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THE USE OF PHOENICS COMPUTATIONAL FLUID DYNAMICS (CFD) CODE FOR GEOTHERMAL RESERVOIRS CONTAINING FLUIDS NEAR THEIR THERMODYNAMIC CRITICAL POINT.

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ABSTRACT

The paper first discusses the real fluids circulating in the earth's crust, and justifies the need to examine the natural convection in a porous medium of a simple pure fluid with properties resembling those near the thermodynamic critical point. The literature on natural convection in a homogenous porous medium between isothermal horizontal plates, the lower one hotter, is then reviewed. Results for comparison are reproduced using PHOENICS. New results for a fluid with temperature dependent expansion coefficient are presented.

INTRODUCTION

The use of the MULKOM-TOUGH family of simulators has been so successful for geothermal reservoir work that one needs a particular reason for using other codes. At the start of this work we had in mind two problems, firstly the flow from one production horizon in a reservoir to another by way of the wellbore, and secondly the natural convection that might occur in geothermal reservoirs containing a fluid near its thermodynamic critical point, where property variations with temperature and pressure are extreme. The first of these problems requires two porous media connected by a fluid filled chamber, for which a fluid mechanics code with a porous medium subroutine is an obvious candidate. Having briefly tackled this problem we continued with PHOENICS on the second problem, with which this paper deals.
In this paper the term "near-critical" is used to signify that the region of interest is limited to super-critical pressures close to the critical point where the specific heat and expansion coefficient have large peaks.

BACKGROUND TO THE PROBLEM

The system H_2O - NaCl - CO_2 is representative of crustal fluids (Bodnar and Costain, 1991). There is evidence from fluid inclusion studies that fluid conditions in some mineral deposits were in the near-critical region, and this has prompted studies of the critical properties of the H_2O - NaCl - CO_2 system (Schmidt, Rosso and Bodnar, 1995) and the H_2O - NaCl system (Bischoff and Pitzer, 1989 and McKibben and McNabb, 1993). Fig 1 shows the locus of the critical point for the H_2O-NaCl system taken from Bischoff and Pitzer (1989), which covers a wide temperature range, from the critical temperature of water at 374°C to the critical temperature of NaCl at about 3600°C.

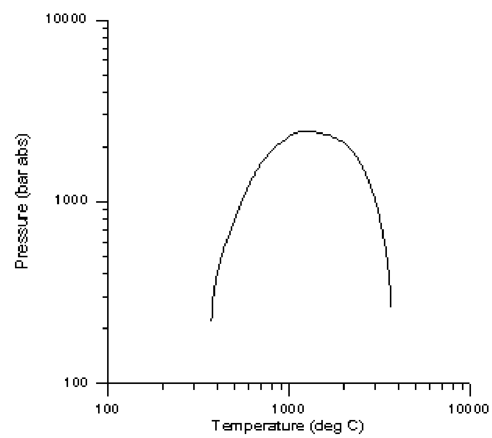


Fig.1 Critical pressure and temperature for the binary mixture H_2O-NaCl, based on Bischoff and Pitzer (1989).

The exact range of NaCl concentrations of crustal fluids is uncertain, but even if limited to solutions with a critical temperature of 800°C, given that concentrations may reduce as fluids convect upwards towards the surface, there is scope for near critical conditions to occur over a large range of depths. Within this temperature range the critical point occurs at pressures between 221 bars for pure water to about 2400 bars for a solution with a critical temperature of 800°C. This pressure range represents a large depth, from about 3,000m to about 20,000 m.

The justification for believing that convection processes in the near-critical region are worth studying in particular comes from studies of heat transfer to near-critical fluids in ducts rather than in porous media. A review of experimental findings was presented by Hall (1971). Neumann and Hahne (1980) stated that natural convection to near-critical CO_2 in a vertical tube showed an effective conductivity "up to 12,000 times the conductivity of copper", implying extremely high Nusselt numbers. Amongst other engineering applications such as cryogenics, at that time there was interest in designing boilers for steam turbine power plant operating at supercritical conditions. In simple terms, it was necessary to know whether the path taken by the water as it was heated could pass near the critical conditions, or whether they could be circumvented. Experiments demonstrated that heat transfer to a fluid in the near-critical region was quite different from that away from that P-T region, due to the extreme variation of properties with temperature and pressure, but particularly temperature. In the main, the thermodynamic and transport properties for a pure fluid show a step change as the saturation line is crossed from the liquid side to the steam side. Above the critical point, the same change occurs but without the step; there is no interface. A "pseudo-critical" line may be drawn on the P-T curve that marks the locus of the maximum slope in the change; this line appears as a short extension of the saturation line beyond the critical point.

