

Extending the Applicability of the iTOUGH2 Simulator to Supercritical Conditions

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ABSTRACT

Supercritical fluids exist near magmatic heat sources in geothermal reservoirs, and the high enthalpy fluid is becoming more desirable for energy production with advancing technology. Furthermore, wells drilled into magma in magmatic geothermal reservoirs have indicated that the heat sources could be located at a shallower depth than assumed in today's standard modeling practices. In geothermal modeling, the roots of the geothermal systems are normally avoided but in order to accurately predict the thermal behavior when wells are drilled close to magmatic intrusions, it is necessary to incorporate the heat sources into the modeling scheme. Modeling supercritical conditions poses a variety of challenges due to the large gradients in fluid properties near the critical zone. This work focused on using the iTOUGH2 simulator to model the extreme temperature and pressure conditions in magmatic geothermal systems. The study is part of a project on investigating the deep roots of geothermal systems, funded by Geothermal Research Group (GEORG). The IAPWS-95 and IAPWS-IF97 thermodynamic formulations were implemented into iTOUGH2 to provide inverse modeling capabilities of high-temperature magmatic geothermal reservoirs. Thus, the operational range of temperature and pressure in iTOUGH2 was extended from 350°C and 100 MPa to 1,000°C and 1,000 MPa when using the IAPWS-95 formulation, and to 800°C and 100 MPa as well as 2,000°C for pressure within 50 MPa, when using the IAPWS-IF97 formulation. In addition, the possibility of extrapolating the IAPWS-IF97 formulation was investigated because the formulation is significantly faster than the IAPWS-95 formulation, which can be extrapolated to high temperatures and pressures with relatively good accuracy. A five-spot geothermal problem was simulated for a subcritical problem, a supercritical problem with temperatures and pressures close to the critical point, and for very high temperature and pressure conditions likely to occur deep in magmatic reservoirs. Both formulations give equivalent results for temperatures up to 800°C and the difference between the formulations was very low even for extreme temperature and pressure conditions at 1500°C and 150 MPa. Hence, the IAPWS-IF97 formulation is recommended instead of IAPWS-95 due to a significantly faster computational speed.

1. INTRODUCTION

Extracting supercritical fluids from geothermal reservoirs is a difficult task but it has promising possibilities for improving the economics of geothermal energy production. At temperatures and pressures above the critical point (374°C and 22.064 MPa), the fluid has multiple power-producing potentials compared to fluid produced in conventional geothermal power plants. The enthalpy is significantly higher at such high temperatures and pressures, and supercritical fluids have greatly enhanced rates of mass transfer due to the increased ratios of buoyancy forces to viscous forces in the supercritical state. Thus, more energy could be produced from a single well extracting supercritical fluids compared to a conventional geothermal well. Deeper wells would be more expensive to drill but for high enough outputs per well, drilling costs and environmental footprint could be decreased due to fewer wells being drilled.

There has been an increasing interest in utilizing supercritical fluids deep in the subsurface, and the feasibility of such energy extraction is likely to increase in the coming years with advancing drilling technologies. The Iceland Deep Drilling Project (IDDP) included plans of drilling geothermal wells to depths of 4-5 km in Iceland at Krafla, Nesjavellir and Reykjanes to reach supercritical fluids at temperatures of 450-600°C, as described by Fridleifsson and Elders (2005). However, the first IDDP well drilled at Krafla in 2009 encountered 900°C hot rhyolitic magma at a depth of only 2.1 km (Fridleifsson et al., 2010). Elders et al. (2014) discuss how this unexpected encounter with magma at a relatively shallow depth has demonstrated possibilities of higher power outputs from the contact zones of intrusions and that it may be possible to extract energy directly from magma in the future. These observations show how the heat source can extend up to a depth shallow enough to greatly influence the hydrology and thermal behavior in the reservoir. Furthermore, these incidents are likely to become more common with increasing drilling depths in magmatic geothermal reservoirs.

