

Modeling and simulation of the porous media pollution

Kenza IRINISLIMANE^{1*}, Kamal MOHAMMEDI²

^{1*}MESOteam/Laboratoire d'Énergétique mécanique et ingénierie, Faculté des sciences de l'ingénieur Université M'Hamed Bougara, Boumerdes 35000, Alger;

²MESOteam/ Laboratoire d'Énergétique mécanique et ingénierie, Université M'Hamed Bougara, Boumerdes 35000, Alger;

*Irinislimane kenza: irinislimanekenza@yahoo.fr

Résumé

Les problèmes de pollution du sol sont courants de nos jours, la présence de polluants pose un problème de toxicité dès lors que ces polluants migrent dans le sol.

De nombreux liquides organiques non aqueux (NAPLs : " Non Aqueous Phase Liquids " en anglais) sont employés en grande quantité par beaucoup d'industries dans le monde entier. Malheureusement, en raison de leur utilisation, ces liquides sont parmi les polluants les plus répandus dans le sol et les eaux souterraines.

Il est malheureusement extrêmement difficile de dépolluer les nappes d'eaux souterraines compte tenu de leur relative inaccessibilité, de leur volume important, leur lenteur d'écoulement. C'est pourquoi la pollution d'une nappe phréatique peut causer un dommage écologique très grave et de longue durée, notamment parce que l'élimination des polluants prend beaucoup de temps.

Dans le contexte des sites pollués, la modélisation numérique est un outil permettant de comprendre le comportement des polluants dans le milieu souterrain et de prédire leur devenir dans l'espace et dans le temps.

L'objectif de mon travail consiste à reproduire, par la simulation, certains phénomènes physiques fréquemment rencontrés dans la réalité et identifier les paramètres qui les gouvernent.

Pour ce faire, on a étudié le problème sur un modèle physique réduit et grâce aux lois de la similitude, les résultats obtenus peuvent s'étendre aux applications réelles.

Mots-clés : milieu poreux, aquifères, pollution, écoulement, simulation numérique.

Nomenclature

Φ : porosity of the milieu

\tilde{c}_i : total concentration of the species in the k mobile and stationary phases, m^3/m^3 PV

ρ_k : density of the pure component k, kg/m^3

n_p : the number of phases

C_{kl} : concentration of component K in the phase liquid m^3/m^3

S_i : saturation of phase liquid m^3/m^3 PV

R_k : term source relative to the bore for the component K

Q_k : injection rate compared to production of the component k.

r_{kl} and r_{ks} : rates of reaction of component k in the liquid(l) and solid (s) phases.

u_l : Darcy velocity of the phase 1 in a multiphase flow, m / s.

k : intrinsic permeability tensor, m²

z : depth, m

k_{rl} : relative permeability of the porous milieu to the phase 1

μ_l : phase 1 viscosity [kg/m²s]

λ_{rlc} : relative mobility of the phase 1

λ_{rtc} : total mobility

C_t : total compressibility

C_k^0 and C_r compressibility of the component

k

and the solid matrix.

Greek symbols

Φ : Porosity

σ : Superficiel tension, N/m²

μ_l : Dynamic viscosity of phase 1, Pa.s

γ_l : Specific weight of phase 1, Kg/m² s²

Abbreviations

DNAPL Dense non aqueous phase liquid

LNAPL Light non aqueous phase liquid

PCE Perchloréthylène

1. Introduction

The study of fluid flows in porous media includes the description and characterization of both the fluid that the environment in which it operates. Due to the terrific development of means of reconnaissance highly heterogeneous subsurface formations, and the improvement opportunities for interpretation of complex data growing computer tool that allows the current problems concern mainly to the heterogeneity of natural porous milieu.

