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Increased Reliability of Supercritical EOS1sc Module in iTOUGH2

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ABSTRACT

A reliable numerical simulator capable of modeling supercritical conditions in geothermal reservoirs is crucial for a better understanding and optimized management of magmatic geothermal systems. This paper describes improvements made to the EOS1sc module in iTOUGH2 for increasing the reliability and speed of the supercritical module. In EOS1sc, the IAPWS-IF97 thermodynamic formulation is used to calculate thermodynamic properties across five regions; liquid, vapor, supercritical, two-phase, and high temperature vapor. Backward equations released for the supercritical region of IAPWS-IF97 were implemented into EOS1sc for calculating specific volume as a function of pressure and temperature. The backward formulation is more reliable than the Newton-Raphson method previously used to iteratively calculate density in the supercritical region and it is approximately eight times faster. In EOS1sc, discrepancies across region boundaries in the IAPWS-IF97 formulation can cause convergence issues. Hence, cubic Bézier curves were implemented to provide a smooth continuous function for thermodynamic properties across the supercritical boundaries. Thereby, poor convergence at intersection points between thermodynamic regions were resolved and the reliability of the supercritical EOS1sc module was increased.

1. INTRODUCTION

Supercritical geothermal fluid has promising possibilities for improving the economics of geothermal energy production due to its increased power-producing potential compared to subcritical fluids. The enthalpy of water increases significantly at temperatures and pressures above the critical point (374°C and 22.064 MPa) and higher rate of mass transfer is possible due to increased ratios of buoyancy forces to viscous forces in the supercritical state (Elders et al., 2014; Fridleifsson et al., 2007). Fridleifsson and Elders (2005) estimated a tenfold increase in energy output per well when utilizing supercritical fluid instead of a conventional well producing subcritical fluid with significantly lower enthalpy. Therefore, the number of wells needed can be reduced by drilling deeper into the ground to reach supercritical fluid and subsequently improving the efficiency per well. For high enough output per well, the improved efficiency could result in lowered drilling costs and a decreased environmental footprint.

Utilization of supercritical geothermal fluid is becoming more desirable with advancing drilling technologies. Deep geothermal wells have reached supercritical fluid in over 25 cases around the world and supercritical systems are currently being investigated in Iceland, Italy, USA, Japan, Mexico, and New Zealand (e.g. Fridleifsson and Elders, 2017; Reinsch et al., 2017; Garcia et al., 2016; Mbia et al., 2015; Espinosa-Paredes and Garcia-Gutierrez, 2003; Kato et al., 1998). The first well of the Iceland Deep Drilling Project (IDDP), well IDDP-1, was drilled at Krafla in 2009 and it encountered 900°C hot rhyolitic magma at a depth of only 2,100 m (Fridleifsson et al., 2010). In 2017, IDDP finished drilling its second well, IDDP-2, to a depth of 4,659 m where it reached supercritical temperatures of approximately 427°C and fluid pressure of 340 bars (Fridleifsson and Elders, 2017). The appearance of supercritical fluids in geothermal wells is likely to become more common with increasing drilling depths. Hence, it is important to be able to create numerical models capable of simulating supercritical conditions to better understand and optimize production of these magmatic geothermal reservoirs.

Simulators suited for modeling pressures and temperatures above the critical point of water include HYDROTHERM (Hayba and Ingebritsen, 1994) and the HOTH2O extension to the STAR simulator (Pritchett, 1995). HYDROTHERM can simulate temperatures up to 1,200°C and pressures up to 1,000 MPa, and the HOTH2O extension to STAR operates for temperatures up to 800°C and pressures up to 100 MPa. In HYDROTHERM, a large lookup table is used to provide fluid densities, viscosities, and temperatures. The lookup table is calculated from steam-table routines of Haar et al. (1984), which were adopted by the International Association for the Properties of Water and Steam (IAPWS) in 1984. The equations by Haar et al. (1984) were later found to manifest substantial weaknesses close to the critical point and when the equations were extrapolated beyond their operational range (Wagner and Pruss, 2002). Other simulators that have been extended to supercritical conditions and are capable of modeling irregular computational grids include the Complex System Modeling Platform CSMP++ (Weis et al., 2014) and codes developed based on the TOUGH2 suite of nonisothermal multiphase flow simulators (Pruess, 1991). The TOUGH2-based codes include the supercritical equation-of-state module EOS1sc by Magnusdottir and Finsterle (2015), supercritical equation-of-state modules by Brikowski (2001) and by Kissling (2004), and the AUTOUGH2 code developed at the University of Auckland (Croucher and O'Sullivan, 2008). Currently, when simulating large-scale three-dimensional supercritical models convergence issues can occur, specifically during phase-changes. O'Sullivan et al. worked on increasing the reliability of the AUTOUGH2 simulator by changing the boundaries of the numerical solution regions, using linear interpolation to blend thermodynamic properties on the boundaries of the supercritical region as well as creating a "two-phase" zone in the supercritical region (2016). The improvements have led to good convergence behavior of three dimensional supercritical systems.

