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Modelling Non-isothermal Flows in Porous Media: A Case Study Using an Example of the Great Artesian Basin, Australia

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Abstract. This paper focuses on physics and mathematics behind the numerical software. Our calculations show that the temperature variation recorded in the Great Artesian Basin significantly affects thermodynamic properties of groundwater such as dynamic viscosity and density. Dynamic viscosity varies by a factor of four within the temperature difference typical of the basin, and water density variation may produce a convective motion in higher permeability regions. We suggest to treat the flow in the higher permeability regions as a non-isothermal flow. A rigorous approach to modelling such a flow will be to invoke the continuity equation for a variable density fluid, the energy equation and the momentum equation in the form of the generalised Darcy's law. Accordingly, numerical packages for simulating non-isothermal flows in porous media should be applied.

1. Introduction

The Great Artesian Basin (GAB) occupies $1,700,000\,km^2$ or 22% of Australia. Its groundwater is of vital importance to economy and environment of the Australian outback regions. The main exploited aquifer of the GAB consists of the Cadna-owie Formation and Hooray Sandstone of the Jurassic and Lower Cretaceous sequence of the aquifers. The horizontal extent of the main aquifer is of the order of 10^6 meters, while its vertical extent is of the order of a few hundred metres with the maximum value of approximately 800 metres. Throughout the GAB area the main aquifer is fairly deep and confined by impervious sediments. Near the basin boundaries it outcrops at the surface underlying permeable sandy sediments. The detailed description of the geology and hydrogeology of the GAB can be found in Habermehl (1980).

Hydrogeological studies of the GAB have been carried out since the 1870's with an abundance of measured data now available for modelling. Measurements taken from numerous water bores in the area have been summarised in Australian Geological Survey Organisation (previously Bureau of Mineral Resources) hydrogeological maps and digital databases. This observation data comprises a good solid foundation for building groundwater models. The purpose of modelling is to develop a computerised model to assist in the management of the GAB and therefore to test various scenarios of groundwater extraction. The computerised model includes all simplifications and assumptions made at the starting step of the modelling process when the conceptual model is build. The conceptual model determines the choice of mathematical equations and a numerical method for solving those equations. This has a major impact on the final numerical results. Therefore, all the assumptions in the conceptual model must be justified.

The aim of this paper is to examine the applicability of the following assumptions to the main exploited aquifer of the GAB:

1. The assumption of isothermal flow.
2. The horizontal flow approximation.

The first assumption reduces the number of dependent variables by eliminating temperature, whereas the second assumption reduces the number of independent variables by eliminating the vertical coordinate. It is important to realise that both aforementioned assumptions exclude the dependence of water thermodynamic properties on temperature from consideration. In what follows we show that these assumptions are not valid everywhere in the main exploited aquifer.

2. Non-isothermal Effects

Significant temperature variation has been recorded in the GAB. Groundwater temperatures in waterbores range from $30°C$ to $100°C$ at the surface (Habermehl, 1980, 86). Geothermal gradients calculated from temperature logs range from $15K/1000m$ to $100K/1000m$ with a mean value of $48K/1000m$ (Pitt, 1982; Cull & Conley, 1983). According to Pitt (1982), more than 75% of these estimates exceed "normal" geothermal gradient of $30K/1000m$ as given in Grant *et al.* (1982). These observations are remarkable and should not be overlooked. Temperature differences in a horizontal direction are as large as $70K$. Such large temperature differences will considerably affect thermodynamic properties of groundwater.

The effect of these temperature differences on water dynamic viscosity and density is examined below.

2.1. Water Properties. Figure 1 shows the dynamic viscosity of water calculated from steam table equations for a range of temperatures typical of the GAB. According to our calculations, dynamic viscosity varies by almost a factor of 4. Since flow velocity is inversely proportional to dynamic viscosity, the dependence of dynamic viscosity on temperature is important. Water density calculated for this temperature range is shown in Figure 2. Although the density change is relatively small, it cannot be neglected.

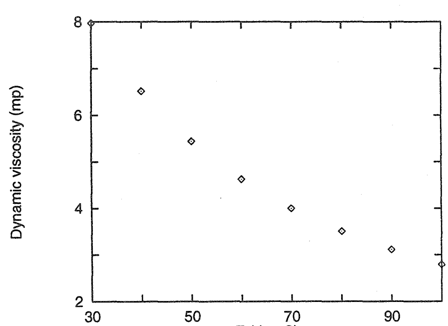

Figure 1. Dynamic viscosity versus T.