The migration of immiscible oil and restoring aquifers where they are present involve multiphase process. At hydrocarbon migration, numerical modeling has allowed a better understanding of the phenomena that act in the gas phase (Baehr, 1987 Faltaand al, 1989) and in liquid form (Guarnacciaand al, 1997, and MoridisPruess, 1995).[1]

2. Pollution of aquifers by NAPLs

Chlorinated solvents and petroleum hydrocarbons, in most cases, are poorly soluble chemicals (miscible) in water. They exist in the aquifer as separate liquid phases, often referred to as non-aqueous liquid phase or NAPL. A NAPL can consist of a single or many components compound. For example, trichlorethylene (TCE) and tetrachlorethylene (PCE) are simple compounds. [2]

The underground water can be of two types: unconfined and confined aquifer .[3]

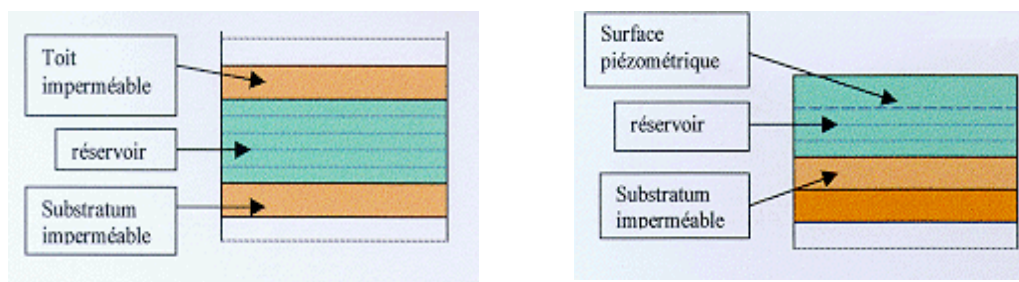


Figure 1: *Nappe captive and unconfined* [3]

Worldwide, all kinds of waste are discharged into the ground or are accidentally spilled on the surface. Fortunately, most hazardous waste is absorbed and broken down by natural processes such as

bacterial activity. However, some are not easily degraded and in some cases, the amount of toxic substances into the soil is such that the natural capacities of the latter to remove pollutants are exceeded, resulting in the pollution of groundwater. The vulnerability of groundwater depends on the type of water, free or captive, and the mode of flow of water in the aquifer. Confined groundwater is better protected by impermeable layers which surmount. Their supply of water is more limited, so easier to protect. Their pollution occurs when the impermeable protective level is pierced by a book (old drilling deep excavation ...). The unconfined aquifers are more vulnerable revenge pollutants from surface can diffuse freely in the soil and the groundwater level to unsaturated area. [2]

3. Trapping NAPLs in groundwater

3.1 Trapping mechanism

During the migration of NAPL in the porous milieu, a party may find themselves trapped under the action of capillary forces; the figure shows the free and trapped NAPL. [2]

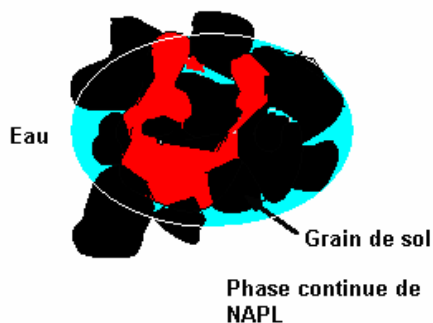


Figure 2: Phase free NAPL (mobile)

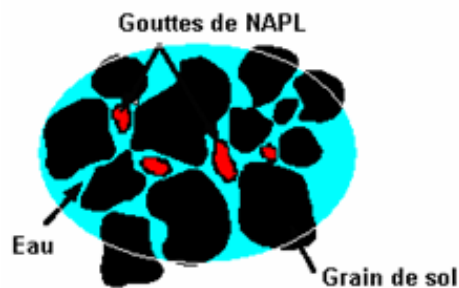


Figure 3: NAPL residual (trapped)