Of the simulators capable of accurately modeling supercritical conditions in geothermal reservoirs, the EOS1sc module in iTOUGH2 (Magnusdottir and Finsterle, 2015) has the highest operational range of 0-800°C for a pressure range of 0-100 MPa and a temperature range of 800-2000°C for pressures within 50 MPa. Additionally, the iTOUGH2 simulator provides a tool for inverse modeling, specifically for parameter estimation, sensitivity analysis, and uncertainty propagation analysis (Finsterle, 2007). In iTOUGH2, an optimization algorithm is used to minimize the objective function, which is the comparison of calculated and observed system state. The minimization algorithm iteratively updates the parameters of the model until the misfit between measured data and the corresponding model output is sufficiently small and the convergence criteria has been reached. The iTOUGH2 simulator is based on the TOUGH2 simulator, which is a numerical simulator for nonisothermal flows of multicomponent, multiphase fluids in porous and fractured media. The mass and energy balance equations describing fluid and heat flow are discretized into strongly coupled nonlinear equations with time-dependent primary variables as unknowns and solved simultaneously using Newton-Raphson iteration. For Newton-Raphson iteration to converge, it is important that the objective function is continuous and smooth.

This paper describes improvements made to the EOS1sc module in iTOUGH2 for increasing reliability, especially during phase changes. First, implementation of backward equations for specific volume as a function of pressure and temperature is discussed. Then, interpolation of thermodynamic properties on the boundaries of the supercritical region are described. Cubic Bézier curves were used for a smooth interpolation between boundaries, avoiding the breakpoints of a linear interpolation that can cause problems during the Newton-Raphson iteration solving for fluid and heat flow in TOUGH2.

2. IMPLEMENTATION OF BACKWARD EQUATIONS FOR SPECIFIC VOLUME

The IAPWS-IF97 industrial thermodynamic formulation for the properties of water and steam is given in terms of five regions nominally defined as liquid, vapor, supercritical, two-phase, and high temperature vapor as shown in Figure 1. Regions 1, 2 and 5 in Figure 1 (liquid, vapor, and high temperature vapor) are individually covered by a fundamental equation for the specific Gibbs free energy given in terms of pressure and temperature. Region 3 (supercritical) is covered by a fundamental equation for the specific Helmholtz free energy and is given in terms of density and temperature and Region 4 (two-phase), i.e., the saturation curve, is given by a saturation-pressure equation. Hence, when crossing the boundary from the liquid or vapor region to the supercritical region, the primary variables are changed from pressure and temperature to density and temperature. Previously, the Newton-Raphson method was used to iteratively calculate density as a function of temperature and pressure. This section describes how backward equations for specific volume as a function of pressure and temperature were implemented into EOS1sc to eliminate the Newton-Raphson method for calculating density and thereby increasing reliability and reducing computational speed.

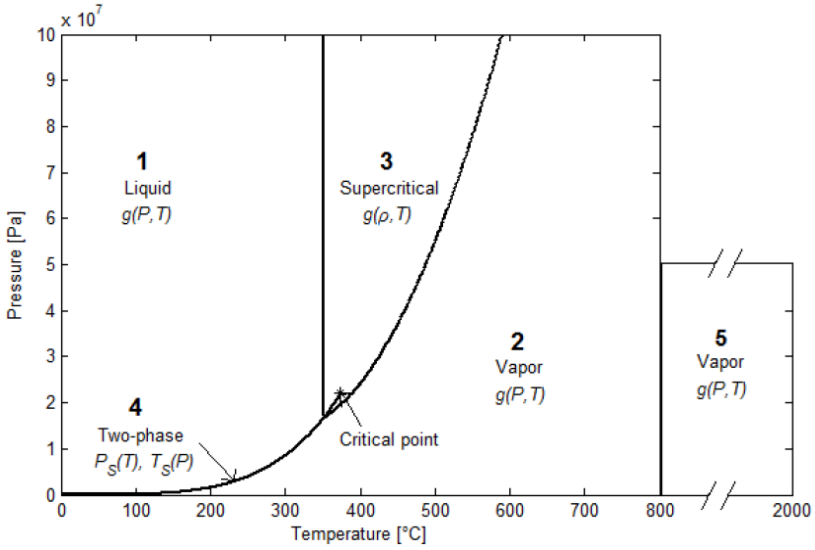

Figure 1: Regions for the IAPWS-IF97 thermodynamic formulation.

