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# THE USE OF COMPUTATIONAL FLUID DYNAMICS (CFD) IN THE STUDY OF TRANSPORT PHENOMENON IN POROUS MEDIA

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**SUMMARY** – Computational fluid dynamics is briefly introduced. Previous results from the prediction of the flow patterns that occur due to natural convection in a porous medium held between parallel plates for various boundary conditions have been reproduced successfully using the PHOENICS CFD code. The code has been used to predict the silica concentration in the same arrangement of porous medium, with dissolution and deposition of solid silica.

## 1. INTRODUCTION

Computational fluid dynamics (CFD) is a numerical technique used to solve the conservation equations governing fluid motion and heat transfer within any given geometry. The development of CFD packages came from the need to create computer programs of a general nature capable of solving these equations for a wide range of geometries and boundary conditions.

In recent years the technique has revolutionised research in many different fields of industry and science. With the increasing speed of computers, PC-based CFD is becoming available for scientists and engineers of all disciplines, a technology once reserved for nuclear and aerospace industries only. At the same time, it has to be recognised that there are cases of CFD being oversold particularly for turbulent flows.

The implementation of CFD for any given fluid dynamic problem falls into three main parts: problem ***definition, solution*** and ***presentation*** of results. Each part is undertaken within a set of subroutines that combine together to form a CFD package.

In defining the problem, all the parameters required by the CFD code should be specified. This is mainly specifying the physical geometry and properties of the media with the optimum type of mesh (grid) and the declaration of boundary conditions of the environment, for example, inlet and outlet for fluid flow and areas of solid where heat transfer from or to the fluid can occur.

The solution of the problem is undertaken at the heart of the CFD code, with a variety of mathematical techniques used to approximate the differential equations into algebraic form, to be solved directly or iteratively and possibly through multilevel iterations.
A post-processor takes the numerical results and displays them as a visual (graphical) presentation of the solution. The post processor is a significant item of software in its own right.
The main difference between specially written software and a CFD code is the varied areas of applications that may be addressed by the code, which is a general tool.

The TOUGH family of reservoir simulators can be classified as a CFD code; it performs the main three functions like all CFD codes. It was specifically designed for fluid flow and heat transfer within the earth's crust.
For this paper the PHOENICS commercial CFD package developed by CHAM (Concentration, Heat and Momentum Ltd. London) was used to solve for natural convection in porous media. PHOENICS (Parabolic Hyperbolic Or Elliptic Numerical Integration Code Series) is a well-known CFD code. It was designed for a very wide range of free fluid problems, but has a porous medium subroutine that has almost never been used. Like most CFD codes it uses the finite volume method (finite domain), which is one of several computational methods used for solving heat transfer and fluid flow problems.

## 2. PREVIOUS INVESTIGATIONS OF NATURAL CONVECTION IN A POROUS MEDIUM BETWEEN PARALLEL PLATES

Natural convection flow in porous media is of interest in a wide range of applications in engineering and science apart from geothermal reservoirs. These include: building and industrial insulation, direct-contact heat exchangers, solar energy storage systems, packed-bed catalytic chemical reactors, nuclear waste disposal systems, cooling of nuclear reactors, enhancement of recovery from petroleum resources, ground water hydrology, dynamics of avalanches in snow layers, drying processes, cooling of electronic components, powder metallurgy and many more, Zarrouk (1999).

In many of these applications, the flow in a porous medium held between horizontal plates has significance.

