house simulator (White and McGuinness, 1991) but a switch to TOUGH2 was made in the early 1990s (White, 1995) and many modelling studies using TOUGH2 have been carried out at IRL since that time.

By the late 1980s UOA had set up a 3-D model of Wairakei (see O'Sullivan et al, 2009). Most of the modifications made to TOUGH2 at UOA have resulted from efforts to build bigger and better models of Wairakei. For example, it was found that the original linear equation solver in MULKOM (MA28) could not handle a model with more than about 500 gridblocks. Therefore conjugate gradient solvers (see Bullivant et al., 1991) were introduced which allowed much larger models to be run. Conjugate gradient solvers were introduced into TOUGH2 at LBNL (Moridis and Pruess, 1998) and IRL (Burnell, 1992) at about the same time. UOA and IRL both independently carried out some work on the thermodynamics routines COWAT and SUPST to speed them up considerably.

Because of interest in the Ohaaki geothermal system, which has high gas content, UOA developed an equation of state (EOS) for mixtures of water and CO_2 (Zyvoloski and O'Sullivan, 1980; O'Sullivan et al, 1985). This became EOS2 in MULKOM, but was replaced in 1997 by an improved version developed by Battistelli et al. (1997).

At IRL the implementation of the capability for modelling chemical reactions with TOUGH2 was pioneered by White and others resulting in the CHEM-TOUGH code (White, 1995). A similar development occurred at LBNL producing TOUGH-REACT (Xu *et al*., 2006).

From the mid-1980s until the present time, the UOA model of Wairakei has grown from a small 3-D model of 301 gridblocks to large complex models of ~50 K gridblocks (O'Sullivan and Yeh, 2007). Similarly IRL are now running large complex models of fields such as Ngatamariki (Clearwater et al, 2011). These achievements were made possible by the effectiveness of TOUGH2, but the process has shown up areas where more research needs to be carried out and where further advances in modelling technology are desirable. These are discussed below.

The fact that TOUGH2 (and its predecessors MULKOM and TOUGH) is so successful and has been so widely adopted for geothermal reservoir modelling and many other applications is a testimony to the good design of the code by Karsten Pruess (Pruess, 1988, 1991, Pruess *et al*., 1999). However it is written in old fashioned FORTRAN and is quite difficult to modify. New versions for modelling gas hydrate, TOUGH+HYDRATE, (Moridis et al., 2008) and carbon sequestration, TOUGH+CO2, (Zhang et al. 2009), have been written in a modern programming language, Fortran 95/2003, but a geothermal version is not currently available and in any case in our opinion more is required than just a rewriting of TOUGH2.

Recently an international working group was set up by the International Parnership for Geothermal Technology (http://internationalgeothermal.org/Working_Groups/Modeling.html) to identify the priorities for future geothermal modelling software and they established the diagram shown in Figure 1 to describe their suggested research aims.

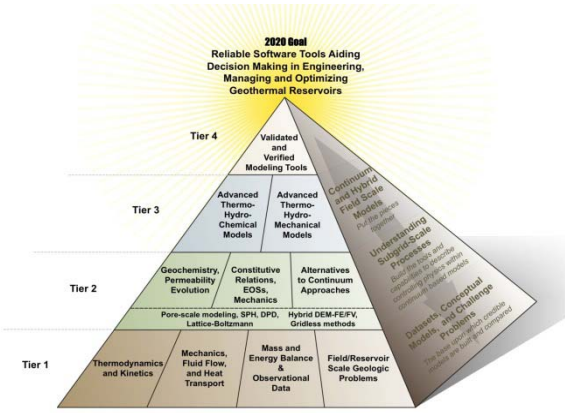

Figure 1: Plan for geothermal modelling research from IGPT.

While we agree with the IGPT report, there are some issues for practical geothermal reservoir modelling in the 21st century that they did not address and the purpose of the present paper is to discuss some of them.

MODELLING COMPLEX GEOLOGIES AND LINKING WITH TOOLS SUCH AS MVS AND LEAPFROG

Recently there has been a rapid uptake of the use of computer based geological models such as MVS and LeapFrog in the geothermal industry. At UOA we have worked with ARANZ, GNS Science and Contact Energy on interfacing LeapFrog with TOUGH2 so that the geological model can be used directly to assign rock-types to a TOUGH2 model (refs) and also so that results from a TOUGH2 simulation can be visualized by LeapFrog. Similarly IRL and Mighty River Power modellers have interfaced geological models created with MVS with TETERAD models.

