2D OR NOT 2D: ARE TWO DIMENSIONS ENOUGH TO ACCURATELY MODEL CONVECTIVE FLUID FLOW THROUGH FAULTS AND SURROUNDING HOST ROCKS?

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ABSTRACT

In many studies of water-rock interaction, convective fluid flow has been invoked to explain diagenetic processes, metamorphism, or hydrothermal mineralisation. Especially fluid convection in faults is increasingly recognised as an important mechanism for fluid flow, heat transfer, and mass transport in hydrothermal systems, because there is often a close spatial relationship between major ore deposits and regional scale faults.

Most numerical studies simulate free convection in 2D only. This is because fluid patterns are more easily recognised with less complicated geometries, less computational time is required, or because some computer codes are restricted to two dimensions. Using the finite difference simulation code SHEMAT, a series of numerical simulations of thermally driven fluid flow have been carried out to investigate the difference in the fluid flow patterns in 2D and 3D models for the same geological architecture.

On the one hand the results show that 2D and 3D models of convection in hydrothermal systems can produce significantly different results when the fault structure cuts the entire system from top to bottom. In this case 2D models represent an oversimplification, and conclusions reached from such investigations are likely to be irrelevant. On the other hand an exception is the existence of an impermeable boundary layer resulting in 2D convection patterns identical to observed 3D fluid flow fields. However, this is observed only if the vertical fault permeability equals the horizontal host rock permeability. In general it is difficult to say when 2D equals 3D. It can therefore be concluded that prediction of convective flow patterns requires the use of 3D architectures.

1 INTRODUCTION

Several driving mechanisms for regional-scale fluid flow have been proposed, including: (1) Topography- or gravity driven flow (Garven and Freeze, 1984); (2) Compaction-driven flow during basin subsidence (Bethke, 1985; Cathles and Smith, 1983); (3) Seismic pumping and tectonically driven flow (Oliver, 1986; Sibson et al., 1975); and (4) Buoyancy-driven flow (Bjørlykke et al., 1988; Cathles, 1981). In many studies of water-rock interaction, buoyancy-driven flow, also called convective fluid flow, has been invoked to explain diagenetic processes, metamorphism, or hydrothermal mineralisation. Fluid convection in faults in particular is increasingly recognised as an important mechanism for fluid flow, heat transfer, and mass transport in hydrothermal systems (Bächler et al., 2003; Zhao et al., 2006), particularly in consolidated and crystalline rocks.

Often, there is a close spatial relationship between major ore deposits and regional scale fault systems. Predicting the location of (as yet) undiscovered deposits requires an understanding of the coupled, physical and chemical processes involved in mineralization. Such understanding may be gained through a combination of conceptual and quantitative models (Ord et al., 2002). Numerical modelling permits investigation of competing hypotheses concerning mineralization, and can be used to reverse-engineer known deposits in order to guide future mineral exploration.

Most numerical studies simulate free convection in 2D only, because fluid patterns are more easily recognised with less complicated geometries, less computational time is required, or computer codes may be restricted to two dimensions. However, it has been shown by Kühn (2004), Kühn and Gessner (2005), and Kühn et al. (2006), that the third dimension can be essential to adequately reproduce fluid flow and heat transfer processes in complex geological architectures. Exceptions are 2D models of high permeability regions with close to radial or linear symmetries, such as damage zones between fault jogs or at fault intersections, giving reasonable results in 2D.

In the work of Kühn and Gessner (2005) vertical 2D dimensional models have been built with (1) a closed system consisting of faults and an aquifer (Kühn et al., 2006), (2) faults connected to an aquifer and the open seafloor (Yang et al., 2004), and (3) faults above an impermeable basement and connection to the open seafloor (Simms and Garven, 2004). These systems, all exhibiting convection through their faults and host rocks were expanded in the third dimension by duplicating the geological architecture of the 2D cross sections. The results of this study show that 2D and 3D models of convection in hydrothermal systems produce significantly different results. It has been shown that in many cases 2D models represent an oversimplification, and conclusions reached from such investigations are likely to be irrelevant. In the case of planar high permeability regions, such as faults and permeable stratigraphic units extending along strike, 2D and 3D modelling outcomes vary significantly. An exception is incorporation of boundary layers with very low permeability, such as for example an impermeable basement, as shown by Simms and Garven (2004), where 2D convection patterns are identical to 3D fluid flow fields. However, it should be noticed that in Simms and Garven (2004) this only occurs, if vertical fault permeability equals horizontal host rock permeability.

