

# Coupling of a two phase gas liquid compositional 3D Darcy flow with a 1D compositional free gas flow

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A model coupling a three dimensional gas liquid compositional Darcy flow and a one dimensional compositional free gas flow is presented. In the porous media  $\Omega = (0, L) \times (\omega \setminus S)$ , the Darcy flow model uses as primary unknowns the gas and liquid pressures  $P^g$  and  $P^l$  as well as the fugacities of the components  $f = (f_i)_{i \in \mathcal{C}}$ :

$$\left\{ \begin{array}{l} \phi \partial_t \sum_{\alpha \in \mathcal{P}} \zeta^\alpha S^\alpha c_i^\alpha + \operatorname{div} \left( \sum_{\alpha \in \mathcal{P}} \zeta^\alpha c_i^\alpha \mathbf{V}^\alpha \right) = 0, \quad i \in \mathcal{C}, \\ \mathbf{V}^\alpha = - \frac{k_r^\alpha(\mathbf{x}, S^\alpha)}{\mu^\alpha} \mathbf{K} \left( \nabla P^\alpha - \rho^\alpha \mathbf{g} \right), \quad \alpha = g, l, \\ S^g + S^l = 1, \quad S^l = S^l(\mathbf{x}, P^l - P^g), \quad \sum_{i \in \mathcal{C}} c_i^\alpha(f, P^g, P^l) = 1, \quad \alpha = g, l. \end{array} \right. \quad (1)$$

In the gallery, the primary unknowns, depending only on the  $x$  coordinate along the gallery and on the time  $t$ , are chosen to be the gas pressure  $p$  and the gas molar fractions  $c = (c_i, i \in \mathcal{C})$ . The set of equations is defined by the following no pressure wave isothermal model where  $\alpha > 0$ ,  $\beta > 0$  are parameters for the pressure drop along the gallery,  $\mathbf{n}$  is the unit normal vector at  $\Gamma = (0, L) \times \partial S$  outward to  $\Omega$ , and  $|S|$  is the surface of the section  $S$  of the gallery.

$$\left\{ \begin{array}{l} \partial_t \left( |S| \zeta^g(p) c_i \right) + \partial_x \left( |S| \zeta^g(p) c_i w \right) = \int_{\partial S} - \sum_{\alpha=g,l} c_i^\alpha \zeta^\alpha \frac{k_r^\alpha(\mathbf{x}, S^\alpha)}{\mu^\alpha} \mathbf{K} \nabla P^\alpha \cdot \mathbf{n}, \\ \sum_{i \in \mathcal{C}} c_i = 1, \quad (\alpha w + \beta |w| w) = -\partial_x p. \end{array} \right. \quad (2)$$

At the interface  $\Gamma$  between the gallery and the porous media the coupling conditions are adaptation to a 1D model in the gallery of [1]. They account for the liquid gas thermodynamical equilibrium, the continuity of the gas phase pressure, and input boundary conditions for the molar gas and liquid fractions obtained by the component fugacities  $f = pc$  in the gallery:

$$P^g = p, \quad f = pc, \quad P^g - P^l = -\zeta^l RT \ln \left( \frac{f_e}{P_{sat}(T) \left( 1 - \sum_{j \in \mathcal{C} \setminus \{e\}} \frac{f_j}{H_j(T)} \right)} \right). \quad (3)$$

This model is applied to the simulation of the mass exchanges at the interface between the Callovo Oxfordian argillite and the ventilation excavated gallery in a nuclear waste geological repository. The convergence of the Vertex Approximate Gradient discretization [2] is analysed for a simplified model coupling the Richards approximation in the porous media and the gas pressure single component equation in the gallery.

## Références

- [1] MOSTHAF K., BABER K., FLEMISCH B., HELMIG R., LEIJNSE A., RYBAK I., WOHLMUTH B., A coupling concept for two-phase compositional porous-medium and single-phase compositional free flow, *Water Resources Research*, 47, 10, 2011.
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