Proceedings World Geothermal Congress 2020+1
Reykjavik, Iceland, April - October 2021

Modeling Analyses of Fluid Flow and Reactive Transport Processes for a Supercritical Geothermal System

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Keywords: Supercritical; Reactive transport; Code development

ABSTRACT

Beyond the critical point of 373.946 ºC and 22.064 MPa, water presents in supercritical state with high density and low viscosity, which is beneficial for geothermal resource development and utilization. According to Cladouhos et al (2018), at a 60 kg/s mass injection rate the energy production of supercritical water at 400 ºC is almost 10 times larger than that at 200 ºC. Supercritical geothermal development is getting more attention recently. However, higher temperature could result in more serious water-rock reactions, affecting the permeability and heat extracting behavior. There is little analysis on super-critical geothermal development, especially on geochemical reaction aspect.

In this work, we develop a multi-phase flow and reactive transport simulation code for supercritical geothermal systems, based on the existing structure of TOUGH2 and TOUGHREACT. IAPWS-IF97（International Association for the Properties of Water and Steam, 2007）is used for calculations of water thermodynamic properties. It can cover the T-P range up to 800 ºC and 100 MPa, and the temperature limit can even extend to 2000 ºC if pressure lower than 50 MPa. For the reactive transport modeling, the largest challenging is the lack of equilibrium constants at high temperature (>300 ºC) for minerals and aqueous species. In this work, SOLTHERM-2011.XPT is introduced, which is developed by Mark Reed and Jim Palandri. It provides the equilibrium constants for minerals and aqueous species under the condition of the density of water larger than 350 kg/m^3. The Icelandic Deep Drilling Project (IDDP-2) is taken as an example to illustrate flow and reactive processes and the heat extraction performance for cold water injection into a supercritical geothermal system.

1. INTRODUCTION

At present, with the development of geothermal energy and the enhancement of drilling capacity, supercritical geothermal has attracted more and more attention. Supercritical geothermal resource refers to that water exists in the supercritical state under the condition of ultra-high temperature and pressure in the deep part of crust (22.064 MPa, 373.946 ºC). Its physical properties are significantly different from the shallow liquid state, and its mobility and thermal extraction efficiency are greatly improved. According to Cladouhos et al. at 60 kg/s mass flow rate, energy extraction in 400 ºC reservoir could be almost 10 times higher than that of 200 ºC reservoir (Cladouhos et al. 2018).

There are many supercritical geothermal projects over the world. Now the drilling and borehole logging work has been finished in IDDP-2 project (Iceland) and DESCRAMBLE Project (Italy). IDDP-2 has reached about 4700 m and 535 ºC; DESCRAMBLE is 2200 m 350 ºC, and extends to 3000 m, reaching supercritical condition.

Since 21st century, Iceland started Iceland Deep Drilling Project (IDDP), tried to conduct the deep drilling to find supercritical geothermal at a proper depth for commercial power generation (Friðleifsson et al. 2014, Fridleifsson and Elders 2005). There are three potential fields, Krafla, Reykjanes, and Hengil. Until now, except Hengil, drilling work both have been completed.

In 2009, IDDP-1 started in Krafla. Original plan was to drill to 4.5 km depth but encountered magma at a depth of 2104 m. Large amount of acid superheated steam corroded the surface equipment. After a flow test, wellhead reached up to 452 ºC, and 14 MPa. After that, some geochemical studies continued to be carried out.

In Dec 2015, IDDP-2 was conducted to deepen the existing wellbore RN-15 in Reykjanes (Fridleifsson et al. 2016). It was completed in Jan 2017, 4659 m depth, about 4500 m in vertical. After 6-day recovery, an unequilibrated bottom temperature is 427ºC, and 34 MPa. According to report of Science Application Group of Advisors (SAGA) on 18 Mar 2018, the equilibrated temperature is about 535 ºC. Several permeable zones were encountered below 3000 m (Friðleifsson et al. 2017, Zierenberg et al. 2017).

