NUMERICAL MODELLING OF GEOTHERMAL RESERVOIRS CONTAINING FLUIDS NEAR THEIR THERMODYNAMIC CRITICAL POINT

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SUMMARY- This work investigates natural convection in geothermal reservoirs containing water near the thermodynamic critical point. The peculiarity in pure water properties near the critical point and the extent **of** the critical region for supercritical pressures are shown. **PHOENICS** commercial computational fluid dynamics (CFD) was used to simulate natural convection in porous media with near critical properties, which are highly temperature dependent. These near-critical properties were modeled by simple algebraic representations. Speculations on the implications of the critical conditions in real geophysical systems are then discussed in view **of** the **results** obtained.

1. INTRODUCTION

The point where the liquid saturation line and vapour saturation line for a pure substance meet on a P-v diagram is called the thermodynamic critical point. At pressures above this point there is no clear division between the superheated vapour region and the compressed liquid region. Phase changes from liquid to vapour or vice versa occur at pressures below this critical point. For pure water the critical pressure and temperature are 221.2 bar abs. and 374.15 °C respectively.

The critical conditions have attracted the attention of researchers from different disciplines over many years. Van der Waals proposed an equation of state for the critical region in 1873. More recently interest in the near-critical region came from several trends in engineering. Some of the early applications investigated were the development of fossil fuel power plants for near-critical conditions and also the use of supercritical pressure water as a coolant in nuclear reactors. Helium at near-critical conditions is used as a coolant for superconductors. In relation to deep geothermal reservoirs, areas of interest are the cooling of magma bodies, formation of seismic boundaries, and ore deposition. Norton and Knight (1977) and Dunn and Hardee (1981) have drawn attention to the possible significance of the near-critical region in geophysical fluid flow and heat transfer.

The occurrence of geothermal prospects that can be developed for major energy extraction is restricted to locations with plate tectonic activity, where the hot rocks and fluid are at accessible depth. At present, wells drilled for geothermal power development reach maximum depths of the order of 3500 m. Assuming hydrostatic pressure and a water level at the ground surface, the maximum pressure that could be reached in such a well is approximately 350 bars, which is above the critical pressure of pure water. The pure water critical conditions are seldom met, and the temperatures reached are much less except in a few cases. However, reservoir conditions of 380 °C and 220 bar abs. have been reported at Nesjavellir field in Iceland by Steingrimsson et al. (1990). At the Kakkonda field in Japan a temperature higher than 449 °C was reported by Yano and Ishido (1990). The existence of near-critical conditions in geothermal reservoirs has also been inferred from the study of fluid inclusion samples (Reyes, 1993).

The presence of dissolved minerals and gases in the geothermal water has the effect of shifting the critical temperature and pressure to higher values and reducing the size of property variation peaks (White et al. 1971) and (Bodnar and Costain, 1991). NaCl is the main dissolved mineral in geothermal fluids, while CO_2 is the main gas. NaCl increases the temperature and pressure of the critical point compared to pure water (Straus and Schubert, 1977). The presence of NaCl also increases electrolyte concentration, increasing the solubility of silica and shifting the quartz solubility maximum to higher temperature and pressure, creating an SiO_2-H_2O sub-system that further influences the critical point (Johnson and Norton, 1991 and Bodnar and Costain, 1991). CO_2 on the other hand increases the pressure but reduces the temperature at which the critical point occurs (Bodnar and Costain, 1991). These shifts increase the likelihood of zones of near-critical fluid having significant size as the concentration of solution varies with depth.

Whilst drilling into a near-critical reservoir would produce interesting results, the focus of this paper is on natural convection at greater depths in the crust. The physical processes by which localized heat flows reach the surface are not yet fully understood. High temperature rocks are anticipated to be plastic and impermeable, and vertical heat fluxes therefore generally low. Near-critical conditions of the type examined in this paper may allow heat to flow laterally to locations from which it can escape vertically.

