MODELING SUPERCRITICAL SYSTEMS WITH TOUGH2: PRELIMINARY RESULTS USING THE *EOS1SC* EQUATION OF STATE MODULE

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ABSTRACT

Supercritical fluid conditions (T>374°C) have been observed at depth in magmatic geothermal systems and are important in the deep heating zones of extensional geothermal systems as well. As interest in the sustainability of mature geothermal fields increases, and as exploration for high temperature resources becomes more attractive, the ability to model an entire field from ground surface to supercritical regions will become crucial. A super-critical equation-of-state module (*EOS1sc*) is under development to extend the range of applicability of *TOUGH2* to such conditions, using a numerical equation of state for pure H_2O, This *EOS1sc* module successfully reproduces sub-critical sample problem results of EOS1 (e.g. RVF, RFP). Large gradients in fluid properties are typical in near-critical point conditions, and therefore convergent supercritical models using *EOS1sc* are currently limited to moderately convective scenarios. Model results for such a system, depicting geothermal production/injection (i.e. forced-convection) under supercritical conditions, based on the *TOUGH2* RFP sample problem, are provided to demonstrate the current capabilities of *EOS1sc*.

INTRODUCTION

Supercritical fluid conditions (T>374°C, Fig. 1) have been observed at depth in magmatic geothermal systems (Kakkonda, Japan; Ikeuchi *et al.*, 1998) and are implied in the deeper portions of extensional geothermal systems as well (Basin and Range, Nevada, USA; Wisian, 2000). As interest in the sustainability of mature geothermal fields increases, and as exploration for high temperature resources becomes more attractive (e.g. Iceland; Fridleifsson and Albertsson, 2000), the ability to model an entire field from ground surface to su-

percritical regions will become crucial. There are currently few options in selecting a supercritical geothermal reservoir modeling computer program. The most commonly-applied programs, *TOUGH2* (Pruess *et al.*, 1999) and *TETRAD* (Vinsome, 1990), are currently limited to sub-critical conditions. The most readily-available supercritical program (*HYDROTHERM*, Hayba and Ingebritsen, 1994) lacks some of the computational and gridding flexibility of *TOUGH2*. Given this situation, a super-critical equation-of-state (EOS) module for *TOUGH2* would be an attractive option; this paper is a report of progress on that task.

That super-critical EOS (*EOS1sc*) is based on the numerical equation of state for pure H_2O (*H2O92*) developed by Johnson and Norton (1991), which in turn is based on the mathematical equations of state developed by Haar *et al.* (1984) and Levelt-Sengers *et al.* (1983). The latter equations provide extremely accurate thermodynamic properties in the critical region. Models of super-critical hydrothermal systems demonstrate strong attraction to near-critical conditions (Norton and Knight, 1977; Brikowski and Norton, 1989; Hayba and Ingebritsen, 1997; Brikowski, 2001), and accurate modeling of these conditions is crucial for accurate modeling of such systems.

SUPERCRITICAL SIMULATORS

Readily available (primarily non-commercial) geothermal reservoir simulation computer programs exhibit a wide variety of capabilities. Selection of the optimal code for application to supercritical geothermal systems is problematic. For the most accurate models of such systems, a code must allow for two or more fluid phases, treat near-critical fluid properties extremely accurately, and ideally consider tracer transport (with water-rock interaction) to further constrain the thermal mod-
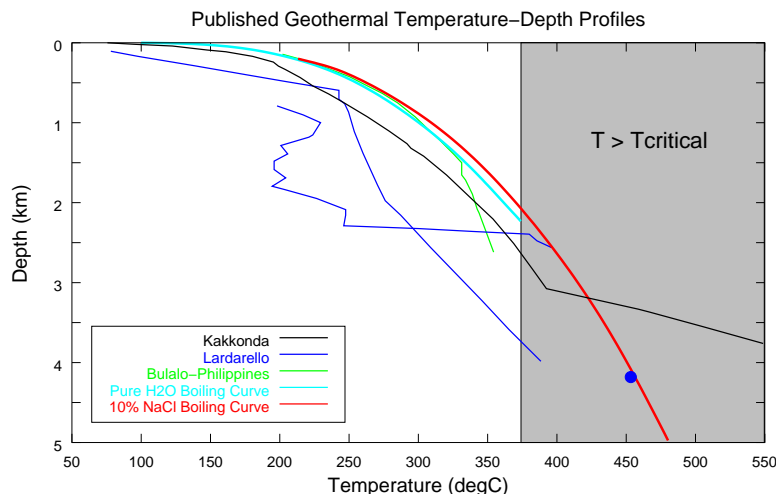
Figure 1: Pressure-depth profiles for deep geothermal systems, after Muraoka *et al.* (2000). Shaded area shows region of supercritical temperatures.