In geothermal reservoir modeling, the heat source is usually assumed to be below the model's depth range, and the model is driven by boundary conditions in the bottom layer of the model. Including the heat source in the model poses a variety of modeling challenges due to the large gradients in fluid properties near the critical point, and due to various unknowns such as the depth range of the water circulation and the time varying spatial distribution of the heat sources. Simulators capable of modeling supercritical conditions 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. However, both simulators are limited to rectangular or radial grids, thus imposing restrictions in representing the complex geometry of magmatic geothermal reservoirs. 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 code (Pruess, 1991). The TOUGH2 based codes consist of the EOS1SC equation of state module by Brikowski (2001), the supercritical equation of state module by Kissling (2004), and the AUTOUGH2 code developed at the University of Auckland (Croucher and O'Sullivan, 2008). The IAPWS-IF97 thermodynamic formulation (Wagner et al., 2000) is used in AUTOUGH2 and the IFC-67 formulation (International Formulation Committee of the 6th International Conference on the Properties of Steam, 1967) is used both in standard TOUGH2, iTOUGH2 and the supercritical version of TOUGH2 by Kissling (2004). The operational ranges for these

thermodynamic formulations are summarized in Table 1. The IFC-67 formulation operates up to 800°C and 100 MPa but the IAPWS-IF97 and IAPWS-95 formulations are significantly more accurate for supercritical conditions. IAPWS-95 operates up to 1,000°C and 1,000 MPa, and the IAPWS-IF97 formulation operates up to 800°C for pressure up to 100 MPa. Additionally, a revised version of IAPWS-IF97 has been released which operates up to 2,000°C for pressure within 50 MPa (International Association for the Properties of Water and Steam, 2007). The temperature of basaltic magma can reach 1,200°C so in order to be able to answer questions relevant to the field management of magmatic geothermal systems, it is important to develop a simulator that can accurately model the high pressures and temperatures of these magmatic intrusions.

This paper describes how the IAPWS-95 (International Association for the Properties of Water and Steam, 2002) and the IAPWS-IF97 thermodynamic formulations were implemented into the iTOUGH2 simulator to test the concept of using IAPWS-95 in a TOUGH2 based code and study the differences between the operational limits of IAPWS-95 and IAPWS-IF97. The IAPWS-95 formulation can be extrapolated to extremely high temperatures and densities, as described by Wagner and Pruss (2002). Moreover, the iTOUGH2 simulator provides capabilities for sensitivity, uncertainty, and inverse modeling analyses, which can be used to examine the relevance of supercritical properties and processes, and to calibrate magmatic geothermal reservoir models. Hence, this extended version of iTOUGH2 could be used to model magmatic intrusions, and some of the unknown model parameters could be estimated using inverse analysis. Yamazaki and Muto (2004) describe how extrapolating the original IAPWS-IF97 formulation to higher temperatures and pressures is limited but in this study the possibility of extrapolating the extended revised version of IAPWS-IF97 was studied. This paper first describes the implementation of the IAPWS-95 and IAPWS-IF97 thermodynamic formulations into iTOUGH2. Then, a geothermal five-spot problem described by Pruess (1991) was simulated for conditions below the critical point, close to the critical point, and for very high temperatures above the critical point. Results using the IAPWS-95 formulation were compared to those using the IAPWS-IF97 formulation.

Table 1: Temperature and pressure range for international thermodynamic formulations.

International standard	Simulator	Temperature range [°C]	Pressure range [MPa]
IFC-67	TOUGH2, iTOUGH2	0-800	0-100
IAPWS-95		0-1,000	0-1,000
IAPWS-IF97	AUTOUGH2	0-800	0-100
Revised region 5 of IAPWS-IF97		800-2,000	0-50