4. Modeling of multiphase displacements under UTCHEM

4.1 The UTCHEM code:

This is a multiphase simulator 3D multicomponent particularly complex. Written in FORTRAN, it is very robust and can be run either on a super computer or workstation. This calculation code digital, still in development at the University of Texas in Austin, was originally developed by Pope and Nelson (1978) to simulate the process of oil recovery by the use of surfactants (surfactants) and polymers [4]. The simulator has the ability to simulate adequately the complex phenomena [5] and also allows us to consider the phenomenon of diffusion between all phases [6] The simulator allows the modeling of more than 19 components: water, oil, surfactant, polymer, alcohol, air, plotters, gels, etc ... which can form up to four (04) fluid phases [5]: a gaseous phase three liquid phases: an aqueous phase (the = 1), an oil phase (l = 2) a microemulsion phase (l = 3).

4.2 Mathematical description

4.2.1 Equation of conservation of mass:

$$\frac{\partial}{\partial t} (\phi \tilde{C}_k \rho_k) + \vec{\nabla} \cdot [\sum_{l=1}^{n_p} \rho_k (C_k \vec{v}_l - \phi S_l \vec{D}_{kl} \cdot \vec{\nabla} C_{kl})] = R_k \quad (1)$$

The total concentration of the species in the k mobile and stationary phases

[m3/ m3 PV] is given by:

$$\tilde{C}_k = \left(1 - \sum_{k=1}^{n_{cv}} \hat{C}_k \right) \sum_{l=1}^{n_p} S_l C_{kl} + \hat{C} \quad \text{pour } k = 1, \dots, n_c \quad (2)$$

$$R_k = \phi \sum_{i=1}^{n_s} S_i r_{ki} + (1-\phi) r_{ka} + Q_k \quad (3)$$

$$\bar{u}_i = -\frac{k_{ri} \bar{k}}{\mu_i} (\bar{\nabla} P_i - \gamma_i \bar{\nabla} z) \quad (4)$$

4.2.2 Pressure Equation:

$$\phi C_t \frac{\partial P_i}{\partial t} + \bar{\nabla} \cdot \bar{k} \lambda_{rTc} \bar{\nabla} P_i = -\bar{\nabla} \cdot \sum_{i=1}^{n_p} \bar{k} \lambda_{rTc} \bar{\nabla} z + \bar{\nabla} \cdot \sum_{i=1}^{n_p} \bar{k} \lambda_{rTc} \bar{\nabla} P_{c1i} + \sum_{k=1}^{n_{cv}} Q_k \quad (5)$$

$$\lambda_{rTc} = \sum_{i=1}^{n_{cv}} \lambda_{rTc} \quad (7)$$

$$C_t = C_r + \sum_{k=1}^{n_{cv}} C_k^0 \tilde{C}_k \quad (8)$$

5. Simulation-Results and Discussion

The product used in our application is Perchloroethylene or PCE is found in many other denominations 1, 1, 2, 2-tetrachlorethylene, tetrachloroethene ethylene tetrachloride, carbon dichloride.

In this application we simulated from a simple model, the behavior of a heterogeneous aquifer, considered as representative of a type of heterogeneity frequently found in nature (stratified milieu). The model used is a simplified physical model, similar to a stack of parallel layers of constant thickness and different characteristics (porosity, permeability).

The milieu considered in this study is a rigid aquifer initially saturated with the pollutant "PCE". The injection of the displacing fluid (aqueous phase) through an injection well, allows to push the contaminant to the recovery wells. The aqueous phase consists of water, of polymer and surfactant.

The injection of a surfactant solution is used to reduce the interfacial tension and decreasing the saturation of residual polluting, and injection of the polymers (often combined with the use of surfactants) increases the viscosity of the water and decreases the mobility ratio to improve sweep efficiency. Exchanges between phases are not taken into account (no phenomenon of diffusion-dispersion) and the tank temperature is invariable (isothermal process).

5.1 Meshing:

The mesh used to discretize the milieu (aquifer) is a three-dimensional Cartesian grid. The finite difference scheme used is the TVD scheme (Total Variation Decreasing); it consists in discretizing the domain into rectangular mesh. Values calculated are average values characterizing the mesh and not the values at the center of the mesh.

