Numerical and mathematical simulation of the influence of the Soret effect on the transport of hydrocarbons chlorinated in a porous media in two-dimension geometry

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Abstract

We require this mathematical and numerical modeling in order to evidence the influence of the soret effect on the transport of hydrocarbons chlorinated in a porous media. Besides the multiphase aspect and the multi-components aspect, we consider, in this study, a third important aspect: Soret effect. Via the method of scaling, we transcribe the equations governing this problem, already written in pore scale, at the macroscopic scale. Since the differential equations established are coupled and nonlinear, the problem will be solved numerically by using a numerical approach based on the finite volume method.

Keywords: Soret effect, Chlorinated hydrocarbons, Multiphase effect, multi-component effect, porous media, unsatured zone, finite volume method

Nomenclature

V	:	Vapor phase;	T	:	Temperature;
β	:	Aqueous Phase;	$C_{i\varphi}$	:	Concentration of species (i) in the φ-phase;
γ	:	Non-aqueous phase;	C_i^{eq}	:	Equilibrium concentration of species (i);
σ	:	Solid phase;	$S_{T\varphi}$	:	Soret coefficient for φ-phase;
φ	:	Phase index representing V and β;	$D_{Ti\varphi}$	:	Molar thermo-diffusion coefficient of species (i) in the φ-phase;
$\vec{v}_\varphi$	:	Fluid velocity in the φ-phase (microscopic scale);	$D_{i\varphi}$	:	Dispersion coefficient of species (i) in the φ-phase;
$\vec{V}_\varphi$	:	Fluid velocity in the φ-phase (macroscopic scale);	$D_{i\varphi}^*$	:	Effective Dispersion coefficient of species (i) in the φ-phase;
$\vec{V}_{i\varphi}$	:	Velocity of species (i) in the φ-phase;	$\rho_\varphi, \rho_\gamma, \rho_\sigma$	:	Density respectively of the φ-phase, γ-phase and σ-phase;
$\omega_{i\varphi}$	:	mass fraction of species (i) in the φ_phase;	$C_{P\varphi}, C_{P\gamma}, C_{P\sigma}$	:	Specific heat capacity respectively of the φ-phase, γ-phase and σ-phase;
α_i	:	mass exchange coefficient of species (i);	I	:	Identity matrix;
$\lambda_\varphi, \lambda_\gamma, \lambda_\sigma$	:	Conductivity coefficients respectively of the φ-phase, γ-phase and σ-phase;	$\alpha_{i\varphi T}$	:	Transverse dispersion coefficient of species (i) in the φ-phase;
$\varepsilon_V, \varepsilon_\beta, \varepsilon_\gamma$	:	Volume fraction respectively of the V-phase, β-phase and γ-phase;	$X_{i\gamma}$	:	Average mole fraction of species (i) in the γ-phase.
R_γ	:	Evaporation quantity;			

1. Introduction

In this paper, we are interested to the influence of soret effect in addition to the multiphase effect on a mixture of the hydrocarbons chlorinated, most used industrially as Trichloroethylene and Tetrachloroethylene. Their low solubility in water constitutes a non-miscible phase [1]. This phase is trapped in the porous matrix and its compounds can be transferred towards the atmosphere especially by diffusion [2] and towards the aquifer by the molecular diffusion and dispersion [3]. Then they affect their qualities and cause a danger to the human health [4].

Several studies are approached the subject of transport of hydrocarbons. But, the majority of these studies is confined with the pure substances (mono component) and without taking into consideration the soret effect and the exchanges inter-phasiques are often neglected [5]. However, we note some recent studies on the subject [6, 7, and 21]. For the vapor phase, this effect was theoretically predicted [24]. Other authors studied the influence of soret effect on a single phase mixture [22].

The originality of this work is to highlight, on geometry of two dimensions, the influence of the soret effect and the multiphase effect on a multi-component mixture or the interactions between the various components make the simulation of transport delicate since the assessments of all the species strongly nonlinear and are coupled. After the establishing of the equations governing our problem on a microscopic scale, we use the method of the volume average [8] and the decomposition of Gray [9] in order to have the equations on a macroscopic scale. Then, we adopt the finite volume method to transform the obtained equations en algebraic ones.

2. Pore scale

On a microscopic scale, the pollutant undergoes some different type of mass transfer, towards the aqueous phase, the vapor phase and possibly towards the solid phase of the porous matrix, which justifies the presence of the pollutant in the three phases and possibly by adsorption in the solid phase [10].

At this scale, the mechanism of dissociation is translated by the transfer of the chemical components of the organic phase towards the aqueous phase. We note in this case, a continuous contribution of molecules solubilized in the aqueous phase and a continuous source containing the pollutant. These transfers can be studied using two mechanisms of dissolution: local equilibrium and non-local one. We adopt the second mechanism of dissociation: not 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 based on fundamental processes. Indeed, the equations governing the problem are deduced from those of conservation of mass, of conservation of energy and transport of aqueous solution.

At the pore scale, each phase can be treated as a continue space. Thus, we established the equations for each phase independently of the others.

2.1. *Equations of flow*

We are witnessing a two phase flow that is the aqueous phase and the vapor phase, so the equations governing this flow on the scale of pore are writing:

$$\mu_\phi \vec{\nabla}^2 v_\phi - \vec{\nabla} p_\phi = -\rho_\phi \vec{g} \tag{1}$$

Where φ represent the vapor phase and the aqueous phase.