Focus of this study is to explore conditions required to match 2D with 3D convection patterns, using the finite difference simulation code SHEMAT (Clauser, 2003). To demonstrate the effect of presence or absence of a basement with low permeability, a series of numerical simulations of thermally driven fluid flow with simple geometries have been carried out.

2 NUMERICAL SIMULATION

2.1 Free convection theory

The Rayleigh number [Ra, Eq. (1)] indicates the tendency towards free convection, that is, flow driven purely by density differences. Ra is based on the ratio of buoyant forces, which drive convective fluid flow, to the viscous forces inhibiting fluid movement.

$$Ra = \frac{\alpha_f g \rho_f^2 c_{pf} kH(T_1 - T_2)}{\mu \lambda_m} \quad (1)$$

In Eq. (1) α_f [K^{-1}] is the thermal expansion coefficient of water (subscript f = fluid), g [m s^{-2}] the gravitational acceleration, ρ_f [kg m^{-3}] the density of liquid water, c_{pf} [J kg^{-1} K^{-1}] the isochoric heat capacity, k [m^2] the permeability, H [m] the characteristic height of the system, (T_1 - T_2) [K] the temperature difference across this height, μ [kg m^{-1} s^{-1}] the dynamic viscosity of water, and λ_m [J s^{-1} m^{-1} K^{-1}] the medium thermal conductivity.

Free convection for an infinitely long and homogenous vertical 2D system with impermeable boundaries of constant temperature and a linear initial thermal gradient across the layer is expected above a critical Ra value of $4\pi^2$ (Lapwood, 1948). A very similar solution for the 3D case is given by Zhao et al. (2003). However, in a 3D system with a fault, as investigated in this study, Ra simplifies to the 2D solution, when the fluid flow pathway (the fault) is too thin for a convection cell to evolve across strike.

2.2 Numerical code.

The Simulator for HEat and MAss Transport (SHEMAT) has been chosen to carry out the numerical simulations, because together with Processing SHEMAT (Kühn and Chiang, 2004) it is an easy-to-use, general purpose reactive transport code for a wide variety of thermal and hydrogeological problems in two and three dimensions. SHEMAT solves coupled problems involving fluid flow, heat transfer, species transport, and chemical water-rock interaction in fluid saturated porous media on a Cartesian grid. In SHEMAT, the different flow, transport, and reaction processes can be selectively coupled. Flow and heat transport are coupled in the way that the fluid parameters density, viscosity, compressibility, thermal conductivity, and thermal capacity are functions of temperature and pressure. A detailed description of the governing equations and code verifications are given by Clauser (2003).

2.3 Numerical model.

The 2D model used in this study is 10 km long (x-direction) and 5km high (z-direction), consisting of one vertical cross section 200 m wide. The 3D model has been derived from the 2D model by multiplying the vertical cross section 24 times, resulting in an entire model width of 5 km (y-direction). Each model element measures 200 m x 200 m x 200 m. One vertical fault zone of 600 m width is defined in the centre of the model (FIGURE 1).

Initial fluid pore pressure conditions are defined to be hydrostatic. The porosity in the entire model is set to 20 % regardless of the rock type or varying permeabilities (TABLE 1). This simplification was done, because prior research (Kühn et al., 2006) showed that the influence of changing porosity on the flow field is negligible. Resulting convection cell patterns stay the same for a range of porosities between 1 % and 20 %. Initial permeabilities have been set to be $7.0 \cdot 10^{-14}$ m^2 in x- and y-direction of the host rock ($k_{x,y}$), as well as in z- and y-direction within the fault ($k_{y,z}$). Permeabilities in z-direction of the host rock (k_z) and in x-direction for the fault (k_x) are 2 orders of magnitude lower to account for the layering in the host rock due to sedimentation and the transition between fault and host rock, respectively.

Temperature at the bottom of the model is 145°C and 20°C at the top reflecting a linear thermal gradient of 2.5°C per 100 m. Rock thermal properties are assumed to be uniform for the entire model with a thermal heat capacity of 2.06 MJ m^{-3} K^{-1} and a thermal conductivity of 2.9 W m^{-1} K^{-1}.

All six boundaries are impermeable, defining a closed box system with no sources or sinks for the pore fluid. Thermal boundaries are set to constant temperature at the top and bottom of the model. The lateral boundaries of the model allow no heat transfer across them, i.e. they are perfectly insulated.