2.1 IAPWS-IF97 backward equations

The IAPWS-IF97 thermodynamic formulation is described by the International Association for the Properties of Water and Steam (IAPWS, 2007). In 2014, IAPWS authorized a revised supplementary release on backward equations for specific volume as a function of pressure and temperature (IAPWS, 2014). These backward equations are for the supercritical region of the IAPWS-IF97 formulation, i.e. region 3 shown in Figure 1, and the operational range of the equations is illustrated in Figure 2. They also include auxiliary equations for a small area very near the critical point shown in Figure 2. The range of validity of the backward equations is defined by:

$$623.15 < T < 863.15 \tag{1}$$

and

$$p_{B23}(T) < p < 100\,MPa \tag{2}$$

where T is temperature [K], p is pressure [MPa] and p_{B23} represents the pressure on the boundary between region 2 and region 3 of IAPWS-IF97. The backward equations consist of 26 subregions, thereof six that are part of the auxiliary equations. Specific volume reaches an infinite slope at the critical point, which makes it difficult to meet consistency requirements set to have the same consistency as when using the Newton-Raphson iterations. This permissible relative tolerance for specific volume, v, is:

$$\left|\frac{\Delta v}{v}\right|_{tol} = 0.001\% \tag{3}$$

The backward equations fully meet this required accuracy that is consistent with using the Newton-Raphson iterations except for a small area. It is infeasible to achieve that consistency requirement for that area due to the complicated structure of specific volume near the critical point. Hence, the small area shown in Figure 2 is instead covered by auxiliary equations with reasonable consistency. The maximum relative difference of specific volume within the auxiliary equations is equal to:

$$\left|\frac{\Delta v}{v}\right|_{\max} = 3.5\% \tag{4}$$

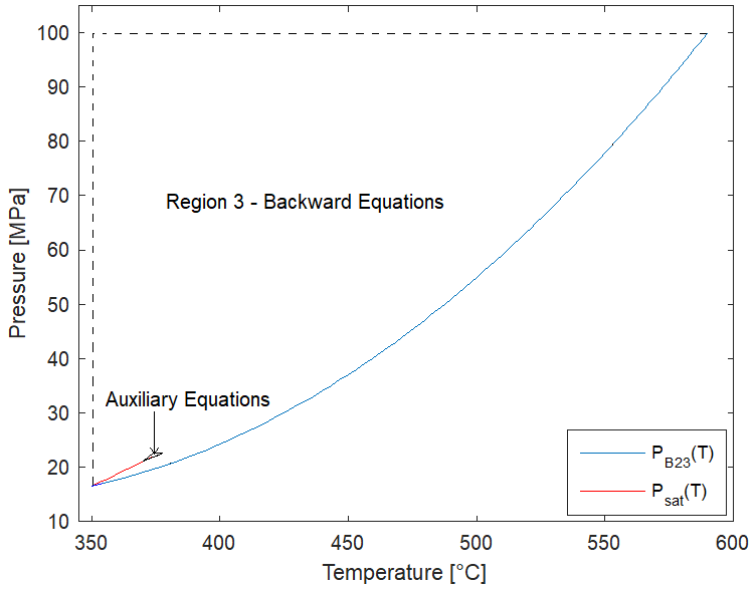

Figure 2: Range of validity of the backward equations and auxiliary equations.

2.2 Increase in computational speed

Backward equations were implemented into the EOS1sc module in iTOUGH2 in order to eliminate the need for Newton-Raphson iterations to calculate density as a function of pressure and temperature. The calculation of density as a function of pressure and temperature is necessary during phase changes across the supercritical region. The first primary variable is pressure for the liquid and vapor regions and it is changed to density while crossing of the supercritical region boundaries. Although the Newton-Raphson method previously used to calculate density is a highly efficient method for finding the roots of a function, an initial value needs to be guessed in the iteration process and a bad initial guess and/or an unsmooth function can yield divergence. Thus, the Newton-Raphson method is less reliable than the backward equations. It is also more time-consuming because during the iteration process, pressure needs to be calculated for each iteration based on pressure and density using the IAPWS-IF97 formulation until a good match has been found.