2.2. *Transport equations*

2.2.1. *Phase* φ

In the case of a single-phase multicomponent mixture, the temperature gradient induces a material displacement effect, in addition to the classical Fick's law. The total flow for the compound in phase is expressed as follows [23]:

$$\vec{J}_{i\phi} = -D_{i\phi} \vec{\nabla}(\rho_\phi \omega_{i\phi}) - D_{Ti\phi} \vec{\nabla} T_\phi \tag{2}$$

The mass balance equations for each mobile phase are:

$$\frac{\partial \rho_\varphi \omega_{i\varphi}}{\partial t} + \vec{\nabla}.(\rho_\varphi \omega_{i\varphi} \vec{v}_{i\varphi)} = 0 \tag{3}$$

$$\vec{\nabla}.\vec{v}_\varphi = 0 \tag{4}$$

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2.2.2. *Phase* γ
This phase is assumed stationary; the mass balance takes the following form:

$$\frac{\partial \rho_\gamma}{\partial t} = 0 \tag{5}$$

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

ρ_ϕ is supposed to be constant. The flow of component can be broken up into two terms: convective term and a diffusive term [11]:

$$\rho_\phi \omega_{i\phi} \vec{v}_{i\phi} = \rho_\phi \omega_{i\phi} \vec{V}_\phi + \vec{J}_{i\phi} \tag{6}$$

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 [12].

2.3.1. *Phase* φ

$$\frac{\partial \rho_\varphi c_{P\varphi} T}{\partial t} + \rho_\varphi c_{P\varphi} \vec{v}_\varphi . \vec{\nabla} T - \vec{\nabla}.\left(\lambda_\varphi \vec{\nabla} T\right) = 0 \tag{7}$$

2.3.2. *Phase* γ

$$\frac{\partial \rho_\gamma c_{P\gamma} T}{\partial t} - \vec{\nabla}.\left(\lambda_\gamma \vec{\nabla} T\right) = 0 \tag{8}$$

2.3.3. *Phase* σ

$$\frac{\partial \rho_\sigma c_{P\sigma} T}{\partial t} - \vec{\nabla}.\left(\lambda_\sigma \vec{\nabla} T\right) = 0 \tag{9}$$

3. Darcy scale
In order to obtain a macroscopic description of the phenomena we want to model and define new effective properties, we need to change the scale, from the microscopic to the Darcy scale. To this end we adopt the method of the volume average. [6, 13, 14].
The description of the phenomena on a macroscopic scale uses the generalized Darcy relation [15] for both mobile phases, the mass balance equations of the two mobile phases, transfer equations of the species in the vapor phases, aqueous and non-aqueous, the equation for the non-aqueous phase and the heat transfer equation.

The equations governing our model become:

3.1. *Equations of flow*
3.1.1. *Phase* φ

$$\vec{V}_\varphi = -\frac{KK_{r\varphi}}{\mu_\varphi} \vec{\nabla}\left(P_\varphi - \rho_\varphi gz\right) \tag{10}$$

$$\vec{\nabla}.\vec{V}_\varphi = 0 \tag{11}$$

3.2. *Transport equations*
3.2.1. *Phase* V

$$\varepsilon_V \frac{\partial C_{iV}}{\partial t} + \vec{V}_V . \vec{\nabla} C_{iV} - \vec{\nabla}. \varepsilon_V D_{iV}^*\left(\vec{\nabla} C_{iV} + S_{TV} \vec{\nabla} T_V\right) + R_\gamma = 0 \tag{12}$$

3.2.2. *Phase* β

$$\varepsilon_\beta \frac{\partial C_{i\beta}}{\partial t} + \vec{V}_\beta . \vec{\nabla} C_{i\beta} - \vec{\nabla}.\left(\varepsilon_\beta D_{i\beta}^*\left(\vec{\nabla} C_\beta + S_{T\beta} \vec{\nabla} T\right)\right) + \alpha_i\left(C_{i\beta} - C_i^{eq} X_{i\gamma}\right) = 0 \tag{13}$$

With :

$$S_{T\phi} = \frac{D_{T\phi}}{D_\phi} \tag{14}$$

3.3. *Equation of evolution of the non-aqueous phase*

$$\frac{\partial \rho_\gamma \varepsilon_\gamma}{\partial t} - \sum_{i=1}^{2} \alpha_i\left(C_{i\beta} - C_i^{eq} X_{i\gamma}\right) - R_\gamma = 0 \tag{15}$$

3.4. *Equation of heat conservation*

In this paper we use the hypothesis which assimilates the porous medium to a single fictive medium and is to admit that throughout the volume element on which an energy balance is performed, the average temperatures of the solid and fluid phases are equal. That is the model most used in the literature [16]. Also, it is satisfactory to describe the transfer of heat in a porous medium when the filtration velocities are low. So, we write:

$$\langle T_V \rangle^V = \langle T_\beta \rangle^\beta = \langle T_\sigma \rangle^\sigma = \langle T_\gamma \rangle^\gamma = \langle T \rangle \tag{16}$$

We also pose:

$$\varepsilon = \varepsilon_V + \varepsilon_\beta + \varepsilon_\gamma \tag{17}$$

$$\left[\varepsilon_V \rho_V c_{PV} + \varepsilon_\beta \rho_\beta c_{P\beta} + (1-\varepsilon)\rho_\sigma c_{P\sigma} \right] \frac{\partial T}{\partial t} + \frac{\partial \left(\varepsilon_\gamma \rho_\gamma c_{P\gamma} \right) T}{\partial t} + \left(\varepsilon_V c_{PV} \vec{V}_V + \varepsilon_\beta c_{P\beta} \vec{V}_\beta \right).\vec{\nabla} T$$
$$- \vec{\nabla}. \left[\left(\varepsilon_V \lambda_V + \varepsilon_\beta \lambda_\beta + \varepsilon_\gamma \lambda_\gamma + (1-\varepsilon)\lambda_\sigma \right) \vec{\nabla} T \right] = 0 \tag{18}$$

