



A New Linearization Technique of the Advection Diffusion Equation for modelling free-Phase NAPL Spreading in Groundwater

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1 Introduction

Many contaminants of the Groundwater have become known as Non-Aqueous Phase Liquids (NAPL): light non-aqueous phase liquid (LNAPL) if the density is less than the density of water or dense non-aqueous phase liquid (DNAPL) if the density is greater than water. Under certain conditions and assumptions like as sharp interface between both phases (e.g. NAPL/Water) the governing equation of free-phase NAPL-spreading in groundwater reduce to a non-linear advection diffusion equation in terms of NAPL thickness. In the case of an immobile groundwater this equation coincides with the well known Boussinesq equation for unsteady groundwater flow.

Numerous and well known solutions are obtained for the linearized Boussinesq equation from [MUSKAT 1948], [CHARNI 1951], [ARAVIN and NUMEROV 1965], [POLUBARINOVA-KOCHINA 1962], [BEAR 1972] which became standard solutions for unsteady groundwater flow modelling. The most widely used technique for linearization is the decomposition of the groundwater thickness $h(x,y,t)$ in a spaced averaged thickness $\bar{h}(t)$ and its deviations $\delta h(x,y,t)$ from the averaged value. In above mentioned works currently, a simple domain averaging method was used to calculate \bar{h} (e.g. groundwater volume per extending area). For small deviations δh (e.g. drainage and storage problems which are typical shallow problems) the obtained results with

linearized equation are closed to the exact solution.

In the last decade several analytical, semi-analytical and numerical solutions for LNAPL lens spreading were obtained using the same linearization method like in the groundwater flow modelling mentioned above [CORAPCIOGLU 1996], [LIAO, ARAL 2000]. It will be shown in the paper that this approach for the LNAPL lens spreading in opposite to the above mentioned groundwater flow can lead to significantly large Errors. A new Weighted Averaging Technique for linearization of the governing equation of LNAPL spreading has been proposed, which reduce substantially these calculation Errors [DAVID 2004]. Consequently through the proposed new linearization technique an improvement of the existing numerical and semi-analytical calculation methods for spreading and migration of the NAPL in groundwater is possible.

Analysis of the reliability of the results obtained on the basis of linearized LNAPL spreading equation

To prove the reliability of the results obtained on the basis of linearized equation we take into account the following representative form of the nonlinear governing equation for free LNAPL spreading in homogeneous unconfined aquifer. The governing equation in term of LNAPL thickness (h_l) over of the ambient groundwater is the following nonlinear Advection Diffusion equation [CORAPCIOGLU et all 1996], [DAVID, 2004]:

$$n_l \frac{\partial h_l}{\partial t} + \vec{q}_w \frac{k_l}{k_w} \nabla(h_l) - k_l \nabla \cdot (h_l \nabla h_l) = 0 \quad (1)$$

k_l, k_w = hydraulic conductivities of LNAPL/water

q_w = Darcy velocity of the groundwater

n_l = effective porosity

If $q_w=0$ eq. 1 coincide with the well known Boussinesq's equation [BEAR 1972] for modelling unsteady groundwater flow in unconfined aquifer in term of the entire groundwater depth h .

Only a small number of exact solutions of this nonlinear equation are known to date which can be used to prove the reliability of approximated solutions.

A very effective approach to obtain solutions is the use of the linearized form of the equation 1. The most widely used technique for the linearization is to introduce a decomposition of the LNAPL thickness h_l in the form

$$h_l(x, y, t) = h_a(t) + \delta h(x, y, t) \quad (2)$$

$h_a(t)$ is the averaged LNAPL phase thickness at time t and δh is the deviation of the h_l from h_a which has been used successfully for groundwater modelling [MUSKAT 1948], [CHARNI 1951], [ARAVIN and NUMEROV 1965], [POLUBARINOVA-KOCHINA 1962], [BEAR 1972]:

$$h_a(t) = \frac{\iint_{\Omega} h_l(x, y, t) d\Omega}{\iint_{\Omega} d\Omega} = \frac{1}{\Omega} \iint_{\Omega} h_l(x, y, t) d\Omega = \left(\frac{V_{ol}}{\Omega} \right)_{LNAPL} \quad (3)$$

where ς indicate the LNAPL spreading area in the (x, y) plane.

[LIO and ARAL 2000] used the same average technique for modelling LNAPL spreading.