els. A variety of matrix solution options and flexible gridding (e.g. finite element) are a distinct advantage when modeling natural systems. It was determined that a modified version of *TOUGH2* would best meet these criteria, but a review of other options is warranted.

HYDROTHERM

Released in 1994, *HYDROTHERM* became the first widely-available geothermal reservoir simulator to include both two-phase and supercritical conditions (Hayba and Ingebritsen, 1994). This finite-difference code is based on the earlier *GEOTHER* (Faust and Mercer, 1979), and utilizes fluid enthalpy and pressure as its primary (dependent) variables. Fluid (pure H_2O) properties are calculated using smoothed bicubic interpolation of lookup tables based on steam table compilations by Haar *et al.* (1984), and an extended equation for fluid viscosities presented by Sengers and Kamgar-Parsi (1984). Solution of the non-linear finite difference equations is accomplished using slice-successive overrelaxation for matrix solution embedded in Newton-Raphson iteration for the non-linear parameters. An example of application of this code is a study of convection in hypothetical pluton settings (Hayba and Ingebritsen, 1997). Likely difficulties in implementing tracer transport and water-rock interaction modeling in a finite-difference formulation precluded the use of this code.

TETRAD

TETRAD is a versatile reservoir simulator primarily concerned with multiphase petroleum and geothermal settings (Vinsome, 1990). Fluid and rock matrix can be compressible. Fluid properties are computed using user-settable values or steam table, and allows for an essentially limitless pressure-temperature-salinity range. Treatment of critical-point phenomena (i.e. termination of the two-phase boundary) would be difficult with such a formulation. *TETRAD* allows for computation of dissolved species transport. The program is based on the finite difference method, with Newton-Raphson iteration and pre-conditioned iterative solution of the matrices. This program has been used for detailed studies of liquid adsorption (Shook, 1994). Probable limitations in treatment of near-critical phenomena made this code unlikely to be the best candidate for this study.

MARIAH

This finite element program was originally written at Sandia National Laboratory for modeling of single phase, incompressible fluid (pure H_2O) flow in sub-critical conditions (Gartling and Hickox, 1982). Since that time it has been extensively modified by this author to treat supercritical (single-phase) conditions (Brikowski and Norton, 1986) using *H2092*. This routine provides continuous, very accurate fluid properties over the range 0-1200 °C and 0-3000 MPa, with particular

accuracy near the critical point. Although computationally intensive, this continuity has proven crucial in obtaining numerical solutions for systems that bracket the critical point of H_2O.

In recent years, *MARIAH* has been modified to include modeling of water-rock interaction and transport of oxygen isotopes (i.e. ^{18}O, Brikowski, 1995), with subsequent application to natural state models of The Geysers (Brikowski and Norton, 1999; Brikowski, 2000, 2001). These models demonstrate the importance of near-critical phenomena in controlling the nature of high-temperature geothermal/hydrothermal systems, and the utility of $\delta^{18}O$-alteration as a tight constraint on models of such systems. While the flexible gridding allowed by the finite-element formulation of *MARIAH* is highly advantageous, the prospect of conversion of this code to treat two-phase compressible fluids was daunting.
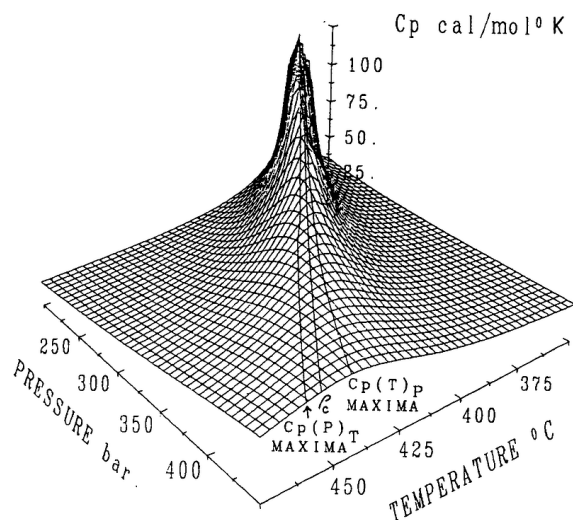
H2092