2. OBJECTIVES

The aim of this work is to investigate the form and behaviour of geophysical flows of near-critical fluid using computer modeling. More specifically, this study concentrates on natural convection in porous medium of fluids close to but just above the critical pressure, where the property variations with temperature are extremely large. The fluid is contained in a rectangular 2-D cell with isothermal bottom and top, the bottom being hotter, and adiabatic vertical walls

3. CRITICAL PROPERTIES OF WATER

At the critical point, pure water exhibits extreme variations of properties with temperature and pressure, but more strongly with temperature. These property variations have the potential to modify various common modes of heat transfer and create unusual flows (Hall 1971). Numerous equations of state for different fluids have been proposed since Van der Waals, but they all fail to represent the critical region as a continuous function of pressure and temperature.
The International Association for the Properties of Water and Steam Industrial Formulation (IAPWS-IF97) previously known as 1967 IFC (International Formulation Committee) has produced accurate properties.

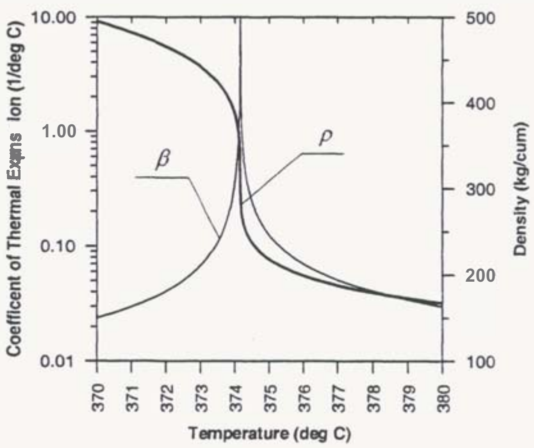

Figure 1. Coefficient of thermal expansion and density of water at the critical pressure (221.2 bar), based on IAPWS-IF97.

Using these with constant pressure of 221.2 bar abs. (the critical pressure) localised peaks in the coefficient of thermal expansion (Figure 1), specific heat capacity (Figure 2) and thermal conductivity (Figure 3) are revealed with change in temperature. A significant drop in density (Figure 1) and dynamic viscosity (Figure 3) and an increase in specific enthalpy (Figure 2) also occur.

It is important to note that the peaks in properties also occur above the critical pressure, but to a lesser extent, and the pressure and temperature of these is called the pseudo-critical point. Significant effects extend to about 1.2 times the critical pressure (Hall, 1971).

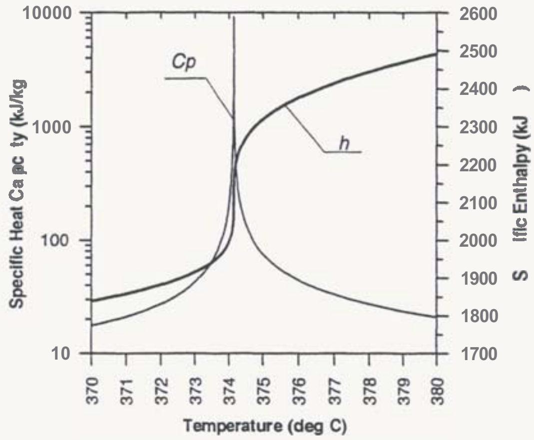

Figure 2. Specific heat capacity and Specific enthalpy of pure water at the critical pressure (221.2 bar), based on IAPWS-IF97.

