GEOTHERMAL SUPERMODELS PROJECT: AN UPDATE ON FLOW SIMULATOR DEVELOPMENT

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**ABSTRACT**

The “Geothermal Supermodels” project is a four-year New Zealand-based research programme, a major part of which is the development of a new open-source, parallelized geothermal reservoir flow simulator, called “Waiwera”. This paper describes recent progress on Waiwera. Features recently added include simulation of non-condensible gases, a flexible framework for modelling source and sink terms, support for radial and two-dimensional models and capillary pressure functions. Numerical performance has been improved via non-dimensionalising the primary thermodynamic variables, and better algorithms for polynomial evaluation. Thermodynamic behaviour has also been improved by implementing more sophisticated algorithms for phase transitions and for non-condensible gas energy of solution. Work has also been done to increase the efficiency of linear equation assembly and also solution, via improved pre-conditioning techniques. We demonstrate the performance of Waiwera via results from a range of benchmark tests.

1. INTRODUCTION

The “Geothermal Supermodels” project is a four-year research programme based in New Zealand, aiming to develop next-generation integrated geothermal modelling tools (Burnell et al., 2015). The flow simulator software design, development workflow and initial development progress were described by Croucher et al. (2015), with a further report on implementation progress and test results presented by Croucher et al. (2016).

The present paper provides an update on flow simulator development progress over the past year, and presents simulation results from seven benchmark test problems. Results from the application of Waiwera to two large-scale geothermal reservoir models are given in a companion paper (O’Sullivan et al., 2017).

2. IMPLEMENTATION PROGRESS

2.1 New features

2.1.1 Non-condensible gases

An equation of state module has been developed in Waiwera for simulating non-isothermal mixtures of water and non-condensible gases (NCGs). Within Waiwera’s object-oriented code framework, this has been implemented as a generic NCG EOS from which specific EOS modules for particular gases can be derived. This approach maximises code re-use and consistency between different NCG modules.

All non-gas-specific code (e.g. for phase transitions) is kept in the generic NCG EOS module, so adding a module for a new gas essentially only involves implementing thermodynamic routines for the particular gas (for computing gas density, enthalpy, mixture viscosity and Henry’s constant for gas dissolution into water).

For any NCG, the gas partial pressure is used as the additional primary thermodynamic variable. The energy of solution of the gas is calculated from the derivative of the logarithm of Henry’s constant with respect to temperature (Himmelblau, 1959), the same approach used by the EWASG EOS module in TOUGH2 (Battistelli et al., 1997).

To date, specific NCG EOS modules have been implemented for the two most commonly simulated gases in geothermal modelling: CO\textsubscript{2} and air. Like TOUGH2’s EWASG EOS module, Waiwera’s water/air EOS behaves slightly differently from TOUGH2’s original water/air EOS modules (EOS3 and EOS4), owing to a more realistic thermodynamic formulation, including a temperature-dependent Henry’s constant and a non-zero energy of solution for air. While the results are in most cases very similar to those obtained using TOUGH2 EOS3 or EOS4, our experiments indicate that this improved formulation can lead to better convergence in natural state models.

2.1.2 Sources and source controls

Geothermal reservoir models often require complex arrangements of sources and sinks, some of which may interact with each other and/or depend on reservoir conditions. This is particularly the case when modelling production runs and future scenarios. In developing the AUTOUGH2 geothermal simulator (Yeh et al., 2012) we added a variety of new generator types to address this problem.

A new and more modular approach has been developed for Waiwera. Instead of providing custom source types for specific situations, sources are kept simple and generic. However their parameters (principally flow rate and enthalpy) are managed by separate “source controls”. Each source may have multiple source controls and these can be chained together to simulate complex behaviour. Alternatively, one source control may manage multiple sources simultaneously.

So far, the following source controls have been implemented: \textit{tables} (for tables of flow rate or enthalpy vs. time), \textit{deliverability} (for controlling flow rates based on a reference pressure), \textit{separators} (for computing flow rates of separated steam and condensate) and \textit{limiters} (for limiting flow rate based on a specified maximum total, steam or condensate flow).

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These four source controls can be combined to mimic the behaviour of most of the AUTOUGH2 geothermal generator types. More types of source controls will be added as needed, and it is envisaged that these could also form the basis of a future surface network modelling system.

