Numerical Simulation to Study the Effects of 
Multiphase and Multi-component on Transport 
of Oil Derivatives in a Porous Media

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Abstract

The numerical model, which we established, described the transport of the derivatives oil in the unsaturated zone of a porous media, leading to the contamination of groundwater. We consider in this study two important purposes: the multi-component effect and the multiphase effect. Based on method of scaling, we rewrite all the equations established already at the pores level in the scale of the aquifers. By using a numerical approach based on the finite volume method, we solved the equations, which described our problem.

**Keywords:** Multiphase effect, multi-component effect, porous media, unsaturated zone, finite volume method

1. Introduction

In the current paper, we studied the phenomena of transport of the oil derivatives; most used industrially such TCE (trichloroethylene) and PCE (tetrachloroethylene), and trapped in the unsaturated zone of the ground. These oil derivatives are volatile and not very soluble in water. They constitute a non-miscible phase, and cause a harmful to the human health [Bohy and al., 2004], [Pankow and al., 1996]. Being given their strong volatility and their immiscibility which reveal the notion of the non-aqueous phase, these species can be transferred towards to the near layers and then to the atmosphere and can affect their qualities [Benremita & Schäfer, 2003].

In the literature, most studies treating the transport of hydrocarbons are devoted to the pure substances (mono-constituent), in addition, the coefficient of mass transfer which characterizes the inter-phase exchanges is often neglected [Khachikian and Harmon, 2000]. One however notes some recent studies on the subject [Coutelieris and al., 2006].

The originality of this study is to establish a numerical code to characterize simultaneously the impact of the multiphase aspect and the presence of several solvents. Indeed, these interactions, which make the simulation of transport delicate since the assessments of all the species, are strongly nonlinear. Firstly, we establish the governing equations of our problem on a microscopic scale. Then, we use the method of volume average [Whitaker, 1991] and the decomposition of Gray in order to have the equations on a macroscopic scale. We adopt a numerical code based on the finite volume method to discretize the obtained equations.

2. Pore scale

On a microscopic scale, the presence of the pollutant in the three phases is due to the fact that each pollutant locally participate in different mass transfer, towards the
aqueous phase, the vapor phase and possibly, towards the solid phase of the porous matrix [Bear, 1987].

The mechanism of dissociation represents the transfer of the chemical compounds of the organic phase into the aqueous phase. One notes a continuous contribution of molecules dissolved in the aqueous phase and one continues source area containing the pollutant on a non-aqueous phase.

These transfers can be studied using two mechanisms of dissolution: local equilibrium and non-local one. We adopt the second mechanism of dissociation: non-local equilibrium where the duration of complete dissolution of the mixture of two chlorinated solvents (TCE and PCE) is much longer and modeling becomes more complex.

The relations, which are necessary to predict and describe the phenomenon of the pollution of underground, concern fundamental processes. Indeed, the governing equations of the problem are the mass conservation, energy conservation and transport of aqueous solution.

At the level of pores, each phase can be treated like a continuous space and the porous media is regarded as a set of more or less imbricates continuous mediums. One established the equations for each phase independently of both others.

2.1 Equations of flow

We attend a diphase flow with knowing aqueous phase and vapor phase, therefore the equations governing this flow at the level of pore are written as:

\[ \mu_p \ddot{v}_p - \nabla \rho_p = -\rho_p \ddot{g} \]  

(1)

Where, \( \varphi \), represents the vapor phase and the aqueous phase

2.2 Transport equations

2.2.1 Phase \( \varphi \)

The equations of weight breakdown for each mobile phase are:

\[ \frac{\partial \rho_{\varphi}}{\partial t} + v(\rho_{\varphi} \omega_{\varphi} \tilde{v}_{\varphi}) = 0 \]  

(2)

\[ \bar{V} \cdot \tilde{v}_{\varphi} = 0 \]  

(3)

2.2.2 Phase \( \gamma \)

This phase is supposed to be motionless; the weight breakdown takes the following shape:

\[ \frac{\partial \rho_\gamma}{\partial t} = 0 \]  

(4)

The relation (3) corresponds to the total weight breakdown of the phase \( \varphi \).

\( \rho_\varphi \) is supposed to be constant. The flow of component can be broken up into two terms: convective term and a diffusive term [Quintard and al, 2006]:

\[ \rho_\varphi \omega_\varphi \tilde{v}_\varphi = \rho_\varphi \omega_\varphi \tilde{v}_\varphi - D_{\varphi} \frac{\partial}{\partial v} (\rho_\varphi \omega_\varphi) \]  

(5)
2.3 Equation of heat conservation

The transfer of energy in porous media, at the level of pores, is defined as being the transfer of heat in the three coexistent phases besides the solid phase, which constitutes the porous matrix [Kaviany, 1999].

