MODELLING TRACERS USING THE WAIWERA GEOTHERMAL FLOW SIMULATOR

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ABSTRACT

The Waiwera parallel, open-source geothermal flow simulator now includes the ability to model the movement of passive tracers in geothermal flows. A new algorithm is used which offers greater flexibility and higher efficiency. Rather than creating special equation-of-state modules for tracers, the tracer equations are solved separately from the flow equations, and as they are linear, this can be done using only a single linear equation solution per time step. This approach also allows arbitrary numbers of tracers to be modelled in conjunction with any equation of state. Either liquid-phase or vapour-phase tracers can be simulated, and temperature-dependent Arrhenius decay can be included.

In this paper we describe Waiwera's new tracer capabilities and demonstrate their performance via benchmark test problems and by application to a field-scale geothermal reservoir model.

1. INTRODUCTION

In many geothermal fields, tracer tests are used to help identify flow paths and estimate reservoir parameters. The ability to model tracers was recently added to Waiwera, a parallel, open-source geothermal flow simulator developed at the University of Auckland (Croucher et al., 2019; Croucher et al., 2020).

Like the TOUGH2 simulator (Pruess et al., 1999) and its derivatives such as AUTOUGH2 (Yeh et al, 2012), Waiwera uses a finite volume numerical method to solve discretised mass and energy balance equations over the model mesh. However, Waiwera has a completely new structured, object-oriented code base and a number of new features aimed at improving the robustness of phase transition behaviour and accelerating natural-state convergence. It is fully parallelised to run on both desktop PCs and supercomputers, so it scales well to very large models.

Both TOUGH2 and Waiwera use a general multi-phase, multi-component formulation which means tracers may simply be added as additional mass components, to be solved for along with e.g. water and energy components. This approach is appealing because tracer capability can be added with minimal coding. However, it has two disadvantages.

The first is that for any equation of state (EOS) module (e.g. water, NCG, energy) an additional EOS is usually needed whenever tracer is to be added, resulting in a proliferation of EOS modules. This is even more problematic when multiple tracers must be simulated simultaneously. Hence, the approach lacks flexibility.

The second disadvantage is that the tracer solution process is embedded in the non-linear solution process used for the fluid flow equations, increasing its size and slowing it down. Passive tracers, present in low concentrations, do not affect the fluid properties and hence can be solved for separately, after the main fluid flow solution process is complete.

Furthermore, the tracer mass balance equations are linear and therefore do not require a non-linear solver. Tracer concentrations can be found by solving a single auxiliary set of linear equations per time step (regardless of the number of tracers), resulting in significant efficiency benefits.

2. METHODS

The mass balance equation for tracer can be written as:

$$\frac{d}{dt}\int_V M^T dV = \int_{\partial V} \mathbf{F}^T . \hat{n}\ dA + \int_V q^T\ dV - \int_V \alpha M^T\ dV$$

where M^T is the mass density of tracer in an arbitrary volume V, $\mathbf{F}^T$ is the flux of tracer through the boundary ∂V, q^T represents tracer source and sink terms (per unit volume) and α is the decay rate of tracer inside V.

A standard finite volume discretisation of this equation leads to its discrete form:

$$\frac{d}{dt}M_i^T = \frac{1}{V_i}\sum_j A_{ij}F_{ij}^T + q_i^T - \alpha_i M_i^T$$

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where M_i^T, q_i^T and α_i are the average values of M^T, q^T and α over a mesh cell volume V_i, A_{ij} is the face area between cells *i* and *j*, and F_{ij}^T is the tracer flux through that area.

For single-phase (i.e. non-partitioning) tracers, present only in phase *p* (e.g. liquid or vapour), the mass term M_i^T can be expressed as:

$$M_i^T = \phi_i S_{i,p} \rho_{i,p} X_i^T$$

where in cell *i*, ϕ_i is the porosity, $S_{i,p}$ and $\rho_{i,p}$ are the saturation and density of phase *p* and X_i^T is the tracer mass fraction to be solved for.