2. METHOD

The IAPWS-95 formulation serves as the international standard for water's thermodynamic properties. The IAPWS-IF97 formulation in AUTOUGH2 is a separate, faster formulation based on IAPWS-95. It is maintained for industrial use and replaces the IFC-67 formulation currently used in standard TOUGH2. Croucher and O'Sullivan (2008) show how the primary variables of the standard TOUGH2 were modified in AUTOUGH2 to account for the supercritical region. In standard TOUGH2, the primary variables are the same as those of the IFC-67 formulation, i.e. pressure and temperature in the single-phase liquid and vapor regions, and pressure and saturation in the two-phase region. Thus, the primary variables are not the same in all regions and they need to be switched when phase boundaries are crossed. The IAPWS-IF97 formulation is given in terms of regions nominally defined as liquid, vapor, supercritical, and two-phase, as shown in Figure 1. The boundaries of the regions are chosen arbitrarily; they are different from the true phase boundaries. In AUTOUGH2, the same primary variables were used as in the IAPWS-IF97 formulation so that the formulation can be used directly without need for iteration. Regions 1-4 in Figure 1 are included in AUTOUGH2 with an operational limit of 800°C and 100 MPa. The primary variables of the IAPWS-95 formulation are different from the IAPWS-IF97 formulation; density and temperature are used for the complete relevant state space. However, in this study the same primary variables were used as in IAPWS-IF97 (which required iterative function inversions for IAPWS-95 outside of the supercritical region), and the IAPWS-IF97 formulation was implemented in a similar way as done in AUTOUGH2 (Croucher and O'Sullivan, 2008). The revised release of the IAPWS-IF97 formulation was used including the fifth region (Fig. 1) to extend the operational limit to 2000°C for pressure at or below 50 MPa.

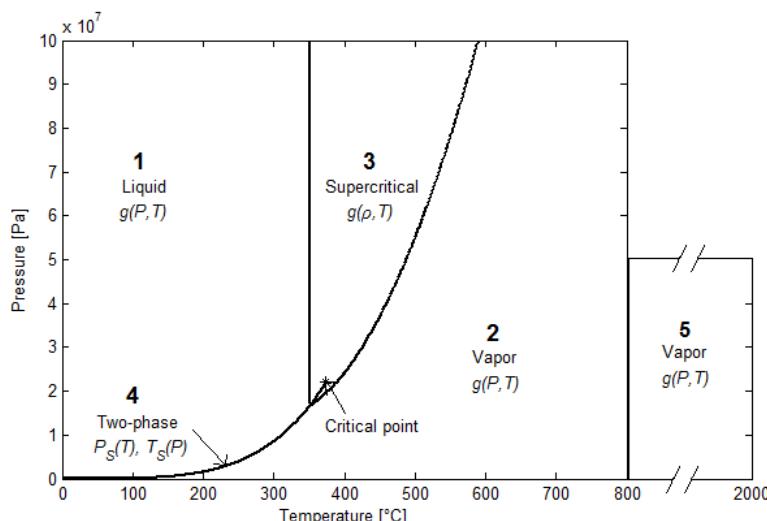


Figure 1: Regions for the IAPWS-IF97 thermodynamic formulation.

Croucher and O'Sullivan (2008) made some necessary changes to the TOUGH2 code to avoid the assumption that the first primary variable is always pressure. The changes were similar to those described by Talman et al. (2004) for simulating geological CO₂ storage. Another factor to take into account is that there is no phase distinction in the supercritical region, which becomes problematic because TOUGH2 bases its calculations on mass and energy balances for each phase. Thus, the saturation line was artificially extended into the supercritical region. Above the extended line the supercritical fluid is nominally designated 'liquid' and below it is called 'vapor', although there is no change in physical properties when the line is crossed in the supercritical region.