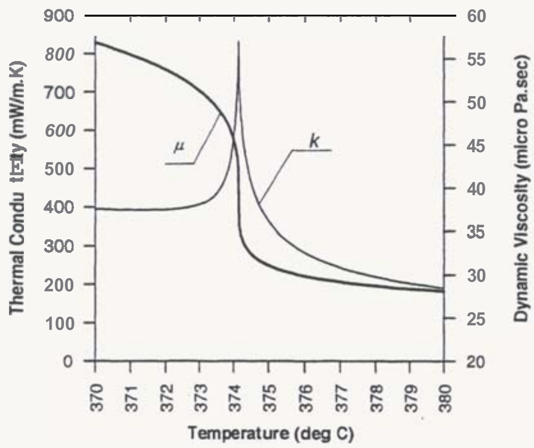

Figure 3. Thermal Conductivity and Dynamic viscosity of pure water at the critical pressure (221.2 bar), based on IAPWS-IF97.

4. PREVIOUS STUDIES ON POROUS MEDIA

The only laboratory experiment to examine natural convection of near-critical pressure fluid in porous media is that of Dunn and Hardee (1981). The experimental apparatus consisted of a 1 litre cylinder with a length to diameter ratio of 7 packed with silica sand and saturated with pure water. The cylinder was fully insulated and the outer sidewall was kept at constant temperature while a platinum wire heated the center line. A hand pump maintained the pressure between 225-245 bar and temperature measurements were taken by thermocouples embedded in the sand radially around the platinum wire.

The measured heat transfer rate near the critical point (**370-380** °C) showed an increase of about 70 times the rate at room temperature.

Cox and Pruess (1990) numerically simulated this experiment using the MULKOM geothermal reservoir simulator and calculated an enhancement in heat transfer rate of **only 5** times that of pure conduction, even though the permeability used was **20** times greater than that reported in the laboratory experiment. This contradiction between experiment and numerical simulation has not been explained. There is no doubt that the experimental arrangement may not have allowed clear conclusions, and experiments with near-critical fluid are difficult because of property variations with pressure and temperature. On the other hand the authors' preliminary experience with MULKOM led them to the belief that it was not ideal for single-phase natural convection studies.

5. THE EQUATIONS GOVERNING FLOW AND HEAT TRANSFER IN POROUS MEDIA

The present work was carried out for 2-dimensional rectangular geometry, for which the governing equations are conservation of mass, momentum and energy:-

$$\frac{\partial v}{\partial y}+\frac{\partial w}{\partial z}=0 \qquad (1)$$

$$v=-\frac{K}{\mu}\frac{\partial P}{\partial y} \qquad (2)$$

$$w=-\frac{K}{\mu}\left(\frac{\partial P}{\partial z}+\rho_f g\right) \qquad (3)$$

$$(\rho Cp)_m\frac{\partial T}{\partial t}+(\rho Cp)_f.\mathbf{v}\nabla=k_m.\nabla^2 \qquad (4)$$

where:

$$(\rho Cp)_m=(1-\phi)(\rho Cp)_r+\phi(\rho Cp)_f$$

$$k_m=(1-\phi)k_r+\phi k_f$$

These equations were solved using the PHOENICS CFD simulator. Experimental measurements in cellular convection of ordinary fluids were replicated using this program for verification Zarrouk (1999b).

6. REPRESENTATION OF NEAR-CRITICAL PROPERTIES FOR THIS STUDY

The central problem in understanding near-critical crustal **flows** is to learn what happens to a fluid that rises into a region of near-critical pressure and temperature. The properties of pure water in the near-critical region described in the IAPWS-IF97 and the 1967 IFC version give good smooth property variations in the near-critical region with full representation of the peaks, but the equations are very complex. Furthermore there is the question of dealing with small variations about high standing values, which was discussed by Cox and Pruess (1990) and is a problem for numerical simulation. To avoid these problems we have "invented" a fluid with property variations with temperature to suit our investigation. The invented fluid has the (constant) properties of atmospheric pressure water with the exception of β and Cp which are anticipated to dominate convection in the near-critical region. The real variation of β and Cp with temperature is much greater than with pressure and these parameters depend only on temperature in the invented fluid.

The assumed β is shown in Figure **4**; when solving with a fine grid the discontinuity in slope is insignificant.