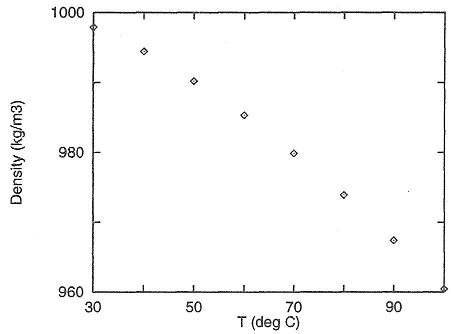

Figure 2. Water density versus T.

2.2. The Onset of Thermal Convection. Figure 2 shows that density of water decreases when temperature increases. In the presence of a downward temperature increase, the buoyancy forces may overcome stabilising effects of the viscous forces and instability may appear in the form of convective flow. The Rayleigh number is normally used as a quantitative measure for the onset of thermal instability.

For the flow in porous media the Rayleigh number can be written in the form (Nield & Bejan, 1992):

$$Ra = \frac{\rho^* g \beta k H \Delta T}{\mu^* \alpha}, \tag{1}$$

where ρ^* is the density of water at some reference temperature, g is gravitational acceleration, β is thermal expansion coefficient for water, k is rock permeability, μ^* is characteristic dynamic viscosity, α is thermal diffusivity of the porous medium, and ΔT is the temperature difference over a distance H.

The critical Rayleigh number for the onset of thermal instability in homogeneous porous media is (Nield & Bejan, 1992)

$$Ra^{cr} = 4\pi^2 \approx 39.48. \tag{2}$$

For the GAB model, $\rho \sim 10^3 kg/m^3$. (Here and in the following "$\sim$" stands for "is of the order of".) We take $H \sim 250m$, then $\Delta T \sim 12K$, where ΔT is calculated from a mean value of geothermal gradient for the basin of $48\, K/1000\, m$. For thermal expansion coefficient of water, steam table equations give the characteristic value of $\beta \sim 10^{-3}K^{-1}$. The characteristic value of dynamic viscosity, as calculated from the steam table equations, $\mu^* \sim 0.5 \times 10^{-3} Ns/m^2$ (Figure 1). Thermal diffusivity of the saturated rock can be calculated using $\alpha = \lambda/(\rho c_p)$, where λ is rock thermal conductivity and c_p is water heat capacity at constant pressure. For the basin sequences, λ is around $3W/mK$ (Cull & Conley, 1983) and c_p is of the order of $0.4 \times 10^4 J/kgK$ (Haar *et al.*, 1984), hence $\alpha \sim 10^{-6} m^2/s$. According to (Habermehl 1980), permeability k ranges from $10^{-14}m^2$ to $10^{-12}m^2$.

Finally we have:

$$Ra \sim 12 \times 10^{13} \times k.$$

When $k \sim 10^{-12}m^2$, the Rayleigh number becomes $Ra \sim 120 > Ra^{cr}$. Therefore, convective flow is likely to develop in the higher permeability regions of the aquifer. The actual flow pattern is not horizontal in the vicinity of these regions, because vertical forces are significant there. Hence, the essentially horizontal flow approximation is not applicable to the aquifer as a whole.

2.3. A Mathematical Model. A mathematical model for the flow in the convective regions includes the continuity equation for a variable density fluid, the energy equation to account for heat transfer, and the momentum equation written in the form (Nield & Bejan, 1992):

$$\overline{V} = -\frac{k}{\mu}(\nabla p - \rho \overline{g}), \tag{3}$$

where $\overline{V}$ is the Darcy velocity vector, p is pressure and $\overline{g}$ is the acceleration vector. Equation (3) is known as the generalised Darcy's law equation. It is used to describe non-isothermal and variable density flows in porous media when the Reynolds number is less than 10 (Bear & Verruijt, 1987; Nield & Bejan, 1992). The concept of potentiometric head is no longer applicable for such flows, and three aforementioned equations involve pressure p and temperature T as dependent variables. The constitutive relationships that describe thermodynamic water properties as functions of temperature must be added to these equations. There has been a number of numerical packages developed for solving these equations, for example TOUGH2 (Pruess, 1991).

Note that the numerical program MODFLOW (McDonald and Harbaugh, 1988) is only applicable to constant density flows. It solves one second order partial differential equation in terms of potentiometric head obtained by combining the continuity equation for a constant density fluid and the Darcy's law equation in the following form:

$$\overline{V} = -K\nabla h. \tag{4}$$

Only in a very particular case where $\rho = const$, equation (4) is identical to equation (3).

Variable density flow modifications of MODFLOW, for example (Kuiper, 1983), do not solve the energy equation and, hence, can only give the first approximation to the reality. By assuming the temperature distribution to be known, they ignore coupling between heat and mass transfer which is the most essential aspect of non-isothermal flows. Thus, MODFLOW and its modifications cannot be used for simulating flow in the convective regions of the GAB.

