Improvements to the AUTOUGH2 Supercritical Simulator
With Extension to the Air-Water Equation-of-State

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ABSTRACT
Developing a numerical simulator capable of reliably modelling supercritical thermodynamic conditions is becoming increasingly important in geothermal reservoir modelling. This work presents improvements that have been made to the supercritical TOUGH2 algorithm developed by Croucher and O’Sullivan (2008) which increase its reliability. The algorithm has also been extended to apply to the air-water equation-of-state (EOS3) and the details of the extension are explained. Large, complex, supercritical geothermal systems can now be simulated using the improved algorithm with domains extending from the brittle/ductile transition all the way up to the surface. Three dimensional simulations of a number of supercritical systems have been carried out successfully and the convergence behaviour of the simulations has been shown to be very good.

1. Introduction
Numerical modelling has become a widely used tool for both the management of geothermal systems and research into the physical processes taking place within them (O’Sullivan et al., 2001; Dipippo, 2016). The range of thermodynamic conditions encountered in numerical models is increasing as a wider range of geothermal systems are modelled and more diverse investigations into their behaviour are carried out. However, most geothermal simulators, including the industry standard TOUGH2 (Pruess, 1991), are limited to modelling temperatures and pressures below supercritical conditions. Simulations of very hot systems such as Krafla in Iceland (Magnusdottir and Finsterle, 2015) and Menengai in Kenya (O’Sullivan et al., 2015) require the use of supercritical thermodynamics. Similarly, investigations into the deep roots of geothermal systems and the interaction of multiple geothermal systems cannot be simulated using subcritical thermodynamics (Burnell et al., 2015).

Several supercritical simulators have been developed in the past including HYDROTHERM (Hayba and Ingebritsen, 1994), the HOTH2O extension to the STAR simulator (Pritchett, 1995) and CSMP++ (Weis, et al. 2014). Brikowski (2001) and Kissling (2004) both developed supercritical equations-of-state for TOUGH2 and Croucher and O’Sullivan (2008) developed a supercritical equations-of-state for AUTOUGH2; the University of Auckland’s version of TOUGH2 (Yeh et al., 2012). The algorithm developed by Croucher and O’Sullivan (2008) was recently implemented in the standard version of TOUGH2 by Magnusdottir and Finsterle (2015).

Despite these advances, there are very few examples of full-scale, three-dimensional simulations of geothermal systems with supercritical conditions present. In the case of the TOUGH2 family of simulators this is possibly because of the well-known convergence issues that often occur during phase changes (O’Sullivan et al., 2013, O’Sullivan et al., 2014). A supercritical equation-of-state contains many more phase changes than a subcritical equation-of-state and hence many more opportunities for convergence issues to arise.
In the work presented here we have used our experiences resolving convergence issues within standard TOUGH2 (O’Sullivan et al., 2013, O’Sullivan et al., 2014) to improve the supercritical equation-of-state developed by Croucher and O’Sullivan (2008). The details of the improvements are given in the following sections along with the extension of the algorithm to create a supercritical air-water equation-of-state. The improved algorithm has been tested on a number of full-scale, three-dimensional simulations of geothermal systems and preliminary results have been published previously (O’Sullivan et al., 2015, O’Sullivan and O’Sullivan, 2016). Examples of the results are given below along with an analysis of the convergence behaviour which shows that the improved supercritical algorithm performs very well. Note that the PyTOUGH library (Croucher, 2011; Wellmann et al., 2012) was used extensively throughout this project to create models, control simulations and visualize results.

2. Changes to the Algorithm

Previous work (O’Sullivan et al., 2013, O’Sullivan et al., 2014) to address convergence issues in the TOUGH2 solution algorithm identified that it is important to maintain continuous thermodynamic properties throughout the solution domain. Discontinuities in the fluid densities have been found to be particularly problematic but discontinuities in any fluid properties should be avoided. In the standard version of TOUGH2 the thermodynamic properties are limited to temperatures less than approximately 350°C which results in only three thermodynamic regions (liquid, vapour and two-phase) and two phase boundaries. For this restricted thermodynamic domain eliminating discontinuities across region boundaries was relatively straightforward.