This is one example of a trend that we expect to continue and increase: namely the interfacing of TOUGH2 with other software. It is likely that results from TOUGH2 simulations will be compared with models of MT, gravity, micro-seismicity, geochemistry and subsidence (see below), for example. This interfacing requires the easy manipulation of TOUGH2 input and output, a task that UOA have recently been addressing with the development of PyTOUGH, an open-source Python scripting library for TOUGH2 (Croucher, 2011; Wellmann et. al, 2012). We expect this kind of flexible and customizable interface for TOUGH2 to be a very important ingredient of geothermal modeling in the future.

ADVANCED TREATMENTS OF WELLS

Wellbore-reservoir interaction

For modelling the future scenarios of geothermal systems, it is usual to operate each production well on deliverability, so that the production rate falls off as the pressure of the reservoir feed block declines. The simplest version of the deliverability formula available in TOUGH2 is

$$q_\beta = \frac{k_{r\beta}}{\nu_\beta} PI\left(p_\beta - p_{wb}\right) \qquad (1)$$

Here, q_β is the mass production rate, $k_{r\beta}$ is the relative permeability, ν_β is the kinematics viscosity and P_β is the block pressure, all for phase β. PI is the productivity index, discussed in detail by Pruess et al. (1999), and P_{wb} is the flowing bottom-hole pressure.

One of the difficulties with using (1) is the fact that for a fixed wellhead pressure, P_{wb} varies with the total mass flow q_m and the flowing enthalpy h_f. To accurately deal with this issue, it is necessary to couple a wellbore simulator with a reservoir simulator. This approach was taken by Hadgu et al. (1995) and Bhat et al. (2005), but has not been generally adopted, probably because the maximum time step permitted is likely to be controlled by wellbore processes and to be impractically small.

An alternative approach introduced by Murray and Gunn (1993) and also implemented in TOUGH2 (Pruess et al., 1999) is to generate a table of flowing bottom-hole pressures defining the function below:

$$P_{wb} = f(q_m, h_f; P_{wh}, z, r_w) \qquad (2)$$

In TOUGH2, this formula is implemented by an interpolation scheme based on tabular data pre-calculated with a wellbore simulator and read for a separate data file. We have used both (2) and a simplified version in the form

$$P_{wb} = f(h_f; P_{wh}, z, r_w) \qquad (3)$$

This is implemented by reading in a table of values of P_{wb} vs h_f and using interpolation. The main use we have made of (3) is in ensuring that production wells in our Wairakei model are switched off when the feedzone enthalpy drops below 763.1kJ/kg (180°C).

A second difficulty with using (1) is that in many cases, geothermal wells have more than one feedzone. Again, the only way to model this situation accurately is to use a coupled wellbore-reservoir simulator. TOUGH2 offers an approximate method for modelling multifeed wells by means of the following formula for calculating the wellbore pressure in layer $l+1$ from that in layer l:

$$P_{wb,l} = P_{wb,l+1} + 0.5g(\rho_l^f \Delta z_l + \rho_{l+1}^f \Delta z_{l+1}) \qquad (4)$$

Here, g is the acceleration of gravity and ρ_l^f is the flowing density in the well opposite layer l. The method used for calculating ρ_l^f is described by Pruess et al. (1999). The wellbore pressure at the deepest layer must be prescribed. At present the multifeed option cannot be combined with a rate and enthalpy-dependent P_{wb} defined by (2).

Control of production and injection

UOA have introduced some minor modifications of the standard deliverability option in TOUGH2. The first option allows for the fact that a geothermal well may be operated in throttled state initially and then opened up over time. To represent this situation, the mass flow is calculated using the following equation:

$$q_m = \min(q_{delv}, q_{\max})$$

Here, q_{delv} is the mass flow calculated using (1), assuming that the well is fully open, and q_{max} is the target maximum flow. The flow restriction can be applied either to the total mass flow or to the total steam flow.