Two general scenarios have been modelled for both the 2D and 3D case. (1) The system as shown and described in FIGURE 1 and (2) this system enlarged by a basement with low permeability.

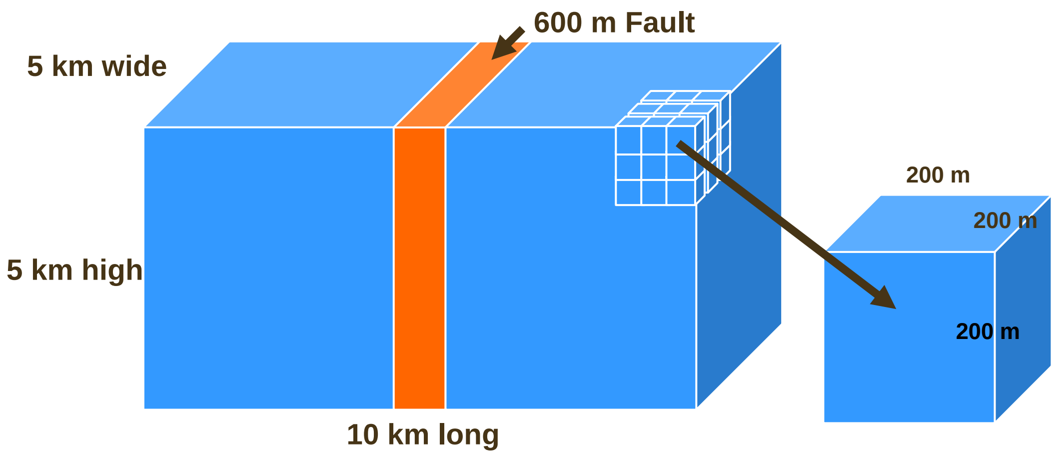

FIGURE 1. General model set-up

TABLE 1. Model parameters.

	Host rock	Fault system	Basement
Porosity (%)	20	20	20
Permeability (m^2): k_x	7.0E-14	7.0E-16	1.0E-18
k_y	7.0E-14	7.0E-14	1.0E-18
k_z	7.0E-16	7.0E-14	1.0E-18
Thermal conductivity (W m^{-1} K^{-1})	2.9	2.9	2.9
Thermal capacity (MJ m^{-3} K^{-1})	2.06	2.06	2.06

3 RESULTS AND DISCUSSION

3.1.1 2D and 3D general fault system.

The resulting flow field of the first scenario, the 2D model without basement, is shown in FIGURE 2. Two convection cells are observed with hot water flowing upward through the fault and cool water flowing down through the less permeable host rock. The resulting temperature distribution is advective, driven by the flow field. As expected, the convection cells are oriented perpendicular to the fault. FIGURE 3 displays the results gained with the general model for the 3D case. Convection now occurs along strike within the fault. In opposite to the 2D case there is no fluid flow observed within the host rock. Because flow only occurs in the fault with its higher permeability the observed fluid velocities are one order of magnitude higher in the 3D model ($3.76{\cdot}10^{-8}$m s^{-1}, Darcy flow) than they are in the 2D model ($4.4{\cdot}10^{-9}$m s^{-1}).

3.1.2 2D and 3D general fault system including impermeable basement.

For the second test scenario a 1 km thick low permeability layer simulating a basement has been added to the system described in FIGURE 1. The permeability of this basement is set to $k = 10^{-18}$ m^2 (TABLE 1) to suppress any fluid flow within this layer. Results of the 2D case (FIGURE 4) display two convection cells, as observed before. However, convection direction is reversed now with hot water flowing upward at the margins of the model and cool water flowing downward through the fault. FIGURE 5 shows that the resulting fluid flow pattern in 3D for the case including an impermeable basement is the same. The resulting Darcy flow velocities of approximately $7{\cdot}10^{-9}$ m s^{-1} for both cases also emphasize the conformity between the 2D and 3D model.