However, a supercritical version of TOUGH2 presented by Croucher and O’Sullivan (2008) covers a much larger range of thermodynamic variables covering four thermodynamic regions (liquid, vapour, supercritical and two-phase) and associated region boundaries. This supercritical equation of state (EOS) was tested by successfully simulating several supercritical flows, but in further testing on more complex supercritical flow problems a number of discontinuities in the thermodynamic properties occurred in the solution domain which lead to poor convergence. The following sections discuss these discontinuities and the changes to the algorithm in the supercritical EOS that have been applied to deal with them.

2.1 Changing the Boundaries of the Numerical Solution Regions

In their work Croucher and O’Sullivan (2008) extended the approach used in standard TOUGH2 and defined the numerical solution regions based on the thermodynamic regions defined in the IAPWS-97 Formulation (Wagner et al., 2000) for calculating thermodynamic properties. They define four thermodynamic regions: 1 liquid, 2 vapour, 3 supercritical and 4 two-phase. In the sub-critical region this approach works well as the boundaries of the thermodynamic regions coincide with physical phase-change boundaries. However, above 350°C the boundaries of the thermodynamic calculation regions do not coincide with phase-change boundaries but instead are arbitrary, having been determined to make the calculation of thermodynamic properties convenient. In fact, there are no physical phase-change boundaries between sub-critical liquid (region 1) or vapour (region 2) and supercritical fluid (region 3).

The boundaries defined for the thermodynamic calculation regions identify where different independent variables are used for the thermodynamic formulae. Within the supercritical region (region 3 in Figure 1a) the thermodynamic properties are calculated using formulae dependent on density and temperature whereas in regions 1 and 2 they are calculated using formulae dependent on pressure and temperature. In their original algorithm Croucher and O’Sullivan (2008) introduced the idea of a supercritical phase and changed phase when crossing into region 3 and as part of the process changed the primary solution variables from pressure and temperature to density and temperature. Unfortunately, there are very small but significant discontinuities in the thermodynamic properties calculated by the different formulae used in regions 1 and 2 and those used in region 3. The differences can be seen in Figure 2 which plots the discrepancies in pressures calculated using formulae from thermodynamic region 1 and formulae from thermodynamic region 3 at 350°C. These values were calculated by calculating the fluid density using the region 1 formula \( \rho(p_{1,T}) \), then using the density to recalculate the pressure using the region 3 formula \( p_3(\rho,T) \) and finally calculating the difference between \( p_1 \) and \( p_3 \). These small discontinuities can cause the original algorithm to encounter difficulties when crossing regions at this boundary.

For the discussion below we also introduce the concept of a supercritical “phase” as well as the usual liquid and vapour phases and we discuss phase changes between liquid and supercritical and between vapour and supercritical. Then the approach in the algorithm presented here is to move the boundaries for the phase changes slightly away from the boundaries of the thermodynamic regions defined by Wagner et al. (2000). This means that the phase changes to and from the supercritical phase take place entirely within thermodynamic calculation region 3 and so there are no inconsistencies in formulae used on either side of the phase boundary. The phase-change boundaries were offset 5°C from the thermodynamic calculation regions. Therefore phase transitions from liquid to supercritical take place at 355°C and the formula for the boundary between regions 2 and 3 was adjusted to be consistent. The resulting formula is:
\[ p_{b23}^{\text{NEW}}(T) = p_{b23}^{97}(T) + 499656.09510250762 \]

Plot (b) in Figure 1 shows the resulting numerical solution regions in terms of pressure and temperature and plot (b) in Figure 3 shows them in terms of density and temperature.

Note also that it was found to be important to retain the previous numerical solution region for each block so that when convergence fails, time step reduction can proceed smoothly.

### 2.2 Blending the Thermodynamic Properties on the Edges of the Supercritical Region

Moving the supercritical phase change boundaries away from boundaries of the thermodynamic calculation regions removes discontinuities that occur during phases changes. However it was found that the small discontinuities in the formulae could still affect convergence when no phase changes were occurring. Therefore a small zone was defined where the thermodynamic properties are determined using a blend of formulae from the subcritical region and

**Figure 1.** Thermodynamic regions in terms of pressure and temperature as defined in IAPWS Industrial Formulation 1997 (a). Numerical solution regions used in the algorithm described in this work (b).