The standard case examined is when the plates are isothermal with the lower one hotter than the upper one. The matrix is rigid. An important issue was the conditions for convection to take place. Horton and Rogers (1945) and Lapwood (1948) showed that for a constant property fluid with the Boussinesq approximation, natural convective motion takes place at or beyond a critical Rayleigh number (Ra,) of $4\pi^2$. The Rayleigh number in porous media (Darcy-Rayleigh number) is:

$$Ra = \frac{g.\beta.K.H.\Delta T}{\nu.\alpha_m} \qquad (1)$$

which is the product of Darcy number ($K/H^2$) by the Rayleigh number for free viscous fluid ($g.\beta.\Delta T.H^3/\alpha.\nu$). Katto and Musuoka (1967) demonstrated both analytically and experimentally that the thermal diffusivity ( a ) in the Ra number of equation (1) must be defined as the effective thermal conductivity of the porous medium divided by the specific heat capacity of fluid, $\alpha_m = k_m/(\rho.Cp)_f$ .

For Ra > Ra, the fluid forms buoyancy driven counter-rotating cells that convect warm water upward and cold fluid downward, (Home and O'Sullivan (1974) and Home (1975)) Several convection cells occupy the space, according to the aspect ratio $\Lambda$=*Length/Height*.

When the porous media between parallel plates is subjected to end-to-end (horizontal) temperature difference, while having adiabatic upper and lower boundaries, a single horizontal convection cell is found to occupy the entire space, Home (1975). Many other cases for different boundary conditions have been examined.

Numerical studies on this topic have been carried out over more than two decades. The solutions in most cases were undertaken using software written specially for the purpose, using a variety of solution procedures. An interesting and essential task was to examine how well these solutions could be reproduced by PHOENICS before moving on to new problems.

## 3. REPRODUCTION OF EARLIER NUMERICAL RESULTS USING PHOENICS.

### 3.1 The equations to be solved.

The system considered in this study is a two-dimensional horizontal porous layer, which is subjected to different boundary conditions. Darcy's law is assumed for homogenous and water saturated porous medium with density variations due to temperature changes treated according to the Boussinesq approximation.

$$\rho = \rho_o\left[1 - \beta(T - T_o)\right]$$

The conservation equations for mass, momentum and energy are:

$$\frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0 \qquad (2)$$

$$\frac{\partial w}{\partial y} - \frac{\partial v}{\partial z} = -\frac{gK\beta}{\nu}\frac{\partial T}{\partial y} \qquad (3)$$

$$\sigma\frac{\partial T}{\partial t} + v\frac{\partial T}{\partial y} + w\frac{\partial T}{\partial z} = \alpha_m\left(\frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2}\right) \qquad (4)$$

where:

$$\sigma = \frac{(\rho Cp)_m}{(\rho Cp)_f} \quad \text{and} \quad \alpha_m = \frac{k_m}{(\rho Cp)_f}$$

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

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

### 3.2 Porous media heated from below

This case is of prime importance to geophysical and geothermal systems as heat travels from the deep hot mantle through the crust to the ground surface.

Temperature contours show steady conduction taking place at first, which breaks up as cellular convection develops into a wavy-form temperature profile with 4 convection cells filling the space (Figure 1). As pointed out by Horne and O'Sullivan (1974), for a horizontally heated porous media, the natural convection regime is greatly influenced by the presence of vertical boundaries. This can be clearly seen in the first time steps, which show that fluid movement starts near the boundaries, Zarrouk (1999).

One of the most important results obtained using PHOENICS, is that the accepted critical Rayleigh number of $4\pi^2$ for the onset of convection is considered to be in a very good agreement with the value obtained, lying between 40 and 60.

*Figure I. Porous medium heated from below (50 ''C) and cooled from the top (20 ''C), Ra=60, A =3.*

For a porous medium heated from above with adiabatic vertical sidewall, no motion of fluid will take place regardless of the value of Rayleigh number, Vadasz *et al.* (1993). This stable case was modelled by inverting the values of temperature in the boundary conditions for Figure 1, with the result shown in Figure 2.