### 2.1.3 Radial and two-dimensional meshes

Waiwera uses an underlying geometric mesh, useful for pre- and post-processing and necessary for rock mechanics. Previously only fully three-dimensional meshes were supported.

More recently, support for radial and two-dimensional meshes has been added. Input specification of radial meshes is straightforward: an external mesh file is specified as usual, representing the two-dimensional \( r - z \) mesh, together with a 'radial' flag. Waiwera then internally computes the cell volumes and face areas for the corresponding radial mesh. The \( r - z \) mesh file can also be used for convenient post-processing and visualisation of output.

#### 2.1.4 Capillary pressure functions

Capillary pressure functions have been added to Waiwera. To date, linear, van Genuchten and piecewise-linear table functions have been implemented. More can easily be added as needed.

#### 2.1.5 Dual porosity (MINC)

Work is under way on including simulation of fractured media in Waiwera via the Multiple INteracting Continua (MINC) method (Pruess and Narasimhan, 1985). The new Waiwera implementation allows users to specify multiple MINC zones in the model mesh with different parameters. All MINC processing of the mesh (i.e. adding cells representing flow in the matrix rock) is done internally by Waiwera, so users do not have to create a separate MINC mesh.

We plan to implement a method similar to that of Zyvoloski et al. (2008) for increasing execution speed of MINC models. This approach takes advantage of the particular sparsity structure of the linear equations arising from the MINC mesh topology, which is locally one-dimensional in the rock matrix, and effectively reduces the linear equation system size back down to that of a single-porosity model on the same mesh.

### 2.2 Numerical improvements

#### 2.2.1 Non-dimensionalised primary variables

At each time step of a Waiwera simulation, a vector containing the updated solution is solved for. Previously this solution vector consisted of “raw” thermodynamic variables in each cell: fluid pressures and temperatures for single-phase water, pressures and saturations for two-phase water, and additional gas partial pressures for simulations involving NCGs.

These thermodynamic variables typically have very different magnitudes. This can cause problems when computing the finite-difference Jacobian matrix, which involves estimating a suitable increment for each variable. Waiwera uses the PETSc library (Balay et al., 2016) to carry out the Jacobian computation. If the variable \( v \) is large enough then PETSc takes the increment \( \Delta v \) as a fixed proportion (e.g. \( \varepsilon = 10^{-3} \)) of the variable itself (\( \Delta v = \varepsilon v \)). However if the variable approaches zero (which can occur for saturations and partial pressures), this would no longer work, because the effects of the increment could become lost in round-off error. Hence, a cut-off value \( v_{\text{min}} \) is used, below which the increment is calculated instead as \( \Delta v = v_{\text{min}} \). The problem then becomes one of choosing the appropriate cut-off value \( v_{\text{min}} \). Selecting a single appropriate value is not possible if the variables have very different magnitudes.

To address this problem we have non-dimensionalised the Waiwera solution vector. Aside from finite differencing considerations, the PETSc documentation also recommends non-dimensionalisation as a way of improving non-linear solver convergence. The non-dimensionalisation used here is a simple scaling, carried out by dividing each variable by a fixed reference scale. The reference scales were determined by experiment to give the best overall performance on a range of different problems. By default, pressures (both fluid pressure and NCG partial pressure) are currently scaled by \( 10^6 \), while temperatures are scaled by \( 10^2 \) (saturations are already non-dimensional and of order unity). This has resulted in considerably improved performance on some problems, particularly simulations that include NCGs.

#### 2.2.2 Phase transitions

Waiwera uses different primary variables to describe the fluid state in different thermodynamic regions, for example pressure and temperature in single-phase pure water, but pressure and vapour saturation for two-phase pure water. During the non-linear solver iterations at each time step, the fluid state may transition from one thermodynamic region to another (e.g. if there is a phase transition). In this case the thermodynamic trajectory of the fluid is temporarily stopped on the boundary between the two regions and restarted using the variables appropriate to the new region.

In the case of pure water, if the fluid boils the new two-phase variables are pressure and vapour saturation. The boundary vapour saturation is set just above zero. However there are various choices that could be made for the boundary pressure. If the old and new fluid states are \( (T_o, P_o) \) and \( (T_i, P_i) \) respectively (see Figure 1), then previously Waiwera set the boundary pressure to \( P_s(T_i) \), the saturation pressure at the new temperature. This is the same choice for the boundary pressure that is made in TOUGH2.