Figure 2: Variation of isobaric heat capacity (C_p) for pure H_2O in the near super-critical region. Looking from high P and T down the critical isochore toward the critical point. C_p reaches infinite value at that point, surface has been truncated for graphical purposes. After Johnson and Norton (1991).

Although not a reservoir simulation code, *H2092* merits separate discussion. Fluid properties reach extrema at the critical point (e.g. isobaric heat

capacity theoretically reaches $+\infty$, Fig. 2). These extrema have a profound effect on fluid dynamics, and accurate treatment of such properties is required for accurate reservoir models that include the critical region. *H2092* uses a Taylor series approximation for Helmholtz free energy outside the critical region, from which most of the remaining fluid thermodynamic properties can be obtained via numerical differentiation (pg. 580, Johnson and Norton, 1991). In the vicinity of the critical point, the alternative Levelt-Sengers equation for thermodynamic potential, which can be treated similarly to obtain fluid properties. Given input T-P or T-ρ, *H2092* computes a total of eighteen fluid thermodynamic properties and ratios. The Taylor series are based on physical considerations of the internal chemistry of the fluid, and as such will be far more accurate than strictly mathematical interpolations of these properties (e.g. International Formulation Committee, 1967). For systems containing critical-point conditions this accuracy is fundamentally important, but it comes at a steep computational cost, since the Taylor series require calculation of many more terms at each P-T point. The code is freely available as a part of the SUPCRT aqueous geochemical modeling package (Johnson et al., 1992).

TOUGH2

This program is a refinement of the MULKOM code system developed over several decades at Lawrence Berkeley National Laboratory. The program employs the integrated finite difference method, allowing for flexible gridding, treats multi-phase subcritical fluid and heat flow, using Newton-Raphson iteration and a user-selectable variety of matrix solution techniques. It has been qualified for use as the unsaturated zone performance assessment code for the Yucca Mountain Nuclear Waste Repository. The flexibility of this program, particularly in terms of two-phase phenomena and matrix solution approaches make it an attractive candidate for supercritical modeling. An extensive bibliography of literature on *TOUGH2* and its applications is available on the Internet at http://ccs.lbl.gov/TOUGH2/BIBLIOGRAPHY.html.

APPROACH

Since no one of the codes described above is capable of modeling supercritical conditions with the

desired level of detail, as well as modeling dissolved species transport and water-rock interaction, some hybrid of the codes will be required. The apparent optimal choice for this hybrid is *TOUGH2*, modified to include first a supercritical equation of state (*H2092*), and later the oxygen-isotope alteration routines from *MARIAH*. The subject of this paper are the results of the first coding phase of the project, in which *H2092* will be adapted as an EOS module, to serve as a plug-in conversion to enable supercritical modeling. The supercritical equation of state module has been designated as "*EOS1sc*", and its structure largely imitates that of the original EOS1 module avaliable with *TOUGH2* (Pruess *et al.*, 1999). The implementation of *EOS1sc* extends the range of *TOUGH2* considerably, currently giving it an applicable range of $0 < T \leq 1000°C$ and $0 < P \leq 1000$ MPa (Fig. 3)
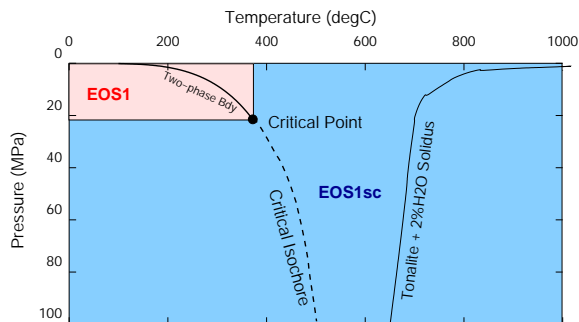