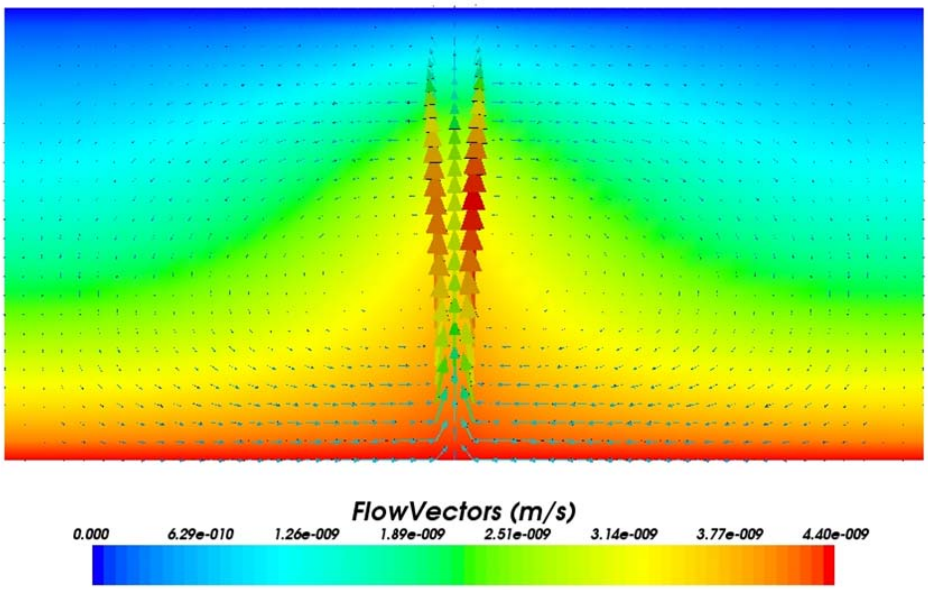

FIGURE 2. The results of the general model in 2D show two convection cells indicated by the velocity vectors with up flow through the fault and down flow through the host rock. The temperature distribution is displayed by the contour colors.

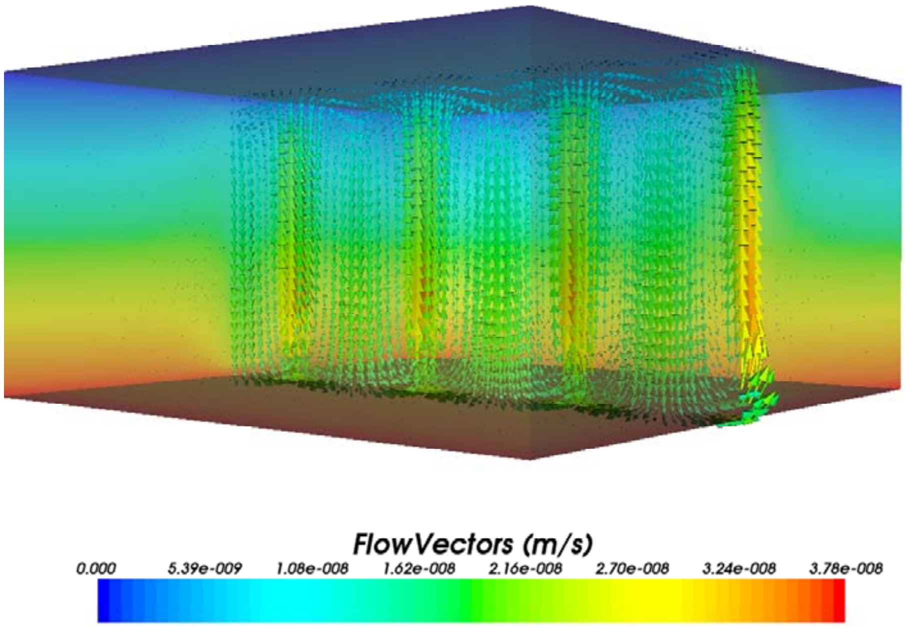

FIGURE 3. The results of the general model in 3D show convection within the fault only.