The expansion coefficient, β, and the specific heat at constant pressure, Cp, show peaks centred on this line and superimposed on the general change from liquid to gas. These peaks decrease in amplitude with increasing distance along the pseudo-critical line away from the critical point. Fig 2 shows the specific heat as a decreasing ridge on the P-T plane, calculated from the properties of pure water as represented by the 1967 IFC Formulation for Industrial Use. The expansion coefficient β has a similar shape.

In a porous medium, the rock matrix specific heat reduces the significance of the peak in the fluid specific heat, but the latter is so large that some effect is likely to remain. The zone occupied by this fluid

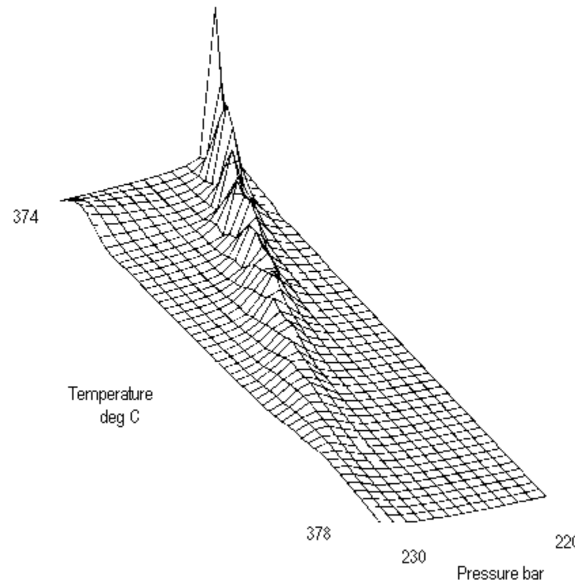


Fig 2 Showing the peak in specific heat Cp of pure water in the near-critical region; expansion coefficient b is similar

may become thermally stabilised as a result.

The expansion coefficient is very large in this region, and may have an influence on local natural convection that might have a controlling or at least a significant effect over a much wider spacial extent. This paper studies the effect of the expansion coefficient in a simplified manner.

The thermodynamic and transport properties of near-critical fluids are being investigated at present because of their applications as solvents (Kiran and Levelt Sengers, 1993). Depending on the nature of the constituent molecules, the critical behaviour has been classified into several groups. Fortunately, H_2O-NaCl appears to have a particularly simple behaviour, two critical points connected by a simple curve as in Fig 1. The inclusion of CO_2 is a major complication. Whilst it has been argued that to study hydrothermal ore deposits it is sufficient to simplify the real case (H_2O - NaCl - CO_2) to H_2O-NaCl rather than H_2O-CO_2, whether this is appropriate for the consideration of convection is open to question. In any event, at present a study of the near-critical convection of a particularly simple pure fluid is all that we are considering.

Interest in geothermal reservoirs with near-critical fluids is not new. Dunn and Hardee (1981) and Hadley (1982) separately carried out some simple experiments on heat transfer from a heated wire to near-critical fluid in a porous medium. One of the lessons of near-critical studies in ducts was the difficulty of designing experiments to give clear cut results, and Dunn and Hardee's experiment is not simple to interpret. Cox and Pruess (1990) modelled this experiment numerically; their numerical approach will be referred to later. Steingrimsson, Gudmundsson, Franzson and Gunnlaugsson (1990) recorded the evidence for temperatures of 380°C in an Icelandic field, and Yano and Ishido (1990) similarly for Kakkonda in Japan. They used the STAR reservoir simulator, and showed how the presence of near-critical fluids could be deduced from transient pressure tests rather than on the natural flow regimes that might exist.