The computational speed of the backward equations was tested and compared to using the Newton-Raphson iteration. A total of 100,000 data points for pressure and temperature randomly distributed over the supercritical region were used to calculate density. First, density was calculating for these points using the Newton-Raphson method and then the same points were used to calculate density using the backward equations. The process was repeated ten times. Each time, the backward equations were on average approximately eight times faster than the Newton-Raphson method.

The number of elements in TOUGH2, i.e. the size/detail of the model, is limited by computing power. Hence, for inverse analysis of large-scale supercritical reservoir models, the computational speed is extremely important. The forward model of TOUGH2 is solved several times during the inverse analysis in iTOUGH2 so it is essential that the TOUGH2 simulation can be solved within reasonable time. In TOUGH2, the mass and energy balance equations describing fluid and heat flow are discretized into strongly coupled nonlinear

equations with time-dependent primary variables as unknowns and solved simultaneously using Newton-Raphson iteration. For the Newton-Raphson iteration to converge it is crucial to be able to quickly and reliably calculate the primary variables in each region. Hence, the increased speed and reliability of the backward equations is of great value. In addition, the numerical consistency of calculating the primary variables is essential for convergence. In order to meet the consistency requirement for EOS1sc listed in Equation 3, the small region around the critical point shown in Figure 2 is not covered by the auxiliary equations in EOS1sc. Instead, Newton-Raphson iteration is used within that small area and the auxiliary equations are used to find a good starting value to yield a quicker and more reliable convergence and a good consistency.

3. INTERPOLATING DENSITY ON BOUNDARIES OF THERMODYNAMIC REGIONS

Another important factor in yielding convergence in a TOUGH2 simulation is the smoothness of the objective function. If the objective function has sharp corners or is discontinuous, the Newton-Raphson iteration can fail. It cannot find the root of the objective function if the function is not differentiable and continuous. This section describes the discrepancy in thermodynamic variables between regions of IAPWS-IF97 that can lead to convergence issues as region boundaries are crossed during TOUGH2 simulations. Interpolation is necessary to provide a continuous function for thermodynamic properties. Linear interpolation is commonly used to connect known data points on either side of an unknown data point with a straight line. However, the straight line used to connect two functions will have breakpoints at each end that can cause problems in the Newton-Raphson iteration. Hence, cubic Bézier curves are used instead providing a smooth continuous function for the thermodynamic properties.

3.1 Discrepancy in formulations for different thermodynamic regions

The IAPWS-IF97 formulation uses different equations to calculate the thermodynamic variables for each of the five regions shown in Figure 1. Hence, there's a possibility of discrepancy between equations at the region boundaries. Although EOS1sc has been tested and works well on several examples (Magnusdottir and Finsterle, 2015), convergence issues were discovered for some large-scale supercritical models. Convergence failures were occurring as the boundary between region 2 and 3 were crossed. On further observation, a discrepancy in pressure between the thermodynamic formulations were noticed at the boundary at 350ºC as shown in Figure 3. For studying the discrepancy between the formulations, density was first calculated for temperature at 350ºC and pressure from 17-100 MPa using the formula for region 1. Then, the calculated density was used to recalculate pressure using the formula for region 3. The difference between pressure calculated on the boundary using formula for region 1, P_1, and pressure calculated using formula for region 3, P_3, is shown in Figure 3. Additionally, the discrepancy in pressure between regions 2 and 3 is shown in Figure 3. Although the discrepancy in pressure between boundaries is relatively small, it can cause difficulties in the Newton-Raphson algorithm when crossing boundaries. As Figure 3 shows, the formulas on each side of the boundaries do not give a consistent difference. The supercritical formula sometimes gives higher pressure and sometimes lower than the formula for region 1 or region 2. In order to make the function smooth across region boundaries, interpolation of the thermodynamic properties is necessary.