**Figure 2.** Discrepancies in pressures calculated using formulae from thermodynamic region 1 and formulae from thermodynamic region 3 at 350°C.

**Figure 3.** Thermodynamic regions in terms of density and temperature as defined in IAPWS Industrial Formulation 1997 (a). Numerical solution regions used in the algorithm described in this work (b).
those from the supercritical region. Figure 2 shows that the two formulae do not have a consistent difference: sometimes the supercritical formulae give higher pressures, sometimes lower. The size of the zone was defined such that there was a consistent difference between the results from subcritical formulae on one side and the results from the supercritical formulae on the other. Then linear interpolation between the two values was used within the transition zone.

For the boundary between thermodynamic calculation regions 1 and 3 this results in the following algorithm:

<table>
<thead>
<tr>
<th>Condition</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T &lt; 350^\circ$</td>
<td>$\rho, u$ calculated using subcritical formulae</td>
</tr>
<tr>
<td>$350^\circ &lt; T &lt; 350.05^\circ$</td>
<td>$\rho, u$ calculated using a linear blend of subcritical and supercritical formulae</td>
</tr>
<tr>
<td>$T &gt; 350.05^\circ$</td>
<td>$\rho, u$ calculated using supercritical formulae</td>
</tr>
</tbody>
</table>

For the boundary between thermodynamic calculation regions 2 and 3 this results in the following algorithm:

<table>
<thead>
<tr>
<th>Condition</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>$p &lt; p_{B23}^{97}(T)$</td>
<td>$\rho, u$ calculated using subcritical formulae</td>
</tr>
<tr>
<td>$p_{B23}^{97}(T) &lt; p &lt; p_{B23}^{\text{Blend}}(T)$</td>
<td>$\rho, u$ calculated using a linear blend of subcritical and supercritical formulae</td>
</tr>
<tr>
<td>$p &gt; p_{B23}^{\text{Blend}}(T)$</td>
<td>$\rho, u$ calculated using supercritical formulae</td>
</tr>
</tbody>
</table>

where $p_{B23}^{\text{Blend}}(T)$ is given by:

$$p_{B23}^{\text{Blend}}(T) = p_{B23}^{97}(T) + 100(T - 350)$$

It is important to note that as a consequence of shifting the numerical boundaries and using the blending described above, there are zones where the primary variables are $p$ and $T$ but the thermodynamic calculations are carried out using formulae in terms of $\rho$ and $T$. In these zones an efficient nonlinear solve is used to invert the formula for $\rho$ and the computational cost is small. However recently the IAPWS Industrial Formulation has provided a new formula for $\rho(p, T)$ in the supercritical region which could be implemented instead of carrying out the nonlinear solve (IAPWS, 2014).

2.3 Creating a “Two-Phase” Zone in the Supercritical Region

In their original algorithm Croucher and O’Sullivan (2008) used a pseudo-saturation line to divide the supercritical region into a “liquid-like” supercritical zone and a “vapour-like” supercritical zone. This allowed the supercritical region to be represented consistently in TOUGH2 which uses an inherently two-phase algorithm. In TOUGH2 a vapour saturation is calculated in all regions and used explicitly in the governing equations. In the liquid region the vapour saturation is zero, in the vapour region it is one and in the two-phase region it is between zero and one. In the standard version of TOUGH2 the two-phase region separates the liquid and vapour region and therefore acts as “blending” region that allows the saturation to transition smoothly from zero to one or vice versa.

The pseudo-saturation line in the original algorithm also provided a mechanism for transitioning from a gas saturation of zero to a gas saturation of one while moving through the supercritical region. However, from a more detailed consideration of the interaction between a supercritical block and sub-critical it became apparent that properties at the interface between the blocks become discontinuous when a sharp transition is used.

In this work we present a “two-phase” zone (3c) in the supercritical region which allows for a smooth transition from “liquid-like” (3a) to “vapour-like” (3b) supercritical fluid. The boundaries of the zone have been defined for numerical reasons and are somewhat arbitrary. However there are some physical arguments for such the existence of this type of zone (Brazhkin and Trachenko, 2012) and the boundaries could be adjusted accordingly.

