E-proceedings of the 36th IAHR World Congress
28 June – 3 July, 2015, The Hague, the Netherlands

NUMERICAL MODEL FOR NAPL MIGRATION IN DOUBLE-POROSITY SUBSURFACE SYSTEMS

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ABSTRACT

The double-porosity concept has been successfully applied by many researchers to simulate fluid flow in oil reservoirs over the past few decades. These oil reservoirs were typically considered to be made of fractured or fissured rock, hence the usance of the double-porosity concept. Nonetheless, double-porosity may also exist in soil either through soil aggregation, or through soil features such as wormholes, cracks and root holes. These attributes in soil that cause the occurrence of double-porosity are also known as secondary porosity features and are akin to the reservoir rock fractures or fissures. In the case of groundwater contamination, the occurrence of double-porosity in soil is highly influential since immiscible fluids have been found to flow preferentially through the secondary porosity features. Ergo, a numerical model for non-aqueous phase liquids (NAPL) migration in double-porosity groundwater systems was developed. This model was modified from the conventional double-porosity model applied in the petroleum industry. The difference is that while the standard double-porosity models usually simulate the fluid flows in both continua making up the double-porosity medium, the double-porosity model presented here focuses the modelling on the secondary porosity features in the soil, therefore making it more pertinent in the context of groundwater contamination. In the modified model, the phase saturations and relative permeabilities are expressed as functions of the capillary pressures. The resultant non-linear governing partial differential equations are solved using numerical methods. The problem is discretized spatially using the Galerkin's weighted-residual finite element method whereas a fully implicit scheme is used for temporal discretization. Verification of the developed model has been done against similar works in the open literature and the preferential flow of NAPL through the secondary porosity features was validated.

Keywords: Dual Porosity, Groundwater Pollution, Immiscible Fluids

1. INTRODUCTION

One of the best sources of freshwater naturally found on earth is groundwater. It is a freshwater supply source for nearly two billion people around the world (UNWWAP, 2012). In areas where groundwater sources yield significant supplies, it can be channeled directly to the surface water supply network. Groundwater also forms an invaluable alternative source in water-stressed areas such as in Mexico City, Calcutta and Cairo (Morris et al., 2003) as well as in areas of smaller communities and isolated industries which do not have access to piped water supply from surface water sources. Even though the value of groundwater to humans has been established, a concerted effort to conserve and protect this precious resource is still lacking in many parts of the world. One main problem is the ease at which groundwater gets contaminated; just a few parts per billion of some chemicals can negate its function as consumable water (Mumford et al., 2008) unless intensive treatment is applied. Another issue is that unlike surface water pollution, groundwater contamination is difficult to detect, difficult to control, and may persist for decades. This is especially true when the contamination is due to non-aqueous phase liquids (NAPL), which is one of the more ubiquitous groups of groundwater contaminants. NAPL can be defined as immiscible, hydrocarbon liquids found in the subsurface (Bedient et al., 1999) which come from crude oil and petroleum-based industries. Though categorized as non-aqueous, the solubilities of the NAPL are sufficient to render huge quantities of groundwater unfit for consumption if they come into contact with the groundwater source.

NAPL contaminants will percolate through the vadose zone before reaching and entering the phreatic zone. Therefore, the unsaturated zone is important in determining how and when contaminants from the soil surface reaches the groundwater table. Some NAPL, including fertilizers and pesticides, require moisture in the soil as well as infiltration of either rain or irrigation water for downward movement. When moving through the vadose zone, NAPL usually leave a fraction of themselves trapped in some or all of the soil pores. This is due to capillary forces working in conjunction with surface tension of the different phases in the subsurface (Mitchell and Soga, 2005). The NAPL might migrate and make contact with the saturated zone if enough is released over time. Subsequent movement of the NAPL once it reaches the phreatic zone is dependent on the density of the NAPL. Light non-aqueous phase liquids (LNAPL) that have densities lower than water will form a layer on the groundwater table, flowing according to the dip of the groundwater surface.