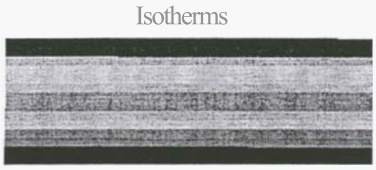


*Figure 2. Porous medium heated from the top (50 ''C) and cooled from below (20°C), A =3.*

### 3.3 Porous medium heated from the side

When the same rectangular geometry is heated along the vertical sides, while having adiabatic upper and lower boundaries, the critical Rayleigh number ($4\pi^2$) is no longer applicable, since the pure conduction equilibrium condition of vertical temperature gradient (horizontal isotherms) is no longer satisfied. Home (1975) showed that the onset of convection is less distinct than heating from below. The natural convection forms a steady unicellular pattern that fills the whole geometry; Figure 3 shows the PHOENICS results.

*Figure 3. Porous medium heated from the side, Ra=60, Λ =3.*

### 3.4 Porous medium with multi-wall heating

In this case vertical and horizontal walls are heated. This reproduces the work by Vadasz *et al.* (1993) for a porous medium having conductive walls along with vertical temperature gradient between the upper and lower walls. The main application for this case is in the study of corner effects in insulation panels.

Two main cases were examined, for an aspect ratio Λ =2.

1- Upper wall is isothermal at 1 ''C and lower wall at 0 ''C, with two sub-cases:
   - a- Side walls at 1.5 ''C and *Ra*=100.
   - b- Side walls at 0.5 ''C and *Ra*=200.

2- Upper wall is isothermal at 0 ''C , and lower wall at 1 ''C, with four sub-cases:
   - a- Side walls at 1.5 ''C and *Ra*=50.
   - b- Side walls at -0.5 ''C and *Ra*=50.
   - c- Side walls at 0.5 °C and *Ra*=100.
   - d- Side walls at 0.5 °C and *Ra*=200.

The results show a perfect match with those reported by Vadasz *et al.* (1993), in nearly all the cases.

Figure 4 shows a perfect match for a 1.5 ''C side wall temperature with a negative temperature gradient and for a *Ra*=100, forming one large cell adjacent to each wall. The side walls are isothermal and the term gradient applies to the difference between upper and lower boundaries. When the side wall temperature is reduced to 0.5 °C for *Ra*=200, two convection cells at each wall were obtained, which also perfectly matches the results of Vadasz *et al.* (1993).

For a positive vertical temperature gradient on the side walls, large cells near the walls change their direction of circulation when the temperature changes from 1.5 ''C to -0.5 for the same *Ra*=50; a perfect match was again produced. When the wall temperature is 0.5 ''C with *Ra*=100 the flow matches the Vadasz *et al.* (1993) results of two counter rotating cells near each wall, Figure 5. On the other hand when *Ra* is raised to 200, our results showed the hot fluid rising from the middle and near the walls of the geometry reaching the top boundary, while cold fluid descends between the rising hot plumes, forming two large cells in the middle and two small ones near the walls, Figure 6. The same case presented by Vadasz *et* al. (1993) showed two rows of convection cells, Figure 6. Intuitively our results look more likely especially if the aspect ratio is increased (A > 2), Zarrouk (1999).

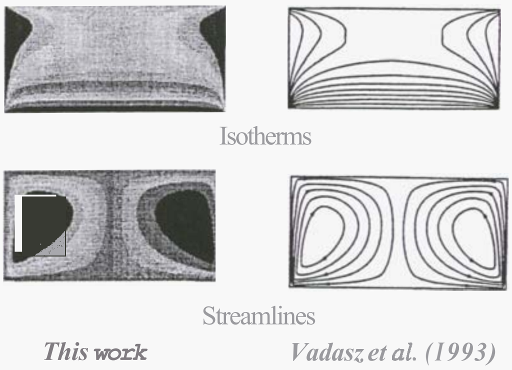
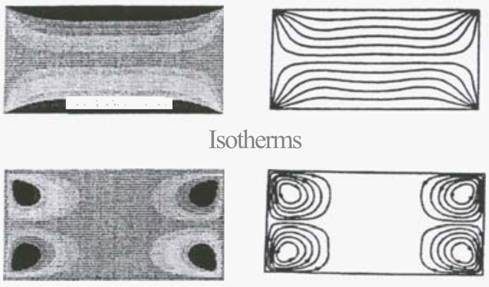
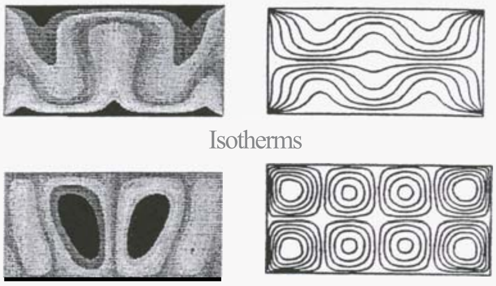