Tables 1: Properties of reservoir

Compressibility of the rock (1/KPa)		0 (undeformable rock)		
Rock porosity		layer 1	layer 2	layer 3
		18%	12%	8%
Permeability of the rock (millidarcy)	X	1000	1000	200
	Y	500	500	200
	Z	70	35	25
Reference pressure (atm)		1		
Initial saturation of the phases	phases	layer 1	layer 2	layer 3
	1	0%	0%	0%
	2	100%	100%	100%

We focus in this study to determine the saturation fields of the fluid phases in the case of the method of recovery of the pollutant (PCE) by injection of an aqueous phase (water, polymer, surfactant). This study examines the influence of the injection of the aqueous phase of the displacement of PCE through the medium under consideration.

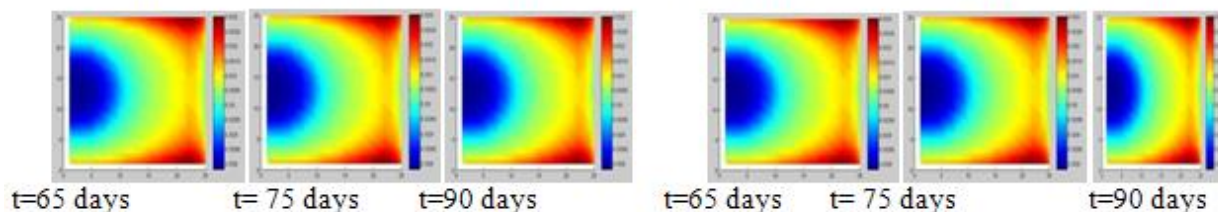
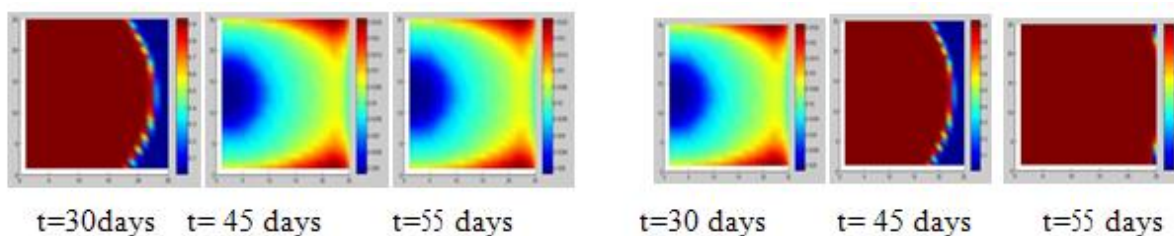
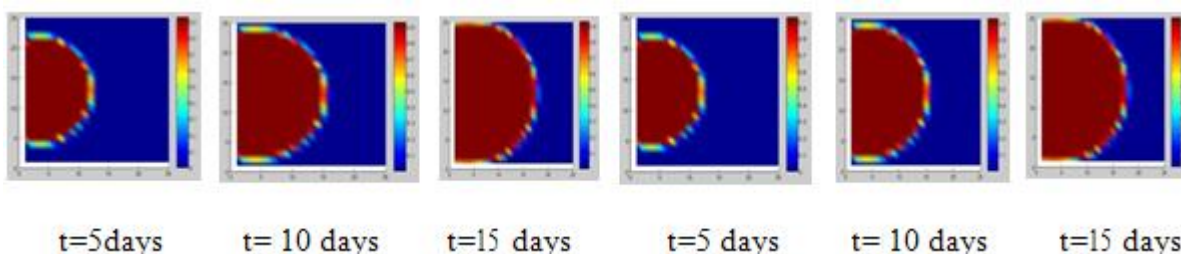


Figure 4: Saturation of the injectable Phase (Water, polymer, surfactant) in the layer 1.