Multiphase flow refers to the condition where the flow consists of two or more fluid phases. Due to the complicated multiphase flow processes, few analytical solutions for NAPL pollution cases can be found (Simoni et al., 2008). This gave rise to the application of numerical simulations in analyzing and solving NAPL-related problems.

Lately, more and more research on double-porosity in soil can be found in the open literature (Ngien et al., 2012). For soil, the double-porosity condition may be caused by several factors such as cracks, soil pipes, root holes and soil fauna (Beven and Germann, 1982). Aggregated soil made up of soil aggregates and inter-aggregate pores also contributes to double-porosity in soil and can be found in agricultural soil as well as naturally. These features in the soil are known as secondary porosity features and act as the paths of least resistance for NAPL flow through soil (Ngien et al., 2012). At present, most multiphase flow models uses single-porosity media in their analysis, which may not be adequate for soils with double-porosity. Therefore, a double-porosity, multiphase flow model for NAPL migration in the subsurface is introduced.

2. THE CONCEPT OF DOUBLE-POROSITY

In the model presented here, the soil is assumed to be an overlap of two continuums, the secondary porosity features and the porous matrix, as shown in Figure 1. The porous matrix has a lower permeability with higher porosity while the opposite is true for the secondary porosity features, which are neither fixed in geometry nor in size.

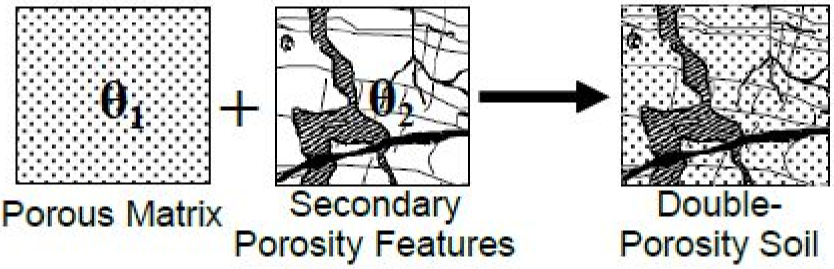

Figure 1. Visualization of the double-porosity.

With the application of external loading, a pressure difference is created between the fluid in the porous matrix and the fluid in the secondary porosity features that culminates in the migration of the NAPL. The exchange of fluids between the porous matrix and the secondary porosity features can be incorporated in a transfer function. The pertinent information in NAPL pollution problems is the first contact of the contaminants with groundwater. Therefore, this double-porosity model will focus the modelling on flow through the preferential pathways of the NAPL contaminants.

3. NUMERICAL FORMULATION

Different from miscible contaminants, immiscible contaminant flow is determined by a combination of surface tension, pressure and gravity (Rahman and Lewis, 1999). In order to describe the processes in mathematical form, the relationship between the hydraulic properties of the phases have to be expressed in functional terms.

In the unsaturated medium, the pores of the soil are assumed to contain air, NAPL and water with the sum of the saturation of all three phases equal to 1. Capillary pressure refers to the pressure discontinuity across a curved interface separating two fluids (Mitchell and Soga, 2005) and is the argument of the phase saturation function in a multiphase system, as presented in Eq. [1].

$$S_\alpha = f(P_{caw}, P_{cnw}, P_{can}) \qquad [1]$$

where $P_{caw} = P_a - P_w$, $P_{cnw} = P_n - P_w$, P_{can} is $P_a - P_n$, P_a is the air pressure, P_w is the water pressure, P_n is the NAPL pressure, and α refers to either w-water, n-NAPL or a-air. The relative permeabilities of each phase are in turn functions of the phase saturations. The expressions for relative permeabilities in this model were obtained from Brooks and Corey (1966) as well as Lujan (1985).