*Figure 4. Porous medium heated from the top (1.0 ''C) and cooled from below (0.0 ''C) with side heating (1.5 ''C), Ra=100, A =2.*



*This work* *Vadasz et al. (1993)*

***Figure 5. Porous medium heated from below (1.0 °C) and cooled from the top (0.0"C) with side heating (0.5°C), Ra=100, Λ =2.***

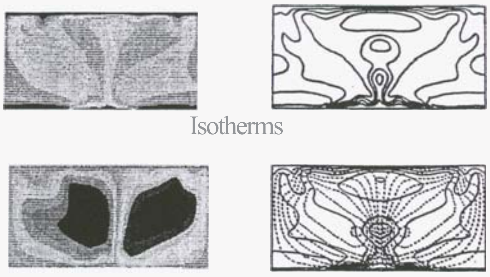


*This work* *Vadasz et al. (1993)*

***Figure 6. Porous medium heated from below (1.0 "C) and cooled from the top (0.0°C) with side heating (0.5°C), Ra=200, Λ =2.***

### 3.5 Oscillatory convection

In this section the case presented by Home and O'Sullivan (1974) for a partially heated lower boundary and Rayleigh number of 750 will be studied. The thermal input is centrally located and occupies half the length of the lower plate. The results obtained using PHOENICS are relatively in good agreement with Home and O'Sullivan's (1974) work (Figure 4), despite a small error (difference) in the length of our heat source. The shape and size of the fluid flow pattern is difficult to compare since it is oscillatory. There is also the limitation in the graphical visualising of the results, arising from the large temperature difference used. This model requires further numerical refining. It would have been interesting to compare the values of $Ra$ at which steady convection becomes oscillatory, which Horne and O'Sullivan found to be $\approx 360$. Figure 4 shows that the streamlines are more developed into two rolls in this work than in Home and O'Sullivan's, but the general agreement is satisfactory.



*This work* *Home et al. (1974)*

***Figure 7. Oscillatory convection in porous medium heated from below, Ra=750, Λ =2.***

## 4. TRANSFER OF HEAT AND SILICA

It has been realised in recent years that it is not always acceptable to neglect the effect of convection on chemical reactions in porous media, Nield and Bejan (1992).

Silica dissolution in water filled porous media has been considered here using chemical kinetics. This model simulates the effect of natural convection in geothermal reservoirs on the dissolution process of silica.

Silica represents the dominant mineral in rocks, and can be found in many forms (Quartz, tridymite, cristobalite, amorphous silica and others), especially in places with hydrothermal activities. Each form has different mechanisms for reaction, dissolution and deposition. In this work only amorphous silica is considered.