We focus on solving this problem in two-dimension geometry. This requires that the velocities will be of decomposed in two components (U and W) such as:

$$\vec{V}_\varphi = U_\varphi \vec{e}x + W_\varphi \vec{e}z \tag{19}$$

The dispersion coefficient is considered as the sum of the coefficient of cinematic dispersion, and the molecular diffusion coefficient [17].

$$D_{UW\varphi} = D_{CUWV\varphi} + \delta_{UV} D^*_{UWV\varphi} \tag{20}$$

The cinematic dispersion tensor is given by the following relation, [Bear, 1972]:

$$D_{C\phi} = \|\vec{V}_\phi\| \left[\alpha_{T\phi} I + \left(\alpha_{L\phi} - \alpha_{T\phi} \right) E_\phi \right] \tag{21}$$

$\left(E_\phi \right)$ is a tensor which depends on the

$$E(\vec{V}_\varphi) = \frac{1}{\|\vec{V}_\phi\|^2} \begin{pmatrix} U_\varphi^2 & U_\varphi W_\varphi \\ U_\varphi W & W_\varphi^2 \end{pmatrix} \tag{22}$$

Where $\left(\|\vec{V}_\phi\| \right)$ is the standard velocity of the phase φ; $\left(\alpha_{L\varphi} \ et \ \alpha_{T\varphi} \right)$ are respectively the longitudinal and transverse dispersivity of phase (φ), and (I) is the unit matrix.

The transverse dispersivity is much smaller than the longitudinal dispersivity, generally one to two orders of magnitude [17]. It is taken generally on the order of one tenth of the value of the longitudinal dispersivity [18].

4. Boundary conditions

The partial differential equations we have developed describe the flow in the unsaturated zone of the soil. So to predict the evolution of the system, it is necessary to define the initial conditions and boundary conditions of the domain considered.

4.1. *Initial conditions*

The initial conditions must be specified on all parts of the domain. These conditions may be expressed in pressure load, in water content or concentration.

At $t = 0$:

$$C_{AV} = 0 \tag{23}$$

$$C_{A\beta} = -(X_{A\gamma} C_A^{eq}) z / L_z + X_{A\gamma} C_A^{eq} \tag{24}$$

$$T = T_0 + (T_1 - T_0) z / L_z \tag{25}$$

$$P_\beta = P_{0\beta} + \rho_\beta gz \tag{26}$$

$$P_V = P_{0V} \left(\frac{T}{T_0} \right)^{\frac{Mg}{R} L_z / (T_1 - T_0)} \tag{27}$$

4.2. *Boundary conditions*

In this study, we choose on the boundary $z = 0$ and $z = Lz$, the conditions of Dirichlet. And on the boundary

$x = 0$ and $x = $ Lx, we choose the conditions of Newmann. These conditions are chosen for constituent concentrations and pressures in the two phases, aqueous vapor, and also for the temperature.

- *Concentration*

$$C_{A\beta}(x,0,t) = X_{A\gamma} C_A^{eq} \tag{28}$$

$$C_{A\beta}(x,L_z,t) = 0 \tag{29}$$

$$\left.\frac{\partial C_{A\beta}}{\partial x}\right|(0,z,t) = \left.\frac{\partial C_{A\beta}}{\partial x}\right|(L_x,z,t) = 0 \tag{30}$$

$$\tag{31}$$

$$\left.\frac{\partial C_{AV}}{\partial x}\right|(0,z,t) = \left.\frac{\partial C_{AV}}{\partial x}\right|(L_x,z,t) = C_V(x,0,t) = C_V(x,L_z,t) = 0$$

- *Pressure*

$$P_V(x,0,t) = P_{0V} \tag{32}$$

$$P_V(x,L_z,t) \qquad pressure\ free \tag{33}$$

$$\left.\frac{\partial P_V}{\partial x}\right|(0,z,t) = \left.\frac{\partial P_V}{\partial x}\right|(L_x,z,t) = 0 \tag{34}$$

$$P_\beta(x,0,t) = P_{0\beta} \tag{35}$$

$$P_\beta(x,L_z,t) \qquad pressure\ free \tag{36}$$

$$\tag{37}$$

$$\left.\frac{\partial P_\beta}{\partial x}\right|(0,z,t) = \left.\frac{\partial P_\beta}{\partial x}\right|(L_x,z,t) = 0$$

- *Temperature*

$$T(x,0,t) = T_0 \tag{38}$$

$$T(x,L_z,t) = T_1 \tag{39}$$

$$\left.\frac{\partial T}{\partial x}\right|(0,z,t) = \left.\frac{\partial T}{\partial x}\right|(L_x,z,t) = 0 \tag{40}$$

Lx and Lz represent the Dimension of the domain studied in the directions $\vec{e}_x$ and $\vec{e}_z$.

5. Method of solution
There are many numerical methods for transforming differential equations into algebraic equations [25-38]. We choose the use of finite volume method [19] of implicit type. The choice of such method is based essentially 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 [20].

