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Multiphase multicomponent modelling of the NAPL transfer in the subsurface using CubiM simulator

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Mass balance equations

By component

The model consists of four α phases: solid phase s , gaseous phase g and two liquid phases w, o , for water and NAPL respectively. Each of these phases is composed of i components and has their own volumetric mass density ρ_α and saturation s_α . The saturations must satisfy the closure relation $\sum_\alpha s_\alpha = 1$. Let the volume fraction be $\epsilon_\alpha = \phi s_\alpha$ with ϕ the porosity. For each component i present in phase α , macroscopic mass conservation equations describing reactive transport and mass transfer exchange of liquid and solid phase species are written as:

$$\partial_t(\epsilon_\alpha \rho_\alpha \omega_{\alpha,i}) + \nabla \cdot (\epsilon_\alpha \rho_\alpha \omega_{\alpha,i} \mathbf{v}_\alpha + \epsilon_\alpha \mathbf{j}_{\alpha,i}) = \epsilon_\alpha r_{\alpha,i} + \sum_{\beta \neq \alpha} e_{\alpha,i}^{\alpha\beta}, \quad (1)$$

where $\omega_{\alpha,i}$ is the mass fraction of component i in phase α , \mathbf{v}_α is the mean pore velocity of phase α , $\mathbf{j}_{\alpha,i}$ is the intrinsic mass dispersion vector, $r_{\alpha,i}$ is the biodegradation rate and $e_{\alpha,i}^{\alpha\beta}$ the rate of mass transfer of species i into the α phase at the $\alpha\beta$ interface including sorption, volatilization and dissolution in $M/(L^3T)$. At the scale of a Representative Elementary Volume (REV) of porous medium, the vector of specific discharge (or Darcy velocity) of each phase at reference pressure for a saturation distribution is given by Muskat law:

$$\mathbf{q}_\alpha = \epsilon_\alpha \mathbf{v}_\alpha = -\frac{kr_\alpha(s_\alpha)}{\mu_\alpha} \mathbf{K}_s \cdot (\nabla p_\alpha - \rho_\alpha \mathbf{g}), \quad (2)$$

where \mathbf{K}_s is the absolute permeability tensor, μ_α is the dynamic viscosity of phase α , kr_α is the relative permeability of phase α , \mathbf{g} the gravitational acceleration vector, p_α is the intrinsic pressure of phase α . The model is completed by the capillary-pressure relationship:

By phase

The mass balance equations for each phase α are obtained by summing equation 1 over all species i present in the given phase α . For example, in the liquid phase one has:

$$\partial_t(\epsilon_\alpha \rho_\alpha) + \nabla \cdot (\epsilon_\alpha \rho_\alpha \mathbf{v}_\alpha) = \epsilon_\alpha r_\alpha + e_\alpha^{\alpha\beta} + \rho_\alpha q_\alpha, \quad (3)$$

where q_α is the sink/source flow rate ($1/T$), $e_\alpha^{\alpha\beta}$ is the rate of mass transfer between α and β phases and r_α is the sum of macroscopic rate production (reactive term) per unit of volume of α phase $M/(L^3/T)$. Volumetric mass density of each phase is considered to be variable with phase composition especially for the NAPL phase. Both phases are supposed to be mobile. CubicM is able to model active transport in both phases, NAPL entrapment, phase consumption due to dissolution and saturated biodegradation. User provide a reference component in each liquid phase (specific mass density, molar mass), (for example H_2O for both NAPL and water phase and nitrogen N_2 in the gas phase).

Aqueous components are subject to local chemical reactions. When chemical reaction are driven by microorganisms (biotic degradation), cubicM supposes that microorganisms are freely available in the porous media. Therefore, cubicM does not simulate biomass evolution.

Numerical scheme using Method-of-Lines approach

For space discretization, a Control Volume Finite Element method previously presented is performed with upstream weighting phase mobilities. For the time discretization, the time-stepping strategy is fully implicit/fully coupled using FLC-BDF scheme for a maximum of robustness and time efficiency. It is performed on fully unstructured meshes using Gmsh mesh generator [1] and produces monotone solutions on highly distorted grids. The method conserves mass locally (vertex centered) in order to get correct shock positions and to manage small concentrations. We obtained for a three-phase flow calculation the semi-discrete systems in (p_g, s_w, s_o) . Writing the weak formulation in terms of coefficient vectors of a system of Ordinary Differential Equations (ODE), or Differential Algebraic Equation (DAE) for the slightly compressible liquids (ρ_l constant), we can re-formulate the time variational term involving M_α in a mass matrix form (transport equation are also provided here) on a control volume i :