Figure 3: P-T Validity Range of eos1 (pink shaded area, Pruess *et al.*, 1999) and *EOS1sc* (blue area). Liquid-vapor solidus of hydrous tonalite magma with 2 wt% H_2O shown to indicate typical magmatic conditions (Whitney, 1975). Dashed line shows approximate location of critical isochore (line of density equal to density at the critical point).

Challenges

A number of conceptual and numerical challenges in this approach were predictable, and were encountered. Most problematic is the termination of the two-phase boundary at the critical point. All of the reservoir simulators listed above utilize phase mass-balances which are computed at every point in the system. Both steam and liquid "disappear" above the critical point, and become an indistinguishable supercritical fluid. At and above the critical point, this requires an artificial

iso-enthalpic "reaction" (e.g. Hayba and Ingebritsen, 1994, p. 8) to convert steam or liquid into fluid. *HYDROTHERM* handles this problem by declaring 50% saturation with identical steam and liquid properties in supercritical regions. Since *TOUGH2* utilizes steam saturation as a primary (dependent) variable along the two-phase boundary, this approach was not an option. Instead an artificial extension to the two-phase boundary was implemented, across which a thermodynamically-neutral reaction of liquid and steam was allowed. Although many orientations for this extension are possible, extending it along the critical isochore (line of density equal to that at the critical point, dashed line, Fig. 3) was conceptually the simplest. A more difficult problem is implied phase transitions (a super-critical cell with sub-critical neighbor). These lead to "subtle and complicated difficulties" (e.g. Pruess *et al.*, 1999, Appendix D) or (e.g. Hayba and Ingebritsen, 1994, p. 8) in computing accurate phase mass balances, and care must be taken to treat interfacial fluxes properly. Variable switching in *TOUGH2* to pressure-saturation along the two-phase boundary becomes somewhat problematic at the critical point. Finally, a problem that will never be completely eliminated is difficult convergence near the critical point. The incorporation of *H2092* is specifically intended to treat extrema in fluid properties accurately, based on the proposition that these extrema are the fundamental controls on fluid circulation and heat transport in deep systems. As a result spatial gradients in fluid properties are larger than with alternative equations of state described above. This leads to increased residuals (errors) in mass and energy balance equations, and increased difficulty in finding convergent solutions for problems with coarse grid and high advective flow rates. At the time of this writing, *EOS1sc* succeeds only in forced-convection problems, where non-linear effects on flow rates are minimized. This restriction will hopefully be resolved in the future.

RESULTS

Tests of *EOS1sc* have been made in two categories. The first are sub-critical models run to confirm that existing capabilities of *TOUGH2* have not been degraded by the application of *EOS1sc*. The second explore the supercritical performance of *EOS1sc*, and are more limited, since successful supercritical runs have only recently been achieved.

Sub-Critical Tests

For general familiarity, the two sample problems distributed with *TOUGH2* that invoke the EOS1 module were run for comparison. These are RFP, the "geothermal five-spot injection/production" problem (sec. 9.4, Pruess *et al.*, 1999), and RVF, the "heat sweep in a vertical fracture" problem. Both runs produce results that are graphically indistinguishable from the EOS1 results (Figs. 4 and 5. In detail, results differ by less than 0.01%, running in double-precision (REAL*8). As expected, a significant difference in run-times is apparent (Fig. 6), with the *EOS1sc* runs requiring 5 to 50 times longer on an SGI O2 R10000 workstation. Since memory usage is small, and disk access minimal in these test problems, similar time differences should be experienced on most computing platforms. Recall that EOS1 has been optimized for speed in sub-critical settings, while *EOS1sc* has been constructed for maximum accuracy in the near-critical region. Users wishing to apply *EOS1sc* should be thoroughly committed to thermodynamic accuracy versus computational speed.

