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Modelling coupled Component Based Multiphase and Reactive Transport Processes in Deep Geothermal Reservoirs using OpenGeoSys

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Abstract

In deep geothermal reservoirs, artificial fracture networks are often stimulated and the enhanced during the well construction, in order to facilitate efficient heat transfer from the host rock to the heat carrying fluid. However, throughout the life span of a geothermal power plant, the geochemical reactions on the fracture surfaces will gradually control the hydraulic and mechanical behavior of the fractures, thus further affect the energy output of the reservoir.

The numerical simulation of such long term behavior of the reservoir imposes several challenges to the modelers. First, it is a coupled non-isothermal system that often contains multiple fluid and solid phases. In addition to that, controlled by the pressure and temperature conditions, phase change process may happen in certain part of the modeling domain. To further increase the non-linearity of the system, the long term fluid-rock geochemical reactions have to be included in the consideration and the model must be able to account for their feedback to the hydraulic and flow field.

Within the framework OpenGeoSys software, we extend the traditional phase volume based multiphase flow module to chemical component based formulations. This allows a further coupling with geochemical processes on the fracture surface. The developed code will be verified against several benchmark cases, which involves non-isothermal multiphase flow involving phase change and mineral-water geochemical reactive transport processes. The simulation of coupled processes in fracture network dominated geothermal reservoirs will also be presented.

1. INTRODUCTION

For the performance analysis of deep geothermal reservoirs, numerical modelling tools are widely employed to simulate the flow processes in the subsurface. With high temperature and pressure in the reservoir, coupled multiphase flow processes often interact with chemical reactions and impose challenges on the numerical models. In order to reproduce the phase change behavior mentioned above in the numerical simulation, there exist so far several different numerical schemes. The most popular one is the primary variable switching method proposed by Wu et al. (2001), which was adopted by the multi-phase flow code TOUGH (Pruess, 2008) and MUFTE (Class et al., 2002). Although this approach works in most scenarios, the governing equations are intrinsically non-differentiable, as the primary variable is changing. This often leads to numerical difficulties. Abadpour et al. (2009) proposed a negative saturation method, in which saturation values less than zero and bigger than one are used to store extra information of the phase transition. Salimi et al. (2012) later extended this method to the non-isothermal conditions and taking the diffusion and capillary forces into account. Although the primary variable switching is avoided, the negative saturation actually does not have a physical meaning and this method cannot be further extended when more than two chemical components are presenting in the system. Therefore, in order to handle the multi-component two phases system that is widely occurred in deep geothermal reservoirs, primary variables of the governing equation must be persistent. Marchand et al. (2013) suggested to use mean pressure and molar fraction of the light component as primary variable. Following their ideas, all the primary variables can be constructed independently of the present phase, which allows the (dis)appearance of any of the two phases, and no unphysical quantities or variables switching are required.

In this work, as the first step of building multi-phase reactive transport model for the geothermal reservoir, we first extend Marchand's (2013) component based multiphase flow system to the non-isothermal condition. The extended governing equations were solved by Newton iterations. The extended model has been implemented into the OpenGeoSys software. To validate the numerical code, one benchmark case --- heat-pipe problem was simulated using OpenGeoSys. The modelling results are compared with semi-analytical solution. Furthermore, details on the numerical techniques were discussed regarding how to solve the highly nonlinear local EOS system. In the end of this paper, general ideas regarding how to include chemical reactions into the current form of governing equations will be introduced.

2. MATHEMATICAL MODEL

2.1 Governing Equation

Different from the traditional multiphase flow equations, which were written based on the volume balance of each phase (Kolditz et al., 2012), we formulate the mass balance equations of each chemical component in the multiphase system. In the simplest case, a multiphase system can be established with two-phases and two-components. Let the subscript α =L, G implying the liquid and gas phase, and the superscript i referring to the corresponding component, the N and S are the molar density and saturation. The general governing equations of the componential mass balance can be written as,

$$\frac{\phi\partial\left(NX^{(i)}\right)}{\partial t}+\nabla\left(N_L X_L^{(i)}v_L+N_G X_G^{(i)}v_G\right)+\nabla\left(N_L S_L W_L^{(i)}+N_G S_G W_G^{(i)}\right)=q^{(i)}. \tag{1}$$

Where the flow velocity v is regulated by the general Darcy's law,

$$v_\alpha=-\frac{Kk_{r\alpha}(S)}{\mu_\alpha}(\nabla P_\alpha-\rho_\alpha g) \tag{2}$$

and the diffusive flux be calculated after the Fick's law,

$$W_\alpha^{(i)}=-D_\alpha^{(i)}\phi\nabla x_\alpha^{(i)}. \tag{3}$$

In the above governing equation, P [Pa] denotes the weighted mean pressure of gas and liquid phase, with each phase volume as the weighting factor. X [-] is the total molar fraction of light component in both fluid phases. When one of the phases disappears, these two primary variables are equal to the pressure and molar fraction of the remaining phase, respectively. These two parameters are then chosen as primary variables. The liquid and gas phase pressure P_L and P_G can be derived from them. Besides, N_L and N_G, which are the molar density [mol/m^{-3}] of two phases can also be calculated. S_L *and* S_G are the saturations [-] of the corresponding phase. $X_L^{(i)}$ and $X_G^{(i)}$ are the molar fraction of *i*-th component in the liquid and gas phase. These eight parameters are secondary variables and determine the state of the system.

