Extending MULKOM to Super-critical Temperatures and Pressures

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Abstract

This paper describes some recent work which aimed at extending the MULKOM geothermal simulator to higher temperatures and pressures. The formulation of Arnold (1970) for the thermodynamic properties of super-critical water has been used to extend the operating range of MULKOM to temperatures of 800°C and pressures of 1000 bars. In addition, work has begun on a high temperature version of MULKOM which includes the transport of salt. We discuss some of the research problems which motivate this work and give examples of situations where high temperatures and pressures are encountered.

1 INTRODUCTION

The simulator MULKOM (Pruess 1982) has been used by the Applied Mathematics Group at Industrial Research Limited (IRL) to create models of a number of New Zealand and overseas geothermal fields. For these models the existing version of MULKOM, which covers the temperature range up to 350°C, has generally been adequate. There are however a number of situations where higher temperatures and pressures are encountered. This paper describes the extension of MULKOM to high temperatures and pressures and looks at some of the situations where this capability is useful.

The exploitation of geothermal fields in New Zealand has so far been mostly from relatively shallow levels, say less than 1.5 kilometres in depth. Recently, however, there has been interest in deeper exploitation of these geothermal fields, as the shallow reserves of heat begin to run out. Temperatures in the vicinity of 400°C may be expected in some of the high temperature fields (for example at Rotokawa) at depths of 3 or 4 kilometres, and this provides one of the main motivations for the work described in this paper.

Even higher temperatures are encountered close to magma bodies. Shallow magma, such as that found in Japan and Hawaii, has been considered as a source of energy by Dunn et al.(1987). These authors have successfully demonstrated an open heat exchanger system for energy extraction from solidified magma. Their numerical experiments involve the flow of super-critical water through a fractured, cooling magma body.

Closely related to this is the study of the hydrothermal systems associated with volcanoes. Isotopic studies of fumarole gases from White Island volcano, New Zealand, (Stewart and Hulston 1975) suggest that the water in these gases is derived at least in part from seawater, but later studies by Giggenbach and Stewart (unpublished) do not support this. A simple model of the White Island system (White and Kissling 1992), also makes this conclusion difficult to understand. Giggenbach (1987) has recently suggested that fumarole gases on White Island come from the interaction of 'rising gas streams and highly saline brines', and a similar mechanism is proposed by Hurst et al.(1991) for heat and chemical transfer into the Crater Lake of Mount Ruapehu, New Zealand.

In addition, there is considerable interest in the origin and structure of the New Zealand geothermal systems. A recent meeting on the Taupo Volcanic Zone (TVZ Heat Transfer Workshop '94, held at Wairakei, New Zealand, in February 1994) brought together experts from many fields to discuss this problem, but no real consensus was reached as to the nature of the heat source for the geothermal fields. It has been argued by McNabb (1992) that a 5 to 7 km deep saline 'hot plate' at a temperature of perhaps 400°C provides a conductive buffer zone between the overlying cooler hydrothermal systems and the deeper, much hotter magmatic regions which ultimately supply heat to the geothermal systems. On the other hand, others have argued for the more conventional picture of isolated magma bodies as the heat source for individual geothermal fields. The former problem is addressed with a simple numerical example in a following section of this paper.

Clearly there are many problems of interest which require such a 'high temperature and pressure' version of MULKOM which is capable of handling either pure water or hot brines. In this paper two high temperature versions of MULKOM are described which can handle precisely these two cases. A basic premise of the work was to make as much use of the existing structure of MULKOM as possible. This meant, for example, retaining the use of pressure and temperature as dependent variables. This created a number of difficulties which are discussed in greater detail in the sections which follow.

2 THERMODYNAMIC and TRANSPORT PROPERTIES of PURE WATER

The original version of MULKOM uses a thermodynamic formulation for pure water taken from Arnold (1970). More recent formulations are available, for example in Johnson and Norton (1991), who summarize recent experimental and theoretical work on the thermodynamic and transport properties of water. In the present work however, the equations of Arnold have been used to maintain compatability with the rest of MULKOM. It is probable that there is no practical difference between the formulae of Arnold and the more recent work.