![Figure 1: Variable switching for boiling phase transition](image)

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However this choice sometimes leads to transition failures and consequent time step reductions. As a result, we have modified Waierwa so that the boundary pressure is now taken from the intersection of the saturation curve $P_s(T)$ and the straight line between the old and new fluid states ($P$, in Figure 1).

Because the saturation curve is non-linear, we use a root-finding algorithm (Brent’s method) to find the intersection point. The computational cost of this is relatively small (typically involving ~5 saturation curve function evaluations) and easily outweighed if any time step reductions are avoided.

A very similar interpolation process is used to find the boundary pressure for transitions from dry steam to two-phase, and for transitions from two-phase to single-phase. The same technique is also applied to phase transitions with mixtures of pure water and NCGs.

The improved behaviour of the new phase transition scheme is illustrated in Figure 2, which shows simulation time step size histories for the 10-cell 1-D vertical column model described by Croucher et al. (2016). This model starts from cold water initial conditions but develops a steam zone at around $10^{13}$ s as a result of hot water (240°C) injected at the bottom. Previously Waierwa, like AUTOUGH2 (version 2.42), reduced time step at this point. TOUGH2 (v.2) reduces time step twice at this same point and later stalls at a time step size of around $10^{13}$ s. However, with the new phase transition scheme Waierwa now runs to a steady state at $10^{13}$ s with no time step reductions at all.

![Figure 2: Time step size history for running a vertical column model with a steam zone to steady state](image)

While a single time step reduction is of relatively little concern, running field-scale geothermal reservoir models to steady state often results in many phase transitions and time-step reductions. The new transition method does not eliminate these altogether, but it does make them significantly less frequent and usually enables reservoir models to reach steady state in many fewer time steps.

### 2.2.3 Polynomial evaluation

Many of the formulae for thermodynamic properties of NCGs are expressed as polynomial functions of temperature. These may be evaluated numerically by explicitly computing the required powers of temperature (as they are in TOUGH2). However, Waierwa employs nested multiplication (“Horner’s method”) for general polynomial evaluation, resulting in fewer arithmetic operations and greater efficiency.

In addition, we have reformulated many of these polynomials so that they are expressed in terms of non-dimensionalised temperature. This reduces rounding errors and in some cases can significantly improve the steady-state convergence of models including NCGs.

### 2.3 Linear equations

#### 2.3.1 Jacobian matrix assembly

Assembly of the finite-difference Jacobian matrix in Waierwa is carried out by the PETSc library, which makes use of a “colouring” scheme to increase efficiency. This decreases the number of residual function evaluations needed, by determining which primary variables can be independently perturbed within a single residual function call (Balay et al., 2016).

In Waierwa the efficiency of this process has been increased further by re-using as much of the residual vector as possible between residual function calls, rather than re-calculating residuals that have not been affected by the perturbed primary variables. For the 31,000 cell Waierwa reservoir model described by Croucher et al. (2016) this resulted in run-time savings of approximately 25%.

#### 2.3.2 Pre-conditioning

We have continued to experiment with improved pre-conditioning techniques for solving the very ill-conditioned linear equations often encountered near steady state in geothermal models. For parallel simulations the Jacobian matrix is usually treated as a partitioned matrix with the partitions distributed over the processors.

Parallel pre-conditioners generally make use of a serial sub-pre-conditioner (e.g. incomplete LU factorisation, or ILU) on each processor. For some models we have found that performance can be greatly improved by changing the parameters of the ILU sub-pre-conditioners. This is discussed in more detail in our companion paper (O’Sullivan et al., 2017).

### 3. BENCHMARK TESTS

#### 3.1 Model Intercomparison Study problems

These benchmark tests are taken from the 1980 Geothermal Model Intercomparison Study (Molloy, 1981). We previously presented results for problems 5 and 6 from this study (Croucher et al., 2016).

#### 3.1.1 Problem 1: Avdonin model

This is a one-dimensional radial problem with steady single-phase flow and unsteady heat transport. Water at temperature 160°C is injected at 100 kg/s into a 170°C reservoir. An analytical solution (assuming constant fluid density, viscosity and heat capacity) was published by Avdonin (1964).