It was concluded that different aspects of the geothermal development chain have to be addressed, and a need for in-depth investigations was formulated (Dobson et al. 2017):

1. Exploration methods for better resource assessment

2. Laboratory experiments for investigate in-situ fluid as well as in-situ rock physical properties

3. Adapted drilling and completion technologies

4. Borehole logging and monitoring instruments and strategies

5. Numerical simulation tools capable of handling supercritical conditions

6. Field laboratories to gain more knowledge about downhole conditions and test technological approaches along the entire

For the aspect of supercritical fluid numerical simulation, because of the drastic changes of water’ s properties in the vicinity critical point, conventional simulators cannot meet the demand. So far, several research teams have developed their simulation programs, including HOTH2O HYDROTHERM, Complex System Modeling Platform (CSMP++) (Driesner et al. 2015), and some programs based on TOUGH (Pruess 1991), such as AUTOUGH, iTOUGH-EOSsc etc.

Among which, HOTH2O (Pritchett 1995) and HYDROTHERM (Hayba and Ingebritsen 1994) both are extension of STAR simulator, using pressure and fluid internal energy as primary variables. Although it meets the supercritical demand, it only supports radial and rectangular mesh, not so flexible for irregular gridblocks simulation. Kissiling developed a supercritical equation of state module for TOUGH based on IFC-67 formulation and equations of Haar et al. Then, the brine effect is considered. It incorporates a description of the complete phase diagram for H2O-NaCl mixtures, including liquid, vapor and solid phases, over a wide range of pressure, temperature and concentration conditions. Croucher and O’Sullivan made some modifications (Croucher and O’Sullivan 2008); original thermodynamic formulation IFC-67 is superseded by IAPWS-97 (Wagner et al. 2000). They used density and temperature as primary thermodynamic variables under supercritical conditions. Then they continued their work, extended their algorithm to apply to the air-water EoS module (EOS3). Now the geothermal systems can be simulated using the improved algorithm with domains extending from the brittle/ductile transition all the way up to the surface (O’Sullivan et al. 2016). Magnusdottir and Finsterle also developed iTOUGH-EOS1sc, a supercritical EoS module for iTOUGH2 using IAPWS-IF97, provided forward and inverse modeling capabilities at supercritical conditions. It presents a better accuracy and higher computational speed (Magnusdottir and Finsterle 2015, Magnusdottir and Jonsson 2018).

In this study, we also developed our own simulation program based on TOUGHREACT and using IAPWS-IF97. We also made some modifications and improvements, and add reactive transport and wellbore function into it.

2. MULTIPHASE FLOW

IAPWS-IF97 [International Association for the Properties of Water and Steam, 2007] is a formulation serves as the international standard for water’s thermodynamic properties calculation. It is an improved version with higher efficiency based on IAPWS-95. The T-P range of IAPWS-IF97 is as Figure 1 shows. In AUTOUGH and iTOUGH-EOS1sc, it supersedes original thermodynamic formulation IFC-67 International Formulation Committee [1967].

The T-P range of IAPWS-IF97 can be separated into 2 parts and 5 regions. First part is within the T-P range of 0~800 °C and 0~100 MPa. It contains 4 regions, different regression equations are applied for different regions. Region 4 is the saturation line, the supercritical point is 647.096 K, 22.064 MPa. The other part is the Region 5, which is suitable for the condition where pressure is below 50 MPa, temperature could be up to 2000 °C.

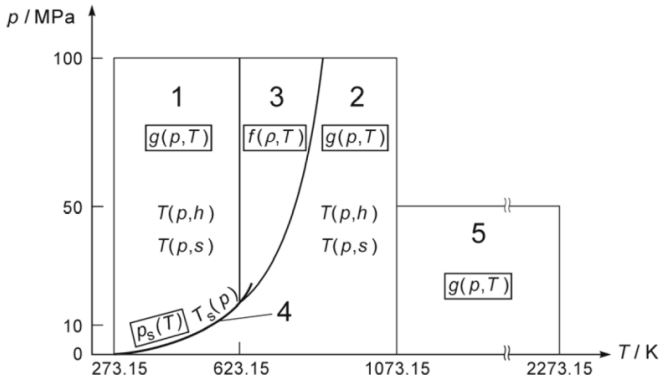

Figure 1: Regions and equations of IAPWS-IF97

The phase diagram of water and corresponding physical properties (Density, viscosity and specific enthalpy) calculated using IAPWS-IF97 is shown as Figure 2.