The flux term can be written as a sum of advection and diffusion terms:

$$F_{ij}^T = X_{ij}^T F_{ij,p} - \left[\phi \rho_p \tau\right]_{ij} D^T \frac{\partial X^T}{\partial n}$$

In the advection term, $F_{ij,p}$ is the total fluid mass flux in phase *p* on the face between cells *i* and *j*, and X_{ij}^T is the effective tracer mass fraction on the face. This is upstream weighted for stability, which does introduce numerical dispersion. While some alternative methods have been proposed which are less dispersive (Oldenburg and Pruess, 2000; Croucher et al., 2004), these have so far not been demonstrated for practical geothermal reservoir models involving multi-phase flows on irregular 3-D meshes.

In the diffusion term, D^T is the tracer diffusion coefficient and the tracer normal gradient is evaluated by finite differencing across the face. The factor pre-multiplying the diffusion coefficient is evaluated on the face by harmonic weighting and is a product of cell porosity, phase density and a "tortuosity" τ.

Various formulations are possible for computing the tortuosity (Pruess et al., 1999). In general, the tortuosity in cell *i* is written as the product of rock and fluid contributions:

$$\tau_i = \tau_{i,0} \tau_{i,p}$$

At present we have adopted a simple "constant diffusivity" tortuosity formulation in which the rock contribution $\tau_{i,0}$ is identically 1 and the fluid contribution for phase *p* is given by:

$$\tau_{i,p} = S_{i,p}$$

Other tortuosity formulations can easily be added to Waiwera in future if desired. However, in many geothermal reservoir models, particularly with coarse meshes, the effect of diffusion is masked to some extent by the numerical dispersion introduced by upstream weighting of the advection term, and also by low-order time stepping schemes such as the commonly used backward Euler method.

For each tracer, the decay coefficient α_i can be assigned a fixed value or evaluated as a function of temperature from the Arrhenius equation:

$$\alpha_i = \alpha^0 e^{-E_0/(RT_i^k)}$$

where α^0 is a reference decay rate, E_0 is the activation energy for the tracer, R is the universal gas constant and T_i^k is the cell temperature in Kelvin.

It can be seen that the discretised tracer mass balance equations are linear in the mass fractions X_i^T. Waiwera computes the mass fractions for all tracers using a single auxiliary linear solve per time step. Different linear solvers and preconditioners (from the PETSc library, https://petsc.org/) may be used for the flow and tracer solution processes, so that optimal configurations can be chosen for each. The flow and tracer solution processes use the same time stepping method (currently Waiwera offers the backward Euler and BDF-2 methods).

3. TESTS AND APPLICATIONS

3.1 Two-dimensional line source problem

A two-dimensional tracer flow problem with an analytical solution was described by Javandel et al. (1984) and used by Oldenburg and Pruess (2000) and Croucher et al. (2004) to test the performance of their tracer codes. It uses a 7 m × 4 m rectangular domain (Fig. 1) with steady unidirectional single-phase flow (0.1 m/day in the *Y*-direction). The diffusion coefficient is 1.162×10^{-8} m^2/s in both directions. Dirichlet tracer boundary conditions ($X^T = 0.01$) are applied along a line at the upstream end ($Y = 0$, $Z > -0.5$).

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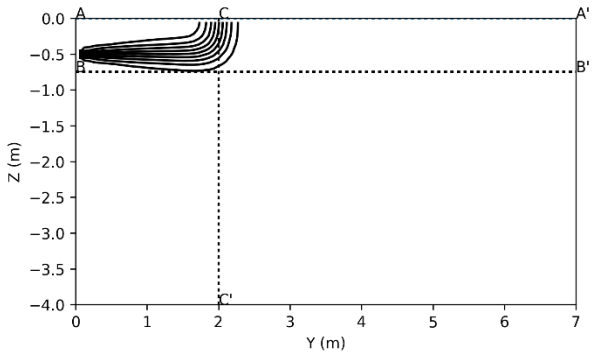

Figure 1: Two-dimensional line source problem with tracer contours (mass fraction × 100) and plotting lines A – A', B – B', C - C'