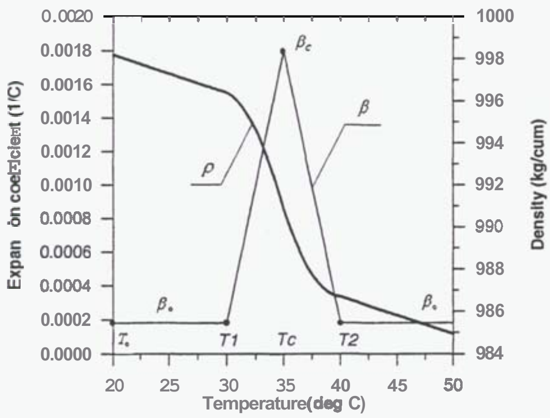

Figure **4.** Typical assumed variation of expansion coefficient with temperature and the resulting variation of density with temperature for ($\beta_c/\beta_\circ=10$).

The form assumed allowed examination of the effects of different peak properties and amplitudes. The equations are:

$\beta=\beta_\circ$=Constant for $T_\circ < T < T_1$ and $T > T_2$ (5)

$\beta = a + bT$ for $T_1 < T < T_c$ and $T_c < T < T_2$ *(6)*

where a and b are specific to the temperature range.

Neglecting variations with pressure, the definition of thermal expansion:

$$\beta=-\frac{1}{\rho}\left(\frac{\partial \rho}{\partial T}\right)_P \qquad (7)$$

allows integration to give a density variation of general form:

$$\rho = \rho_x e^{b(T^2 - T_x^2) + a(T - T_x)} \quad (8)$$

where ρ_x, **a, b,** and T_x can be expressed in terms of $\rho_\circ$, T_1, T_c, T_2, $\rho(T_1)$, $\rho(T_c)$ and $\rho(T_2)$. Solutions were carried out with different amplitudes of the peak, characterised as $\beta_c/\beta_\circ$.

A similar form has been assumed for ***Cp***, and the enthalpy variation with temperature that results can similarly be arrived at by integration (Figure 5).

$$h = h_\circ + Cp_\circ(T - T_\circ) \text{ for } T_\circ < T < T_1 \text{ and } T > T_2 \quad \textbf{(9)}$$

$$h = h_1 + \frac{e}{2}(T^2 - T_1^2) + f(T - T_1) \text{ for } T_1 < T < T_2 \quad (10)$$

where e and f are again specific to the temperature range. Figure 5 shows ***Cp*** and the corresponding enthalpy for $Cp_c/Cp_\circ = 10$.

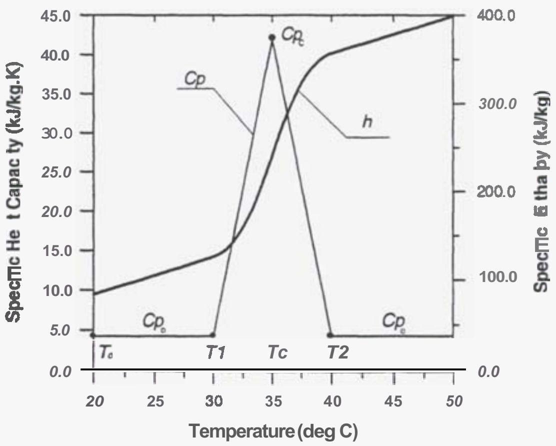

Figure 5. Typical assumed variation of specific heat capacity with temperature, for ($Cp_c/Cp_\circ$=10).