On multiphase flow simulation, we made some improvements in following aspects:

1) Primary variables for ZONE 3 ;

2) Treatment of supercritical state;

3) Relative permeability and capillary;

The details are discussed below:

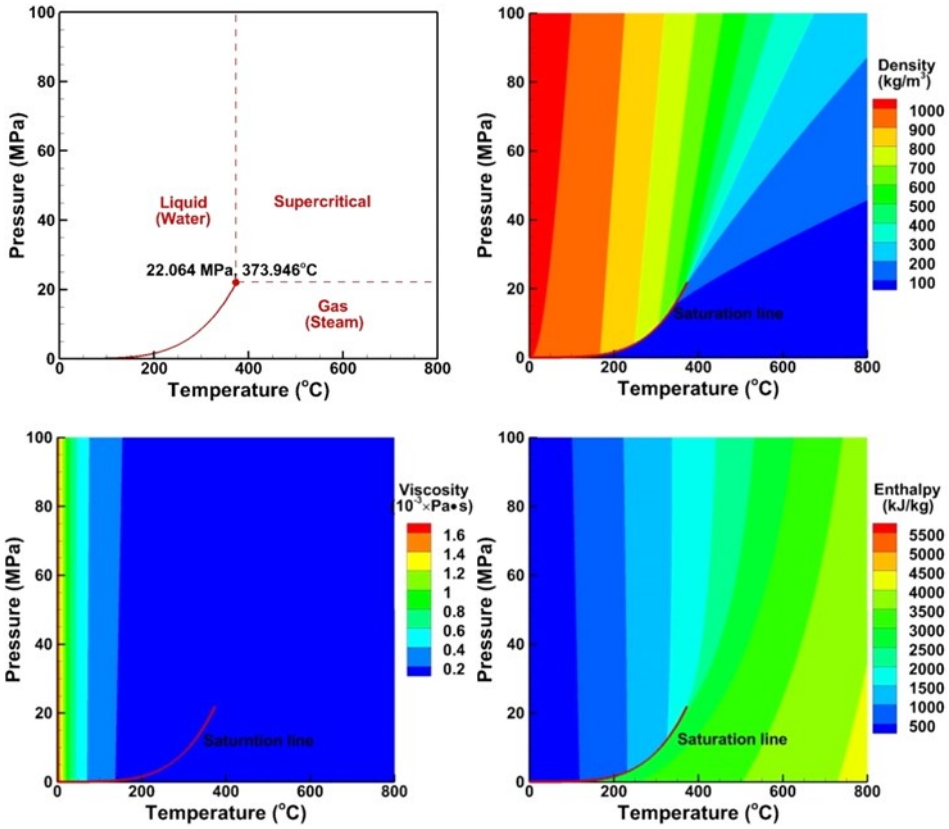

Figure 2: Phase diagram and physical properties (density, viscosity and enthalpy) of water calculated by IAPWS-IF97

2.1 Primary variables for ZONE 3

As discussed above, a series of very complicated regression equation are derived to calculate the properties of water or steam based on some primary variables. For Zone 1, 2, 5, pressure and temperature are selected as the primary variables. However, for ZONE 3, it covers water/steam two phase states, i.e. one variables combination may corresponds to two series of properties. Therefore, P, T is no longer suitable for ZONE 3; density and temperature combination is selected, as

$$\frac{f(\rho,T)}{RT} = \emptyset(\delta,\tau) = n_1 \ln\delta + \sum_{i=2}^{40} n_i \delta^{I_i} \tau^{J_i} \quad (1)$$

AUTOUGH and iTOUGH-EOS1sc also adopt it. In our code, to follow the structure of original TOUGH-EOS1, P-T combination is retained for supercritical state. Therefore, the new EOS module structure is totally the same with original EOS1, beneficial for users to familiar with.