For most geothermal projects, as the total production from a group of wells falls away, make-up wells are introduced. UOA have included the automatic introduction of make-up wells as an option in TOUGH2. A group of wells is given "DMAK" as a well-type, the current wells are given a positive PI, and the make-up wells are given a negative PI. The total mass flow (or steam flow) is compared with a target value, and when the total falls below 95% of the target, a make-up well is added. If the addition of the new well means that the target flow is exceeded then it is throttled back so that the target is exactly met (an alternative option is allowed so that flow in all wells is reduced by a small fraction so that the target is exactly met).

Other options that would make TOUGH2 easier to use in simulating production for geothermal systems are: to be able to assign a particular well to a named separator, to be able to use a complex time schedule for wells on deliverability, and to be able to specify the separation process for each well (e.g., single flash, double flash, or binary plant). These options are not essential in terms of their effect on the reservoir behavior, but they would make it easier to carry out simulations of complex future scenarios without having to stop and restart the simulation several times. Again the development of a complex schedule of production and injection for a TOUGH2 simulation of a future scenario is probably better achieved with a customizable PYTHON script or a customizable subroutine rather than through trying to anticipate all possibilities within the specification of the GENER module in TOUGH2.

MODELLING THE TOP OF THE SYSTEM - SURFACE FEATURES, GROUNDWATER LEVELS AND CAPPING STRUCTURES

In the UOA model of Wairakei (O'Sullivan *et al*., 2009) the unsaturated zone is incorporated by using an air-water EOS and extending the model up to the ground surface. Some other geothermal models take the water table as the top of the model. The approach used for the Wairakei model works satisfactorily, but does not track the movement of the water table very accurately, since the minimum layer thickness is 25 m. It would be useful to be able to handle the water table in a geothermal model similarly to the way unconfined aquifers are included in groundwater models.

A more sophisticated approach is required than for groundwater modelling as the surface where $P = P_{atmospheric}$ may be partly boiling. Nevertheless, having the top surface of a model, either water or steam, able to move up or down through a gridblock would be a very useful advance in accurately representing near-surface behavior, such as the development of large areas of steaming ground.

Similarly, improved models of surface features such as hot springs and geysers would be useful. Some modelling studies of surface features have been carried out (see Kissling and White, 2006, Sapatdji et al., 1994), but these local models have not been coupled with large-scale reservoir models. Currently, we use the DELV option to represent the hot springs as wells on deliverability, whose flow drops off as the pressure and/or enthalpy of the feed zone declines.

MODELLING MOVING FRONTS, BOILING ZONES, AND CHEMISTRY

TOUGH2 uses the finite volume method with upstream weighting of key properties that must be evaluated at block boundaries, such as relative permeabilities and flowing enthalpies. While this procedure leads to a robust and stable computational method it also results in the introduction of numerical dispersion. At UOA we have carried out some numerical experimentation on using the Euler-Lagrange method (Croucher and O'Sullivan, 2004), but only for single-phase flows. Potentially a similar approach could be used for two-phase flows and in particular to track the expansion and contraction of boiling zones. However it may be difficult to implement such an approach on a general 3D unstructured grid.

The phase change algorithm in TOUGH2 works well for models that involve pure water but for models with a second gaseous component, say CO2 or air, then sometimes simulations tend to stall when one block in a two-phase state experiences difficulty in changing to all liquid conditions. Sometimes we have used manual intervention to force the phase change which is a clumsy solution to the problem and a more sophisticated control of this type of phase change is required.

Much work has been carried out at IRL on including chemistry in TOUGH2 simulations (Burnell, 1992, White, 2005). The goal is to provide further constraints to the modelled reservoir flow processes by matching changes in chemistry within the reservoir. Chemistry is fully coupled with TOUGH2; chemical species are advected with the calculated mass flow, and changes in chemistry and dissolution and precipitation alter the flow characteristics. Adding the extra equations to describe the chemistry results in very large model systems which are very time-consuming to solve. This type of modelling is currently suited to models with small grids or short production-scale times.

MODEL CALIBRATION

Background

The greatest challenge facing the geothermal modelling community is improvement in model calibration techniques. The calibration process involves two stages (O'Sullivan et al., 2001, Mannington et al., 2004).