7. NUMERICAL RESULTS

For the property variations of Figures **4** and **5** with $\beta_c/\beta_\circ = 10$ and $Cp_c/Cp_\circ = 10$, the results **show** an unsteady fluid-motion taking place (Figure *6),* resulting in an unsteady temperature distribution. Near-critical temperature fluid occupies most of the space. Though the solution is numerically stable, it is found that no steady state is reached and the patterns continue to change. Figure **7** shows the results after **18000** seconds where the critical specific heat capacity and density **is** following the temperature distribution. Increasing the ratios of **both** $\beta_c/\beta_\circ$ and $Cp_c/Cp_\circ$ caused numerical instability initially. The decision of whether the unsteadiness is numerical instability or a real fluid flow and heat transfer effect was crucial. **PHOENICS** uses the whole field residuals method for convergence.

$$\sum R(\Phi)_{x,y,z} = \text{Constant} \quad (11)$$

$$\frac{\Phi_i^{n+1} - \Phi_i^n}{\lambda} = R(\Phi)_i^n \quad (12)$$

where: R is the residual of variable Φ **at the end** of solution and λ is the relaxation parameter.
By careful numerical investigation on the solution controls (linear relaxation, and number of iterations) and from experience in watching the solution develop and how the residuals decrease and also from mesh refinement study, we believe that the results obtained so far are representative of the near-critical region, for the given assumptions.

If we consider $\psi = f(\beta_c, Cp_c, \frac{d\beta}{dT}, \frac{dCp}{dT})$, where ψ is the stream function, β_c and Cp_c represent the amplitude of the peak in those properties, then the value of ***Ra*** based on plate temperature difference cannot be used alone to distinguish flow regimes. So the onset of unsteady convection probably depends on the amplitude as well as the width of the property peaks.

8. DISCUSSION OF RESULTS

The implications of natural convection in porous media with near-critical fluid for geophysical systems have led to several speculations. Straus and Schubert **(1977)** noted that these conditions might occur beneath geothermal fields, most likely above shallow magma bodies in the crust. Nevertheless as the magma continues to rise towards the surface, maintaining a critical pressure will become unlikely especially in an unconfined geothermal system under hydrostatic pressure, and as two-phase conditions form (White **1971** and Dunn and Hardee **1981). Dunn** and Hardee (1981) suggested that the intense convection could significantly weaken a porous or a fracture-controlled permeable medium, due to enhanced rock dissolution. The solubility of some species becomes very high at near-critical conditions; this is the basis of supercritical separation in process engineering. The increase in permeability due to rock dissolution would also mean an increase in the ability of the geothermal **system** to transfer energy (Bodner and Costain **1991).**

A question that arose at the outset of this work **was** whether an isolated layer of convection cells could occur due to high $\beta_c/\beta_\circ$ and $Cp_c/Cp_\circ$ ratios, between plates that were spaced far apart and had a small temperature difference, so that the ***Ra*** value based on the plate temperature was less than $4\pi^2$. This question has not yet been answered. This might be an important issue in geophysical terms. In the Taupo Volcanic Zone (TVZ) of New Zealand, there are many geothermal resources lying close together but with separate resistivity boundaries. There has been speculation that these are the result of cellular convection above a deep "hot plate" (McKibbin 1993). The mechanism for lateral heat flow to create such a plate has not been satisfactorily explained. *An* isolated layer of counter-rotating convection cells would provide a mechanism for lateral heat flow. It is possible that the magma intrusions are **localised** effects and the near-critical regions provide the means of expanding the effects of magma intrusions laterally.

The heat transfer coefficient in the near-critical zone (the effective conductivity) would be very high and with the high specific heat would keep the zone at almost uniform temperature, since the vertical heat transfer rate is restricted. This has been demonstrated in our work, Figure *6.*

From Figure 6, it is clear that the critical zone is confined within the upper and lower temperature boundaries allowing lateral expansion only. Whether it is possible for cellular convection to take place below and above the critical zone is still open to some question, since the geometry used is not large enough to show such effect clearly.

9. CONCLUSIONS

- It appears that the cellular convection does occur in fluids with near-critical properties, but the convection is always unsteady, probably due to the very rapid change of property with temperature.
- It has not been fully proven by this study, but there are indications that the critical property region exists as a thin layer with the ability to transfer heat laterally.