The IAPWS-95 formulation is based on the specific Helmholtz free energy f and is divided into an ideal-gas part φ^0 and a residual part φ^r where,

$$\frac{f(\rho, T)}{RT} = \varphi^0(\delta, \tau) + \varphi^r(\delta, \tau) \quad (1)$$

with $\delta = \rho/\rho_c$ and $\tau = T/T_c$ where ρ is the mass density, T is the absolute temperature, c denotes the critical point, and R is the specific gas constant. The free energy formulation (Equation 1) works for the complete relevant state space but the following Maxwell construction has to be added to this formulation when the values of ρ and T lie inside the two-phase region to calculate the saturation pressure p_s and the densities ρ' and ρ'' of pure water and pure vapor,

$$\frac{p_s}{RT\rho'} = 1 + \delta' \varphi^r_\delta(\delta', \tau) \quad (2)$$

$$\frac{p_s}{RT\rho''} = 1 + \delta'' \varphi^r_\delta(\delta'', \tau) \quad (3)$$

$$\frac{p_s}{RT\rho''} \left(\frac{1}{\rho''} - \frac{1}{\rho'} \right) - \ln \left(\frac{\rho'}{\rho''} \right) = \varphi^r(\delta', \tau) - \varphi^r(\delta'', \tau) \quad (4)$$

where

$$\varphi^r_\delta = \left[\frac{\partial \varphi^r}{\partial \delta} \right]_\tau \quad (5)$$

Equations 2-4 are solved simultaneously to calculate the saturation pressure as well as the vapor and water densities. An extensive description of this formulation can be found in the revised release on the IAPWS-95 formulation 1995 for the thermodynamic properties of ordinary water substance for general and scientific use (International Association for the Properties of Water and Steam, 2002).

Junglas (2008) describes how the IAPWS-95 standard was implemented in the WATER95 program library for MATLAB, and a similar method was used in this study to implement IAPWS-95 into iTOUGH2. A schematic illustration of how the density and internal energy are calculated in this study using IAPWS-95 outside of the supercritical region is provided in Figure 2. The function that calculates density, ρ , is used to iteratively evaluate density, because the primary variables of the IAPWS-95 formulation are density and temperature.

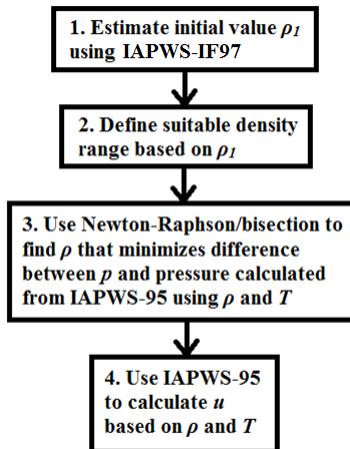


Figure 2: Schematic illustration of how the density ρ and internal energy u is calculated based on temperature T and pressure p using IAPWS-95 in iTOUGH2.

First, an initial density value, ρ_I , is calculated based on temperature and pressure. The IAPWS-IF97 formulation is used to calculate ρ_I if $T \leq 1200^\circ\text{C}$ and the constraints listed in Table 2 are used for $T > 1200^\circ\text{C}$ where $p1100$ is the lower limit of pressure for $\rho = 1100 \text{ kg/m}^3$ and $p800$ is the upper limit of pressure for $\rho = 800 \text{ kg/m}^3$. Then, the lower limit of density is set as $0.8 \times \rho_I$ and the upper limit is set as $1.2 \times \rho_I$. If needed, this range is incrementally increased until the difference between the pressure given and the pressure calculated using IAPWS-95 based on the upper limit of density has an opposite sign to the difference between the pressure given and the pressure calculated based on the lower limit of the density. That way, the root of the function describing the difference between the pressure given and the pressure calculated using IAPWS-95 can be found within the density range using a combination of the Newton-Raphson and bisection methods (Press, 1992) to determine the density corresponding to the pressure

given (task three in Figure 2). Once the density has been calculated, the internal energy is calculated based on pressure and density using the IAPWS-95 formulation.

Table 2: Start value for density for $T > 1200^{\circ}\text{C}$.