Table 1:

Code	Primary Variables
AUTOUGH / iTOUGH-EOS1sc	**(P, T) for liquid/gas** **(P, Sg) for two-phase** **(ρ, T) for supercritical**
Present	**(P, T) for liquid/gas/supercritical** **(P, Sg) for two-phase**

Because the primary variables are not the same with thermodynamic formulation, an iterative procedure is needed for calculation. To improve the calculation efficiency, Newton-Raphson iteration is applied, in most cases, 2-4 times iterations could get convergence, except the zone around critical point. At critical point, $\partial\rho/\partial P \rightarrow \infty$, a squeeze method is applied.

For subcritical condition, the equation has multiple roots. One for gas and one for liquid, the third is a wrong root that should be excluded. The wrong one is picked via a derivate of $\partial\rho/\partial P$, it should always be positive.

2.2 Treatment of supercritical state

For AUTOUGH and iTOUGH-EOS1sc, they both were developed based on TOUGH2. In TOUGH2, the flow of each phase are calculated separately. They adopted virtual extended saturation line to calculate in supercritical condition (Figure 3). i.e. supercritical state is artificially divided into two parts. The relative permeability for all phases is set 1.

Here, in our code, the supercritical condition is regarded as a third state and convertible. If its neighbor block is gas, we regard it as gas. If its neighbor block is liquid, we regard it as liquid.

However, no matter the virtual extended saturation line method or our present, both face the discontinuity of relative permeability and capillary function around the point.

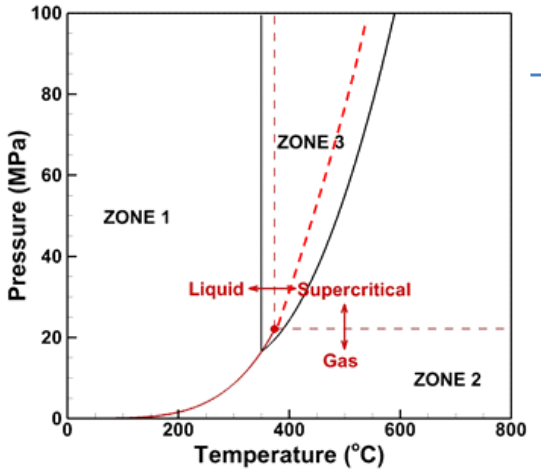

Figure 3: Virtual extended saturation line treatment for supercritical state

2.3 Relative permeability and capillary

The third problem is the discontinuity of relative permeability and capillary function around critical point.

Darcy velocity of single-phase flow is calculated assuming fluid flows through the whole cross-section; porosity is not in consideration, as Equation (2). While for multiphase flow, it should be corrected, if we take the phase saturation into account. However, multiphase coexistence would affect each other; retard the velocity of other phases. The mutual effect is relative permeability, as the Krb in Equation (3)

$$F = -k\frac{\rho}{\mu}(\nabla P - \rho g) \tag{2}$$

$$F_\beta = -k\frac{k_{r\beta}\rho_\beta}{\mu_\beta}\left(\nabla P_\beta - \rho_\beta g\right) \tag{3}$$

Most studies on relative permeability are carried out for water-air in vadose zone, or water-oil in petroleum engineering. The phases are stable, and the physical properties of each phase do not change significantly. Many models are setup for these problems. However, it may be not suitable for supercritical geothermal system. The reason is that, along the saturation line, the properties of gas and liquid are getting more and more similar (Figure 4). It tends to integrate into one phase; the mutual effect on different phases should be weakened, relative permeability gets closer to phase saturation.