The basic dissolution/deposition reaction for silica in water (temperature dependent only) is:

$$Si02 + 2H_2O \leftrightarrow H_4SiO_4 \quad \text{(Silicic acid)}$$

**Solid** **Aqueous**

Modelling temperature dependent reaction in a porous media will be considered by starting from the law of natural growth, which states that "The quantity of a certain material increases at a rate proportional to the amount of that quantity" which has the general form:

$$\frac{dC}{dt} = -Kr.(C - Ce)^n \qquad (5)$$

Where $Kr$ in the reaction rate coefficient given by the Arrhenius equation:

$$Kr = A.e^{-\frac{E_a}{RT}} \qquad (6)$$

The governing equation for silica transfer is based on the classical theory of Brownian diffusion developed by Einstein and later workers concerned with the random migration of isolated colloidal particles or large solute molecules due to interacting with molecules of the suspending fluid, (Zarrouk 1999).

The transient mass-transfer equation can be written in a form identical to the Fourier law of thermal diffusion, referred to as Fick's law of mass diffusion.

$$\frac{\partial C}{\partial t}+V.\nabla C = \nabla.(D\nabla C) \qquad (7)$$

For silicic acid **($H_4SiO_4$)** in water.
$D$ = 1E-09 $m^2$/sec, Fleming (1986).

Since there is no fluid flow within the solid rock, the porosity of the solid matrix should be considered. Equation (7) is multiplied by the porosity ($\phi$) to yield:

$$\phi\frac{\partial C}{\partial t}+\phi.V.\nabla C = \phi\nabla.(D\nabla C) \qquad \textbf{(8)}$$

Using the Dupuit-Forchheimer relation, $v = V\phi$ and using $D_m = \phi D$ for the mass diffusion of the porous medium, Equation (8) will become:

$$\phi\frac{\partial C}{\partial t}+v.\nabla C = \nabla.(D_m\nabla C) \qquad \textbf{(9)}$$

When considering the rate of increase in concentration due to chemical reaction, of equation (9) it becomes:

$$\phi\frac{\partial C}{\partial t}+v.\nabla C = \nabla.(D_m\nabla C)+\phi.Kr.(C-Ce)^n \qquad (10)$$

By substituting $K$ from equation (6):

$$\left.\begin{aligned}&\phi\frac{\partial C}{\partial t}+v.\nabla C = \nabla.(D_m.\nabla C)\\&+A.\phi(C-Ce)^n.\exp\left(\frac{-Ea}{R.T}\right)\end{aligned}\right| \qquad \textbf{(11)}$$

This equation is based on the following:

- Rock porosity is constant and porosity at an interface is equal to the volume porosity.
- The chemical reaction does not generate energy within the porous media.
- The chemical reaction is temperature-dependent only.

In order to model the dissolution of amorphous silica in a water-saturated porous medium heated **from** below with the same geometry and conditions of section 3.2, Equation (11) is solved together with equations of mass, momentum and energy comservation.

Empirical relations for the polymerisation and dissolution of amorphous silica obtained by Fleming (1986) are used for the reaction term, representing silica solubility ranging from 100 to 200 ppm as listed below:

$$\frac{-dC}{dt} = K_{sr}(C-C_e)^3 \qquad (12)$$

Where: $K_{sr} = k_{sr}A_s\Gamma_e^2C_e^{-2}$

and $k_{sr}\Gamma_e^2 = A_{sr}\exp\frac{-E_{sr}}{RT}$

Reaction activation energy $E_{sr}$ = 13.5 ±1.8 kcal/mole = 56.48 ±7.5 kJ/mole, Fleming (1986). The equilibrium silicic acid solubility concentration will be calculated from the relation given by Fournier and Rowe (1977).

$$\text{Log } C_e = \frac{-731}{T}+4.52 \qquad \textbf{(13)}$$

Initial conditions and approximations:

- The pH, salinity and any other ions in the geothermal fluid have no effect on the reaction.
- Since the initial temperature of water is 20 °C, the initial concentration of silica is calculated at this temperature (115 ppm) using equation (13).
- The fluid considered is single component pure water, with no thermohaline convection effects from the dissolved silica or any other minerals.