2.3.1 Phase $\phi$

$$\frac{\partial \rho_{\phi} c_{p\phi} T}{\partial t} + \rho_{\phi} c_{p\phi} \bar{V}_\phi T - \bar{V} (\lambda_{\phi} \bar{V} T) = 0$$

(6)

2.3.2 Phase $\gamma$

$$\frac{\partial \rho_{\gamma} c_{p\gamma} T}{\partial t} - \bar{V} (\lambda_{\gamma} \bar{V} T) = 0$$

(7)

2.3.3 Phase $\sigma$

$$\frac{\partial \rho_{\sigma} c_{p\sigma} T}{\partial t} - \bar{V} (\lambda_{\sigma} \bar{V} T) = 0$$

(8)

3. Darcy scale

The description of the phenomena on a macroscopic scale uses the generalized Darcy relation [Dullien, 1992] for the two mobile phases, the equations of mass conservation of the two mobile phases, and the transfer equations of the species in the vapor phases, and the conservation equation of the temperature.

At the level of Darcy, one gathers the equations of the temperature (6), (7) and (8) to have only one equation. The equations, which govern our model, become:

3.1 Equations of flow

Phase $\phi$

$$\bar{V}_\phi = - \frac{KK_{\phi}}{\mu_{\phi}} \bar{V} (\rho_{\phi} - \rho_{\phi} g z)$$

(9)

$$\bar{V} \bar{V}_\phi = 0$$

(10)

3.2 Transport equations

3.2.1 Phase $V$
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\[ \varepsilon_\gamma \frac{\partial C_{i\gamma}}{\partial t} + \vec{v}_i \cdot \vec{\nabla} C_{i\gamma} - \vec{v}_i \left( \varepsilon_\gamma D_{i\gamma} \vec{\nabla} C_{i\gamma} \right) + R_\gamma = 0 \]  \tag{11}

3.2.2 Phase \( \beta \)

\[ \varepsilon_\beta \frac{\partial C_{i\beta}}{\partial t} + \vec{v}_i \cdot \vec{\nabla} C_{i\beta} - \vec{v}_i \left( \varepsilon_\beta D_{i\beta} \vec{\nabla} C_{i\beta} \right) + \alpha_\beta (C_{i\beta} - C_{i\beta}^{eq}) = 0 \]  \tag{12}

3.3 Equation of evolution of the non-aqueous phase

\[ \frac{\partial \rho_i}{\partial t} - \sum_{\gamma=1}^{i} \alpha_\gamma (C_{i\gamma} - C_{i\gamma}^{eq}) - R_\gamma = 0 \]  \tag{13}

3.4 Equation of the temperature

We pose: \( \varepsilon = \varepsilon_\gamma + \varepsilon_\beta + \varepsilon_\gamma \)

\[ \begin{bmatrix} \varepsilon_\gamma \rho_i c_{pv} + \varepsilon_\beta \rho_i c_{ph} + (1 - \varepsilon) \rho_\sigma c_{\sigma \rho} \end{bmatrix} \frac{\partial T}{\partial t} + \frac{\partial \left( \varepsilon_\gamma c_{pv} \vec{v}_i \right) T}{\partial t} + \left( \varepsilon_\gamma c_{pv} \vec{v}_i + \varepsilon_\beta c_{ph} \vec{v}_i \right) \frac{\nabla T}{\nabla} \]

\[ \vec{v}_i \left( \left( \varepsilon_\gamma \lambda_\gamma + \varepsilon_\beta \lambda_\beta + \varepsilon_\gamma \lambda_\gamma + (1 - \varepsilon) \lambda_\sigma \right) \frac{\nabla T}{\nabla} \right) = 0 \]  \tag{14}

We are interested to solve this problem using one-dimensional geometry. Indeed, speed is given according to the longitudinal axis:

\[ \vec{v}_o = W_o \vec{z} \]  \tag{15}

The linear dispersion of the scatter coefficient takes the following shape [Quintard and al, 2006]:

\[ D_{\omega \rho} = D_{\omega \rho} + \alpha_\omega \| \vec{v}_\rho \| / l \]  \tag{16}

4. Boundary condition

The solution of the partial derivative equations, which describe the flow in the unsaturated zone of the ground, requires the definition of the initial conditions and the boundary conditions. We choose the conditions of Dirichlet, these conditions express that during an injection of aqueous solution on the surface of the ground, this one is subjected immediately and regularly to a concentration \( C_{i\gamma}^{eq} \).

4.1 Initial condition

At \( t=0 \) \( T = T_0, C_{i\beta} = C_{i\beta}^{eq} X_i, \) and \( C_{iv} = 0 \)

4.2 Boundary conditions
At $z = 0$ \quad $T_{(0,0)} = T_0$,

At $z = L$ \quad $T_{(L,L)} = T_i$ and $C_i = C_f = 0$

5. Method of solution

There exist many numerical methods, which make it possible to transform the differential equations into algebraic equations. We choose the use of the method of finite volume method [Patankar, 1980], [Gueraoui and al, 2008] of implicit type. The choice of such method is based primarily on reasons of stability and thus of time-saver of calculation.