Arnold's formulation divides the temperature-pressure space into a number of separate regions, as shown in figure 1. For each of these regions the formulation gives the functional relationship between temperature, pressure, density, entropy and internal energy of pure water. These functions are designed to ensure continuity of the thermodynamic properties and their derivatives across the region boundaries. (This continuity is necessary in order to guarantee the accuracy of the Jacobian matrix, which is generated numerically in MULKOM).

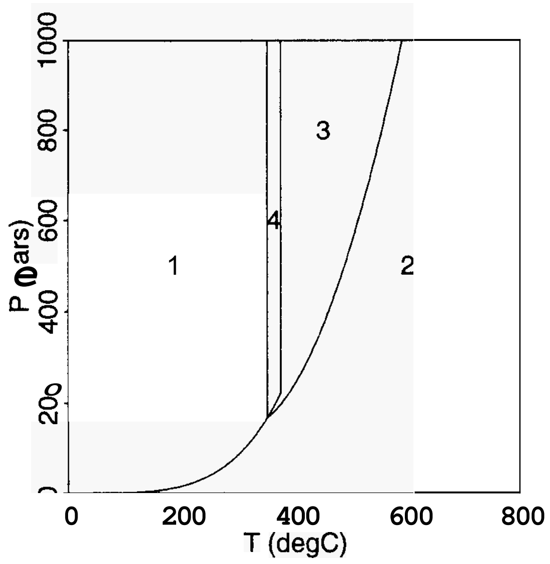

Figure I. The thermodynamic formulation of Arnold (1970). Standard MULKOM uses regions 1 and **2** for temperatures below 350°C.

Figure **2** shows the typical behaviour of the thermodynamic properties, (in this case the density, but others are similar) as a function of temperature and pressure. Below the critical point the density is discontinuous across the saturation line, with the size of the 'jump' becoming smaller as criticality is approached. Above the critical point, the fluid properties are smooth (differentiable) in P-T space and there is no liquid - vapour distinction.

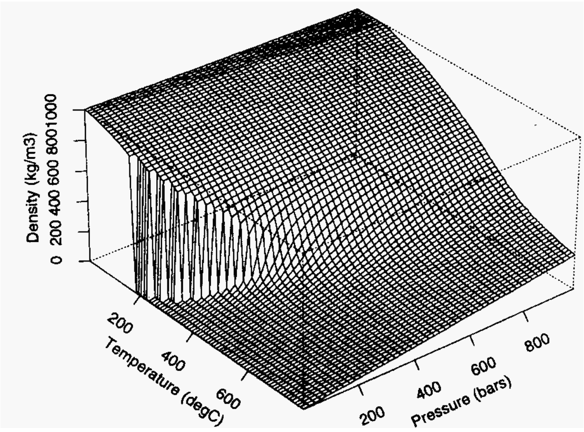

Figure **2.** The density of water in pressure-temperature space. Below 374.15°C the density is discontinuous across the saturation line. The density surface is clipped above 1000 kg/m^3.

Besides the density and internal energy, we also require the dynamic viscosity and thermal conductivity of water. MULKOM uses rather simple formulae for these quantities, which are not satisfactory in the super-critical region. In their place, we have used the expressions given by Schmidt (1979), which express the dynamic viscosity and thermal conductivity of water in terms of temperature and density. These algorithms are 'universal' in the sense that they apply (at least) over the complete P-T space shown in figure 1. We therefore do not require separate routines to calculate the viscosity or thermal conductivity of steam and liquid water, as in the original MULKOM.