### 4.1 Results

The early time steps of the solution, Figure 8, show that the isosolutal lines are similar to the temperature contours because convection cells have not yet been formed. As the solution proceeds, high isosolutal lines will follow the direction of the flow between the convection cells. The concentration distribution will become stable at a steady state in which there is continuous dissolution in the bottom and deposition on top. Since heat has a much higher diffusivity than $SiO_2$, the temperature variations across the cell are much less distinct than the isosolutes variations (Figure 8).

It is possible to link the concentration of silica to the porosity of the media and produce porosity contours, which will show locations where channel effects will be introduced due to dissolution, similarly other locations will show reduced porosity due to silica deposition. If this can be achieved, the medium will no longer be considered as homogeneous or isotropic, invoking the possibility of deviation from the Darcian flow. It is also possible to consider the effects of other chemical parameters and components (eg. pH, NaCl, $CO_2$, etc.) and link them through chemical kinetics to silica polymerisation/dissolution process and possibly to fluid properties.

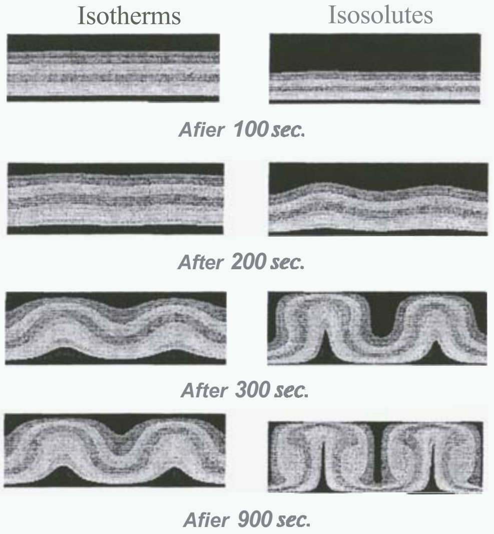


*Figure 8. Transient solution for Silica dissolution in a porous medium heated from below (50°C) and cooled from top (20°C), Ra=60, A =3.*

## CONCLUSIONS

CFD in general and PHOENICS in particular appears to give very good results for modelling laminar natural convection in porous media.

PHOENICS is capable of modelling mass transfer problems such as rock alteration or mineral deposition.

## NOMENCLATURE

| | |
|---|---|
| $A$ | the pre-exponential factor in $sec^{-1}$. |
| $A_s$ | specific surface area (area/volume) = **4200** $cm^2/cm^3$. |
| $A_{sr}$ | Arrhenius pre-exponential factor given as $\ln A_{sr} = 13.7 \pm 2.7 \Rightarrow A_{sr} = 890911.2$ |
| $C$ | the concentration in mg of chemical reactant per kg of the fluid mixture (ppm). |
| $Ce$ | the equilibrium concentration in ppm. |
| $Cp$ | specific heat at constant pressure |
| $D$ | mass diffusivity in $m^2/sec$. |
| $E_a$ | the activation energy in J/mole. |
| $E_{sr}$ | surface rearrangement reaction activation energy. |
| $g$ | acceleration due to gravity |
| K | permeability |
| k | thermal conductivity |
| $Kr$ | reaction rate coefficient in $sec^{-1}$. |
| $k_{sr}$ | surface rearrangement reaction constant. |
| $n$ | reaction order. |
| P | pressure. |
| $R$ | universal gas constant (**8.31** J/mole.°K) |
| $Ra$ | Darcy-Rayleigh number |
| T | temperature |
| t | time |
| $v$ | velocity in y direction (horizontal) |
| $w$ | velocity in z direction (vertical) |
| y, z | spacial coordinates |
| $\phi$ | porosity |
| $\mu$ | dynamic viscosity |
| $\rho$ | density. |
| A | aspect ratio |
| $\Gamma_e$ | equilibrium silicic acid surface concentration. |

### *Suffixes*

| | |
|---|---|
| $f$ | fluid |
| $m$ | mixture |
| $r$ | rock |
| $o$ | initial state |

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