5.1. *Flow equation*
The equations of flow of the vapor phase and the aqueous phase in discrete form are given by:

$$U_{V(I,j)}^{t+\Delta t} = \frac{\chi_V}{\Delta x}\left[P_{V(i,j)}^{t+\Delta t} - P_{V(i-1,j)}^{t+\Delta t}\right] \tag{41}$$

$$W_{V(i,J)}^{t+\Delta t} = \frac{\chi_V}{\Delta z}\left[P_{V(i,j)}^{t+\Delta t} - P_{V(i,j-1)}^{t+\Delta t}\right] - \chi_V \rho_V g \tag{42}$$

$$U_{\beta(I,j)}^{t+\Delta t} = \frac{\chi_\beta}{\Delta x}\left[P_{\beta(i,j)}^{t+\Delta t} - P_{\beta(i-1,j)}^{t+\Delta t}\right] \tag{43}$$

$$W_{\beta(i,J)}^{t+\Delta t} = \frac{\chi_\beta}{\Delta z}\left[P_{\beta(i,j)}^{t+\Delta t} - P_{\beta(i,j-1)}^{t+\Delta t}\right] - \chi_\beta \rho_\beta g \tag{44}$$

5.2. *Transport equations*
5.2.1. *Phase v*
The transport equation in the vapor phase in discretized form is written:

$$a_{PV}C_{V(i,j)}^{t+\Delta t} + a_{EV}C_{V(i+1,j)}^{t+\Delta t} + a_{OV}C_{V(i-1,j)}^{t+\Delta t} + a_{NV}C_{V(i,j+1)}^{t+\Delta t} + a_{SV}C_{V(i,j-1)}^{t+\Delta t} = -a_{RV} \tag{45}$$

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With:

$$a_{PV} = \left[\varepsilon_V \Delta x \Delta z + \left[\left(\varepsilon_V D_{UUV}^{t+\Delta t}\right)_e + \left(\varepsilon_V D_{UUV}^{t+\Delta t}\right)_o\right]\frac{\Delta z \Delta t}{\Delta x}\right]$$

$$a_{EV} = \frac{1}{2}U_{V(i,j)}^{t+\Delta t}\Delta z \Delta t - \left[\left(\varepsilon_V D_{UUV}^{t+\Delta t}\right)_e\right]\frac{\Delta z \Delta t}{\Delta x} - \frac{1}{4}\left[\left(\varepsilon_V D_{iWUV}^{t+\Delta t}\right)_n - \left(\varepsilon_V D_{iWUV}^{t+\Delta t}\right)_s\right]\Delta t$$

$$a_{OV} = -\frac{1}{2}U_{V(i,j)}^{t+\Delta t}\Delta z \Delta t - \left[\left(\varepsilon_V D_{UUV}^{t+\Delta t}\right)_o\right]\frac{\Delta z \Delta t}{\Delta x} + \frac{1}{4}\left[\left(\varepsilon_V D_{iWUV}^{t+\Delta t}\right)_n - \left(\varepsilon_V D_{iWUV}^{t+\Delta t}\right)_s\right]\Delta t$$

$$a_{NV} = \frac{1}{2}W_{V(i,j)}^{t+\Delta t}\Delta x \Delta t - \frac{1}{4}\left[\left(\varepsilon_V D_{iUWV}^{t+\Delta t}\right)_e - \left(\varepsilon_V D_{iUWV}^{t+\Delta t}\right)_o\right]\Delta t$$

$$a_{SV} = -\frac{1}{2}W_{V(i,j)}^{t+\Delta t}\Delta x \Delta t + \frac{1}{4}\left[\left(\varepsilon_V D_{iUWV}^{t+\Delta t}\right)_e - \left(\varepsilon_V Di_{AUWV}^{t+\Delta t}\right)_o\right]\Delta t$$

$$a_{RV} = \begin{bmatrix} -\varepsilon_V C_{V(i,j)}^t \Delta x \Delta z + \overline{R}_\gamma \Delta x \Delta z \Delta t + \left[-\frac{1}{4}\left(\varepsilon_V D_{iUWV}^{t+\Delta t}\right)_e \Delta t - \frac{1}{4}\left(\varepsilon_V D_{iWUV}^{t+\Delta t}\right)_n \Delta t\right]C_{iV(i+1,j+1)}^{t+\Delta t} + \\ \left[\frac{1}{4}\left(\varepsilon_V D_{iUWV}^{t+\Delta t}\right)_e \Delta t + \frac{1}{4}\left(\varepsilon_V D_{iWUV}^{t+\Delta t}\right)_s \Delta t\right]C_{iV(i+1,j-1)}^{t+\Delta t} + \left[+\frac{1}{4}\left(\varepsilon_V D_{iUWV}^{t+\Delta t}\right)_o \Delta t + \frac{1}{4}\left(\varepsilon_V D_{iWUV}^{t+\Delta t}\right)_n \Delta t\right]C_{iV(i-1,j+1)}^{t+\Delta t} + \\ \left[-\frac{1}{4}\left(\varepsilon_V D_{iUWV}^{t+\Delta t}\right)_o \Delta t - \frac{1}{4}\left(\varepsilon_V D_{iWUV}^{t+\Delta t}\right)_s \Delta t\right]C_{iV(i-1,j-1)}^{t+\Delta t} - \\ \left[\frac{1}{2}S_{TWV(i,j)}^{t+\Delta t}\left(\varepsilon_V D_{iUUV}^{t+\Delta t}\right)_e\left(T_{(i+1,j)}^{t+\Delta t} - T_{(i,j)}^{t+\Delta t}\right) - \frac{1}{2}S_{TWV(i,j)}^{t+\Delta t}\left(\varepsilon_V D_{iUUV}^{t+\Delta t}\right)_o\left(T_{(i,j)}^{t+\Delta t} - T_{(i-1,j)}^{t+\Delta t}\right)\right]\frac{\Delta z \Delta t}{\Delta x} - \\ \left[\frac{1}{2}S_{TWV(i,j)}^{t+\Delta t}\left(\varepsilon_V D_{iUWV}^{t+\Delta t}\right)_e\left(T_{(I+1,J+1)}^{t+\Delta t} - T_{(I+1,J)}^{t+\Delta t}\right) - \frac{1}{2}S_{TWV(i,j)}^{t+\Delta t}\left(\varepsilon_V D_{iUWV}^{t+\Delta t}\right)_o\left(T_{(I,J+1)}^{t+\Delta t} - T_{(I,J)}^{t+\Delta t}\right)\right]\Delta t - \\ \left[\frac{1}{2}S_{TUV(i,j)}^{t+\Delta t}\left(\varepsilon_V D_{iWUV}^{t+\Delta t}\right)_n\left(T_{(I+1,J+1)}^{t+\Delta t} - T_{(I,J+1)}^{t+\Delta t}\right) - \frac{1}{2}S_{TUV(i,j)}^{t+\Delta t}\left(\varepsilon_V D_{iWUV}^{t+\Delta t}\right)_s\left(T_{(I+1,J)}^{t+\Delta t} - T_{(I,J)}^{t+\Delta t}\right)\right]\Delta t \end{bmatrix}$$