The functional forms were determined so that boundaries between the single-phase regions and the two-phase regions were continuous when viewed in density/temperature space (see Figure 3b). They were also chosen to ensure a unique value of density could easily be found for every temperature. To achieve this, the pseudo-liquid saturation line and the pseudo-gas saturation line begin slightly below the critical temperature ($0.1^\circ$C). This allows the algorithm to avoid the zone very close to critical point where the pressure is not unique for a given temperature and range of densities (Figure 4a). Plot (b) shows that for temperatures in this zone it can be difficult for the algorithm to determine the saturation densities accurately as there are three solutions to $p = p_{sat}$, all in very close proximity.

Hyperbolic functions in temperature/density space were selected to represent the pseudo-saturation lines. This allowed them to have very steep gradients close to the critical point which approximately match the gradients encountered
in the true saturation lines at \((T_{\text{critical}}-0.1)\)°C. Figure 5 shows the pseudo-saturations lines close to the critical point in both pressure/temperature and density/temperature space. Their functional forms are as follows:

\[
\rho_{\text{sc}} = \frac{T_{\text{C}} - T_{\text{asy}}}{T - T_{\text{asy}}} \left[ \rho_{\text{off}} - m_{\text{C}}(T_{\text{C}} - T_{\text{asy}}) \right] + m_{\text{C}}(T - T_{\text{asy}}) + \rho_{\text{C}} - \rho_{\text{off}}
\]

\[
\rho_{\text{og}} = \frac{T_{\text{G}} - T_{\text{asy}}}{T - T_{\text{asy}}} \left[ -\rho_{\text{off}} - m_{\text{G}}(T_{\text{G}} - T_{\text{asy}}) \right] + m_{\text{G}}(T - T_{\text{asy}}) + \rho_{\text{G}} + \rho_{\text{off}}
\]

where \(T_{\text{C}}, T_{\text{G}}, \rho_{\text{C}}, \) and \(\rho_{\text{G}}\) are the temperatures and densities at the intersections between the true saturation lines and the pseudo-saturation lines (see Figure 5b). For this work \(T_{\text{C}} = T_{\text{G}} = (T_{\text{critical}}-0.1)\)°C. The slopes of the pseudo-saturation lines are given by \(m_{\text{C}}\) and \(m_{\text{G}}\), their offset from the critical density is given by \(\rho_{\text{off}}\) and vertical asymptote which is used to control their gradients at CL and CG is defined by \(T_{\text{asy}}\). The values used in the algorithm presented here were as follows:

\[
m_{\text{C}} = 2 \quad m_{\text{G}} = 1
\]

\[
\rho_{\text{off}} = 10 \text{ kg/m}^3 \quad T_{\text{asy}} = (T_{\text{critical}}-0.4)\text{°C}
\]

Despite possible physical justifications (Brazhkin and Trachenko, 2012), in this work the supercritical two-phase region does not represent a physical change in the fluid properties but is simply a mechanism for achieving numerical stability. As such the governing equations are the same throughout region 3 and the primary variables used is the algorithm do not change within this region. Instead the temperature and density of the supercritical fluid are used to calculate the pseudo-saturation at all locations within region 3. Thus for any given temperature the saturation is calculated as follows:

\[\vdots\]
<table>
<thead>
<tr>
<th>Condition</th>
<th>S\textsubscript{gas}</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\rho &lt; \rho_{\text{eq}})</td>
<td>(S_{\text{gas}} = 1.0)</td>
</tr>
<tr>
<td>(\rho &lt; \rho &lt; \rho_{\text{eq}})</td>
<td>(S_{\text{gas}}) calculated using linear interpolation</td>
</tr>
<tr>
<td>(\rho &gt; \rho_{\text{eq}})</td>
<td>(S_{\text{gas}} = 0.0)</td>
</tr>
</tbody>
</table>

### 2.4 Including Air in the Supercritical Algorithm

In order to model geothermal systems from the surface down to the brittle-ductile transition zone the supercritical algorithm must be modified to enable it to represent the unsaturated vadose zone near the surface. In standard TOUGH2 this can be achieved by including air as an additional component in the governing equations. Including air the supercritical algorithm could be achieved in several ways. One approach could be to only include air in the shallow zones of the model and track an internal boundary with the rest of the domain where only pure water exists. However, determining the depth to which air is transported is challenging as is handling an internal boundary.