(i) Natural State Modelling

(ii) History Matching

In natural state modelling, the permeability structure and location of the deep inflow are guessed, and then a simulation of the model to steady state is carried out. This steady state is assumed to be the natural or pre-exploitation state of the geothermal system that has developed over geological time (a concept that is open to some debate). Then the natural state temperature and the location of the surface outflows are compared to the measured data. If the match is not satisfactory, then adjustments are made to the permeability structure and deep inflows, and the process is repeated, possibly many times.

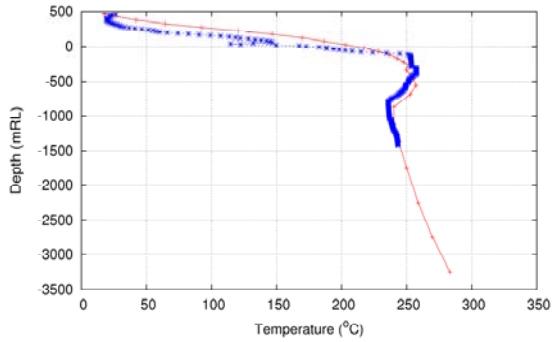

Figure 2. Natural state temperatures in one well for the Wairakei model (data - blue symbols, model - red line)

Once a reasonable natural-state model has been obtained (see Figure 2 for example), the results are used as the initial conditions for a simulation of the production and injection history, with the measured mass flows being assigned to the appropriate model blocks. Then the pressure and enthalpy changes predicted by the model are compared to the data, and adjustments are made to the permeabilities and porosities to improve the model (Figures 3 and 4).

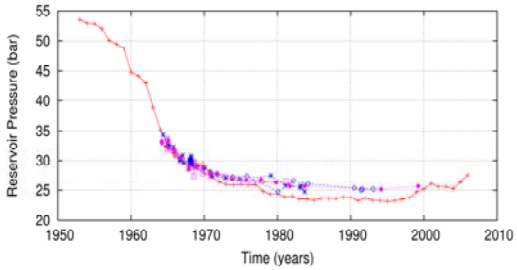

Figure 3. Pressure decline in the western borefield for the Wairakei model (data - blue symbols, model - red line)

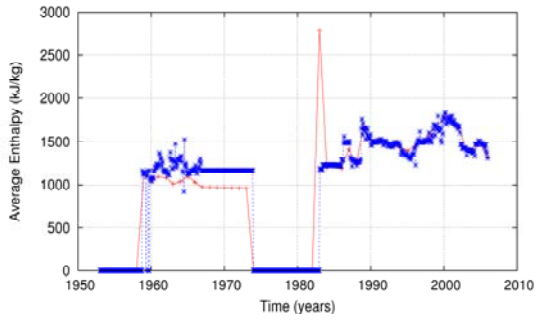

Figure 4. Enthalpy changes for one well in the Wairakei model (data—blue symbols, model—red line)

The process described above is appropriate for a convective geothermal system where the fluid is moving in the natural state. It is not so useful for warm water systems or hot dry rock (EGS) systems, where conduction is the only heat-transfer mechanism and the reservoir fluid (hot water) does not move.

In hot water systems, the reservoir does not boil during production, and the production enthalpy does not change. However, in systems like Wairakei and Mokai (New Zealand), there is considerable boiling, and enthalpy changes are very useful for model calibration.

We have used three calibration techniques:

(i) Manual calibration

(ii) Inverse modelling with iTOUGH2 (Finsterle, 2007abc)

(iii) Statistical sampling methods (Cui et al., 2007)

Suggestions for improving these methods will be discussed below.

Improved Manual Calibration

The basic idea of manual calibration is to determine where the model fit to the data is worst, and then to adjust the model structure to improve the fit. This is a slow process, because after each adjustment of the structure, the model must be re-run (possibly both the natural state and history match), and the results re-checked against the data. In some cases, it may not be obvious which reservoir parameters should be adjusted to improve the model, and then the skill and experience of the modeler can assist the process.

To speed up manual calibration and to make it less dependent on the modeller, an "expert system" approach may be useful—and this is one of our current research themes. The idea is to codify the various strategies followed by a modeller and to apply them in a systematic fashion. For example, in a natural state model, if block I is too hot, then the following steps should be followed:

(i) Check flow directions for all connections between block I and other blocks.
(ii) For flows into block I, if the neighboring block J is hotter, then decrease the permeability of block J. If block J is colder than block I, then increase the permeability of block J.
(iii) Repeat for all blocks sending fluid into block I.