THE MODEL

The present problem has been posed as a 2-dimensional rectangular area 0.3m by 0.1m, occupied by a homogenous rigid porous medium with constant properties. The long sides of the "box" are horizontal and the short ones vertical. Both horizontal surfaces are isothermal, the lower one hot and the upper cool. The vertical sides are adiabatic. The geometry and boundary conditions thus represent a classical natural convection problem, of laboratory scale, on which there is extensive literature. A structured grid with non-uniform spacing has been used, with ratio 1.3, to create a finer mesh near the walls. Two grids have been used, 70 by 30 and 140 by 60.

REVIEW OF LITERATURE ON NATURAL CONVECTION BETWEEN HORIZONTAL PARALLEL PLATES

The requirement here is to establish whether our results are "correct" by comparison with previous work. A comprehensive review is presented by Nield and Bejan (1992), from which we have drawn the following.

For the model specified, with constant $\beta = \beta_0$ and all other matrix and fluid properties constant, similarity is governed by the Rayleigh-Darcy number,

$$Ra = (g\,\beta_0\,K\,H\,\Delta T)/\mu\,\alpha_m \qquad (1)$$

where $\alpha_m = k_m/(\rho Cp)_f$

Various numerical solutions have been produced and with supporting experimental work the general conclusions are :-

- for $Ra < 4\pi^2$ there is no motion.
- for $4\pi^2 < Ra < 240$ to 300 stable cellular convection occurs in the form of counter-rotating rolls.
- for larger values of Ra there is oscillatory convection.

The oscillatory regime, which might have been considered merely a numerical artefact, is well confirmed by several different approaches using different methods of solution, and by experimental work.

RELEVANT FEATURES OF PHOENICS

PHOENICS (parabolic, hyperbolic or elliptic numerical integration code series) is a commercially available package based on the work of D B Spalding and colleagues. Version 2.1.3 was used.

Continuity, momentum and energy equations are written in finite difference form for a fixed volume, summing over all surfaces, with interpolation to interfaces.

PHOENICS was written as a general purpose program, and the input files are therefore lengthy; there is an input language, although particular properties, for example, can be provided as Fortran routines. Output arrangements are sophisticated. Several solution procedures are provided, although for our problem with significant nonlinearities, a "slabwise" procedure is mandatory. Consider the situation where conditions are specified at any one time for all blocks. For a particular horizontal row i, this solution method solves using old values for the rows i+1 and i-1 immediately above and below. When the solution moves to deal with row i+1, the values used for row i are the old values not the new ones. When all rows are completed all old values are replaced with new ones and another "sweep" through the rows is undertaken.

The required time step is specified, together with the number of sweeps at each time step (typically 100).

The version of PHOENICS used treats the momentum equation for porous medium flow in the usual Darcy law manner, but treatment of the thermal properties is unusual. Presumably this is because the code has not been used much for porous media. The input specification allows for only one set of thermal properties and a porosity to represent fluid and rock. The energy equation has the form :-

$$(\rho Cp)_m\,\partial T/\partial t + (\rho Cp)_f\,v\,\partial T/\partial y + \ldots = k_m\,\nabla^2 T + \ldots \quad (2)$$

The thermal conductivity of the rock-fluid mixture is the arithmetic mean form :-

$$k_m = (1-\phi)k_r + \phi\,k_f \qquad (3)$$

The group $(\rho Cp)_m$ is similarly defined as

$$(\rho Cp)_m = [(1-\phi)\rho_r + \phi\rho_f].[\,(1-\phi)Cp_r + \phi Cp_f] \qquad (4)$$

Taking the density of fluid and rock as 1000 kg/m^3 and 2500kg/m^3 respectively and the specific heats as 4200 J/kgK and 1000 J/kgK respectively with porosity of 5% gives :-

$$(\rho Cp)_m = 2.8 \times 10^6 \quad \text{and} \quad (\rho Cp)_f = 4.2 \times 10^6$$

so that setting them equal is a poor assumption. This assumption can be totally avoided only if the value of the fluid specific heat is such as to make both groups equal.