When non-isothermal condition is considered, a heat balance equation can be added, considering the gas and liquid phase has the same temperature.

$$\frac{\partial[(1-\phi)\rho_s c_s T+\phi S_l\rho_l c_l T+\phi(1-S_l)\rho_g c_g T]}{\partial t}$$
$$-\nabla[\rho_g c_g T\frac{Kk_r^g}{\mu_g}(\nabla p_g+\rho_g g)]-\nabla[\rho_l c_l T\frac{Kk_r^l}{\mu_l}(\nabla p_l+\rho_l g)]-\nabla\cdot(k_T\nabla T)=Q_T \tag{4}$$

In the above equation, the phase density ρs, ρl, and heat capacity cg, cl are all temperature and pressure dependent. Compared to the primary variable switching Wu and Forsyth (2001) and the negative saturation Salimi et al. (2012) approach, the choice of P and X as primary variables fully covers all three possible status of the two phase system, i.e. the single-phase gas, two-phase, and single-phase liquid regions. Instead of switching the primary variable, the non-linearity of phase change behavior is removed from the global PDE system, and embedded into the solution of local EOS.

2.2 Equations of State (EOS)

As seen from Eq. (1), if the P and X serve as the primary variables of the governing equation, then the secondary variables P_L, P_G, N_L, N_G, S_L, S_G, $X_L^{(i)}$, and $X_G^{(i)}$, which are dependent on P and X, have to be re-calculated whenever P and X are changed. We assume the thermodynamic equilibrium of the multiphase system is reached, then the Equations of State (EOS) are formulated according to the three phase states,

$$S=0 \quad \wedge \quad x_l^{(1)}\le X_m(P,0) \tag{5}$$

$$0\le S\le 1 \quad \wedge \quad X_m(P,S)-x_l^{(1)}=0,\quad x_g^{(1)}-X_M(P,S)=0 \tag{6}$$

$$S=1 \quad \wedge \quad x_g^{(1)}\ge X_M(P,1) \tag{7}$$

We define the minimum function,

$$\varphi(a,b):=\min\{a,b\} \tag{8}$$

Then Eq. (5) to (6) can be transformed to,

$$F(1)=\varphi(S,X_m(P,S)-x_l^{(1)})=0 \tag{9}$$

$$F(2)=\varphi(1-S,x_g^{(1)}-X_M(P,S))=0 \tag{10}$$

$$F(3)=\frac{SN_g(X-x_g^{(1)})+(1-S)\ N_l(X-x_l^{(1)})}{SN_g+(1-S)\ N_l}=0 \tag{11}$$

The above equations need to be solved locally on each node of model domain, with P and X as input parameter, saturation S, molar fraction of light component in the gas phase $X_g^{(1)}$, molar fraction of light component in the liquid phase $X_l^{(1)}$ as unknown. The other secondary variables can be derived from these 3 variables.

2.3 Numerical Settings

For a two-phase, two components non-isothermal multiphase flow system, we solve the global governing equation (1) to (4), with local EOS system of Eq. (9) to (11) simultaneously satisfied. To handle the nonlinearities, a nested Newton scheme is implemented. For the global equations, the time is discretized with the backward Euler scheme, and Galerkin finite element discretization was applied in the space. After each global Newton iteration, the EOS system is solved on each node of the model domain. For the local problem, a Newton scheme with line-search was applied. This numerical scheme has been implemented into the open-source scientific software OpenGeoSys (Kolditz et al., 2012).

3. MODELLING EXAMPLES AND RESULTS

3.1 The heat-pipe problem (Non-isothermal flow)

The heat pipe problem (Fig. 1) is a widely used benchmark for the demonstration of non-isothermal multi-phase flow processes. Initially, the 2.25 m long heat pipe was partially saturated with a S_w value of 0.5. The temperature of the column was set to70 °C. On the right hand side of the column, a heater will produce constant heat flux, which raises the water temperature in the vicinity up to the boiling point. When the temperature is beyond 100 °C, liquid phase water evaporates and is turned into steam. The steam then flows towards left under the pressure gradient. When the steam is in contact with the cold water and its temperature is lowered, it undergoes condensation and flows backwards to the right. Udell and Fitch produced analytical solution that can be used for model validation. Detailed description of the heat problem description and the parameters used can be found in their paper (Udell and Fitch, 1985).

Here in this work, we have adopted a 2D rectangular mesh with 325 triangular elements and 208 nodes. On the right hand side boundary, a Neumann boundary condition of 100 J/m/s is imposed on the heat transport equation (4), representing the heater. Time discretization of 1 day is applied during the period from 1 to 100 days. Afterwards, this value gradually increased to 100 days along with the simulation until 30 years.