Figures 3 shows modelled temperature results vs. time at radius 37.5 m from the well. Results from the analytical solution as well as from AUTOUGH2 (v. 2.42) and S-Cubed (from the original study) are shown for comparison. There is very good agreement between the three numerical simulators, while the analytical results are slightly different. This is probably because they assume constant fluid
properties whereas the numerical simulators more realistically allow these properties to vary with temperature and pressure.

Figure 4 shows the modelled temperatures vs. radius at time $10^9$ s. Once again there is good agreement between the results from the three numerical simulators.

Figure 4: Temperature vs. radius at time $10^9$ s for Avdonin problem

3.1.2 Problem 2: Radial well test

This is again a one-dimensional radial problem, but simulates production. There are three different cases: case (a) simulates single-phase flow, while cases (b) and (c) simulate two-phase flow. In case (c) a flashing front develops and propagates away from the well. For cases (b) and (c) a semi-analytical similarity solution is available (O'Sullivan, 1981). We simulated all three cases, but for the sake of brevity present only the results for the most demanding case (c) here.

We used a slightly modified version of the mesh specified in the original study. The original mesh specified the positions of the “nodes”. However, it is not geometrically possible to construct a finite-volume mesh with cell centres at the specified nodal positions. The original mesh also used a relatively coarse discretisation near the well (the first cell having 0.5 m radial size). We used a mesh with slightly smaller innermost radial mesh sizes of 0.3, 0.4 and 0.6 m, and increasing logarithmically after that, with a total of 33 cells as opposed to the original 26.

Figures 5 and 6 shows the pressure and liquid saturation solutions as a function of the similarity variable $z = t / r^2$. Again, there is good agreement between the three numerical simulators, but they do not match the semi-analytical solution very well at larger values of $z$ (e.g. near the well). Molloy (1981) suggested that the match might be improved if a finer mesh were used. Our mesh was slightly finer than that used in the original study, but this did not improve the match with the semi-analytical solution.

Figure 5: Pressure solution for radial well test case (c)

Figure 6: Liquid saturation solution for radial well test case (c)

3.1.3 Problem 4: Expanding two-phase zone

This is a one-dimensional vertical model, 2 km deep, with an initially hydrostatic water column disturbed by constant-rate mass withdrawal from the bottom over a 40-year period. The upper half of the model has lower permeability, and the initial temperature profile is piecewise linear with temperatures of 310°C at the bottom, 290°C in the middle and 10°C at the top. This problem is sufficiently complex that there is no analytical or semi-analytical solution available. Hence we compare the Waiauera results with those from the S-Cubed and AUTOUGH2 simulators.

Figures 7 and 8 show the modelled pressure and liquid saturation histories at depth 1550 m. Again the three numerical simulators give very consistent results. The agreement at other depths (not shown here) was similarly very good.

3.2 Lumped-parameter CO$_2$ problem

This simple problem was described by O’Sullivan et al. (1985) and effectively simulates the effect of CO$_2$ on...
depletion from a lumped parameter model. It provides a simple but useful first benchmark for testing a simulator’s water-CO₂ mixture thermodynamics.

The single 1 m³ cell is initially at temperature 260°C, vapour saturation 0.2 and CO₂ partial pressure 30 bar. Fluid is produced at a constant rate of 5 kg/s. Two different sets of relative permeability curves were used to show their effect on the solution; for our benchmarking purposes we simulated only the case using the Corey curves.

The modelled pressure history is shown in Figure 9, together with results from AUTOUGH2 and the original MULKOM results. Once again there is excellent agreement between Waiwera and the other numerical simulators.

### 3.3 CO₂ column problem

For a more complex CO₂ test we used the vertical column steady-state model from O’Sullivan et al. (1985). The column is 1 km deep with a caprock zone (permeability 0.5 mD) extending to a depth of 300 m, below which is a reservoir zone with permeability 20 mD. Atmospheric conditions at 10°C are prescribed at the top, and heat and mass are injected at the bottom (2 kg/s per km², with enthalpy 1300 kJ/kg). The model is run from isothermal hydrostatic initial conditions (with no CO₂) to a steady state.

O’Sullivan et al. (1985) presented results from the MULKOM simulator for five cases with increasing CO₂ content in the injected fluid. However it is not entirely clear how much CO₂ was injected in each case. Their figures 10 and 11 indicate that the cases corresponded to partial pressures of CO₂ of 0, 0.1, 1, 5 and 20 bar, but the text suggests that these values may have referred to percentage mass fractions of injected CO₂. The reported partial pressures at the bottom of the model are also not consistent with the labelled values of input partial pressure.