Works by Rahman and Lewis (1999) in multiphase flow as well as Ghafouri and Lewis (1996) in double-porosity were referred to in obtaining the governing equations for the current model. Incompressible, immiscible fluid behaviour in porous media was obtained by combining Darcy's linear flow law with the mass conservation balance for each fluid phase in the multiphase system, as shown in Eq. [2].

$$-\nabla \rho V = \textit{Rate of Fluid Accumulation} \qquad [2]$$

where ρ is the density of the fluid and V is Darcy's velocity. Further information on the elements influencing the fluid accumulation rate within the multiphase system can be found in Rahman and Lewis (1999). Movement of the fluids between the two porosities is encapsulated in a transfer function, shown in Eq. [3], that is based on fluid pressure in the secondary porosity features. Coupling of this type can be based on an individual parameter of a single continuum (Lewandowska et al., 2008).

$$\frac{\rho\bar{\alpha}kk_rP}{\mu} \qquad [3]$$

By combining Eqs. [2] and [3] as well as integrating the factors for fluid accumulation, the governing equation for multiphase immiscible flow in double-porosity soil as shown in Eq. [4] is obtained.

$$-\nabla^T\left[k\frac{\rho_\alpha k_{r\alpha}}{\mu_\alpha B_\alpha}\nabla(P_\alpha+\rho_\alpha gh)\right]+\phi\frac{\rho_\alpha}{B_\alpha}\frac{\partial S_\alpha}{\partial t}+\phi\rho_\alpha S_\alpha\frac{\partial}{\partial t}\left(\frac{1}{B_\alpha}\right)+\phi\frac{S_\alpha}{B_\alpha}\frac{\partial\rho_\alpha}{\partial t}-P_\alpha\frac{\rho_\alpha\bar{\alpha}kk_{r\alpha}}{\mu}$$
$$+\rho_\alpha Q_\alpha+\frac{\rho_\alpha S_\alpha}{B_\alpha}\left[\left(m^T-\frac{m^TD_T}{3K_s}\right)\frac{\partial\varepsilon}{\partial t}+\left(\frac{1-\phi}{K_s}-\frac{m^TD_Tm}{9K_s^{\,2}}\right)\frac{\partial\bar{p}}{\partial t}+\frac{m^TD_T}{3K_s}c\right]=0 \qquad [4]$$

where Q is the external sinks or sources. The continuity equation for each fluid phase can be obtained by substituting the subscript α in Eq. [4] with the letters as mentioned in the description for Eq. [1].

Prescribed values were used as the initial and boundary conditions of the current model. The governing equations were discretized spatially using finite elements and temporally using finite difference. The unknowns in the spatial discretization are associated with the nodes surrounding the perimeter of each element. Galerkin's weighted-residual method and the Gauss theorem were used to form a weak formulation of the governing equations before transforming the second spatial derivatives. A set of non-linear, ordinary differential equations in time were used to obtain the primary unknowns in the form of the fluid pressures in the system. An implicit scheme was applied on the unknown-dependent non-linear coefficients, and the final solution was obtained through iterations in each time step.

4. MODEL VERIFICATION AND VALIDATION

A two-dimensional, multiphase flow example simulating NAPL leakage in the subsurface was used to validate the current double-porosity model. The migration of the NAPL comes from a continuous source at the soil surface, and the cross-section as well as boundary conditions of the example are as shown in Figure 2. LNAPL was applied as the leaked fluid.

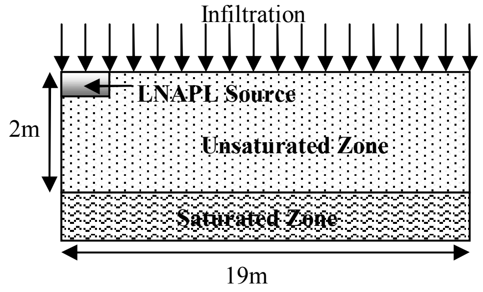

Figure 2. Schematic diagram of soil domain and boundary conditions.