Constraint	Start value for density
$p > p_{I100}$	$\rho_I = 1200 \text{ kg/m}^3$
$p_c < p \leq p_{I100}$	$\rho_I = 1000 \text{ kg/m}^3$
else if steam and: $p < 5 \times 10^4 \text{ Pa}$ $p > 100 \times 10^5 \text{ Pa}$ $5 \times 10^4 \text{ Pa} \leq p \leq 100 \times 10^5 \text{ Pa}$	$\rho_I = 0.1 \text{ kg/m}^3$ $\rho_I = 100 \text{ kg/m}^3$ $\rho_I = 1 \text{ kg/m}^3$

The IAPWS-95 formulation added to iTOUGH2 was compared to published values from the NIST Chemistry WebBook (National Institute of Standards and Technology, 2005) and the WATER95 program library for MATLAB, both based on the IAPWS-95 formulation. Junglas (2008) compared WATER95 to the NIST Chemistry WebBook for a set of randomly chosen values scattered over the state space which led to identical results, but differences were found for densities along the saturation curve very close to the critical point. Similarly, the IAPWS-95 formulation in iTOUGH2 gave identical results to WATER95 and the NIST Chemistry WebBook for randomly selected values, but very close to the critical point there were differences for the densities along the saturation curve. Results are summarized in Table 3. Junglas (2008) rounded the WATER95 values to the same precision as the NIST WebBook values to show that the differences between the values were small. He also demonstrated that the WATER95 values fulfill the Maxwell condition much better than the NIST WebBook values. The small differences between values using the IAPWS-95 formulation in iTOUGH2 and the WATER95 values for $T \geq 373.94^{\circ}\text{C}$ were found to be due to differences in numerical treatment between FORTRAN and MATLAB.

Table 3: Comparison of the IAPWS-95 formulation added to iTOUGH2, the WATER95 values, and the NIST WebBook.

T [°C]	p _s [MPa]	ρ' , IAPWS-95 in iTOUGH2	ρ' , WATER95	ρ' , NIST	ρ'' , IAPWS-95 in iTOUGH2	ρ'' , WATER95	ρ'' , NIST
373.86	22.041	356.07	356.07	355.85	287.78	287.78	287.56
373.9	22.052	349.50	349.50	349.32	294.37	294.37	294.20
373.93	22.060	340.39	340.39	340.27	303.46	303.46	303.35
373.94	22.062	333.94	333.96	333.90	309.89	309.90	309.84
373.945	22.064	327.13	327.18	327.16	316.75	316.80	316.79

The IAPWS-IF97 formulation accurately describes the pressure and temperature on the entire saturation curve while being significantly faster than the IAPWS-95 formulation. Thus, IAPWS-IF97 was used to calculate the saturation pressure and temperature for all examples in this study, including the ones where IAPWS-95 was used to calculate thermodynamic properties for other phase regions.

3. RESULTS

A geothermal five-spot problem described by Pruess (1994) was modeled to compare the thermodynamic formulations IAPWS-IF97 and IAPWS-95. The five-spot well pattern shown in Figure 3 has a high degree of symmetry so only one-eighth of the pattern including one injector and one producer were modeled. The reservoir was modeled as a homogeneous porous medium with thickness 305 m, porosity 0.01, and permeability $6 \times 10^{-15} \text{ m}^2$. The grain density of the rock was set as 2650 kg/m^3 , the specific heat was set as $1000 \text{ J/kg}^{\circ}\text{C}$, and the heat conductivity was defined as $2.1 \text{ W/m}^{\circ}\text{C}$. First, a subcritical version of the problem was modeled and the IAPWS-95 formulation compared to the IAPWS-IF97 formulation as well as the IFC-67 formulation in standard TOUGH2. Then, supercritical versions were modeled with temperature and pressure close to the critical point and with very high temperature and pressure that are likely to occur in magmatic intrusions. Yamazaki and Muto (2004) describe how region 2 (Fig. 1) with operational limit of 800°C and 100 MPa can be extrapolated to higher temperature and pressure with better accuracy than region 5 of the original IAPWS-IF97 formulation which has an operational limit of 2000°C for pressure below 10 MPa. However, the possibility of extending the formulation was very limited. Thus, the results when using the IAPWS-95 formulation in iTOUGH2 to model the supercritical problem were compared to those obtained when extrapolating region 2 of the IAPWS-IF97 formulation. Furthermore, the possibility of extrapolating region 5 of the revised version of IAPWS-IF97 formulation (Fig. 1) was studied and results compared to IAPWS-95.