Figure 5: RVF (vertical fracture heat-sweep) test results using EOS1 (line) and *EOS1sc* (points) in *TOUGH2*. See Pruess *et al.* (sec. 9.3, 1999) for details of problem specification.
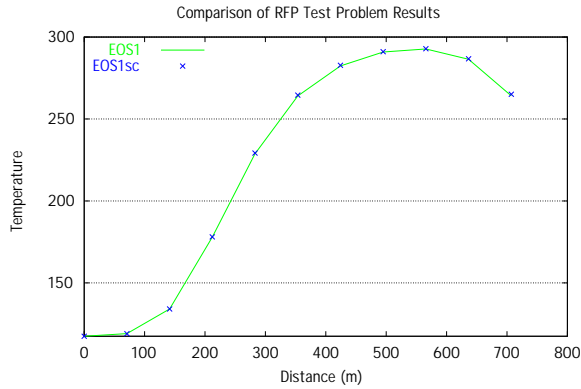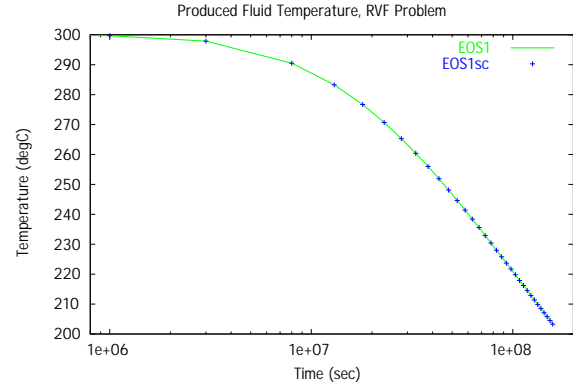

Figure 4: RFP (geothermal 5-spot well) test results for EOS1 (line) and *EOS1sc* (points) in *TOUGH2*. See Pruess *et al.* (sec. 9.4, 1999) for details of problem specification.

Supercritical Tests

For familiarity, RFP, the sub-critical EOS1 sample problem treating the "five-spot" injection/production geometry was extended to supercritical conditions. Starting conditions in the reservoir were specified similar to those found at the bottom of well WD-1a at Kakkonda, Japan
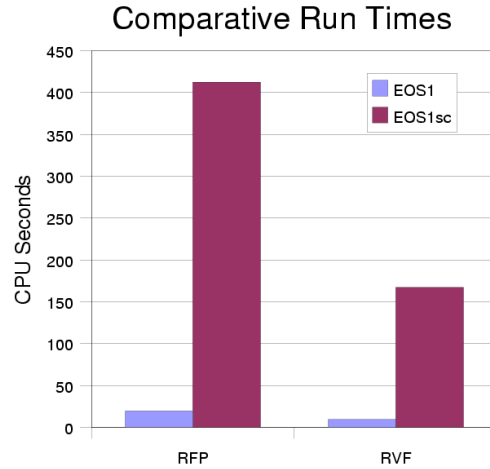

Figure 6: Comparative run times, EOS1 (blue) and *EOS1sc* (magenta). *EOS1sc* runs require 5-10 times more CPU time, since series-based computation of water properties is extremely accurate but time-consuming.
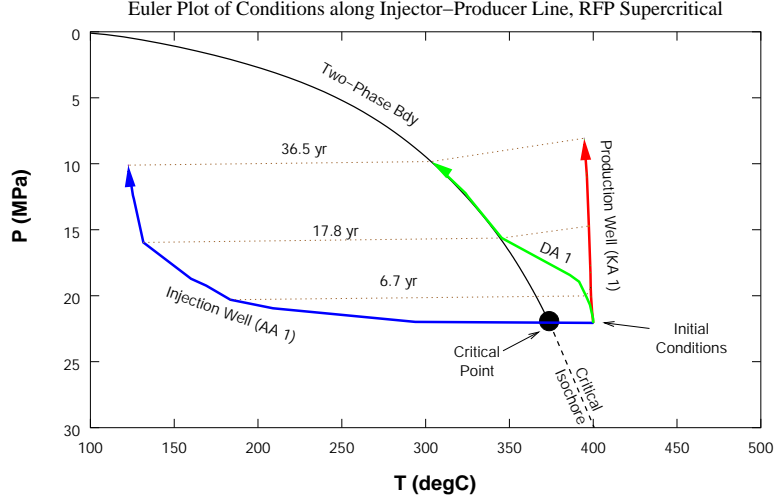
Figure 7: Supercritical RFP test results using *EOS1sc*. Variation of P-T conditions with time at three points along injector-producer line. Points at representative times connected by dashed lines. Injector point migrates rapidly from supercritical initial conditions through critical point to cool liquid conditions. Intermediate point "DA 1" follows boiling curve, production point show isothermal depressurization.