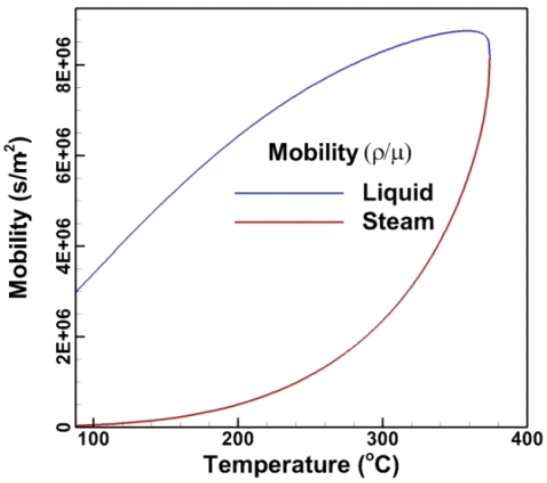

Figure 4: Mobility of gas and liquid state along saturation line

In most cases, relative permeability of each phase is lower than phase saturation, as Figure 5, and krg+krl is less than 1, assuming an element is in two-phase state and infinitely approaches critical point, there exists a numerical discontinuity when a phase change occurs, from two-phase state to supercritical. Therefore, we deduce that approaching the critical point, mutual effect should be weakened, and phase saturation may better characterize two-phase flow under that condition.

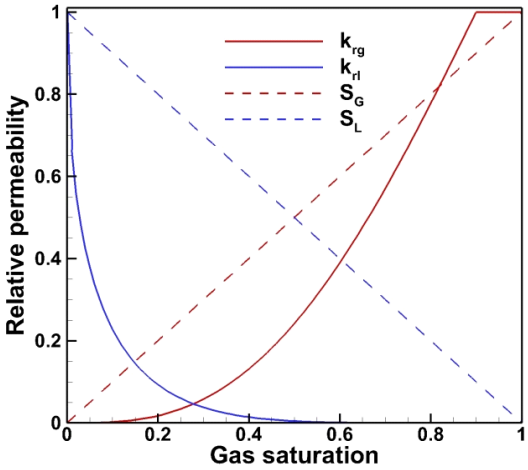

Figure 5: Sketch of relative permeability and corresponding phase saturation

Therefore, it is assumed the function of relative permeability and capillary pressure should be weaken. The ideal value is corresponding phase saturation. A linear interpolation between phase saturation and relative permeability is given.

$$k_{r\beta} = \frac{T}{T_c} S_\beta + \frac{T_c - T}{T_c} k_{r\beta}, \quad T_C = 373.946℃ \tag{3}$$

2.4 Test example

The example is from Magnusdottir and Finsterle (2015), a "five-spot" geothermal field as Figure 6, only 1/8 is simulated, one injection and one production well. Reservoir thickness is 305 m; porosity and permeability is 0.01 and 6×10^{-15} m^2. Fixed mass flow rate is 3 L/s, both for injection and production. An observing point, the gray gridblock, is set between injection and production well.

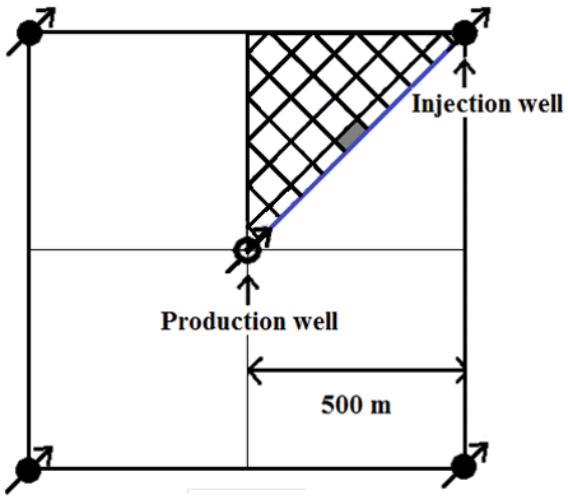

Figure 6: "Five-spot" geothermal conceptual model

The P-T profile evolution is shown as Figure 7. It could be seen the result of our present code fits well with that of Magnusdottir and Finsterle. As cold water being injected and hot water extracted. The pressure and temeprature of whole reservoir goes down.