In this work we opt to include air throughout the domain, accepting that its mass fraction will be very small at depth and careful treatment will be required to ensure the mass of air is conserved. In standard TOUGH2 Air-Water equations-of-state, the air is treated as a passive scalar in the liquid phase but contributes to the enthalpy, viscosity and density of the vapour phase (O’Sullivan et al., 2013). To ensure consistency with this approach air is treated as a passive scalar in the “liquid-like” supercritical region but contributes to the enthalpy, viscosity and density of the “vapour-like” phase.

The extensions to the various phase changes that ensure the consistent handling of the air component are described in the following section.

### 2.5 Handling Phase Changes

The changes described in the preceding sections help to ensure that thermodynamic properties are continuous and consistent throughout the domain. However, even with consistent continuous thermodynamic properties phase changes must be handled carefully and accurately if discontinuities are to be avoided. In the supercritical algorithm there are many more possible phase changes as shown in Figure 6. A brief outline of each of these phase changes are discussed in the following subsections and the approach for handling them in this work is presented. In each case the treatment of the air component is explained.

#### 2.5.1 Phase Change A – Liquid to Two-Phase

If the vapour pressure is less than the saturation pressure for the given temperature then the vapour phase evolves and primary variables are changed to pressure, temperature and vapour saturation. In previous versions of TOUGH2 both the temperature and the partial pressure of air are held constant during the phase change. In the algorithm presented here a set of nonlinear equations are solved to calculate the temperature and the partial pressure of air at the point the vapour pressure dropped below the saturation pressure.

#### 2.5.2 Phase Change B – Liquid to Supercritical

If the temperature is greater than 355°C then the liquid phase changes to a “liquid-like” supercritical phase and the primary variables are changed to density, temperature and air mass fraction. No adjustments are made to temperature or air mass fraction.

#### 2.5.3 Phase Change C – Vapour to Two-Phase

If the vapour pressure is greater than the saturation pressure for the given temperature then the liquid phase evolves and the primary variables are changed to pressure, temperature and vapour saturation. In previous versions of TOUGH2 both the temperature and the partial pressure of air are held constant during the phase change. In the algorithm presented

![Figure 6. Density and temperature plot indicating the various phase changes.](image-url)
here a set of nonlinear equations are solved to calculate the temperature and the partial pressure of air at the point the
vapour pressure increased above the saturation pressure.

2.5.4 Phase Change D – Vapour to Supercritical
If the temperature is greater than 355°C and the pressure increases past the $p^{\text{NEW}}_{B23}$ boundary then the vapour phase
changes to a “vapour-like” supercritical phase and the primary variables are changed to density, temperature and air mass
fraction. The density is adjusted to be a small amount larger than at the boundary and interpolate the air mass fraction to
the same point. These adjustments ensure that the fluid does not pass from region 2, through region 3 straight to region 4
when the temperature is between 355°C and $T_{\text{critical}}$.

2.5.5 Phase Change E – Supercritical to Liquid
If the temperature is less than 355°C then the “liquid-like” supercritical phase changes to a liquid phase and the
primary variables are changed to pressure, temperature and air mass fraction. The temperature is adjusted to be a small
amount less than 355°C, interpolate the density and air mass fraction to the same point and then calculate the correspond-
ing pressure. These adjustments ensure that the fluid does not pass from region 3, through region 1 straight to region 4.

2.5.6 Phase Change F – Supercritical to Vapour
If the temperature is greater than 355°C and the pressure decreases below the $p^{\text{NEW}}_{B23}$ boundary then the “vapour-
like” supercritical phase changes to a vapour phase and the primary variables are changed to pressure, temperature and
air mass fraction. No adjustments are made to temperature or air mass fraction.

2.5.7 Phase Change G – Supercritical (pure “liquid-like” or pure “vapour-like”) to Two-Phase
If the temperature drops below the temperature on the boundary between regions 3 and 4 then the supercritical
phase changes to two-phase and the primary variables are changed to pressure, temperature, and vapour.