Several rules of this kind are currently used by modelers, but need to be formalized. There are many challenges to overcome in order to make such an expert system work, and there are several unanswered questions. For example: will it converge to a good solution in a reasonable time? It is worth noting that simple iterative methods for the numerical solution of Laplace's equation, that have some similarities with the process described above, have a convergence rate that is dependent on the choice of a relaxation parameter.

Another problem with the process discussed above is the local nature of the adjustments proposed. In some cases it may be necessary to change the permeability over quite a large section of the model, in order to change the flow pattern sufficiently to achieve the required temperature change. In principle, it would be possible to track all streamlines entering the block in question and to adjust permeabilities along the streamlines.

With a scheme for local adjustment of permeabilities, based on fitting relatively sparse downhole temperatures, there is the problem of deciding whether to make a local or a global change. For example, if the rule suggests that rock-type IGNIM should have its horizontal permeability increased in block J, then should this change be implemented in all blocks with IGNIM as a rock-type? Or should a new sub-rock-type IGNIX with a higher horizontal permeability be assigned to block J? Possibly both options should be tried, and the new rock-type IGNIX should only be accepted if it produces a substantially better result. That is, there should

be some penalty discouraging fragmentation of the rock-types.

Improved Inverse Modelling

The basic idea of the inverse modelling approach, available through iTOUGH2 (Finsterle, 2007abc) for example, is to solve a nonlinear optimization problem. The unknowns are selected model parameters, and the objective function is the sum of squares of the difference between the model results and given data. What distinguishes inverse modelling of geothermal reservoirs from more traditional nonlinear optimization problems is the complexity of the calculation for the objective function, i.e., through the forward problem, which requires a TOUGH2 simulation.

The iTOUGH2 code is a very comprehensive package. It offers several optimization methods (Gauss-Newton, Levenberg-Marquardt, Downhill Simplex, Simulated Annealing, Grid Search) and very complete sensitivity analysis. Similar functionality has been achieved with the FEHM geothermal simulator (Zyvoloski, 1992) and the PEST inverse modelling code (Doherty, 2005). However, unanswered questions remain. Some are general and relate to the use of nonlinear least squares (see Fox, 2009). These will be discussed further in the next section.

Other problems are more specific to the application of iTOUGH2 to the calibration of geothermal models. In general, we have found iTOUGH2 to be a very useful tool for improving models that are already quite good. Conversely, if a model is not already fitting the data well, iTOUGH2 will probably not produce a model that is much better.

The difficulty with using iTOUGH2 (or any inverse modelling code) in calibrating a geothermal model is the choice of the variable parameters. At one extreme, each block in the model could be assigned different x, y, z permeabilities and porosities. This would result in a huge number of unknown parameters and is currently impractical. The simpler approach, and that which is usually used with iTOUGH2, is to assign a relatively small number of rock-types and then use the permeabilities and porosities of a subset of these rock-types as the parameters to be optimized. (See for example, Porras et al., 2007, Kiryukhin et al., 2008.) However, even if the optimal values for all parameters, for all rock-types, are determined by iTOUGH2, the resulting model is probably not going to be the best possible.

It might be possible to produce a better model by subdividing the zone assigned, say, to rock-type IGNIM into two new zones, labeled IGNIA and IGNIB, for example. Then iTOUGH2 could be re-run optimizing the parameters for IGNIA and IGNIB independently. We have had some success with this technique (Omagbon and O'Sullivan, 2011), but what is required is a more systematic approach with, say, an outer XiTOUGH2 code, or a Python script, that controls the re-assignment of rock-types and calls iTOUGH2 to optimize parameter values for each new rock-type structure.