5.2.2. *Phase β*

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

$$a_{P\beta}C_{\beta(i,j)}^{t+\Delta t} + a_{E\beta}C_{\beta(i+1,j)}^{t+\Delta t} + a_{O\beta}C_{\beta(i-1,j)}^{t+\Delta t} + a_{N\beta}C_{\beta(i,j+1)}^{t+\Delta t} + a_{S\beta}C_{\beta(i,j-1)}^{t+\Delta t} = -a_{R\beta} \tag{46}$$

With:

$$a_{P\beta} = \alpha_{i(i,j)}^{t+\Delta t}\Delta x \Delta z \Delta t + \varepsilon_V \Delta x \Delta z + \left[\left(\varepsilon_\beta D_{UU\beta}^{t+\Delta t}\right)_e + \left(\varepsilon_\beta D_{UU\beta}^{t+\Delta t}\right)_o\right]\frac{\Delta z \Delta t}{\Delta x}$$

$$a_{E\beta} = \frac{1}{2}U_{\beta(i,j)}^{t+\Delta t}\Delta z \Delta t - \left[\left(\varepsilon_\beta D_{UU\beta}^{t+\Delta t}\right)_e\right]\frac{\Delta z \Delta t}{\Delta x} - \frac{1}{4}\left[\left(\varepsilon_\beta D_{AWU\beta}^{t+\Delta t}\right)_n - \left(\varepsilon_V D_{iWU\beta}^{t+\Delta t}\right)_s\right]\Delta t$$

$$a_{O\beta} = -\frac{1}{2}U_{\beta(i,j)}^{t+\Delta t}\Delta z \Delta t - \left[\left(\varepsilon_\beta D_{UU\beta}^{t+\Delta t}\right)_o\right]\frac{\Delta z \Delta t}{\Delta x} + \frac{1}{4}\left[\left(\varepsilon_\beta D_{iWU\beta}^{t+\Delta t}\right)_n - \left(\varepsilon_\beta D_{iWU\beta}^{t+\Delta t}\right)_s\right]\Delta t$$

$$a_{N\beta} = \frac{1}{2}W_{\beta(i,j)}^{t+\Delta t}\Delta x \Delta t - \frac{1}{4}\left[\left(\varepsilon_\beta D_{iUW\beta}^{t+\Delta t}\right)_e - \left(\varepsilon_V D_{iUW\beta}^{t+\Delta t}\right)_o\right]\Delta t$$

$$a_{S\beta} = -\frac{1}{2}W_{\beta(i,j)}^{t+\Delta t}\Delta x \Delta t + \frac{1}{4}\left[\left(\varepsilon_\beta D_{iUW\beta}^{t+\Delta t}\right)_e - \left(\varepsilon_\beta D_{iUW\beta}^{t+\Delta t}\right)_o\right]\Delta t$$

$$a_{R\beta} = \begin{bmatrix} -\varepsilon_\beta C_{\beta(i,j)}^t \Delta x \Delta z - \alpha_{i(i,j)}^{t+\Delta t}X_i C_{(i,j)}^{eq\,t+\Delta t}\Delta x \Delta z \Delta t + \\ \left[-\frac{1}{4}\left(\varepsilon_\beta D_{iUW\beta}^{t+\Delta t}\right)_e \Delta t - \frac{1}{4}\left(\varepsilon_\beta D_{iWU\beta}^{t+\Delta t}\right)_n \Delta t\right]C_{i\beta(i+1,j+1)}^{t+\Delta t} + \left[\frac{1}{4}\left(\varepsilon_\beta D_{iUW\beta}^{t+\Delta t}\right)_e \Delta t + \frac{1}{4}\left(\varepsilon_\beta D_{iWU\beta}^{t+\Delta t}\right)_s \Delta t\right]C_{i\beta(i+1,j-1)}^{t+\Delta t} + \\ \left[+\frac{1}{4}\left(\varepsilon_\beta D_{iUW\beta}^{t+\Delta t}\right)_o \Delta t + \frac{1}{4}\left(\varepsilon_\beta D_{iWU\beta}^{t+\Delta t}\right)_n \Delta t\right]C_{i\beta(i-1,j+1)}^{t+\Delta t} + \left[-\frac{1}{4}\left(\varepsilon_\beta D_{iUW\beta}^{t+\Delta t}\right)_o \Delta t - \frac{1}{4}\left(\varepsilon_\beta D_{iWU\beta}^{t+\Delta t}\right)_s \Delta t\right]C_{i\beta(i-1,j-1)}^{t+\Delta t} - \\ \left[\frac{1}{2}S_{TW\beta(i,j)}^{t+\Delta t}\left(\varepsilon_\beta D_{iUU\beta}^{t+\Delta t}\right)_e\left(T_{(i+1,j)}^{t+\Delta t} - T_{(i,j)}^{t+\Delta t}\right) - \frac{1}{2}S_{TW\beta(i,j)}^{t+\Delta t}\left(\varepsilon_\beta D_{iUU\beta}^{t+\Delta t}\right)_o\left(T_{(i,j)}^{t+\Delta t} - T_{(i-1,j)}^{t+\Delta t}\right)\right]\frac{\Delta z \Delta t}{\Delta x} - \\ \left[\frac{1}{2}S_{TW\beta(i,j)}^{t+\Delta t}\left(\varepsilon_V D_{iUW\beta}^{t+\Delta t}\right)_e\left(T_{(I+1,J+1)}^{t+\Delta t} - T_{(I+1,J)}^{t+\Delta t}\right) - \frac{1}{2}S_{TW\beta(i,j)}^{t+\Delta t}\left(\varepsilon_\beta D_{iUW\beta}^{t+\Delta t}\right)_o\left(T_{(I,J+1)}^{t+\Delta t} - T_{(I,J)}^{t+\Delta t}\right)\right]\Delta t - \\ \frac{1}{2}S_{TU\beta(i,j)}^{t+\Delta t}\left(\varepsilon_\beta D_{iWU\beta}^{t+\Delta t}\right)_n\left(T_{(I+1,J+1)}^{t+\Delta t} - T_{(I,J+1)}^{t+\Delta t}\right) - \frac{1}{2}S_{TU\beta(i,j)}^{t+\Delta t}\left(\varepsilon_\beta D_{iWU\beta}^{t+\Delta t}\right)_s\left(T_{(I+1,J)}^{t+\Delta t} - T_{(I,J)}^{t+\Delta t}\right)\Delta t \end{bmatrix}$$