2.5.8 Phase Change H – Supercritical (mixture of “liquid-like” and “vapour-like”) to Two-Phase
If the temperature drops below (T_{\text{critical}}-0.1)°C while the supercritical pseudo-saturation is between zero and one
then the supercritical phase changes to two-phase and the primary variables are changed to pressure, temperature and
vapour saturation. Interpolation is used to determine the density and air mass fraction at the point where the temperature
dropped below (T_{\text{critical}}-0.1)°C. These values are used to calculate the fluid properties and hence the accumulation of
mass, energy and air for the block. The temperature is set to a small amount less than (T_{\text{critical}}-0.1)°C and the new pressure
calculated based on the saturation. The new pressure and temperature are used to calculate fluid properties and solve
for the gas saturation ensuring that the accumulation of mass, energy and air are conserved for the block. This approach
is necessary because the pseudo-saturation is a numerical tool and is not related to the actual two-phase gas saturation
and cannot be converted directly.

2.5.9 Phase Change I – Two-Phase to Liquid
If the vapour saturation drops below zero then the vapour phase disappears and the primary variables are changed to
pressure, temperature and air mass fraction. Interpolation is used to find the values of pressure and temperature when the
vapour saturation dropped below zero. The equivalent saturation pressure is calculated and hence the partial pressure of air.

2.5.10 Phase Change J – Two-Phase to Gas
If the vapour saturation increases above one then the liquid phase disappears and the primary variables are changed
to pressure, temperature and air mass fraction. Interpolation is used to find the values of pressure and temperature when the
vapour saturation increases above zero. The equivalent saturation pressure is calculated and hence the partial pressure of air.

2.5.11 Phase Change K – Two-Phase to “liquid-like” Supercritical
If the vapour saturation drops below zero then the vapour phase disappears and the primary variables are changed
to density, temperature and air mass fraction. Interpolation is used to find the values of pressure and temperature when the
vapour saturation dropped below zero. The equivalent saturation pressure is calculated and hence the partial pressure of air.

2.5.12 Phase Change L – Two-Phase to “vapour-like” Supercritical
If the vapour saturation increases above one then the liquid phase disappears and the primary variables are changed
to density, temperature and air mass fraction. Interpolation is used to find the values of pressure and temperature when the
vapour saturation increased above zero. The equivalent saturation pressure is calculated and hence the partial pressure of air. The density is limited so that the fluid does not pass from region 4, through region 3 straight to region 2.

2.5.13 Phase Change M – Two-Phase to Supercritical

If the vapour saturation is between zero and one but the temperature increases above \((T_{\text{critical}}-0.1)°C\) then the fluid changes to the supercritical phase and the primary variables are changed to density, temperature and air mass fraction. Interpolation is used to find the pressure, density and vapour saturation where the temperature increased above \((T_{\text{critical}}-0.1)°C\). The equivalent saturation pressure is calculated and hence the partial pressure of air and it is converted to air mass fraction using the fluid properties.

3. Results

The supercritical algorithm for the air-water equation-of-state that is described in the previous sections has been successfully used to simulate several large-scale geothermal systems (O’Sullivan et al., 2015, O’Sullivan and O’Sullivan, 2016). The plots in Figure 7 reproduce results from a natural state simulation of a large, supercritical geothermal system (O’Sullivan and O’Sullivan, 2016). They show that extensive areas of the model domain are supercritical with pressures over 60 MPa and temperatures in excess of 400°C. The convergence behaviour for the final calibration simulation are presented in Figure 8 showing that the algorithm performed well, achieving a large final time step size without any convergence issues.

4. Conclusion

Improvements to the supercritical TOUGH2 algorithm developed by Croucher and O’Sullivan (2008) have been presented. The algorithm has also been extended to apply to the air-water equation-of-state (EOS3) and the details of the extension explained. Large, supercritical geothermal systems can now be simulated using the improved algorithm with domains extending from the brittle/ductile transition all the way up to the surface. Three dimensional simulations of a number of supercritical systems have been carried out successfully (O’Sullivan and O’Sullivan, 2016) and the convergence behaviour of the simulations has been shown to be very good.
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References