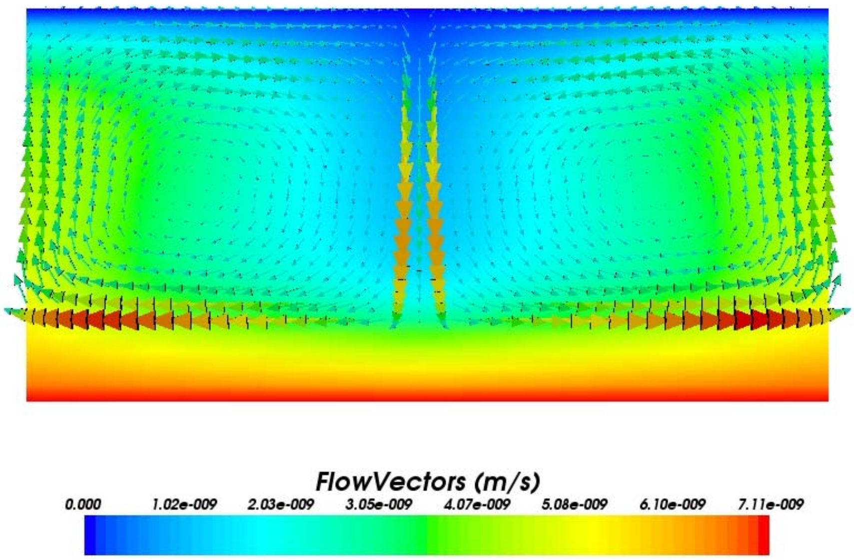

FIGURE 4. Results of the 2D model with basement of low permeability. The convection direction is now reversed with up flow at the margins and down flow through the fault.

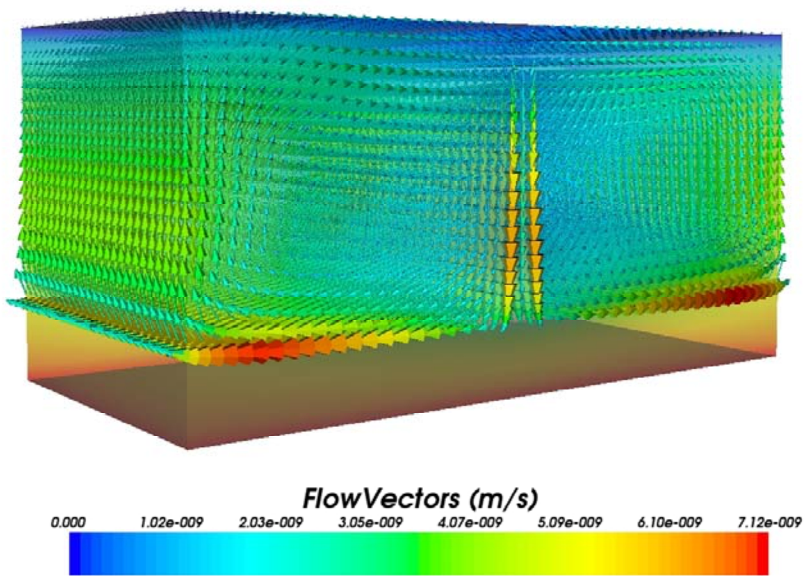

FIGURE 5. Results of the 3D model with basement of low permeability. The observed fluid flow pattern is identical with the 2D case. Convection cells are perpendicular to the fault zone.

4 CONCLUSION

In many studies of water-rock interaction, convective fluid flow has been invoked to explain diagenetic processes, metamorphism, or hydrothermal mineralization. Especially fluid convection in faults is increasingly recognised as an important mechanism for fluid flow, heat transfer, and mass transport in hydrothermal systems, because there is often a close spatial relationship between major ore deposits and regional scale faults.

Many numerical studies simulate free convection in 2D only, because fluid flow patterns are more easily recognised with less complicated geometries, and less computational time is required. However, it has been shown in previous studies that the third dimension can be essential to adequately reproduce fluid flow and heat transfer processes in complex geological structures. The focus of the presented work has been to elaborate the effect of the presence or absence of a basement with low permeability. The finite difference simulation code SHEMAT has been applied to perform numerical simulations of thermally driven fluid flow and investigate the difference of fluid flow patterns in 2D and 3D models for the same geological architecture.

On the one hand the results show that 2D and 3D models of convection in hydrothermal systems can produce significantly different results when the fault structure cuts the entire system from top to bottom. In this case 2D models represent an oversimplification, and conclusions reached from such investigations are likely to be irrelevant. Under these circumstances 3D models are absolutely essential to describe the flow field. On the other hand an exception is incorporation of an impermeable basement, resulting in 2D convection patterns identical to observed 3D fluid flow fields. However, this is observed only if the vertical fault permeability equals the horizontal host rock permeability. In general it is difficult to say when 2D equals 3D. It can therefore be concluded that prediction of convective flow patterns requires the use of 3D architectures.

With respect to predictive mineral discovery, further investigation is essential. The range of parameters to be examined with regard to the question if modelling in two dimensions is enough to accurately describe convective fluid flow through faults and surrounding host rocks will be enlarged. In many cases 2D and 3D convection are very different from each other but in some instances they are identical.

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