Statistical Sampling

As mentioned above, there are some fundamental problems with inverse modelling based on a least-squares-errors approach (see Fox, 2009). One difficulty is that a global optimum or even a local optimum found by a nonlinear optimization technique may not be a "good solution," in the sense that the optimal parameter values may not be what a reservoir engineer expects or finds acceptable. What is really required is to identify a region of the multidimensional parameter space where "good" solutions are likely to be found. The statistical sampling tool for doing this is the Markov Chain Monte Carlo (MCMC) technique (see Cui *et al.*, 2006, 2011). The trouble with MCMC is that it requires a very large number of samples to be taken, or, in the context of geothermal modelling, a very large number of forward runs of TOUGH2 have to be carried out.

UOA have applied MCMC to calibrating a simple single-layer model using data from an extended test of a geothermal well. This is the same problem previously investigated with iTOUGH2 by Finsterle et al. (1997). We have also applied MCMC to a model of the Mokai geothermal system with some success (Cui *et al.*, 2011). After two weeks of computation, the best natural state model produced by MCMC matches the downhole temperatures slightly better than the manually calibrated model.

Further advances with the MCMC technique are required to make it practically useful for calibrating geothermal models. Currently, we are investigating the use of a hierarchy of models ranging from a coarse grid to a fine grid, and we are investigating parallel rejection algorithms. As with inverse modelling techniques (e.g., iTOUGH2), MCMC is ideal for implementation on a cluster of computers in a distributed memory configuration. In the future, it may be possible to use a cluster of multicore processors, each running a parallelized version of TOUGH2 (see Moridis et al, 2008, Zhang et al, 2009).

None of the three methods discussed above can presently automatically deliver a well-calibrated model of a geothermal field.

VERY DEEP SYSTEMS AND SUPERCRITICAL FLUIDS

Large-scale models

Almost all models of geothermal systems do not include the whole of the large-scale convective system. Thus, the base boundary condition must include some input of very hot water, corresponding to the upflow zone of the convective plume. It would be better to make the model large enough so that the whole convective system is contained in the model, and then the permeability structure would have to be compatible with the flow and temperature structure. We have recently moved somewhat in this direction with our model of Wairakei-Tauhara by adding extra layers, so that it is now 4 km deep. Probably more layers, extending the model down to 6–7 km, should be added and a larger area included.

Improved EOS

The use of deeper models leads to the need for a thermodynamic EOS that can handle higher pressures and temperatures. IRL developed a supercritical EOS for pure water, firstly for MULKOM and then for TOUGH2 (Kissling, 1995) and later extended it to include mixtures of H2O and NaCl (Kissling, 2005). UOA have implemented the IAPWS-97 thermodynamic formulation (Wagner et al., 2000), including the supercritical capability valid for pressures up to 100 MPa and temperatures up to 800˚C

(Croucher and O'Sullivan, 2008). This improvement allows for models of high temperatures and pressures to be used, provided that the fluid can be approximated as pure water. It would be very useful for models of other fields (such as Ohaaki and Ngawha) to have an EOS for mixtures of water, carbon dioxide, and sodium chloride that is accurate for temperatures and pressures ranging from atmospheric up to supercritical (pure water) conditions. This would require the extension of the range of validity of the ECO2N fluid property module (Pruess, 2005).

Another EOS option that is required for modelling "gassy" geothermal fields such as Ohaaki and Ngawha, particularly in a carbon-conscious world, is one that can handle mixtures of water, air, and carbon dioxide. We have used a five-component EOS that can handle a mixture of water, methane, and air (broken down into its major components of N_2, O_2 and CO_2) for modelling coalbed methane extraction. Dropping the methane from this EOS would provide one possible approach, but the resulting module would include one more component than is really necessary.

FLUID ROCK INTERACTIONS

Subsidence

At present, subsidence is a significant concern at the Wairakei-Tauhara geothermal field (Allis et al., 2009). To model subsidence, we have used temperature and pressure changes calculated with TOUGH2 as input for a rock-mechanics simulation using the ABAQUS package (ABAQUS, 2003). We had some success in matching the occurrence of the subsidence bowls (see Yeh and O'Sullivan, 2007). The results for the Wairakei bowl are shown in Figure 5.