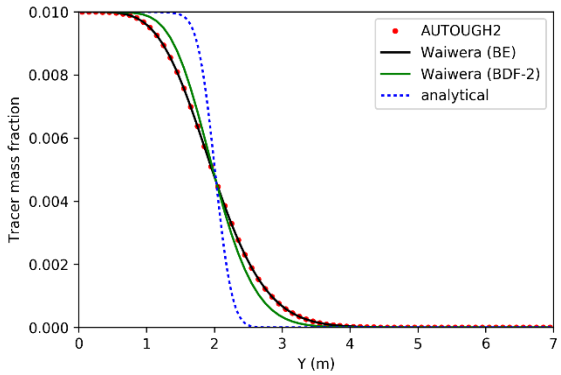

Figure 2: Two-dimensional line source problem, results along line A – A'

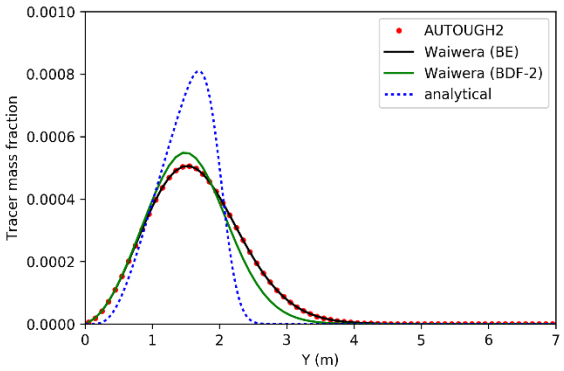

Figure 3: Two-dimensional line source problem, results along line B – B'

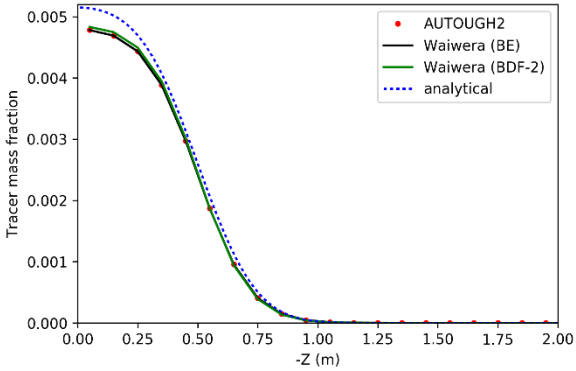

Figure 4: Two-dimensional line source problem, results along line C – C'

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As in Oldenburg and Pruess (2000) and Croucher et al. (2004), a regular rectangular mesh with uniform spacing 0.1 m in both directions is used. The mesh Péclet number is approximately 10, so the problem is advection-dominated. A constant time step size of 19.2 hours is used and the model is run for 20 days. Fig.1 also shows the contours of the analytical solution (mass fractions from 0.001 to 0.01).

Figures 2 – 4 compare the AUTOUGH2, Waiwera and analytical solutions along the lines A – A' (Z = 0), B – B' (Z = -0.75) and C – C' (Y = 2) shown in Fig. 1. Waiwera results are given for both the backward Euler (BE) and BDF-2 time stepping methods.

The Waiwera results with backward Euler time stepping are identical to the AUTOUGH2 results. This is expected, because although the solution approach is different, the underlying numerical methods are essentially the same. These results display the numerical dispersion expected for an advection-dominated problem, with artificial smoothing of the tracer front along A – A' and damping of the peak along B – B'. The results along C – C' are closer to the analytical solution because there is no flow, and hence no numerical dispersion, in the Z direction. The peak damping on the C – C' plot is caused by the numerical dispersion in the Y direction.

The Waiwera results with BDF-2 time stepping show slightly less numerical dispersion. Although its computational cost is essentially the same as backward Euler, BDF-2 is a second-order method with lower truncation error. However, its stability region is smaller than that of backward Euler, so under some conditions it can produce oscillatory solutions, which may be unacceptable (particularly in the flow solution). The results indicate that, for this problem, some of the numerical dispersion is caused by the backward Euler time stepping, but most is caused by the upstream weighting in the flux term.