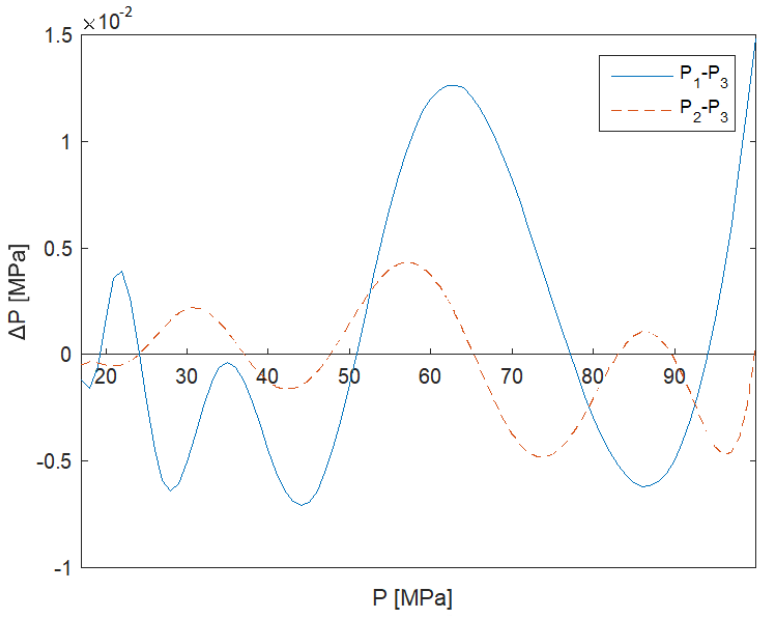

Figure 3: Discrepancies in pressure calculated using thermodynamic formulations for region 1 (P_1) and for region 3 (P_3), and discrepancies in pressure between formulations for regions 2 (P_2) and 3.

3.2 Linear interpolation and Bézier curves

Interpolation is a method for constructing a function for estimating unknown data points within the range of discrete set of data points. This section describes linear interpolation and cubic Bézier curves for interpolating between the thermodynamic formulas given in

IAPWS-IF97 for different regions. For two given points (x_0, y_0) and (x_1, y_1), linear interpolation yields a straight line between the points. For a value x in the interval (x_0, x_1), the value y along the straight line is given as,

$$y = y_0 + (x - x_0)\frac{y_1 - y_0}{x_1 - x_0} \tag{5}$$

A cubic Bézier curve is defined by four points D_0, D_1, D_2, D_3. The curve will start at point D_0 and end at point D_3. Points D_1 and D_2 are control points that are merely to provide directional information and the curve will likely not pass through these points. First, the curve will go from D_0 in the direction towards point D_1, initially with the same slope as between D_0 and D_1. Then, D_2 will determine the direction it goes towards point D_3. Eventually as it reaches point D_3 it will have the same slope as between D_2 and D_3. The distance between points D_2 and D_3 determines how fast the curve moves towards D_1 before turning towards D_2 and D_3. A cubic Bézier curve is given by:

$$B(t) = (1-t)^3 D_0 + 3(1-t)^2 t D_1 + 3(1-t)t^2 D_2 + t^3 D_3 \ , \ 0 \le t \le 1 \tag{6}$$

The difference between linear and cubic Bézier interpolations is further illustrated in Figure 4. The linear interpolation gives a straight line from point (x_0, y_0) to point (x_1, y_1). Breakpoints in the function exist at these points as shown in Figure 4. However, the cubic Bézier curve provides a continuous smooth curve connecting the two functions from point D_0 to point D_3. The slope of the Bézier curve initially has the same slope as the first function and eventually reaches the same slope as the second function. Therefore, breakpoints that cause the formulation to be unsmooth are avoided by using cubic Bézier curves instead of linear interpolation.

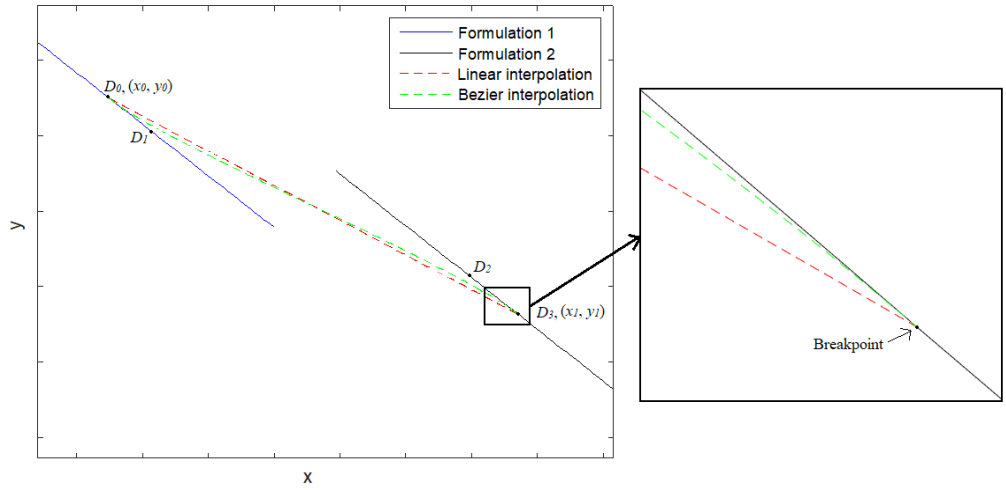

Figure 4: Linear interpolation compared to Bézier curves for interpolating between two functions.