Various authors have pointed out that some of the properties of water, when expressed in terms of pressure and temperature, become singular at the critical point, (see for example Johnson and Norton 1991). Probably the most significant of these are the thermal conductivity and dynamic viscosity, both of which (theoretically) are infinite at the critical point. Figure 3 shows the thermal conductivity in the vicinity of the critical point. In practice, the singularities in these functions (particularly the dynamic viscosity) are weak and they seem to create no numerical problems. The gradients are still quite large however, and MULKOM responds by taking very small timesteps in the near-critical region. Provided that these 'singular' properties are *smooth* functions of pressure and temperature, it seems possible to approach almost arbitrarily close to the critical point in P-T space.

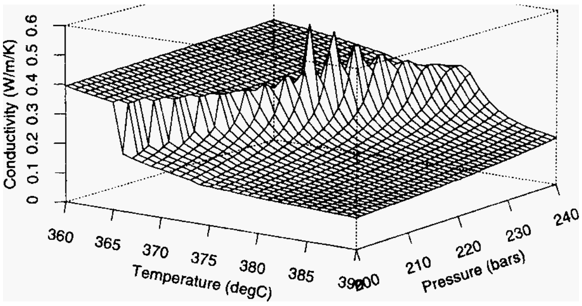

Figure 3. The thermal conductivity of water in the vicinity of the critical point. The highest peak corresponds to the the weakly singular behaviour at the critical point. The smaller peaks on either side are due to the discrete sampling of the surface near the singularity.

3 MODIFYING MULKOM

There are several ways to approach the modelling of super-critical fluids numerically. These have generally involved the use of different sets of dependent variables. For example White (unpublished) has experimented with the use of density and temperature as dependent variables. This approach however, was not successful as the density of liquid water is almost independent of the pressure for some of the P-T space of interest in geothermal problems. Another approach, described by Faust and Mercer (1977), is to use pressure and enthalpy. This has the advantage that there is no singular behaviour in the fluid properties at the critical point. This is obviously attractive from the numerical point of view. In this paper we want to use the existing structure of MULKOM, and so retain the use of pressure and temperature as dependent variables.

Although Arnold's formulation does extend up to 800°C, MULKOM itself is constrained to work only up to 350°C. Strictly speaking, for single phase steam systems, the thermodynamic functions are defined up to 800°C, and so provided one stays within the valid pressure range, (Region *2* in figure 1) satisfactory results can be obtained. MULKOM will also allow single phase liquid water for pressures up to 1000 bars and temperatures below 350°C (Region 1). For two-phase conditions below the critical temperature, 374.15°C, the saturation line defines the boundary between pure vapour and pure liquid states.

Several difficulties arise if one considers how to include the rest of the pressure- temperature space (Regions 3 and 4) within the existing framework of MULKOM. First of all, for these regions, the thermodynamic variables are defined in terms of temperature and density (T and p), rather than temperature and pressure (T and P) as in regions 1 and **2.** Because MULKOM uses T and P as the dependent variables in single phase regions, this means a numerical 'inversion' of the formulations for regions 3 and 4 is necessary. Thus, given T and P, our extended MULKOM solves a non-linear equation for the appropriate value of the density p. This is accomplished quite efficiently by using

Newton's method. There was initially some concern over the CPU time that this would involve, but profiling shows that the overhead is actually quite small.

Some care must be taken to ensure that the Newton iterations converge to the ***correct*** value of density, as the formulations do seem to exhibit multiple roots, particularly near the critical point. Generally this was not a problem as the spurious roots were clearly unphysical, but just below (cooler than) the critical point the 'vapour' and 'liquid' densities become numerically nearly equal, and this poses a real problem. Eventually, the approach taken was to divide the whole of regions 3 and 4 into small 'cells', each with a carefully choosen 'starting' density for the Newton iteration. These starting values were derived by numerical experiment, and ensure that the density is a smooth function of P and T close to the critical point. The structure of the cells is completely arbitrary, they need only be small enough to ensure correct convergence of the density with the single defined starting value.

