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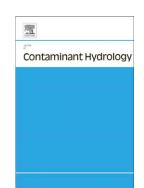
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## **ACCEPTED MANUSCRIPT**

# Comparison of theory and experiment for NAPL dissolution in porous media

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#### Abstract

Contamination of groundwater resources by an immiscible organic phase commonly called NAPL (Non Aqueous Phase Liquid) represents a major scientific challenge considering the residence time of such a pollutant. This contamination leads to the formation of NAPL blobs trapped in the soil and impact of this residual saturation cannot be ignored for correct predictions of the contaminant fate. In this paper, we present results of micromodel experiments on the dissolution of pure hydrocarbon phase (toluene). They were conducted for two values of the Péclet number. These experiments provide data for comparison and validation of a two-phase non-equilibrium theoretical model developed by Quintard and Whitaker (1994) using the volume averaging method. The model was directly upscaled from the averaged pore-scale mass balance equations. The effective properties of the macroscopic model were calculated over periodic unit cells designed from images of the experimental flow cell. Comparison of experimental and numerical results shows that the transport model predicts correctly - with no fitting parameters - the main mechanisms of NAPL mass transfer. The study highlights the crucial need of having a fair recovery of pore-scale characteristic lengths to predict the mass transfer coefficient with accuracy.

#### Keuwords:

Porous media, NAPL dissolution, Upscaling, Volume averaging method

#### List of symbols

 $A_{ij}$  Interface between the *i*- phase and *j*- phase (i,j:  $\omega, \beta, \gamma, k$ )

 $\mathbf{b}'_{\beta}$  Dimensionless form of the closure variable  $\mathbf{b}_{\beta}$ , (-)

 $C_a$  =  $\frac{\|\mathbf{v}_{\beta}\|\mu_{\beta}}{\sigma_{\beta\gamma}}$ , Capillary number, (-)

 $c_{A\beta}$  Pore scale concentration of species A in the  $\beta$  phase, (kg  $m^{-3}$ )

 $\langle c_{A\beta} \rangle$  Averaged concentration of species A in the  $\beta$ - phase, (kg  $m^{-3}$ )

 $c_{A\beta}^{eq}$  Concentration of species A in the  $\beta$ - phase in equilibrium with  $\rho_{\gamma}$ , (kg  $m^{-3}$ )

 $c_f$  Circularity, (-)

 $c_0$  Injected concentration in the complex 2D geometry, (kg  $m^{-3}$ )

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