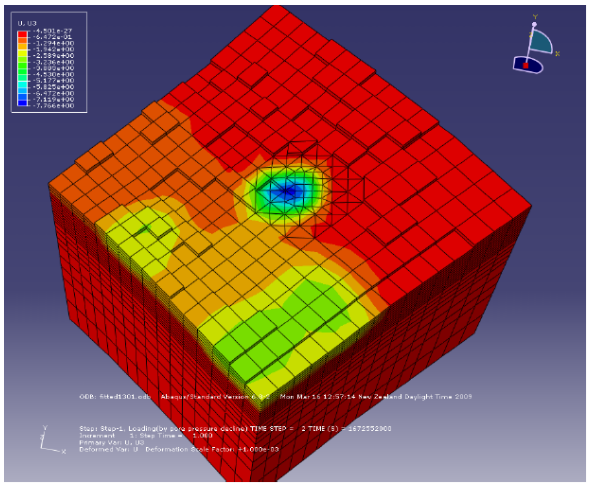

Figure 5. Model results for the Wairakei subsidence bowl.

The methods we have used for linking TOUGH2 and ABAQUS are very similar to those used by Rutqvist and Tsang (2003) and Pruess et al. (2004) for linking TOUGH2 and FLAC3D. The main problem to be dealt with is the interpolation of temperature and pressure data from the block-centered TOUGH2 grid onto the finite element grid used by ABAQUS. At Wairakei the pressure and temperature changes are quite uniform over a large area, and therefore interpolation from the TOUGH2 grid on to a finer grid for the ABAQUS model is not difficult.

Enhanced geothermal systems

More challenging coupled fluid-rock interactions need to be modelled. For example, modelling the spreading of a fracture zone created by hydraulic fractures as part of a hot dry rock (or EGS) project is a problem that needs to be solved. Planners of EGS projects need to be able to calculate the size and permeability of the fractured zone created by hydraulic fracturing. The FEHM code includes some fluid-rock interaction capability that was used in a study of the Hijiori hot dry rock site (Tenma *et al.*, 2008, Kelkar *et al.*, 2012).

Brittle-ductile zone

Some interesting studies of heat and mass transfer through and near the ductile zone, below geothermal systems, have been carried out by Fussels et al. (2009) and Regenauer-Lieb et al. (2009). Kissling et al (2009) included a Mohr-Coulomb yield condition into TOUGH2 which, together with an assumed regional strain rate based on GPS measurements, gave a depth to the brittle-ductile transition beneath a TVZ-like heat source of ~ 8km. This transition depth is consistent with that inferred from the drop off of seismicity in the Taupo area. Further work (e.g Ellis and Kissling, 2011) used a partial coupling between TOUGH2 and the rock mechanics code SULEC (Ellis et al 2011) to investigate the formation of geothermal systems above an evolving continental rift similar to the TVZ.

NUMERICS

As models get larger and more complex, the demand for improved computational speed and more accuracy follow. As pointed out by Pritchett (2007), processing power has increased dramatically, and its cost has decreased considerably. One feature of the present scene is the advent of cheap multicore computers, with quad-core computing becoming almost standard. Even 16-core machines are now relatively inexpensive. The recent development of parallel versions of TOUGH2 (Zhang *et al.*, 2003) and TOUGH+ (Zhang *et al.*, 2009) are able to take advantage of these new multicore machines. Distributed memory clusters may not be so effective for parallelizing TOUGH2, but are very useful for speeding up iTOUGH2.

In various geothermal models that we have set up, the grids cause numerical problems when two small blocks join one large block. Pruess and Garcia (2000) showed how to improve computational accuracy when joining a coarse grid to a fine grid, but their work only considered simple grid structures. More research is required to generalize this approach for complex grids.

Mesh generation remains an issue for complex models. For 2-D models, triangulation can always be achieved, and in 3-D a general tetrahedral grid can be created. But better tools are still required for creating well-conditioned grids containing mostly quadrilaterals in 2-D or their equivalent in 3-D.

Another important topic related to the use of complex modelling software such as TOUGH2 is the input/output file format. The output from TOUGH2 is written to a formatted text file which is reasonably human-readable. However, simulation output is now more commonly viewed and analysed via post-processing software (e.g. graphical interfaces or scripts), particularly for large models, so human-readability has become less relevant than machine-readability. As model sizes increase, formatted text output

files become very large and slow to parse. There are now other file formats designed for efficient storage of this kind of data, e.g. HDF5 (Benger, 2009), and it would make sense for a next-generation geothermal simulator to take advantage of them. Using an established file format rather than a software-specific one also means the simulator output can potentially be read transparently by other software, which is important for a modular approach to simulation.