3.2 One-dimensional advection-diffusion-decay problem

To verify Waiwera's ability to simulate decaying tracers, a simple one-dimensional test model was set up, 100 m in length, with steady single-phase liquid flow (2.4 m/day). To ensure the numerical model performance is determined by the diffusion and decay processes, rather than numerical dispersion, a relatively fine mesh (0.5 m cells) and large diffusion coefficient (3×10^{-5} m^2/s) are used, giving a mesh Péclet number of 0.46. Tracer mass fractions are held constant at 0.01 at the upstream end. The model is run for 20 days with a time step size of 0.1 days.

Figure 5 shows the final Waiwera results (with BDF-2 time stepping) for two cases, one with no tracer decay and the other with constant decay coefficient $\alpha = 2 \times 10^{-7}$ s^{-1}. (For clarity, as the mesh is relatively fine, results are shown only for every fourth cell.) AUTOUGH2 results are shown for the no-decay case (decay is not available in the standard TOUGH2 tracer EOS modules). The model results are compared with the analytical solution published by van Genuchten and Alves (1982).

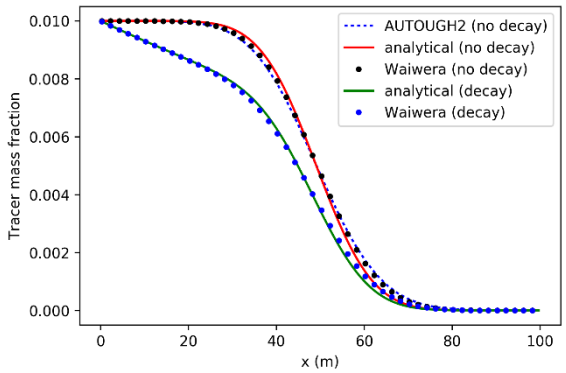

Figure 5: Results for advection-diffusion-decay problem

For the no-decay case, both the AUTOUGH2 and Waiwera results are close to the analytical solution, with only a small amount of numerical dispersion. For the case with decay included, the Waiwera results display the expected reduction of tracer concentrations with respect to the no-decay case and are again in very good agreement with the analytical solution.

3.3 Full-scale production model

Waiwera is being used for ongoing simulations of the full-scale production model (field name withheld for client confidentiality reasons) reported in Croucher et al. (2019). This is a large, complex model with accurate forecasts required for both deep and near-surface geothermal conditions. A non-isothermal air-water equation of state is needed to model the unsaturated zone, and MINC is used to model flow in fractured media. The highest resolution meshes used for this model currently contain approximately two million cells.

Recently work with this model has included simulations of tracer tests involving five different tracers. Initially this was done by developing an EOS module for Waiwera which included water, air, energy and five tracers, giving a total of eight degrees of freedom per cell. This approach was feasible but required significantly increased run-time compared with the non-tracer cases, even when run using several hundred parallel processes on the NeSI "Māui" Cray XC50 supercomputer. As well as increasing the size of the systems of linear equations to be solved, the non-linear solver used for the flow solution process also converged more slowly, which sometimes led to time-step size reductions.

The new Waiwera tracer capability outlined in section 2, using a tracer solution process separate from the flow solution, was then tested on this model. The five tracers were all liquid-phase tracers, and no diffusion or decay was applied. The simulation was carried out using a medium-resolution version of the model containing approximately 350,000 cells (including MINC), giving a total of almost 2.9 million degrees of freedom for the original tracer-EOS approach and just over 1 million degrees of freedom for the flow solution of the new separated tracer solution approach. In both cases the model was run using 160 parallel processes on the Māui supercomputer.

Here we show results from a representative one-month period extracted from the full-length tracer test simulation. Table 1 shows the run times and time step counts for the original and the new approaches. The separated-tracer simulation was approximately 6.5 times faster than the tracer-EOS simulation and required 2.4 times fewer time steps. In the separated-tracer simulation the linear equations for tracer were solved very rapidly, typically in no more than 4 iterations. The tracer solution process used a GMRES linear solver, while Bi-CGStab was used for the linear equations in the flow solution process, with a block Jacobi preconditioner for both.

Figure 6 shows the model time step sizes used by the original and new tracer approaches for this simulation. It can be seen that for the new approach, time step sizes are no longer limited by the tracer solution process and are up to four times larger in some parts of the simulation. This contributes significantly to speeding up the simulation (though it will also result in slightly more numerical dispersion in the computed solution).