3.1 Subcritical Conditions

For the subcritical problem, the initial temperature for the reservoir was set as 300°C , the initial pressure was set as 8.593 MPa, and the initial liquid saturation was defined as 0.99. Fluid with enthalpy 500 kJ/kg was injected into the reservoir at a rate of 24 kg/s and produced at the same rate. The reservoir was simulated using standard TOUGH2 with the IFC-67 formulation, and iTOUGH2 with the IAPWS-95 and IAPWS-IF97 formulations. Figure 4 shows the temperature profile after 36.5 years at the elements along the line connecting the injection and production wells. All three thermodynamic formulations operate at these subcritical conditions and all simulators give equivalent results.

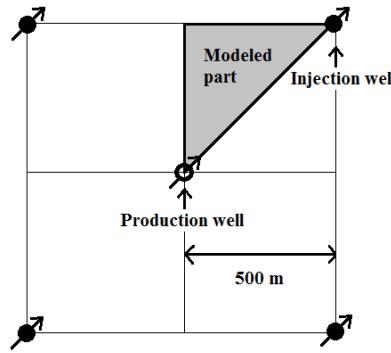


Figure 3: Five-spot injection/production problem showing the modeled part in grey.

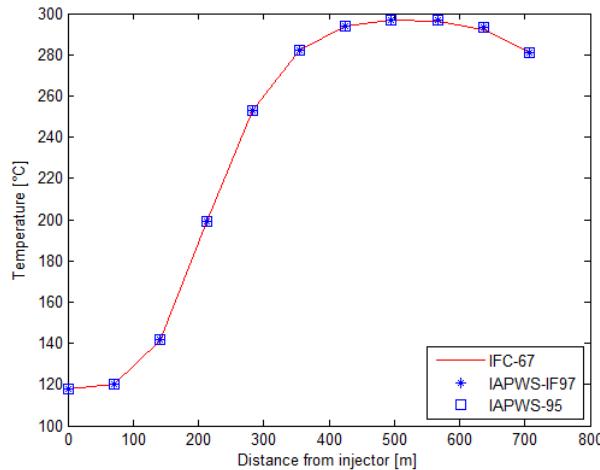


Figure 4: Temperature profile after 36.5 years along a line connecting the injector and the producer.

3.2 Supercritical Conditions Close to the Critical Point

The five-spot geothermal problem was modeled for supercritical conditions close to the critical point of water, which is at 374°C and 22.064 MPa. The initial temperature of the reservoir was raised to 400°C, and the initial pressure was increased to 22.06 MPa. The injection and production rates were decreased to 7.2 kg/s in accordance to conditions modeled by Croucher and O'Sullivan (2008), and the injection enthalpy of 500 kJ/kg was retained. Figure 5 shows the pressure-temperature diagram for the injector and producer modeled up to 36.5 years. In standard iTOUGH2, the IFC-67 thermodynamic formulation does only run for temperatures up to 350°C so for this case the results using iTOUGH2 with the IAPWS-95 formulation were only compared to those using the IAPWS-IF97 formulation in iTOUGH2 as well as to using AUTOUGH2. The results were equivalent, as expected, because the IAPWS-IF97 formulation is an approximation of the IAPWS-95 formulation.