5.3. *Equations of evolution of the not-aqueous phase*
The equation of evolution of the not-aqueous phase in discretized form is written:

$$\rho_{\gamma(i,j)}^{t+\Delta t}\varepsilon_{\gamma(i,j)}^{t+\Delta t} = \rho_{\gamma(i,j)}^{t}\varepsilon_{\gamma(i,j)}^{t} + \sum_{i=1}^{2}\left[\alpha_{i(i,j)}^{t+\Delta t}C_{i\beta(i,j)}^{t+\Delta t}\Delta t\right] - \sum_{i=1}^{2}\left[\alpha_{i(i,j)}^{t+\Delta t}X_{i}C_{i}^{eqt+\Delta t}\Delta t\right] + \left[\overline{R}_{\gamma}\Delta t\right] \tag{47}$$

5.4. *Equation of heat conservation*
The conservation equation of heat in discretized form is written as:

$$a_{PT}T_{(i,j)}^{t+\Delta t} + a_{ET}T_{(i+1,j)}^{t+\Delta t} + a_{OT}T_{(i-1,j)}^{t+\Delta t} + a_{NT}T_{(i,j+1)}^{t+\Delta t} + a_{ST}T_{(i,j-1)}^{t+\Delta t} = -a_{RT} \tag{48}$$

With:

$$a_{PT} = \left((\rho c_{P})^{*} + \left((\rho c_{P})_{\gamma}\right)_{(i,j)}^{t+\Delta t}\right)\Delta x\Delta z + \left(\left(\lambda^{*t+\Delta t}\right)_{e} + \left(\lambda^{*t+\Delta t}\right)_{o}\right)\frac{\Delta z\Delta t}{\Delta x} + \left(\left(\lambda^{*t+\Delta t}\right)_{n} + \left(\lambda^{*t+\Delta t}\right)_{s}\right)\frac{\Delta x\Delta t}{\Delta z}$$

$$a_{ET} = \frac{1}{2}\chi_{U(i,j)}^{t+\Delta t}\Delta z\Delta t - \left(\lambda^{*t+\Delta t}\right)_{e}\frac{\Delta z\Delta t}{\Delta x} - \frac{1}{4}\left(\left(\lambda^{*t+\Delta t}\right)_{n} - \left(\lambda^{*t+\Delta t}\right)_{s}\right)\Delta t$$

$$a_{OT} = -\frac{1}{2}\chi_{U(i,j)}^{t+\Delta t}\Delta z\Delta t - \left(\lambda^{*t+\Delta t}\right)_{o}\frac{\Delta z\Delta t}{\Delta x} + \frac{1}{4}\left(\left(\lambda^{*t+\Delta t}\right)_{n} - \left(\lambda^{*t+\Delta t}\right)_{s}\right)\Delta t$$

$$a_{NT} = \frac{1}{2}\chi_{W(i,j)}^{t+\Delta t}\Delta x\Delta t - \frac{1}{4}\left(\left(\lambda^{*t+\Delta t}\right)_{e} - \left(\lambda^{*t+\Delta t}\right)_{o}\right)\Delta t$$

$$a_{ST} = -\frac{1}{2}\chi_{W(i,j)}^{t+\Delta t}\Delta x\Delta t + \frac{1}{4}\left(\left(\lambda^{*t+\Delta t}\right)_{e} - \left(\lambda^{*t+\Delta t}\right)_{o}\right)\Delta t$$

$$a_{RT} = \left[-\left((\rho c_{P})^{*} + \left((\rho c_{P})_{\gamma}\right)_{(i,j)}^{t}\right)T_{(i,j)}^{t}\Delta x\Delta z - \frac{1}{4}\left(\begin{array}{c}\left(\left(\lambda^{*t+\Delta t}\right)_{e} + \left(\lambda^{*t+\Delta t}\right)_{n}\right)T_{(i+1,j+1)}^{t+\Delta t} - \left(\left(\lambda^{*t+\Delta t}\right)_{e} + \left(\lambda^{*t+\Delta t}\right)_{s}\right)T_{(i+1,j-1)}^{t+\Delta t} - \\ \left(\left(\lambda^{*t+\Delta t}\right)_{o} + \left(\lambda^{*t+\Delta t}\right)_{n}\right)T_{(i-1,j+1)}^{t+\Delta t} + \left(\left(\lambda^{*t+\Delta t}\right)_{o} + \left(\lambda^{*t+\Delta t}\right)_{s}\right)T_{(i-1,j-1)}^{t+\Delta t}\end{array}\right)\Delta t\right]$$