Simulation	Run time (minutes)	Time step count
Original (tracer-EOS)	17:39	346
New (separated-tracer)	2:43	143

Table 1: Run times and time step counts for one-month full-scale production model tracer test simulation

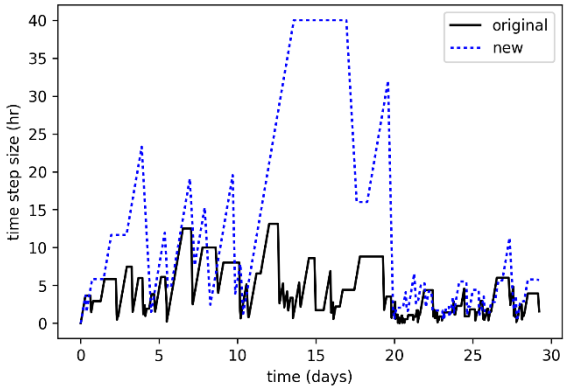

Figure 6: Time step size history for one-month full-scale production model tracer test simulation

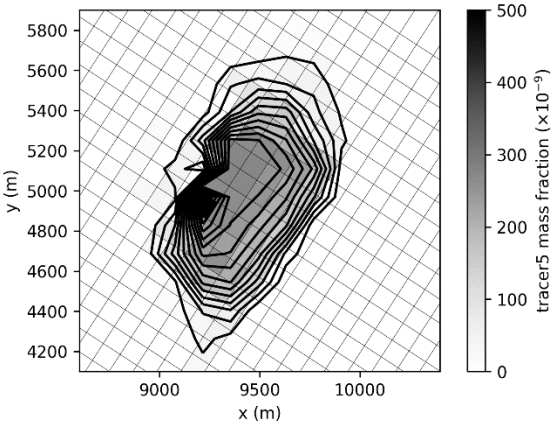

Figure 7: Contours of final tracer 5 mass fraction at elevation 0 m from one-month full-scale production model tracer test simulation (original)

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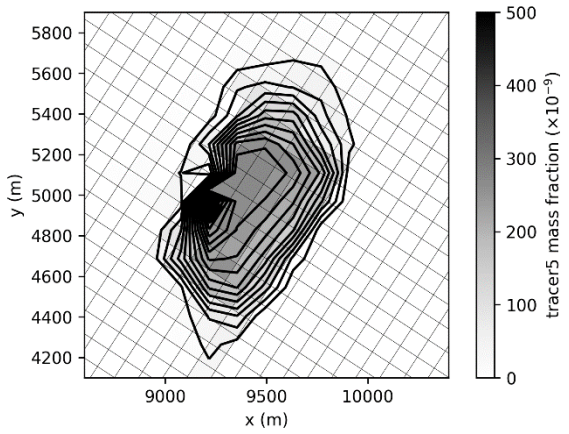

Figure 8: Contours of final tracer 5 mass fraction at elevation 0 m from one-month full-scale production model tracer test simulation (new)

Figures 7 and 8 show contours of one of the tracers ("tracer 5") at elevation 0 m at the end of the run, for the original and new tracer simulations respectively. The computed solutions show small differences attributable to the differences in time stepping, but are otherwise very similar. Results for the other tracers also showed good agreement between the original and new tracer solution approaches.

4. CONCLUSION

We have added passive tracer modelling capability to the Waiwera geothermal flow simulator using a new approach which separates the tracer solution process from the flow solution process. This approach has several advantages, including higher computational efficiency and the ability to model any number of tracers in conjunction with any equation of state. Diffusion and temperature-dependent decay effects have been included, as well as the ability to model either liquid- or vapour-phase tracers.

Benchmark test problems have shown very good agreement between Waiwera tracer results and both analytical solutions and TOUGH2 results. Waiwera's new tracer capability has also been tested on a complex field-scale reservoir model, run in parallel on a supercomputer. The results were comparable to those from a more conventional EOS-based tracer approach, but the new separated approach gave substantially reduced run times and better time-stepping behaviour.

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