3.3 Density interpolated between thermodynamic regions using cubic Bézier curves

Cubic Bézier curves were implemented into the EOS1sc module. These interpolation curves provide a smooth continuous curve connecting the IAPWS-IF97 thermodynamic formulations of region 3 to the formulations of regions 1 and 2 as shown for density in Figure 5. Table 1 summarizes the slopes of the lines in Figure 5 and a comparison to the slopes of a linear interpolation. The Bézier curve starts with the same slope as the line of the formulation for Region 1, which is equal to 1.708. Then, the curve slowly starts deviating from the line and it ends with the same slope as the line of the formulation for Region 3, which is equal to 1.715. Hence, breakpoints associated with linear interpolation are avoided. For a linear interpolation between Region 1 and Region 3, the slope of the interpolation line is 1.594 and breakpoints are present at the start and end points of the line. Therefore, by using cubic Bézier curves the convergence issues due to the discrepancies in thermodynamic properties shown in Figure 3 are avoided making EOS1sc more reliable.

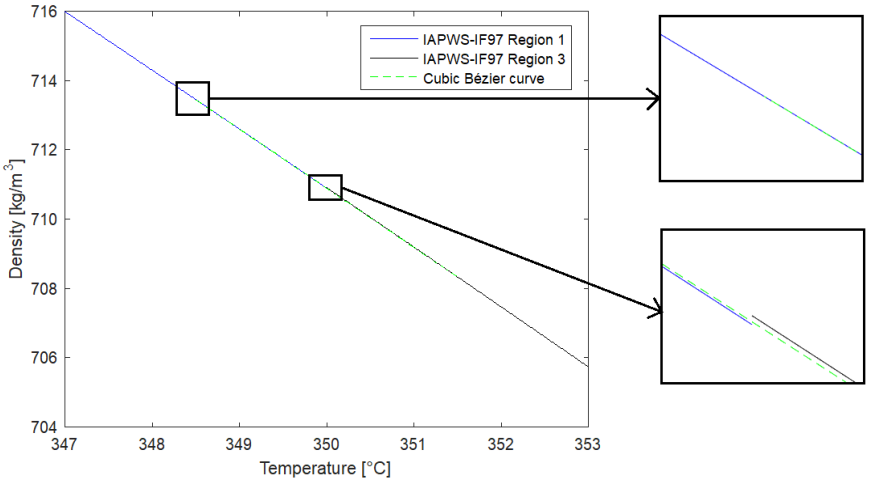

Figure 5: Cubic Bézier curve used to interpolate between Region 1 and Region 3 of the IAPWS-IF97 formulation.

Table 1: The slope of density curves

	Slope of line
Region 1	1.708
Region 3	1.715
Linear	1.594
Bézier 1	1.708
Bézier 3	1.715

4. CONCLUSION

The EOS1sc module in iTOUGH2 was improved by increasing the speed and reliability of the module. First, backward equations for calculating specific volume as a function of pressure and temperature for the supercritical region of the IAPWS-IF97 thermodynamic formulation were implemented into EOS1sc. Newton-Raphson method was previously used to iteratively calculate density as a function of pressure and temperature whenever boundaries of the supercritical regions were crossed and the primary variables were changed from pressure and temperature to density and temperature. The backward formulation is more reliable than the Newton-Raphson method and it is approximately eight times faster. Then, cubic Bézier curves were implemented to eliminate convergence issues due to discrepancies in thermodynamic formulations at the boundary of the supercritical region. The thermodynamic formulation used for the supercritical region does not give the same thermodynamic properties as the formulation for liquid or vapor at the boundaries of the supercritical region. The Newton-Raphson iteration used in iTOUGH2 to solve the mass and energy balances relies on the formulation being smooth and continuous to reach convergence. As the region boundaries are crossed, the Bézier curve provides a smooth continuous formulation for the thermodynamic properties. Hence, poor convergence at intersection points between the thermodynamic regions are avoided and the EOS1sc is more reliable. Future work includes testing the speed and convergence improvements on a full-scale three-dimensional supercritical geothermal system.

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