The simulation results are plotted along the horizontal cross-section along the model domain. Temperature and water saturation profiles at day 1, 10, and 100 are shown in Figure 4, respectively. As the heat flux was continuously introduced on the right hand side boundary, the temperature keeps rising. After 1 day, the boundary temperature has already exceeded 100°C, and water in the pore space begins to evaporate and was turned to steam. This is also reflected by the drop of water saturation on right side. After 10 days, the point of phase transition has shifted to the middle of the column, and steam keeps evaporating and move to the left, while liquid water was flowing back towards right. After 100 days, the system is approaching the steady-state, where the three regions, including single phase gas, two phases and single phase liquid, co-exist and can be distinguished. The appearance of gas (steam) phase and the disappearance of the liquid water phase on the right hand side boundary are considered to be associated with the phase transition phenomenon.

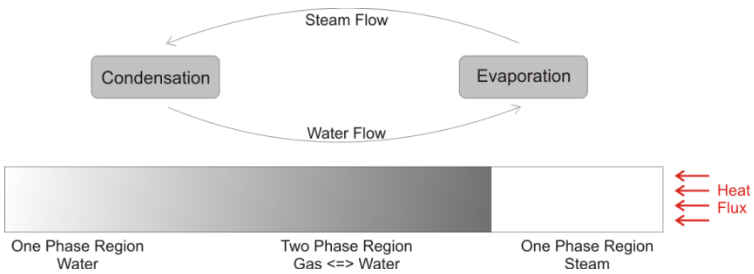

Figure 1: Modelling domain and phase change process involved in the heat pipe problem.

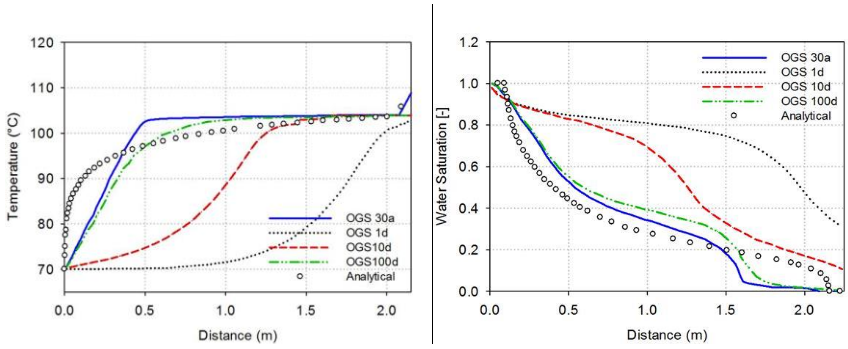

Figure 2: Simulated temperature and water saturation profile of the heat pipe problem after 100 days. Comparison made between OpenGeoSys results and analytical solution of Udell and Fitch (1985).

4. DISCUSSION AND CONCLUSIONS

4.1 Discussions

Following the discussions in section 2.2, one notices that the choice of mean pressure and light component molar fraction as primary variable will alleviate the discontinuous behavior of the global governing equations. Accordingly, it becomes the job of the local EOS system to handle the non-linear transition of phase properties induced by the phase change process. After observing the EOS system of Eq. (5) to (7), it is mathematically a non-linear root finding problem with unequal constrains imposed on the saturation value. When using standard Newton iterations to solve it, the saturation values cannot be guaranties to stay within the range from 0 to 1. Beyond this range, the saturation value becomes physically unfeasible, and the local governing equations no longer hold, which prevents a valid solution to be found.

Our strategy of handling Eq. (5) to (7) is to transform them to Eq. (9) to (11), by using the complementary formulation. When saturation is less than zero or bigger than one, the other argument of the minimization function will be chosen, which effectively prevents the saturation value from moving into unphysical regions. This transformation will result in a local Jacobian matrix that might be singular. Therefore a pivoting action has to be performed before the Jacobian matrix is decomposed to calculating the size of Newton steps. In our test, the complementary transformation is effective for most P and X values, when the starting value of Newton iteration is close to the solution. This is indeed the case during the global simulation, because the primary variables in two adjacent time steps do not change much. However, the saturation values are still not strictly controlled within the range of [0, 1] and the non-linear iterations can still go divergence when the starting values are far away. An alternative approach is to treat the EOS system as a nonlinear optimization problem with constrains. Initial tests show that the optimization algorithms as Trust-Region method is more robust in solving such a local problem, but the calculation time will be considerably longer.

4.2 Conclusions and Outlook

In this work, the component based multiphase flow formulation proposed by Marchand et al. (2013) has been successfully extended to include the non-isothermal condition. The numerical scheme has been implemented into the OpenGeoSys code. The modelling results have been verified by comparing to the results from other models, and also against analytical solutions. It is shown that, the method is capable of handling non-isothermal phase change processes. Currently, we are working to include equilibrium reactions, such as the mineral dissolution and precipitation, into the local EOS system. As our global mass-balance equations are already component based, one governing equation can be written for each basis component. Pressure, temperature and molar fractions of the chemical components can be chosen as primary variables. In the near future, the coupled code is expected to simulate reactive multiphase flow problems in deep geothermal reservoirs.

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