Trying the simulations with the labelled values interpreted as partial pressures, we found that the model would not run to steady state on either AUTOUGH2 or Waiwera. Interpreting them as percentage mass fractions, the model would run to steady state (except for the 20% case), and while the CO₂ partial pressures matched the original MULKOM results reasonably well, the vapour saturations were considerably lower than those from MULKOM (by a factor of around 2 for the 5% case). This suggests there may be further uncertainty around the reported model parameters.

We ran the model using the specified linear relative permeability functions (from figure 4 in the original paper) and injected CO₂ mass fractions of 0.1%, 1% and 5%. Figure 10 shows the modelled steady-state CO₂ partial pressures vs. elevation for each of the three cases. There is excellent agreement between the Waiwera and AUTOUGH2 results, and the match with the original MULKOM results is reasonable considering the uncertainty around the input parameters. O’Sullivan et al. (1985) also
did not give any details of their model mesh. We experimented with several meshes and found this had a noticeable effect on the solution. The results shown used a mesh with 30 m cells in the caprock zone and 35 m cells in the reservoir.

To run the 0.1%, 1% and 5% cases to steady state ($t = 10^{15}$ s), Waiwera took 44, 51 and 87 time steps respectively. The corresponding AUTOUGH2 (v. 2.42) simulations took 72, 97 and 198 time steps, i.e. approximately twice as many in each case. Waiwera’s more rapid steady-state convergence for this model is due mainly to the modified phase transition algorithm (section 2.2.2).

### 3.4 One-dimensional infiltration problem

This problem, taken from the TOUGH user’s guide (Pruess, 1987) is an isothermal air-water problem simulating infiltration into a horizontal tube of partially saturated soil. A semi-analytical solution is available.

The model mesh is only 20 cm long, with 0.5 cm cells. Pressure and temperature boundary conditions are applied at the left-hand end, and the initial vapour saturation is specified as 0.56 inside the model domain. Linear relative permeability and capillary pressure functions are used.

Figure 11 plots the modelled liquid saturations vs. distance along the tube at times 0.01, 0.06 and 0.11 days. The Waiwera results match both the AUTOUGH2 results and the semi-analytical solution (digitised from figure 7 in Pruess (1987)) very closely.

#### Figure 11: Liquid saturation vs. distance for 1-D infiltration problem

### 3.4 Heat pipe problem

This is the “radial heat pipe” problem from the TOUGH2 user guide (Pruess et al., 1999), which simulates a cylindrical 3 kW heater in a porous medium containing a mixture of water, steam and air. A 120-cell one-dimensional radial mesh is used, with logarithmically increasing cell sizes, and fluid conditions are held constant at the boundary ($r = 10$ km). Van Genuchten relative permeability and capillary pressure functions are used.

Figures 12 – 14 show the modelled temperature, vapour saturation and vapour air mass fraction results vs. radius after 10 years. The Waiwera results are practically indistinguishable from the results from AUTOUGH2 and TOUGH2 (digitised from figure 19 in Pruess et al. (1999)).

#### Figure 12: Temperature vs. radius after 10 years for radial heat pipe problem

#### Figure 13: Vapour saturation vs. radius after 10 years for radial heat pipe problem

#### Figure 14: Vapour air mass fraction vs. radius after 10 years for radial heat pipe problem

### 4. CONCLUSIONS

Significant new functionality has been added to Waiwera over the past year, chiefly radial model capability, the new source and source control framework, and the NCG EOS modules.

We have also made a number of numerical improvements, mostly designed to achieve better convergence in steady-state models. The most important of these are non-dimensionalisation of the primary variables and the improved phase transition algorithm. With these improvements Waiwera is now able to reach steady states...
in many fewer time steps than was previously the case with either Waiwera or AUTOUGH2.

In this paper we have demonstrated the results of our ongoing work to validate Waiwera using benchmark problems. The excellent agreement between the results of Waiwera and those from analytical or semi-analytical solutions, and from previous simulators, can give users confidence in the validity of Waiwera’s results.

Our companion paper (O’Sullivan et al., 2017) further demonstrates Waiwera’s capabilities in application to real geothermal reservoir models.

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