3. REACTIVE TRANPSORT

3.1 Thermodynamic database

For common reactive transport modeling program, such as TOUGHREACT, GWB, PHREEQC etc, cannot meet the demand of supercritical simulation, because they are all restricted by the availability of thermodynamic (logK) data files with a temperature range of 0 – 300 °C and pressures on the critical curve for water.

In this work, SOLTHERM-201.XPT is employed, which is a thermodynamic database developed by Mark Reed and Jim Palandri and maintained by University of Oregon. It contains the data of aqueous species, minerals, and gases, including data for stoichiometry, equilibrium constants log K(T,P), aqueous activity coefficients, fugacity coefficients, and water enthalpy. These data include REE aqueous species and minerals. These data are used by programs SOLVEQ-XPT, CHIM-XPT, and GEOCAL-XPT. It is applicable under the condition of 0<T<600 °C, 0<P<1000MPa and density larger than 350 kg/m^3.

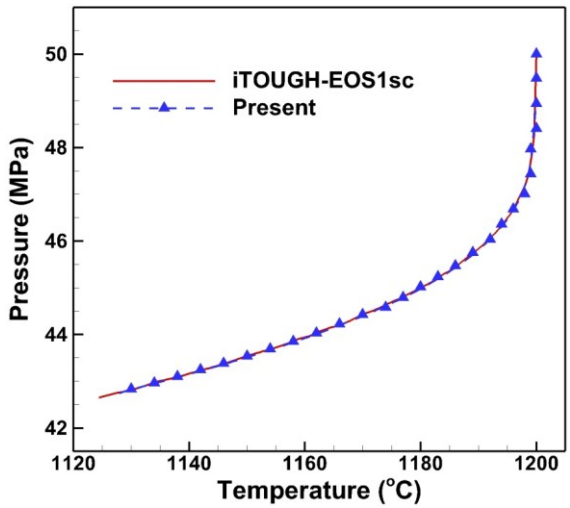

Figure 7: P-T profile of observing point of iTOUGH-EOS1sc and present code

3.2 Implement method

In TOUGHREACT, Log(K) is considered as a function of temperature at a reference pressure P0, Pressure effect on log(K) is not taken into account. Log(K) is expressed as a*ln(Tk) + b + c*Tk + d/Tk + e/Tk2, where Tk is absolute temperature (K), and log and ln stand for base 10 and natural logarithms, respectively. where, a, b, c, d and e are regression coefficients that are provided in thermodynamic database. If all coefficient values are omitted, Log(K) value at different temperatures should be given, the coefficients will be internally regression computed from the data.

While in SOLTHERM-2011.XPT, effect of temperature and pressure on log(K) are both considered. They are listed in a table, tabulated on a grid of (T, P) values, where water presents in liquid phase and density higher than 350 kg/m^3. The saturation line covers the diagonals of a series of consecutive quadrangles in the table.

4. CONCLUSION

In this study, a supercritical EoS module has been developed. Similar to AUTOUGH and iTOUGH-EOS1sc, it is also based on TOUGH structure, and IAPWS-IF97 thermodynamic formulation is employed. There are also some modifications and improvements. In present code, primary variables are totally the same with original TOUGH2-EOS1. In addition, we proposed the effect of pressure and temperature on relative permeability and capillary pressure should be taken into consideration

SOLTHERM-2011.XPT is introduced to extend the upper temperature limitation for supercritical simulation. An example of geothermal field is given for testing. The results of reactive transport modeling of our present code fit well with original TOUGHREACT v2.0-EOS1 module, but there still some difference. The main reason is thermodynamic data of aqueous species and minerals in SOLTHERM-2011.XPT is not exactly with original database. In fact, the data in any database is somewhat different with each other's. The other is the temperature effect on Log(K). The error accumulation for react transport modeling is significant.

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