The principle of this method consists in integrating the equations to solve on a control volume centered in space and on an interval of time [Versteeg and Malalasekera, 1995].

5.1 Equation of flow

The equations of flow of the vapor phase and the aqueous phase in discretized form are written:

$W_{Vp}^{i+1}_j = \chi_i \left[ \frac{P_{Vp}^{i+1} - P_{Vp}^i}{2\Delta z} - \rho_f g \right]$

$W_{Vp}^{i+1}_j = \chi_p \left[ \frac{P_{Vp}^{i+1} - P_{Vp}^i}{2\Delta z} - \rho_p g \right]$

5.2 Transport equations

5.2.1 Phase $V$

The transport equation in the vapor phase in discretized form is written:

$A C_{Vp}^{i+1} + B C_{Vp}^{i+1} + C C_{Vp}^{i+1} = D$

5.2.2 Phase $\beta$

$A = \frac{W_{Vp}^{i+1} - \varepsilon_i}{2\Delta z} \left[ \frac{D_{Vp}}{2} + \frac{D_{Vp}}{2} \right] \frac{\Delta t}{\Delta z}$

$B = \varepsilon_i \left[ \frac{D_{Vp}}{2} + 2D_{Vp} + D_{Vp} \right] \frac{\Delta t}{\Delta z}$

$C = \frac{W_{Vp}^{i+1} - \varepsilon_i}{2\Delta z} \left[ \frac{D_{Vp}}{2} + \frac{D_{Vp}}{2} \right] \frac{\Delta t}{\Delta z}$

$D = \varepsilon_i C_{Vp} - \bar{R}_{Vp} \Delta t$
The transport equation in the aqueous phase in discretized form is written:

\[
AC_{iE}^{t+\Delta t} + BC_{iP}^{t+\Delta t} + CC_{iD}^{t+\Delta t} = D
\]

\[
A = \frac{W_{iE}^{t+\Delta t}}{2\Delta z} - \frac{\varepsilon_{\rho}}{2} \left[ D_{iE}^{t+\Delta t} + D_{iD}^{t+\Delta t} \right] \frac{\Delta t}{\Delta z} + \beta_{\rho} \Delta t
\]

\[
B = \frac{W_{iP}^{t+\Delta t}}{2\Delta z} - \frac{\varepsilon_{\rho}}{2} \left[ D_{iP}^{t+\Delta t} + 2D_{iD}^{t+\Delta t} + D_{iD}^{t+\Delta t} \right] \frac{\Delta t}{\Delta z} + \beta_{\rho} \Delta t
\]

\[
C = \frac{W_{iD}^{t+\Delta t}}{2\Delta z} - \frac{\varepsilon_{\rho}}{2} \left[ D_{iD}^{t+\Delta t} + D_{iD}^{t+\Delta t} \right] \frac{\Delta t}{\Delta z} + \beta_{\rho} \Delta t
\]

\[
D = \varepsilon_{\rho} C_{iD}^{t+\Delta t} + \alpha_{\rho} C_{iD}^{t+\Delta t} \Delta t
\]

5.3 Equations of evolution of the not-aqueous phase

The equation of evolution of the not-aqueous phase in discretized form is written:

\[
\rho_{iP}^{t+\Delta t} V_{iP}^{t+\Delta t} = \rho_{iP}^{t} V_{iP}^{t} + \alpha_{\rho} \left( C_{iP}^{t+\Delta t} \Delta t - C_{eq}^{t+\Delta t} \right) + \overline{R}_{iP}^{t+\Delta t} \Delta t
\]

5.4 Conservation equations of heat

The conservation equation of heat in discretized form is written as:

\[
AT_{iE}^{t+\Delta t} + BT_{iP}^{t+\Delta t} + CT_{iD}^{t+\Delta t} = D
\]

\[
A = \frac{\Delta t}{4\Delta z} \left[ X_{i} \left( W_{iE}^{t+\Delta t} + W_{iD}^{t+\Delta t} \right) + X_{i} \left( W_{iE}^{t+\Delta t} + W_{iD}^{t+\Delta t} \right) \right] - \frac{\Delta t}{\Delta z} X_{i}
\]

\[
B = X_{i} \left( W_{iP}^{t+\Delta t} + W_{iD}^{t+\Delta t} \right) + X_{i} \left( W_{iP}^{t+\Delta t} + W_{iD}^{t+\Delta t} \right) \frac{2\Delta t}{\Delta z} X_{i}
\]

\[
C = \frac{\Delta t}{4\Delta z} \left[ X_{i} \left( W_{iE}^{t+\Delta t} + W_{iD}^{t+\Delta t} \right) + X_{i} \left( W_{iE}^{t+\Delta t} + W_{iD}^{t+\Delta t} \right) \right] - \frac{\Delta t}{\Delta z} X_{i}
\]

\[
D = \left( X_{i} + X_{i} \right) R_{iP}^{t+\Delta t}
\]
6. RESULTATS

Figure 1 : Evolution of the profile $C_{\text{pmax}}$ according to $Z$ (t=Tp/2, Es=0,25)