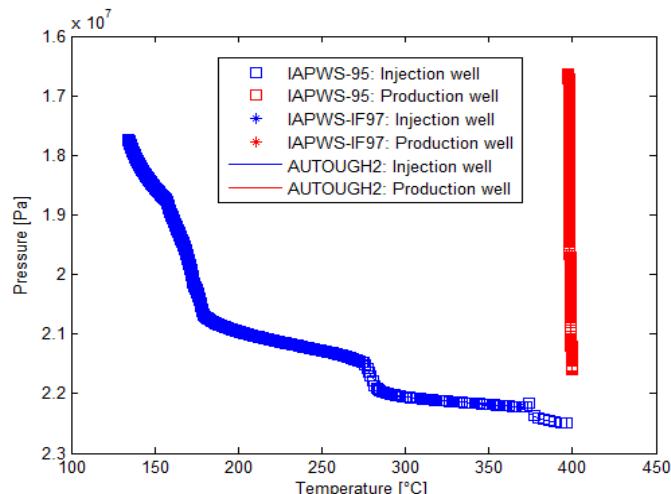


Figure 5: Pressure-temperature diagram for the injector and the producer for supercritical conditions close to the critical point.

3.3 Supercritical Conditions with Extreme Pressure and Temperature

In magmatic geothermal reservoirs, the pressure and temperature at great depths near magmatic intrusions can be very high. Hence, the previously studied five-spot problem was also modeled for extreme pressure and temperature conditions. The applicability of using the IAPWS-95 thermodynamic formulation compared to using the IAPWS-IF97 formulation was studied. The injection and production rates were set as 48 kg/s, and the enthalpy of the injected fluid was set as 3000 kJ/kg. The initial temperature of the reservoir was set as 1100°C, and the initial pressure was set as 90 MPa. Yamazaki and Muto (2004) showed the limitations of extending the original IAPWS-IF97 formulation above the operational temperature range of 0-800°C. Although, the formulation could be extended to higher temperatures at low pressures by extrapolating region 2 (Fig. 1) instead of region 5 of the original IAPWS-IF97 formulation, the deviation of IAPWS-IF97 from IAPWS-95 became high for the pressures and temperatures likely to occur in magmatic intrusions. Figure 6 shows the pressure-temperature diagram for the element located in the middle between the injector and producer for 55 years of production. Extrapolating region 2 of the IAPWS-IF97 formulation gives different results than the IAPWS-95 formulation, and the deviations in thermodynamic properties would be larger for higher temperatures (Yamazaki and Muto, 2004). Thus, region 2 of the IAPWS-IF97 formulation could not be used to accurately model such high temperatures and pressures likely to be present deep in magmatic geothermal reservoirs.

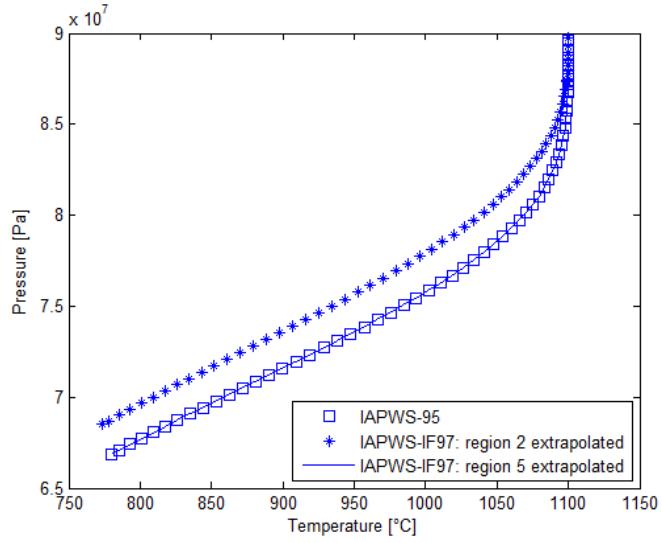


Figure 6: Pressure-temperature diagram for the element in the middle between the injector and the producer for supercritical conditions with initial temperature at 1100°C.