6. Results

In the figure 1 is carried the variation of the density of the non-aqueous phase according to time, t, at the position $x = \frac{1}{2} L_x$ and $z = \frac{1}{2} L_z$. It is noted that this density decreases with time. We can explain this decrease by inter-phase exchange between different pollutants.
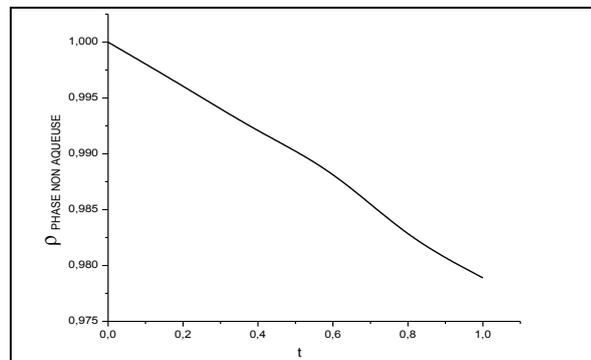
Figure 1: Evolution of the profile of ρ_{γ} according to "time t" ($z = \frac{1}{2} L_z$ and $x = \frac{1}{2} L_x$)
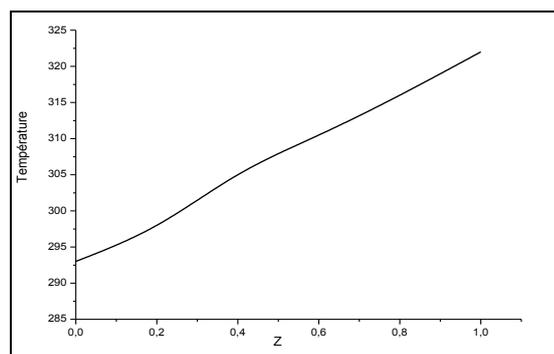
Figure 2: Evolution of the temperature profile according to z, at $x = \frac{1}{2} L_x$ and $t = \frac{3}{4} T_p$

The evolution of the temperature profile as a function of depth z at time $t = \frac{3}{4}\ T_p$ and at the halfway the horizontal dimension of studied domain is illustrated in Figure 2. Note that the temperature increases gradually as z increases which is checked physically and by other authors.
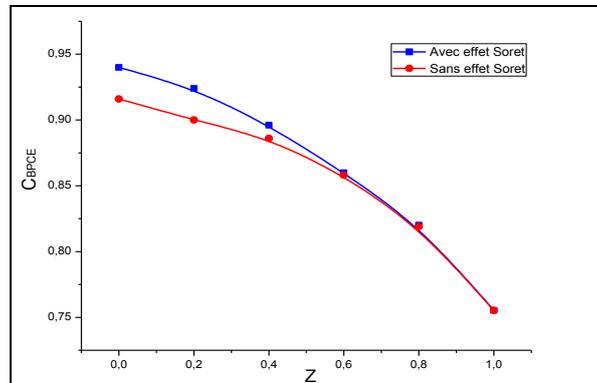
Figure 3: Evolution of the concentration profile of PCE in Aqueous phase according to z, at $x = \frac{1}{2}\ L_x$ and $t = \frac{3}{4}\ T_p$
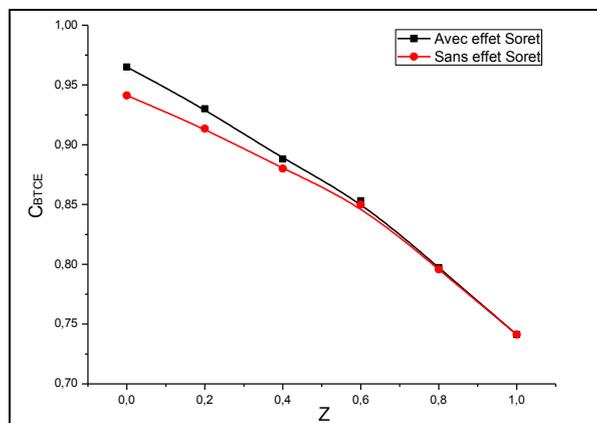
Figure 4: Evolution of the concentration profile of TCE in Aqueous phase according to z, at $x = \frac{1}{2}\ Lx$ and $t = \frac{3}{4}\ T_p$

The influence of soret effect on the concentration profiles respectively of Trichloroethylene and Tetrachloroethylene, as a function of depth, z, at time $t = \frac{3}{4}\ T_p$ and halfway of the horizontal dimension of the area of study is given in Figures 3 and 4. We note that: in a given instant and a given section, the Soret effect leads to an increase in concentrations more particularly in the zone near the surface.
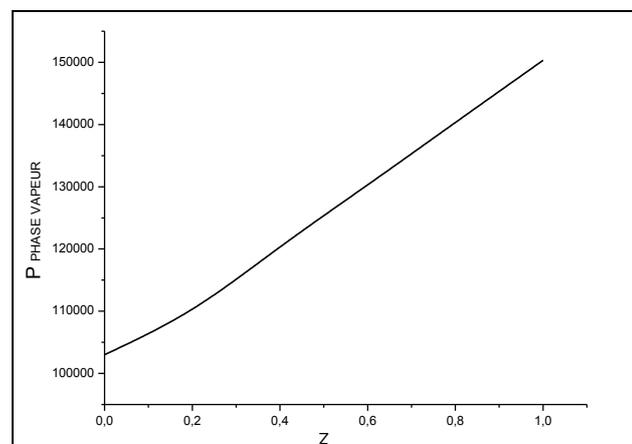
Figure 5: Variation of the vapor pressure according to z, at $x = \frac{1}{2}\ Lx$ and $t = \frac{3}{4}\ T_p$