At super-critical temperatures and pressures, there is only one 'phase' of water; the distinction between liquid and vapour ceases to have any meaning. This means it is possible (figure 4) to move continuously from a pure liquid state to a pure vapour state (from region 1 to region 2) without crossing the saturation line by simply going 'around' the critical point (path A). In this process there is a *continuous* change in the water properties (density and enthalpy) along this path in P-T space. In the sub-critical region the same final result can be achieved by simply crossing the saturation line directly as shown in path B on the figure. On this path there is a discontinuous change in water properties as the saturation line is crossed

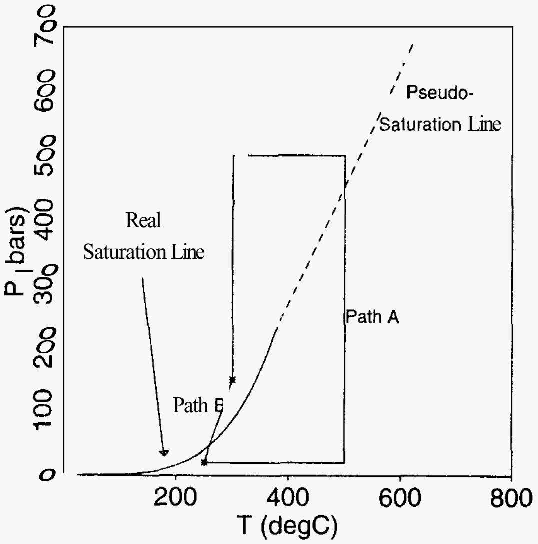

Figure 4. Possible paths (between *'s) in P-T space. On path A it is possible to move from pure liquid to pure vapour with a continous change in fluid properties. By moving on path B however the properties of water change discontinuously across the saturation line.

MULKOM, in its standard form, is only set up to deal with the latter case. **As** the saturation line is crossed the liquid saturation S_l is introduced as a new dependent variable, as P and T are related on the saturation line. How then, are we to accommodate the possibility of the first, super-critical, continuous path? A simple means of effecting this behaviour is to extend the saturation line 'artificially' beyond the critical point, as shown by the dotted line in figure 4. By considering all of the fluid below this line to be a vapour ($S_l = 0$), and all that above to be liquid ($S_l = 1$), the existing phase changing algorithm in MULKOM can be used without significant modification. The only difference (from the sub-critical region) is that in the super-critical region the change from 'vapour' to 'liquid' has no associated change in fluid properties. It must be emphasised that this 'pseudo' saturation line has no physical significance whatsoever, it is merely a computational device to permit the type of behaviour shown in path A in figure 3. For the same reason, the placement of the line is entirely arbitrary.

In general, in crossing the real saturation line, a path like B in figure 3 will move along the saturation line until (say) the appropriate value of enthalpy is obtained, and will then jump into the single phase vapour region. This corresponds to an element of fluid (say a liquid) beginning to boil, and then finally boiling completely and leaving the saturation line. In moving along the saturation line, the vapour saturation S_v is introduced as a new dependent variable by MULKOM. It will change from 0 to 1 as the path moves along the saturation line, that is as boiling proceeds. In the super-critical region no such movement along the saturation line will occur, as the fluid properties are identical on either side of this line, although the vapour saturation will still change from 0 to 1.

4 HOTBRINES

Geothermal fluids in New Zealand typically contain about 1000mgkg of salt. This concentration is sufficiently low that the thermodynamic properties of the fluid are not appreciably changed. In more extreme situations, perhaps where significant boiling occurs, however, this is no longer the case and thermodynamic functions specific to these concentrated 'brines' must be used. **As** a general rule, for brines containing less than about 10%NaCl by weight, the critical point and fluid properties do not differ significantly from those of pure water. The thermodynamic properties of sodium chloride brines have been described in detail by Pitzer et al. (1984).

At IRL an empirical fit to the brine properties has been added to both the original and high temperature versions of MULKOM, as described by Burnell and White (unpublished). It is intended to implement the more complete thermodynamic description of Pitzer et al. in the near future. The phase digram for H_2O - NaCl systems has been described by McKibbin and McNabb (1993). At higher concentrations, two separate phases of brine occur as 'halite' saturated vapour or liquid. A partial implementation of this phase diagram and associated thermodynamic properties is described by McNabb et al. (1993), who demonstrated the development of a 'heavy brine' layer in an idealised model of a mid-ocean ridge.