Next, the same five-spot problem was simulated by extending region 5 of the revised IAPWS-IF97 formulation and the results are equivalent to those when using the IAPWS-95 formulation (Fig. 6). The main disadvantage of using the IAPWS-95 formulation is the relatively slow computational speed. The IAPWS-IF97 formulation is significantly faster: the CPU time decreases by a factor of 10 for this case when using IAPWS-IF97 instead of IAPWS-95. However, the advantage of the IAPWS-95 formulation is that it can be extrapolated to extremely high temperatures and densities (Wagner and Pruss, 2002). Hence, the possibility of extrapolating region 5 of the revised IAPWS-IF97 formulation to even higher temperature and pressure was studied. The initial temperature and pressure of the previous five-spot problem was increased to 1,500°C and 150 MPa. The pressure-temperature diagram for the element located in the middle between the injector and producer after 55 years of production is shown in Figure 7. Even at such high temperature and pressure conditions, the IAPWS-95 formulation and the revised IAPWS-IF97 formulation with region 5 extrapolated give similar results. The difference in density at 1,500°C and 150 MPa between the two formulations is approximately 0.1% and the difference in internal energy is close to 0.02%. Extrapolating region 2 to such high temperature and pressure gave unphysical thermodynamic properties and the simulation did not converge. Thus, it is recommended to use the revised IAPWS-IF97 formulation instead of IAPWS-95 for faster computational speed and to extrapolate region 5 of the formulation if needed. However, for very high temperature and pressure conditions, it is important to study further the uncertainty of extrapolating the thermodynamic formulation.

4. CONCLUSIONS

The IAPWS-95 and IAPWS-IF97 thermodynamic formulations were added to the iTOUGH2 simulator to extend the applicability of the TOUGH2 based code to temperatures and pressures above 800°C and 100 MPa. Such extreme conditions are likely to occur in magmatic geothermal reservoirs where the heat sources can reach relatively shallow depths. Four versions of a five-spot geothermal problem were simulated and results obtained by using the IAPWS-95 formulation were compared to those using the IAPWS-IF97 formulation. First, subcritical conditions and supercritical conditions close to the critical point were modeled and the results using IAPWS-95 and IAPWS-IF97 were identical. Then, supercritical problems were studied with high temperature and pressure conditions. The results demonstrated that the IAPWS-IF97 formulation with region 2 extrapolated deviates from the IAPWS-95 formulation but the revised IAPWS-IF97 formulation with region 5 extrapolated gives equivalent results. Thus, it is recommended that the revised IAPWS-IF97 formulation be used instead of IAPWS-95 because of its significantly higher computational speed.

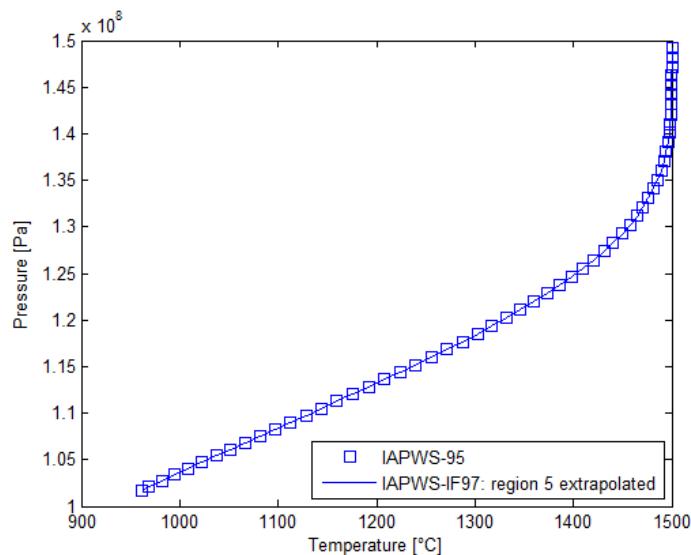


Figure 7: Pressure-temperature diagram for the element in the middle between the injector and the producer for supercritical conditions with initial temperature at 1500°C.

Future work will use this extended version of iTOUGH2 to include the heat sources when modeling magmatic geothermal reservoirs and use inverse modeling to estimate the unknown parameters in the model. That way, comprehensive magmatic geothermal reservoirs can be modeled to answer questions relevant to the field management of these supercritical systems.

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