REPRESENTATION OF THE FLUID PROPERTIES

The properties of pure water described in the 1967 IFC Formulation for Industrial Use give good smooth property variations in the near-critical region, with full representation of the peaks, but the equations are complex. Furthermore there is the question of dealing with small variations about high standing values, which was discussed by Cox and Pruess (1990), who interpolated from a property table. To avoid these problems we have "invented" a fluid with property variations with temperature to suite our investigation.
There are two properties that are anticipated to dominate convection in the near-critical region, β and Cp. The variation of β and Cp with temperature is greater than with pressure. The central problem in understanding near-critical crustal flows is to learn what happens to a fluid that rises and as a result of temperature changes experiences a greatly increased expansion coefficient and specific heat, and with further rising and cooling experiences a similar decrease.
The invented fluid has the properties of atmospheric pressure water with the exception of β and Cp. The assumed variation of β with temperature is representative of a near-critical pure fluid, and is as follows:-

$$\beta = \beta_0 = \text{constant for } T_0 < T < T_1 \qquad (5)$$

$$\beta = A_1 + B_1 T \quad \text{for } T_1 < T < T_c \qquad (6)$$

$$\beta = A_2 + B_2 T \quad \text{for } T_c < T < T_2 \qquad (7)$$

$$\beta = \beta_0 = \text{constant for } T > T_2 \qquad (8)$$

Neglecting variations with pressure,
the definition of

$$\beta = -1/\rho\,(d\rho/dT)$$

allows integration to give density variations of

$$\rho = \rho_0 \exp(-\beta_0 (T-T_0)) \quad \text{for } T_0 < T < T_1 \qquad (9)$$

$$\rho = \rho_0 \exp(-\beta_0 (T-T_0)) \quad \text{for } T > T_2 \qquad (10)$$

and a variation of general form

$$\rho=\rho_n \exp(b(T^2-T_n^2)+a(T-T_n)) \qquad (11)$$

for the linear variations of β with temperature between T_1 and T_2, where ρ_n , b , a , and T_n can be expressed in terms of ρ_0 , T_1 , T_c , T_2 , $\rho(T_1)$, $\rho(T_c)$ and $\rho(T_2)$.
The resulting density variation is shown in Fig 3.

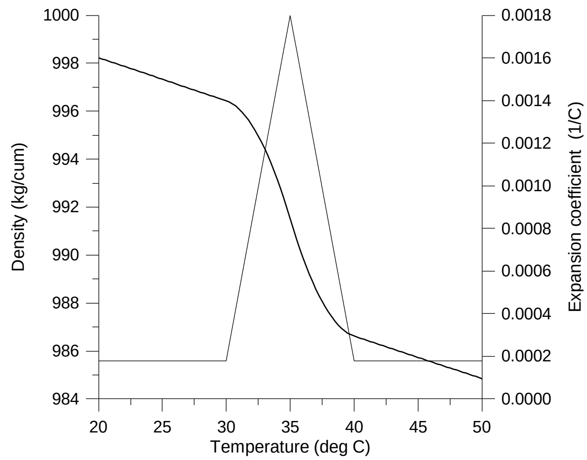


Fig 3 Typical assumed variation of expansion coefficient with temperature, and the resulting variation of density with temperature.

For specific heat the enthalpy variation with temperature can similarly be arrived at by integration, although it has not been used yet because of the current restrictions on Cp discussed above.
Attempts were made to find a continuous function to represent the β and ρ variations of Fig 3, but were unsuccessful with a fine grid the discontinuities in slope are considered not to have an influence.

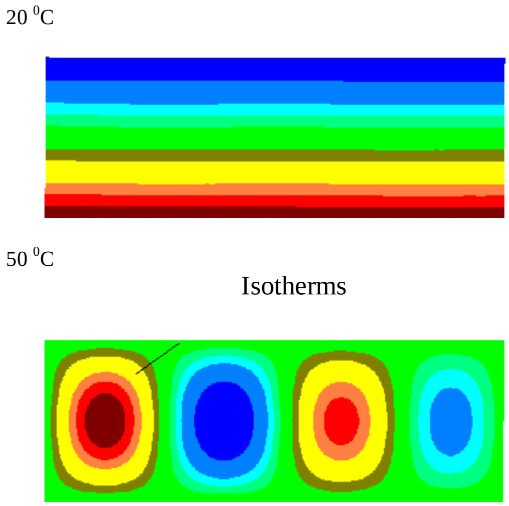
INITIAL CONDITIONS

The fluid was everywhere at the temperature of the cool upper surface (20 °C).