5 NUMERICAL EXAMPLE

In this section, we present a simple model which is hoped represents most of the salient features of a typical New Zealand geothermal field. This is based on the idea that these fields are single 'plume' structures, with the heat source being an extended saline 'hotplate' at a depth of 5 to 7 kilometres. Details of this model are given in McNabb (1992). We are particularly interested in the parameter values (depth of hot plate, permeability, porosity etc.) necessary to obtain such a hydrothermal system. The model presented here has cylindrical symmetry to avoid excessive CPU times, and also uses only pure water, as opposed to brines, for the same reason. The hot plate in this model is therefore postulzted ***a priori*** rather than forming as a natural consequence of the phase behaviour of H_2O-NaCl systems, as proposed by McNabb (1992).

In the model, a cylinder of rock 5 km deep and 10 km in diameter is divided into 10 x 10 elements, each 500 m x 500 m in cross-section. The hot plate at the base of this cylinder supplies heat at a rate of 140 MW. The initial pressure distribution is cold hydrostatic, and the outer boundary is also maintained at this pressure. Fluid can flow into this system from the base and outer boundary, and from rainfall (1 m/year). Outflow from the system is to the 'atmosphere' (at 1 bar and 10°C), over an an area of about 12 km^2, typical of a New Zealand geothermal field such as Wairakei. The outflow rate is about 100 kg/s. The (homogeneous) permeability and porosity of the rock are 2 md and 0.1 respectively, and the thermal conductivity is **2** W/m/°C. To initiate the formation of a convective plume the pressure and temperature of the central 4 km of the hot plate were perturbed by +1 bars and +10°C respectively.

Figure **5** shows the temperature contours for this model. These are calculated for a time approximately 3×10^5 years after the 'cold' start. The temperature at the base has reached 490°C, ie in the supercritical region. The temperature gradient to a depth of 1 kilometer is about the same as that found at Wairakei, and there is a small boiling zone in the top 500 m of the plume. The plume therefore resembles, at least superficially, a typical liquid dominated geothermal field. It is intended to more fully search the 'parameter space' in the hope of understanding more about the nature of the New Zealand geothermal fields. This work will also include the hot brines.

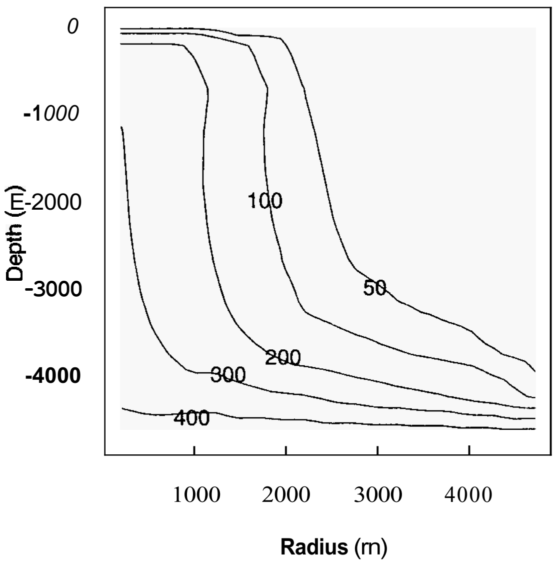

Figure **5**. Temperature contours for the idealised model for a geothermal field, at a time of 3×10^5 years from the start. The temperatures are given on the contours in degrees Celsius.

6 CONCLUSIONS

In this paper the implementation of a 'super-critical' version of MULKOM is described. Some of the geophysical research areas motivating this work are also discussed. Finally, a very preliminary model for a 'typical' New Zealand geothermal field is given.

7 ACKNOWLEDGEMENTS

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