Figure 2 : Evolution of the profile $C_{\text{pce}}$ according to $Z$ (t=Tp/2, Es=0,25)

Figure 3 : Evolution of the profile of $C_{\text{pce}}$ according to time $t$ (Z=1/2, Es=0,25)
Figure 4: Evolution of the profile of $\rho_\gamma$ according to the mass fraction of PCE

Figure 5: Evolution of the profile of the temperature according to $Z$ (with $t=\frac{T}{2}$)

Figure 6: Evolution of the profile of the pressure according to $Z$ (with $t=\frac{T}{2}$)
Figures 1 and 2 illustrate the evolution of the concentration of pollutants in question (TCE and PCE) in the aqueous phase according to depth $Z$ at the moment $t=\frac{T_p}{2}$ ($T_p$ is the duration of follow-up of the phenomenon and $E_s=0.25$, porosity). We notice that the concentration decreases with the depth and it is obvious since one moves away from the source and consequently more and less pollutants arrive at the distant depths.

Figure 3 represents the evolution of the profile of the concentration of component TCE in the aqueous phase according to time $T$ with a section $z=l/2$ depth. We see that progressively time passes; there is an accumulation of pollutant to this section. This result is in perfect agreement with the results got by other authors [Hami and al., 2001].

On figure 4, one notes for a mixture of TCE and PCE, the density of the mixture varies little and linearly with the mass composition of the components. These results are similar to those found by other authors [Quintard and al., 2006].

On figure 5, we notice that the temperature increases as $Z$ increases, which is checked physically and by other authors [Ghouli and al., 2009].

On figure 6, we present the evolution to a given moment and within the space of the pressure. We note that the pressure increases more than one approaches the tablecloth [Ghouli and al., 2009].

By comparing figure 1 and figure 7, we observe, that at a given moment and at a given point of space, that if the porosity of the medium decreases then the concentration of the component in this phase decreases. This result can be explained owing to the fact that the bulk fraction of the aqueous phase increases.
7. CONCLUSION

The established code gives us the possibility to simulate the process of transport of pollutants in the unsaturated zone of a porous media. We solved the obtained equations in one-dimensional geometry. The obtained results are in perfect agreement with those of other authors who deal with the same problem.

8. NOMENCLATURE

$V, \beta, \gamma$ and $\sigma$: Identify the phases respectively: vapor, aqueous, non-aqueous and solid

$\varphi$: Index of phase representing $V$ and $\beta$

$\tilde{v}_{\varphi}$: The speed of the phase $\varphi$ in scale pore

$\tilde{v}_{\varphi}^r$: The speed of phase $\varphi$ at Darcy scale

$\tilde{v}_{\varphi}$: The speed of pollutant I in phase $\varphi$

$\omega_{\varphi}$: The mass fraction of pollutant I in phase $\varphi$

$\alpha_i$: Coefficient of mass transfer between $\beta - \gamma$

$R_\gamma$: The evaporated quantity

$T$: Temperature

$C_{\varphi}$: Concentration of pollutant I in phase $\varphi$

$C_{\varphi}^{eq}$: Concentration at the equilibrium of pollutant I

$D_{\varphi}^*$: Effective dispersion coefficient of pollutant I in phase $\varphi$

$D_{\varphi}$: Corrected effective dispersion coefficient of pollutant I in phase $\varphi$

$\rho_\varphi, \rho_\beta, \rho_\sigma$: Bulk masses respectively $\varphi, \beta$ and $\sigma$ phases

$c_{\rho_\varphi}, c_{\rho_\beta}, c_{\rho_\sigma}$: specific heats respectively of the phases $\varphi, \beta$ and $\sigma$

$\lambda_\varphi, \lambda_\beta, \lambda_\sigma$: Coefficients of conductivity respectively of the phases $\varphi, \beta$ and $\sigma$

$\epsilon_\gamma, \epsilon_\beta, \epsilon_\sigma$: Bulk fractions respectively of the vapor phases, aqueous and non-aqueous

$\alpha_{i\varphi}$: The transverse scatter coefficient in the phase $\varphi$

$I$: identity matrix

$X_{\varphi}$: Average molar fraction of I in the phase $\gamma$
REFERENCES


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