Non-isothermal compositional two-phase Darcy flow: numerical modeling of high energy geothermal systems with soil-atmosphere boundary condition

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Introduction
Taking into account the influence of shallow water levels (vadose zone, water table fluctuations...) is notoriously challenging when modelling the natural state of high temperature geothermal systems. We investigate a new formulation for the non-isothermal compositional gas liquid Darcy flows and its coupling with an advanced soil-atmosphere boundary condition. The model and its formulation are applied on the Bouillante high temperature geothermal field (Guadeloupe, French West Indies) which shows temperatures around 250°C below 300m deep and soil with near boiling conditions in some places.

Non-isothermal compositional liquid-gas Darcy flow model
We developed a two-phase (liquid, gas) compositional model with the set of components noted as $C$. $C$ typically contains a water component which can vaporize into the gas phase, a set of gaseous components which can dissolve into the liquid phase (typically air) and a salt component as geothermal fluids are brines whose physical properties depend on salinity. Then, our formulation of the model is based on the pressures $P_g$ and $P_l$, the saturations $S_g$ and $S_l$, the temperature $T$ and the phase molar fractions $C_\alpha = (C_\alpha^i)_{i \in C}$, with $\alpha = g, l$, as the set of unknowns. Doing so, all physical laws can be directly expressed using subsets of this set of variables. It is also a very natural choice in single phase regions which are usually dominant in geothermal applications. No switch of variables is required as this choice of unknowns is combined with an extension of the phase molar fractions of an absent phase by the molar fractions at thermodynamic equilibrium with the present phase. This implies that the set of unknowns does not depend on the set of present phases. More precisely, the phase transitions are expressed as complementary constraints involving the saturations and the molar fractions

$$S_\alpha(1 - \sum_{i \in C} C_\alpha^i) = 0, \quad S_\alpha \geq 0, \quad 1 - \sum_{i \in C} C_\alpha^i \geq 0, \quad \alpha = g, l$$

combined with the equality of the liquid and gas fugacities for each component. It results that the non-linear system can be solved using semi-smoothed Newton algorithms [1].

Soil-atmosphere boundary condition
The interaction between the flow in the porous medium and the atmosphere plays an important role in geothermal flows. Nevertheless the coupling between the porous medium and surface flows would not be computationally realistic for geothermal time and space scales. This is why we focus on an advanced soil-atmosphere boundary condition. This soil-atmosphere boundary condition is based on mole and energy balance equations expressed at the interface (figure 1). The model takes into account two coupling processes: the vaporization of the liquid phase and the convective molar and energy transfer in the atmosphere (of coefficients $H_m$ and $H_T$) [2, 3], and a liquid outflow condition. Both coupling processes are combined into a single boundary condition assuming that the liquid phase does not accumulate at the surface. Are also considered the net radiation ($R_n$) and the precipitation recharge (defined by the flow rate $q^{\text{rain}}$, the rain molar fractions $C_{\alpha}^{\text{rain}}$ and the rain molar enthalpy $h^{\text{rain}}$). At the interface, the model states the continuities of the component molar and energy normal fluxes, gas molar fractions $C_g$, gas pressure $P_g$ and temperature $T$. The far field atmospheric conditions are defined by the constant molar fractions $C_{\alpha}^{\text{atm}}$, the temperature $T_{\text{atm}}$ and the pressure $P_{\text{atm}}$.

The model introduces two unknowns at the interface which are the gas and liquid molar flow rate on the atmosphere side. They are respectively noted $q^{g,\text{atm}}$ and $q^{l,\text{atm}}$ and are oriented positively outward from the porous-medium domain. On the porous-medium side, thermodynamical equilibrium is assumed as soon as the liquid phase is present. Even when the gas phase is absent, gas molar fractions and pressure at the interface
are extended by their values given by the equilibrium with the liquid phase. Taking into account the effect of capillary pressure, the liquid outflow condition is shown to amount to the following complementary constraints:

\[
\begin{align*}
(P^g - P^l)q_{l,atm}^l &= 0, \\
(P^g - P^l) &\geq 0, \\
q_{l,atm}^l &\geq 0,
\end{align*}
\]

which is obtained from the thermodynamic equilibrium and the continuity of the gas phase at the interface.

Numerical simulation

The time integration is based on a fully implicit Euler scheme to avoid severe restrictions on the time steps. First, the system of equations is discretized using a finite volume discretization in space with a Two-Point Flux Approximation (TPFA) of the Darcy and Fourier fluxes combined with a phase based upwind scheme for the approximation of the mobilities, molar fractions and enthalpies. Assuming isotropic permeability field, a Voronoi mesh satisfying the admissibility condition of TPFA schemes at both inner and boundary faces is built. The TPFA scheme is robust but not adapted to complex geology and geometry. This motivates to study the combination of the TPFA scheme with a Vertex based MultiPoint Flux Approximation. The coupling between both schemes is performed to ensure the consistency and stability of the combined scheme. This approach allows to benefit from the TPFA scheme on parts of the domain which can be meshed using Cartesian cells with anisotropic permeability aligned with the axes, and restricts the MPFA scheme to the remaining parts of the domain with more complex geology or geometry such as faults or pinch-out.

The numerical efficiency of the formulation and the soil-atmosphere evaporation-outflow boundary condition are studied on several 1D and 2D test cases including in particular a 2D cut of the Bouillante high energy geothermal field in Guadeloupe with both air-water and air-water-salt thermodynamic systems.

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References