$$\underbrace{\begin{pmatrix} M_{gg} & M_{gw} & M_{go} \\ M_{wg} & M_{ww} & M_{wo} \\ M_{og} & M_{ow} & M_{oo} \end{pmatrix}}_{\mathbf{A}_i} \underbrace{\begin{bmatrix} \frac{\partial p_g}{\partial t} \\ \frac{\partial s_w}{\partial t} \\ \frac{\partial s_o}{\partial t} \end{bmatrix}}_{\partial y_i / \partial t} = \underbrace{\begin{bmatrix} -G_g(\mathbf{p}_g(t), \mathbf{s}_w(t), \mathbf{s}_o(t)) - Q_g(\mathbf{p}_g(t), \mathbf{s}_w(t), \mathbf{s}_o(t)) \\ -G_w(\mathbf{p}_g(t), \mathbf{s}_w(t), \mathbf{s}_o(t)) - Q_w(\mathbf{p}_g(t), \mathbf{s}_w(t), \mathbf{s}_o(t)) \\ -G_o(\mathbf{p}_g(t), \mathbf{s}_w(t), \mathbf{s}_o(t)) - Q_o(\mathbf{p}_g(t), \mathbf{s}_w(t), \mathbf{s}_o(t)) \end{bmatrix}}_{FC} \quad (4)$$

$$\begin{pmatrix} \epsilon_g \frac{\rho_g}{P_g} & -\phi \rho_g & -\phi \rho_g & \epsilon_g \rho_g \left(1 - \omega_1^g \frac{M_g}{M_1}\right) & \epsilon_g \rho_g \left(1 - \omega_2^g \frac{M_g}{M_2}\right) & \epsilon_g \rho_g \left(1 - \omega_3^g \frac{M_g}{M_3}\right) & \times & \times & \times & \times \\ \times & \phi \rho_w & \times & \times & \times & \times & \times & \times & \times & \times \\ \times & \times & \phi \rho_o & \times & \times & \times & \times & \times & -\epsilon_o \rho_o^2 \left(\frac{1}{\rho_1} - \frac{1}{\rho_{sol}}\right) & -\epsilon_o \rho_o^2 \left(\frac{1}{\rho_2} - \frac{1}{\rho_{sol}}\right) \\ \times & \times & \times & \epsilon_g \rho_g & \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \epsilon_g \rho_g & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \epsilon_g \rho_g & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times & \epsilon_w \rho_w & \times & \times & \times \\ \times & \times & \times & \times & \times & \times & \times & \epsilon_w \rho_w & \times & \times \\ \times & \times & \times & \times & \times & \times & \times & \times & \epsilon_o \rho_o & \times \\ \times & \times & \times & \times & \times & \times & \times & \times & \times & \epsilon_o \rho_o \end{pmatrix}$$

Figure 1: Three-phase flow and transport A-matrix formulation

Test case: fate of the NAPL plume: dissolution and degradation

The test case presented here consists in simulating the dissolution mechanisms NAPL / water with 2 compounds: PCE and TCE. The test case is realized on a 3D bar of 250 m length, (50×10) m² of section. It is a single phase flow with a porous media saturated with water. The presence of an immobile NAPL (composed of a mixture of 2 species) induces dissolution and transport mechanisms of the dissolved compounds in water. The adsorption / desorption mechanisms and biodegradation are also taken into account.

We notice the decrease of the mass fractions in the two blocks linked to a lower permeability. The mass fractions of PCE and TCE in water are close to equilibrium after one year. The effect related to the release in the water of the adsorbed species (dotted) is for the moment masked by the predominant dissolution and degradation (order 1). Quantity of vinyl chloride plume at 365 days and water streamlines are presented in figure 2. Dissolved mass fraction are overestimated because volatilization is not taken into account (quality limit $0.5 \mu\text{g/l}$).

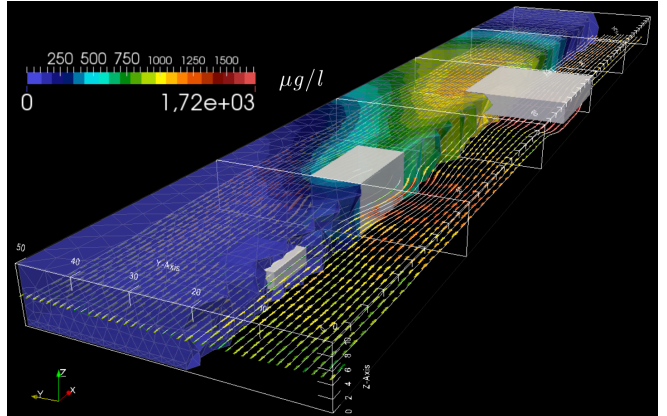


Figure 2: Vinyl Chloride plume at 365 days and water streamlines [2]

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