Based on Figure 2, water is infiltrating throughout the surface of the soil domain whereas the leakage is situated at the top left of the domain. The side boundaries were fixed as impermeable while atmospheric pressure was ascribed to the bottom boundary. In the scenario, the gas phase was considered negligible. The soil domain which is 19m long and 2m in height was discretized into 40 rectangular elements of varying sizes. 0.269 was chosen as the shape factor $\bar{\alpha}$ value. The results obtained from the current model are compared with the results from Rahman and Lewis (1999) who applied a single-porosity model on the same example as described in this article.

Figure 3 and Figure 4 shows the initial water saturation in the current model and Rahman and Lewis' model, respectively. It can be seen that the initial water saturation levels are similar for both models, which should be the case since regardless of whether the soil is double-porosity or single-porosity, the physical parameters applied in both models were the same.

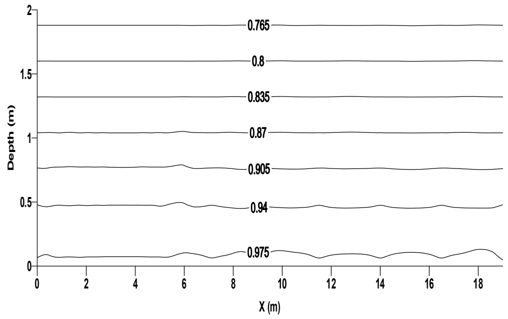

Figure 3. Water saturation at t = 0 for present model

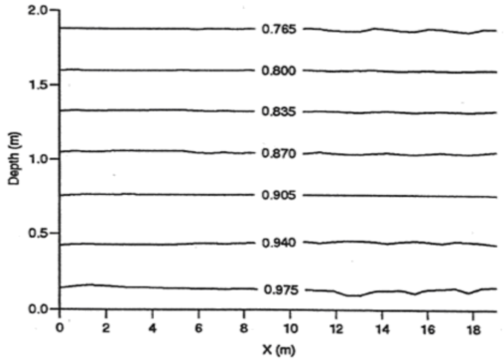

Figure 4. Water saturation at t = 0 for Rahman and Lewis' model

Figure 5 depicts the final water saturation profile for the present model after a simulation time of 3.17 years. Compared to Figure 3, the saturation level has increased due to the boundary condition of constant water infiltration applied. This is also the case for Rahman and Lewis' single-porosity model as shown in Figure 6, where the NAPL was found above the saturated zone as it is lighter than water.

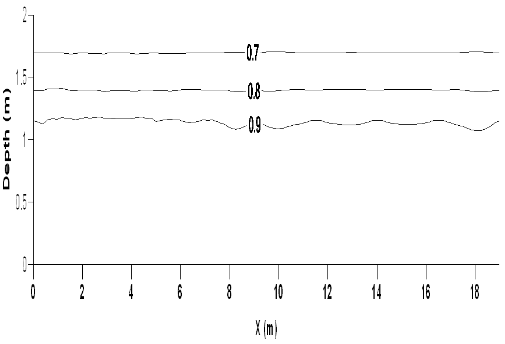

Figure 5. Water saturation at t = 3.17 years (present model)

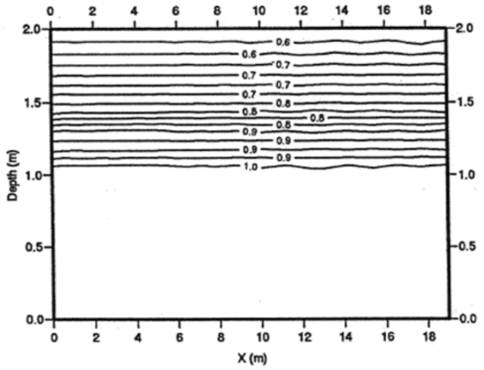

Figure 6. Water saturation at t = 3.17 years (Rahman and Lewis' model)

Figure 7 and Figure 8 shows the NAPL infiltration process happening between the initial and final NAPL saturation stages of the current model. By comparing Figure 7 where the NAPL saturation contours were at 1000 seconds with Figure 8, which portrayed the NAPL saturation after 115.74 days, it is clear that due to the constant infiltration input the NAPL levels in Figure 8 has risen in the domain following the rise in water table and are more saturated above a depth of 0.5m compared to Figure 7.