2.4. Potentiometric Surfaces. As mentioned above, the concept of potentiometric head is not applicable to non-isothermal flows. However, to some limited extent it can be used for constructing potentiometric surfaces. An important point is to distinguish between interpolated and calculated heads. Interpolated heads are derived from measurements. Hence, they do not involve computational errors due to a use of equation (4) instead of equation (3). Also, the dynamic viscosity variation does not affect interpolated potentiometric heads because the definition of potentiometric head does not include μ. The only effect we need to consider in the case of interpolated heads is variation in water density with temperature.

Let us obtain a quantitative estimate for the effect of temperature variation on the interpolated potentiometric head h.

By definition

$$h = \frac{p}{\rho g} + z, \tag{5}$$

where z is the vertical coordinate. In equation (5) we assume $\rho = \rho(T)$. As shown in Figure 2, water density does not vary significantly with temperature. If the density change due to temperature is small, then the Boussinesq approximation can be used (Nield & Bejan, 1992):

$$\rho = \rho^*[1 - \beta(T - T^*)], \tag{6}$$

where ρ^* is the density of water at some reference temperature T^*. For the sake of simplicity, we take $\beta = const.$

Equation (6) in a dimensionless form is

$$\frac{\rho}{\rho^*} = (1 - \theta\hat{T}), \tag{7}$$

where $\hat{T} = (T - T^*)/\Delta T$ is dimensionless temperature and $\theta = \beta\Delta T$ is the buoyancy factor (Pestov, 1997).

The buoyancy factor, θ, can be used as a quantitative estimate for the impact of temperature variation on the interpolated potentiometric head. For the GAB we have $\Delta T = 70K$ for the longitudinal convection. According to our calculations, $\beta \sim 0.73 \times 10^{-3}K^{-1}$. Finally we have $\theta \sim 5\%$ to 6%. Thus, for the interpolated potentiometric head an error due to the assumption of isothermal flow does not exceed 6%. Note that for the calculated head an error due to neglecting temperature variation may be much larger.

3. Conclusions

This paper has examined the applicability of the assumption of isothermal flow and the essentially horizontal flow approximation to the main exploited aquifer of the GAB (Cadna-owie/Hooray aquifer). As the above assumptions neglect the dependence of water thermodynamic properties on temperature, they are not applicable everywhere in the aquifer considered.

According to our calculations, the dynamic viscosity of water changes by a factor of 4 within the GAB horizontal temperature difference of $70K$. Since hydraulic conductivity is inversely proportional to dynamic viscosity, the dependence of dynamic viscosity on temperature cannot be neglected.

Density variation with temperature, although relatively small, cannot be neglected either. Our calculations show that in the higher permeability regions of the aquifer with $k \sim 10^{-12}m^2$ density variation may produce the convective flow. In such regions forces acting in the vertical direction are not negligible and the vertical flow component is significant. The essentially horizontal flow assumption involves two conditions: (1) the aquifer horizontal dimension must be much larger than its vertical dimension, and (2) forces acting in the vertical direction must be much smaller than those acting in the horizontal direction. As the second condition does not hold in the convective regions, the assumption of essentially horizontal flow is not valid everywhere in the main exploited aquifer.

The mathematical model for non-isothermal flow includes the continuity equation for a variable density fluid, the energy equation, and the Darcy's law equation in a general form as given by equation (3). In the case of single phase flow, these three equations can be reduced to two second order partial differential equations in terms of pressure p and temperature T.

The mathematical model for isothermal flow consists of the continuity equation for a constant density fluid and the Darcy's law equation in terms of head h as given by equation (4). It can be reduced to one second order partial differential equation for one dependent variable h.

It is generally accepted that the flow in the convective regions is neither horizontal nor isothermal. Therefore, the mathematical model for non-isothermal flows in porous media should be used to model such regions. The corresponding numerical packages for simulating non-isothermal multidimensional flows in porous media should be applied.

Outside the convective regions, the flow can be assumed to be horizontal and, as the first approximation, the constant density flow model can be used. The dependence of dynamic viscosity on temperature can be included either by calibrating hydraulic conductivity values against measurements or by introducing effective hydraulic conductivity $K_{eff} = K\mu(T^*)/\mu(T)$. Here $\mu(T)$ must be calculated from numerical steam table equations using measured and interpolated temperatures. There is no need to use variable density modifications since variable density effects are insignificant outside the convective regions. For calibrating purposes it is advisable to use the most recent measurements, since the application of the isothermal model is limited to periods of time during which water thermodynamic properties remain unchanged (Kuiper, 1983). The computerised model of this type is computationally less expensive and will give reasonable predictions over periods of time during which only the pressure changes occur. It is not advisable to use isothermal models for transient simulations.

4. Acknowledgements

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