(Ikeuchi *et al.*, 1998), albeit ignoring the very high salinities encountered at those depths. This test is meant to simulate the conditions that might be encountered in production from a barely supercritical reservoir, e.g. as proposed by Fridleifsson and Albertsson (2000) and modeled by Yano and Ishido (1998). Problem specifications are identical to the RFP problem included in the *TOUGH2* distribution, except that rock initial temperature is set to 400°C, pressure at 22.06 MPa (critical point is located at 373.917 °C, 22.046 MPa, Levelt-Sengers *et al.*, 1983). Fluids at 100 °C are injected at the center of the 5-spot grid, and are withdrawn at an identical rate at the corner of the grid. Non-convergence (using the solver settings given in the distributed RFP file) forced reduction of the pumping rate from 3 kg/sec steam in the subcritical case, to 0.9 kg/sec. Grid refinement was not attempted, but would presumably allow convergence for the higher pumping rate. P-T conditions in the reservoir sweep across the critical point, with the injection point moving rapidly to lower temperatures, then all points moving more slowly upward to lower pressures (Fig. 7). Intermediate points (e.g. element "DA 1", blue line, Fig. 7) quickly migrate to the two-phase boundary, and proceed along it until the end of the simulation. Since the P-T profile between injector and producer (dashed lines, Fig. 7) migrate across the critical point, implied phase transitions are encountered in the grid

and are successfully treated by *EOS1sc*.

SUMMARY

A supercritical equation of state for pure H_2O has been developed for use with *TOUGH2*. This module extends the range of *TOUGH2* to beyond typical silicic magma solidus conditions, thereby allowing the modeling the entirety of magmatic and other high-temperature geothermal systems. Deep exploration and concerns about sustainable management of geothermal resources require that these deep roots of the system be considered. Preliminary testing of the module indicates that it preserves existing accuracy of *TOUGH2* at subcritical conditions, and successfully extends the modeling capabilities to supercritical conditions. Most problematic are systems that contain the critical point, e.g. any system with atmospheric conditions at the top, and supercritical conditions at depth. Difficult solution convergence owing to accurate treatment of fluid property extrema near the critical point currently limits the capability of *TOUGH2* with *EOS1sc* to settings that involve forced convection, or limited fluid velocities. Ongoing testing and software modification is addressing these issues.

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ACKNOWLEDGMENTS

REFERENCES

Brikowski, T. H., 1995. Isotope-calibrated hydrothermal models: Geothermal implications of a model of the Skaergaard Intrusion. Geotherm. Resour. Council Transact. 19, 171–176.

Brikowski, T. H., 2000. Using isotopic alteration modeling to explore the Natural State of The Geysers geothermal system, USA. In: Proceedings of the World Geothermal Congress, pp. 2045–50, kyushu-Tohoku, Japan.

Brikowski, T. H., 2001. Deep fluid circulation and isotopic alteration in The Geysers geothermal system: Profile models. Geothermics 30 (1), 8, in press.

Brikowski, T. H., Norton, D., 1986. Consequences of magma chamber geometry on the thermal history of mid-ocean ridges. EOS 67, 1021.

Brikowski, T. H., Norton, D., 1989. Influence of magma chamber geometry on hydrothermal activity at mid-ocean ridges. Earth Planet. Sci. Lett. 93, 241–255.

Brikowski, T. H., Norton, D., 1999. An isotope-calibrated natural state model of The Geysers geothermal system: Initial results. Geotherm. Resour. Council Transact. 23, 347–350.