RESULTS

Results for comparison with previous work

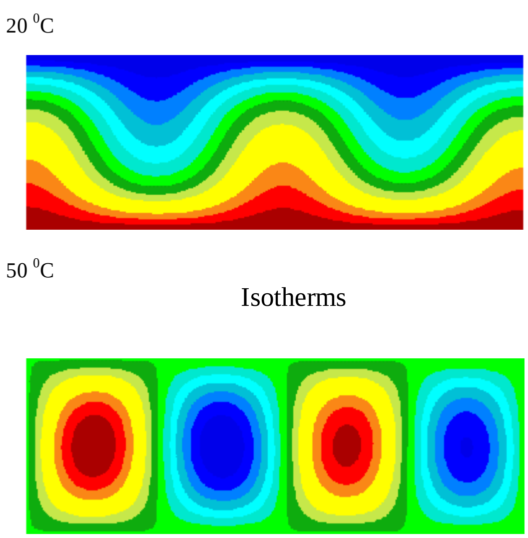
Solutions were first carried out with the Boussinesq approximation and a constant β of 1.8×10^{-4}, the value for atmospheric pressure water. A total time of 2000s was examined, in 100s time steps.
No convection occurred at Ra = 41, but there was convection at Ra = 61, and all results reported here are for this value
The results are shown in Fig 4.



Streamlines

Fig 4 Convection at Ra = 61 with the Boussinesq approximation after 400s

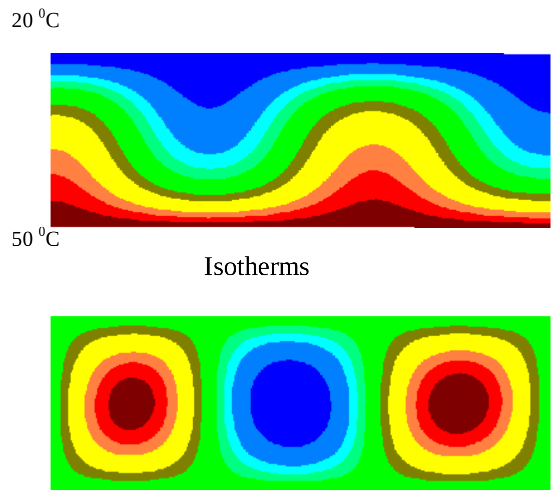
After 400s the convection is just developing, the isotherms are still near-horizontal but the streamlines are well developed and the stream functions are small. By 900s the steady state was reached and the results are shown in Fig 5. The program was run to 2000s as a check.



Streamlines

Fig 5 Convection at Ra = 61 as for the same conditions as Fig 4 but after 900s

Using the same initial and boundary conditions a new set of calculations was carried out for the same constant β but without the Boussinesq approximation and with the density represented by eqn 9 for all values of T. The results are shown in Fig 6 .



Streamlines

Fig 6 Convection at Ra = 61 as for the same conditions as Fig 5, after 900s, but without the Boussinesq approximation.

In this case the transient development is faster and the final solution is different, there being only 3 cells instead of 4. The convection is of similar magnitude to that with the Boussinesq approximation solutions, with a stream function of 2.3 x 10^{-6} compared to 1.9 x 10^{-6}.

Results with supercritical-like properties

The values of T_1, T_c and T_2 were set at 30, 35 and 40 °C respectively. β_0 was set at 1.8 x 10^{-4}, the value used above, and the ratio β_c/β_0 was varied.

For β_c/β_0 = 2 , four cells developed quickly, so that at 200s the stream function was already 2.8 x 10^{-6}; by 1000s the isotherms were more exaggerated but the stream function was only slightly higher at 3.1 x 10^{-6}. For β_c/β_0 = 10, six cells developed, as shown in Fig 7 (overleaf).

For β_c/β_0 = 20 eight cells developed, with higher velocities and stream functions, but otherwise similar in form to Fig 7.