MODEL MANAGEMENT

Models of a geothermal system often have multiple versions. For example there are likely to be a natural state model, a production history model and models for one or more future scenarios. Thus there are multiple copies of the model, a situation that can easily lead to errors in version control. A goal for the future is to maintain multiple versions of a model without having multiple copies of the whole model. This problem, and others we have mentioned above, could be addressed by a "plug and play' approach to geothermal modelling, represented diagrammatically in Figure 6.

With this system a simulation of a geothermal system would not be driven by a single data file but rather by a suite of files and procedures, controlled by a PYTHON script. The modelling system should also recognise that there are many sub-tasks besides a TOUGH2-like simulation. A few obvious tasks are:

- Mesh generation
- Creation of the finite volume computational grid (geometrical information contained in ELEME and CONNE in TOUGH2)
- Population of the computational grid with geological information i.e. assignment of rock-types
- Time-step control
- Production and injection wells
- Boundary conditions

Within any new simulator replacing TOUGH2 there will be some key computational tasks to perform, for example:

- Assembly of the mass and heat balance equations (and possibly balance equations for extra components) and the calculation of residuals and the Jacobian matrix
- Control of the Newton-Raphson updating process
- Solving large systems of linear equation
- Phase change implementation
- Equations of state

Our aim is to have separate subroutines or procedures for carrying out each of the tasks in the two lists above (and probably others as well). As long as there is a clear and well-documented specification of the inputs and outputs for each subroutine then a selection of them can be put together to carry out a TOUGH2-like simulation or to pre- or post-process data for the simulation, or to interface with some other software.

Thus our preferred replacement for TOUGH2 is not a single large simulator but rather a library of subroutines or procedures that can be assembled in some way, say either by compiling a group of FORTRAN, C or C++ subroutines or by using a scripting language such as PYTHON to assemble them.

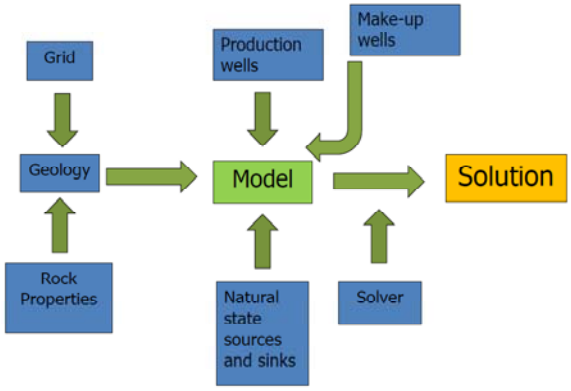

Figure 6. "Plug and play" architecture for geothermal modelling.

This is a style of computing successfully implemented in the NAG computational library (http://www.nag.com/) and used in software libraries such as PETSc (http://www.mcs.anl.gov/petsc/) or Trilinos (http://trilinos.sandia.gov/).

Such a system would allow flexibility, easy updating and easy customisation. For example it would allow easy experimentation with :

- Alternative linear equation solvers
- Analytic calculation of the Jacobian matrix
- Customisable complex production and injection schedules
- New numerical techniques such as the Euler-Lagrange method

CONCLUSION

It seems to us that it is now time for an update of the TOUGH2 code, a simulator that has served the geothermal modelling community very well for four decades. To some extent this aim has been met with the introduction of TOUGH+ (Moridis et al., 2008) but in our opinion this does not go far enough as it is just a re-write of TOUGH2 in a modern computing language. Instead we favour the introduction of a library of subroutines or procedures, a selection of which can be used to carry out a TOUGH2-like simulation but also allow many of the other tasks associated with geothermal modelling to be carried out.

In the past TOUGH2 and its predecssors were so cheap to purchase that it was effectively an open-source code and this is probably one of the main reasons it has been adopted by many different groups world-wide, many of whom have contributed to the development of TOUGH2. On the other hand TOUGH+ is a high-priced commercial code.

Our plan for a library of subroutines to replace TOUGH2 is to make it entirely open-source, and to allow it to grow as users add new subroutines. The only discipline required would be the following of certain protocols with regard to the specification of input and out for each new subroutine or procedure.

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