

## FURTHER IMPROVEMENTS IN THE CONVERGENCE OF TOUGH2 SIMULATIONS

JOHN O'SULLIVAN\*, ADRIAN CROUCHER\*, ANGUS YEH\* AND  
MIKE O'SULLIVAN\*

\* Department of Engineering Science, University of Auckland, Private Bag 92019, Auckland 1142,  
New Zealand, jp.osullivan@auckland.ac.nz, www.des.auckland.ac.nz

**Key Words:** *TOUGH2, convergence, inverse modelling, geothermal reservoir modelling.*

Numerical modelling has become an important tool in managing geothermal systems and planning their exploitation for renewable energy production. The TOUGH2 simulator has been the industry standard tool for developing numerical models for many years. It includes several different equation-of-state modules and thus can be used for modelling many different kinds of geothermal fields as well as other complex sub-surface flow problems such as carbon sequestration and nuclear waste storage. Under certain conditions TOUGH2 simulations stall at a relatively small time step size and are unable run up to the very large times required for a natural state simulation. This behaviour leads to slow model development and also poses a significant obstacle to inverse modelling using iTOUGH2 or PEST as forward simulations are more computationally expensive and may not finish. In previous work the authors identified and analysed conditions leading to stalled simulations and proposed corrections to the air-water and CO<sub>2</sub>-water equation-of-state modules to eliminate the behaviour.

While these improvements prevent simulations from stalling at small time steps they do not prevent a limiting time step size from occurring as simulations approach a large simulation time. This behaviour is observed often, affects all equation-of-state modules and can add significant computational time to simulations. Improvements to the convergence criteria used by the TOUGH2 algorithm during its internal Newton-Raphson iteration are proposed following an analysis of the algorithm's behaviour as the time step size becomes very large. The results presented show that this improvement can dramatically reduce the total simulation time for all equation-of-state modules. In particular the improvement can reduce the computational time required for calculating numerical derivatives during inverse modelling by an order of magnitude. This has a profound effect upon our ability to carry out inverse modelling and uncertainty analysis of numerical models of large-scale, real geothermal systems.