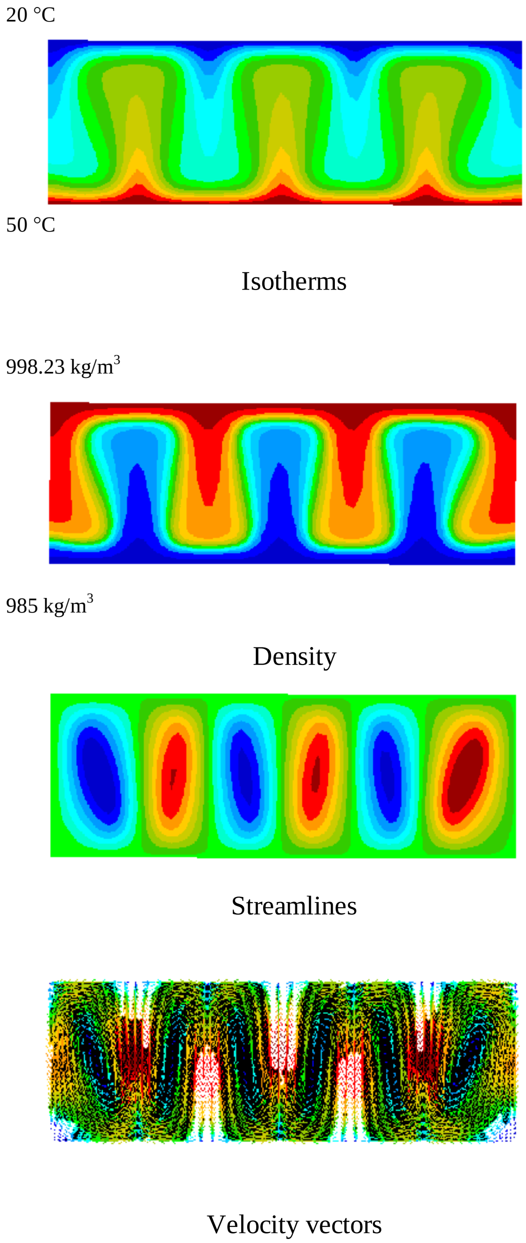


Fig 7 Convection at Ra=61, for b_c/b_0 = 10 after 2000s

DISCUSSION

Constant b results

The comparison with the accepted value of $4\pi^2$ (or 39.5) for the onset of convection is considered to be very good, with a value obtained lying between 41 and 61.

The Boussinesq approximation resulted in 4 cells (Fig 5) while the non-Boussinesq approximation for the same conditions resulted in only 3 cells (Fig 6)., while the stream function values are almost equal. This can only be assumed to be representative of the Boussinesq approximations eg that lateral density variations have some effect on the flow regime.

New results

The variation of β with temperature that has been used does not change the general form of the cellular convection, but a close examination of Fig 7 reveals several significant differences. The cells are tilted to follow the shape of the isotherms, which enclose a relatively large area of "near-critical" fluid. The high density fluid near the top plate streams downwards and flattens out in an anvil-like manner, and vice-versa for the hot fluid.

A question that arose at the outset of this work was whether an isolated layer of convection cells could occur due to a high β_c/β_0 ratio between plates that were spaced far apart and had a small temperature difference, so that the Ra value was less than $4\pi^2$. This case has not yet been examined. This might be an important issue in geophysical terms. In the Taupo volcanic zone 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" (McNabb, 1992). The mechanism for lateral heat flow has not been satisfactorily explained. A isolated layer of counter-rotating convection cells would provide a mechanism for lateral heat flow.

CONCLUSIONS

PHOENICS appears to give satisfactory results for the modeling of natural convection in porous media between isothermal parallel planes heated from below. It therefore appears to be a suitable tool for investigating near-critical natural convection in geothermal reservoirs.

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NOMENCLATURE

A, A_1, A_2	coefficients of β variation
B, B_1, B_2	coefficients of β variation
a,b	coefficients of ρ variation
Cp	specific heat at constant pressure
g	acceleration due to gravity
H	vertical height between plates
K	permeability
k	thermal conductivity
P	pressure
Ra	Rayleigh number
T	temperature
t	time
v	velocity in y direction
y	spacial coordinate
α	thermal diffusivity
β	thermal expansion coefficient
ϕ	porosity
μ	kinematic viscosity
ρ	density

Suffixes

c	critical
f	fluid
m	mixture
r	rock