Figure 5, represents the evolution of the pressure profile of the vapor according to z, at time $t = \frac{3}{4}T_p$ and halfway of the horizontal dimension of the studied domain. It is noted that the pressure increases gradually as one moves away from the surface $z = 0$. This result is checked experimentally.
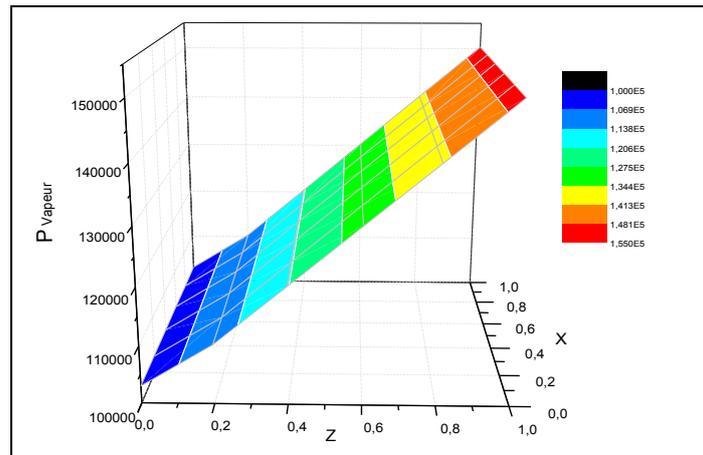
Figure 6: Spatial profile of Vapor pressure phase at $t = ½T_p$

In Figure 6, which shows the spatial profile of the pressure in the vapor phase at time $t = ½ T_p$. It is found that the variation of the pressure is high in the vertical direction and varies only very slightly in the horizontal direction.
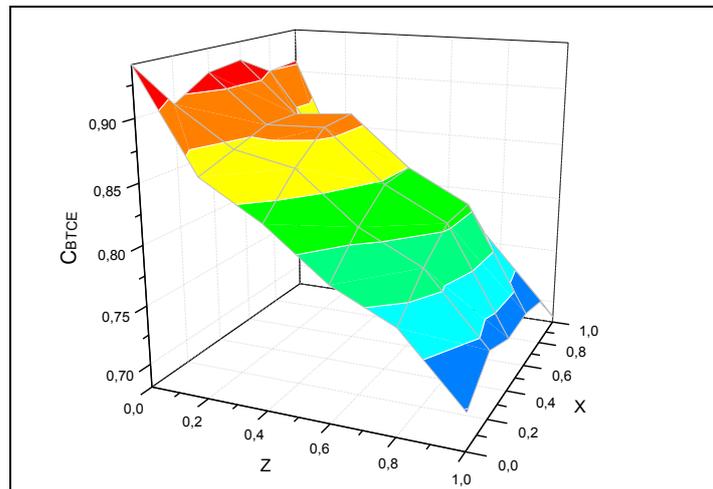
Figure 7: Spatial profile of the TCE concentration in the aqueous phase at $t = ½T_p$

The figure 7 shows the spatial profile of the concentration of trichloroethylene in the aqueous phase at time $½T_p$, it is noted in this figure that the concentration experienced following variations as well as the horizontal direction according to vertical direction. Depending on the depth this variation is very important.
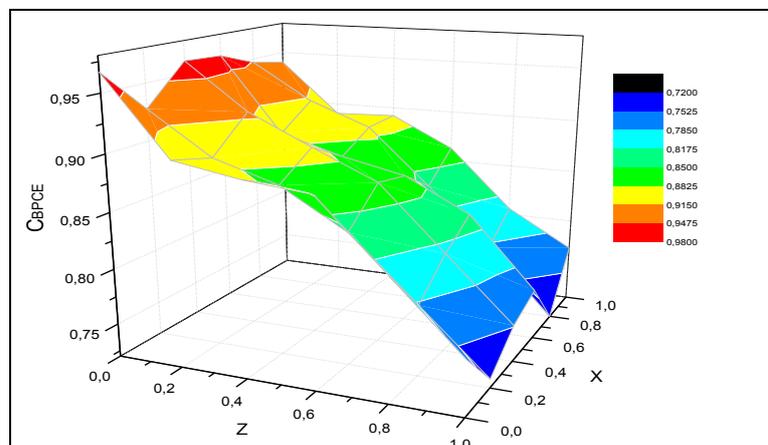
Figure 8: Spatial profile of the PCE concentration in the aqueous phase at $t = ½T_p$

The figure 8 shows the spatial profile of the concentration of tetrachlorothylene in the aqueous phase at time $t = \frac{1}{2}T_p$. As can be seen in this figure that the concentration experienced variations in both directions and that variation is very important according to the depth.

Conclusion

We considered in this paper, in addition to the multiphase aspect and multi-component, a third aspect: soret effect, and We presented the results of our numerical code that gives us the possibility to simulate the process of pollutant transport in the unsaturated zone of a porous media. The equations that determine there are solved in a two-dimensional geometry. The results obtained are in perfect agreement with those of other authors who deal with the same problem.

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