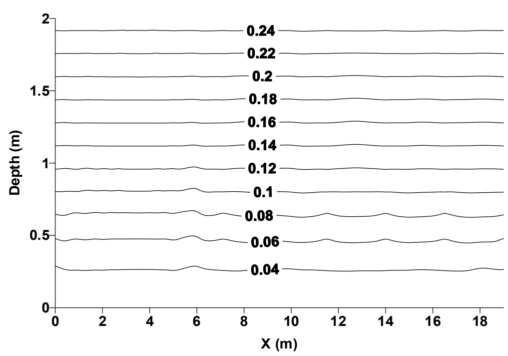

Figure 7. LNAPL saturation at t = 1000 seconds

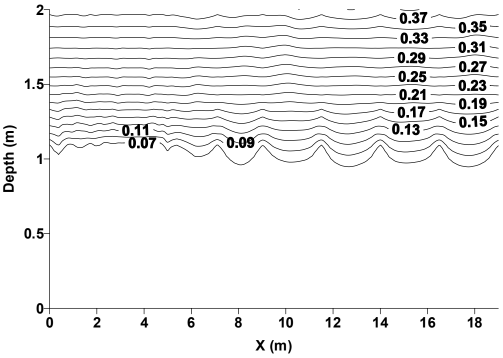

Figure 8. LNAPL saturation at t = 115.74 days

In order to show the changes in NAPL saturation more clearly, a cross-section of the present model from top to bottom was extracted. Figure 9 depicts the final NAPL saturation state along the cross-section. An apparent difference between the NAPL saturation above and below the depth of 1.45m can be observed when the graph lines representing the current model as well as Rahman and Lewis' model are compared. Above 1.45m, the NAPL saturation predicted by Rahman & Lewis exceeds the NAPL saturation predicted by the current model at the surface of the domain but going further down the depth, the two graph lines eventually converged at the depth of 1.45m. Going further down the depth, the converse occurred with the NAPL saturation predicted by the present model exceeding the NAPL saturation predicted by Rahman and Lewis (1999). At the depth of 1m, the two graph lines converged again due to residual NAPL saturation being reached. It is shown from this comparison that the NAPL, in this case LNAPL, flows preferentially through the secondary porosity features in the system.

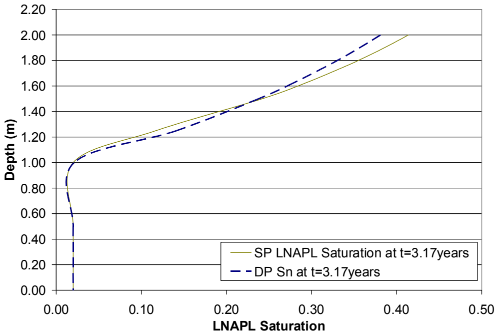

Figure 9. Saturation profile of LNAPL vs soil depth

5. CONCLUSION

A numerical model for NAPL migration in double-porosity subsurface systems has been developed. Analysis was performed to demonstrate the model's capability for two-dimensional applications. It is concluded that the processes and mechanisms happening in the subsurface has been validated based on previous works and NAPL was found to flow preferentially through the secondary porosity features of the simulated domain.

ACKNOWLEDGMENTS

The authors wish to thank their respective universities for the support received and a special note of appreciation to the Department of Research and Innovation, Universiti Malaysia PAHANG for helping with the conference presentation of this paper. The work within is related to the RDU130139 and RDU130382 research grants.

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