Figure 5: Saturation of the injectable Phase (Water, polymer, surfactant) in the layer 2.

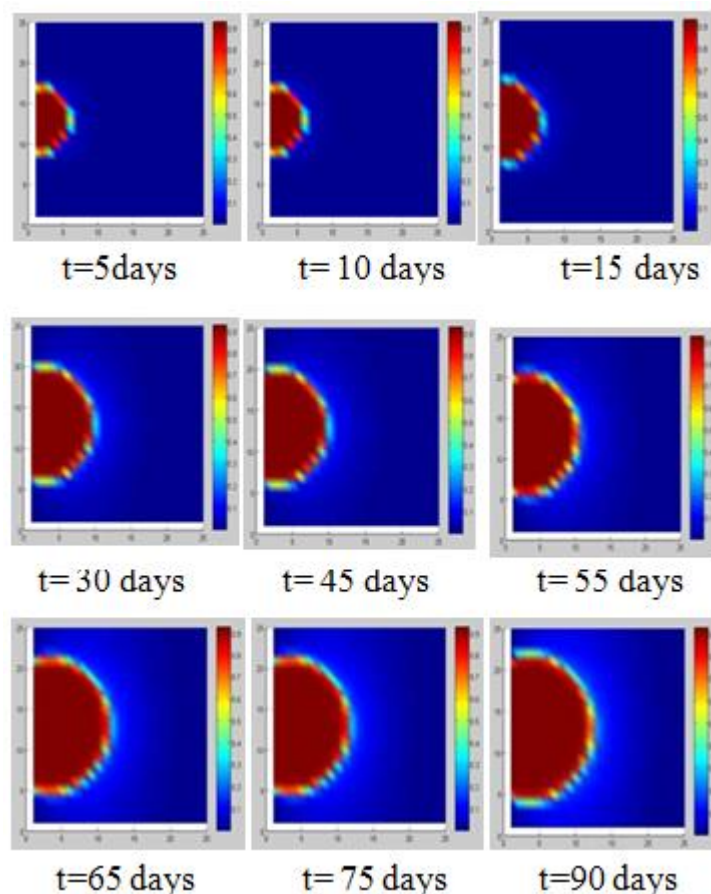


Figure 6: Saturation of the injectable Phase (Water, polymer, surfactant) in the layer 3.

From the figures (4), (5) and (6), we find that the injected aqueous phase moves quickly in the most permeable layers (1 and 2). So the permeability plays an important role in the movement of fluids through the aquifer. The Variation of the saturation of the aqueous phase is initially recorded in the vicinity of the injection well of the same phase. Thereafter the spread of this phase front across the milieu is circular in shape, and forming surfaces iso-saturations. In layer 3, wherein the porosity and permeability is low, and also because the depth to which is the displacement of the moving fluid is very long.

Behind the displacement front, saturation occurs in this phase to a maximum value in the injection well that is complementary to the residual saturation PCE. From the injection well, the saturation of the latter is gradually increased until the onset of the steady state, and stabilized at this value.

By approaching the right boundary, the aqueous phase which serves to push the pollutant moves more southerly along flow axis see Figures (4, 5.6) recovery wells. We also note that the vicinity of the two lateral boundaries is not completely swept away by the latter in the layer 1 and 2 before the first 30 days of the simulation, and in this phase 3 layers reaches the center of the aquifer after 90 days.

6. Conclusion

Unfortunately, it is extremely difficult to clean up underground water due to their relative inaccessibility, their large volume, and flow slowly. Therefore the pollution of groundwater can cause a very serious ecological damage and long-term, especially because the pollutant removal takes time.

The study of fluid flows in porous milieu includes the description and characterization of both the fluid that the environment in which it operates. Due to the tremendous development of means of reconnaissance highly heterogeneous subsurface formations, and improving opportunities for interpretation of complex data and growing software tool that allows the current issues related mainly to the heterogeneity of natural porous media.

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