Faust, C. R., Mercer, J. W., 1979. Geothermal reservoir simulation: 1. Mathematical models for liquid- and vapor-dominated hydrothermal systems. Water Resour. Res. 15, 23–46.

Fridleifsson, G. O., Albertsson, A., 2000. Deep geothermal drilling on the Reykjanes Ridge: Opportunity for international collaboration. In: Proceedings of the World Geothermal Congress 2000, International Geothermal Organization, pp. F7–5, paper R0882.

Gartling, D. K., Hickox, C. E., 1982. MARIAH-A finite element computer program for incompressible porous flow problems : User's Manual. Tech. rep., Sandia National Labs.

Haar, L., Gallagher, J. G., Kell, G. S., 1984. NBS/NRC Steam Tables. Hemisphere Publishers, Washington, D.C.

Hayba, D. O., Ingebritsen, S. E., 1994. The computer model HYDROTHERM, a three-dimensional finite-difference model to simulate ground-water flow and heat transport in the temperature range of 0 to 1,200 degrees C. Wri 94-4045, U. S. Geol. Survey, Denver, CO.

Hayba, D. O., Ingebritsen, S. E., 1997. Multiphase groundwater flow near cooling plutons. J. Geophys. Res. 102 (6), 12235–12252.

Ikeuchi, K., Doi, N., Skagawa, Y., Kamenosono, H., Uchida, T., 1998. High-temperature measurements in well WD-1a and the thermal structure of the Kakkonda geothermal system, Japan. Geothermics 27 (5/6), 591–607.

International Formulation Committee, 1967. A formulation of the thermodynamic properties of ordinary water substance. IFC Secretariat, Düsseldorf, Germany.

Johnson, J. W., Norton, D., 1991. Critical phenomena in hydrothermal systems: State thermodynamic, electrostatic, and transport properties of H_2O in the critical region. Am. J. Sci. 291, 541–648.

Johnson, J. W., Oelkers, E. H., Helgeson, H. C., 1992. SUPCRT92; a software package for calculating the standard molal thermodynamic properties of minerals, gases, aqueous species, and reactions from 1 to 5000 bar and to 1000 degrees C. Computers & Geosciences 18 (7), 899–947.

Levelt-Sengers, J. M. H., Kamgar-Parsi, B., Balfour, F. W., Sengers, J. V., 1983. Thermodynamic properties of steam in the critical region. J. Phys. Chem. Ref. Data 5 (1), 1–51.

Muraoka, H., Yasukawa, K., Kimbara, K., 2000. Current state of development of deep geothermal resources in the world and implications to the future. In: Iglesias, E., Blackwell, D., Hunt, T., Lund, J., Tmanyu, S. (eds.), Proceedings of the World Geothermal Congress 2000, International Geothermal Association, pp. 1479–1484.

Norton, D., Knight, J., 1977. Transport phenomena in hydrothermal systems: Cooling plutons. Am. J. Sci. 277, 937–981.

Pruess, K., Oldenburg, C., Moridis, G., 1999. TOUGH2 User's Guide, Version 2.0. Report LBNL-43134, Lawrence Berkeley Nat. Lab, Berkeley, CA.

Sengers, J. V. L., Kamgar-Parsi, B., 1984. Representative equations for the viscosity of water substance. J. Physical and Chemical Reference Data 13, 185–205.

Shook, G. M., 1994. Effects of adsorption on exploitation of geothermal reservoirs. Geotherm. Resour. Council Transact. 18, 339–346.

Vinsome, K., 1990. TETRAD User Manual. Dyad Engineering,, Calgary, Alberta, Canada.

Whitney, J. A., 1975. The effects of pressure, temperature and χ_{H_2O} on phase assemblage in four synthetic rock compositions. J. Geol. 83, 1–31.

Wisian, K. W., 2000. Insights into Extensional Geothermal Systems from Numerical Modeling. Geotherm. Resour. Council Transact. pp. 281–286.

Yano, Y., Ishido, T., 1998. Numerical Investigation of Production Behavior of Deep Geothermal Reservoirs at Super-Critical Conditions. Geothermics 27 (5/6), 705–721.