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Nomenclature

a, b	coefficients of ρ variation
Cp	specific heat at constant pressure

e, f	coefficients of h variation
g	acceleration due to gravity
h	specific enthalpy
K	permeability
k	thermal conductivity
P	pressure
R	residuals
Ra	Darcy-Rayleigh number
T	temperature
t	time
v	velocity in y direction (horizontal)
w	velocity in z direction (vertical)
y, z	spacial coordinates
β	themal expansion coefficient
ϕ	porosity
μ	dynamic viscosity
ρ	density
Φ	general field variable

Suffixes

c	critical
f	fluid
m	mixture
n	time step
r	rock
$\circ$	initial state

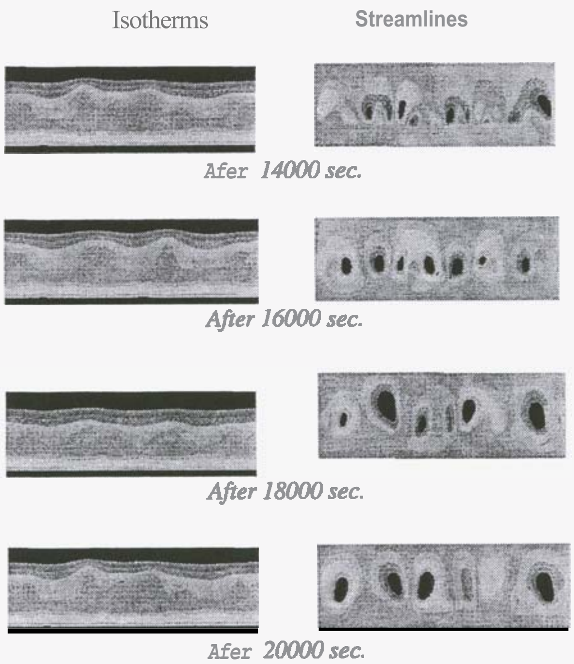

Figure 6. Transient results for $\beta_c/\beta_\circ = 10$ & $Cp_c/Cp_\circ = 10$.

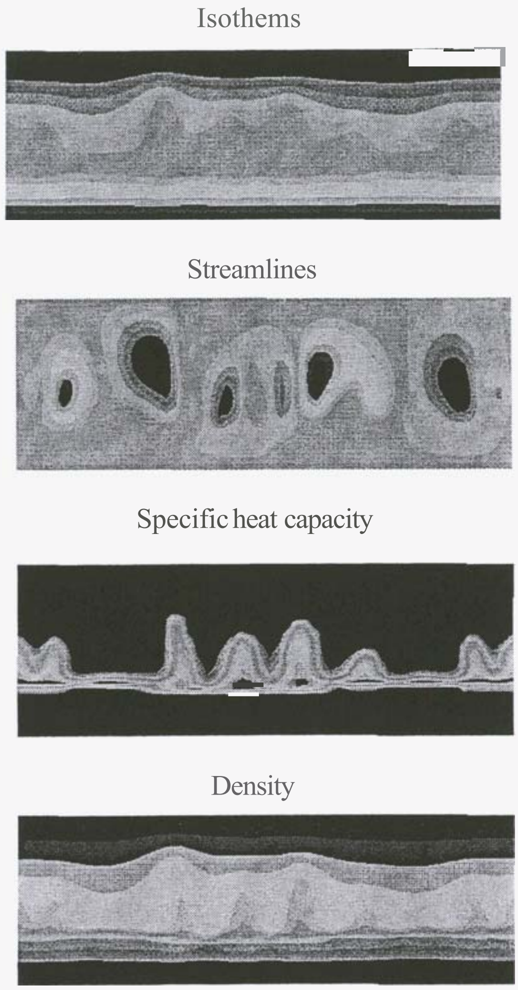

Figure 7. Detailed results for $\beta_c/\beta_\circ = 10$ & $Cp_c/Cp_\circ = 10$ after 18000 sec.