To prove the reliability of the linearization with this simple averaging method 3 the linearized solution will be compared with the exact analytical solution of the nonlinear equation 1. For the comparison, a radial symmetrically LNAPL spreading on the horizontal groundwater (i.e. $q_w=0$) will be take into account, for which an exact analytical solution exist.

The considered LNAPL lens at the time $t=0$ (i.e. initial conditions) is

$$t = 0, h = h(r, 0) = h_o \left(1 - \frac{r^2}{a_o^2}\right), r = \sqrt{x^2 + y^2} \quad (4)$$

The (exact) analytical solution has the following form

$$h_l(r, t) = h_o \cdot \left[\frac{\left(1 + \frac{8 \cdot k_f \cdot h_o \cdot t}{n_e \cdot a_o^2}\right)^{0,5} - \left(\frac{r}{a_o}\right)^2}{\left(1 + \frac{8 \cdot k_f \cdot h_o \cdot t}{n_e \cdot a_o^2}\right)} \right] \quad (5)$$

For the numerical application the following parameters are used:

- $h_0=0.30\text{m}$; $a_0=5.00\text{m}$
- $n_e=0.25$;
- $k_l=4\text{m/day}$; $k_w=4\text{m/day}$
- $q_{wx}=0$

It is assumed that the LNAPL mound volume (V_l) remain constant. For the solutions of the linearized equation 1 the analytical method, the Simple Explicit FD Method

and the MacCormack predictor-corrector Method are applied. To prove the influence of the discretization of different numerical methods several space discretization ($\Delta x = \Delta y = 0.5 - 2.0$ m) and time steps ($\Delta t = 0.01 - 0.2$ day) have been taken into account. The observed differences between different methods and different discretization steps are not of great significance. To calculate the average thickness, the simple average technique 3 was used. The obtained results using the exact solution 5 and the above mentioned methods, for $\Delta x = \Delta y = 1.0$ m, $\Delta t = 0.1$ day was realized. The results shows that the deviations of the results obtained with the linearized equation from the exact solution are relatively large, especially in the central area, where the maximally error amount to 30-80%. We can conclude that the use of the simple average technique 3 to calculate the average free phase thickness leads to relative large errors for the LNAPL thickness profiles.

Proposal and prove of a new weighted average technique to estimate the average free product thickness for the linearized free LNAPL transport equation

To reduce the errors of the LNAPL thickness a new average technique for the free product thickness will be proposed and tested.

The above mentioned simple average technique 3 with its consequence assume that the deviations $\delta h(x,y)$ to the averaged thickness $h_a(t)$ on the LNAPL spreading area ζ are constant weight with a weighting function identically with a unit. The calculated results shown that this assumption (i.e. the simple average technique) leads to relative large errors for the LNAPL thickness, especially in the zone where the thickness has higher values (i.e. in the central area in the case of an axial symmetrically spreading. This observation suggests that a new type of weighting of the deviations is necessary. The proposed weighting function can be select as equal to the LNAPL thickness $h(x,y,t)$:

$$\iint_{\Omega} h_l(x, y, t) \delta h_l(x, y, t) d\Omega = 0 \quad (6)$$

That implies fundamentally, that we give more weight for the deviations area with higher free product thickness where the error is higher.

Replacing in 6 $\delta h_l(x,y,t)$ with 2 one obtain a new weighted average thickness defined as

$$h_a(t) = \frac{\iint_{\Omega} h_l^2(x, y, t) d\Omega}{\iint_{\Omega} h_l(x, y, t) d\Omega} \quad (7)$$

To prove of the new average technique, defined as 7, the same numerical application as in section 2 was realised. That obtained deviations (errors) from the exact solution

are relatively small (i.e. about 2-3%). This was confirmed with numerous other examples. Consequently we can conclude that the proposed averaging technique for the linearized equation leads to much better results for the LNAPL spreading and migration.

Conclusions

The governing equation for the LNAPL spreading is a nonlinear partial differential equation, which can be linearized to a two-dimensional advection-dispersion equation with time-dependent dispersion coefficients. For the semi-analytical and numerical solutions of the linearized equation, the estimation of the LNAPL averaged thickness at each time step is necessary. We demonstrated that the most widely average technique used in the literature (i.e. the average thickness is calculated as the LNAPL lens volume per unit area of the lens) can lead to large error. Consequently a new weighted averaging technique is proposed. Comparisons of the results obtained with the exact solution and linearized solutions shows that the proposed weighted averaging technique, in opposite to the simple average technique, is closed to the exact solutions. Consequently the proposed weighted averaging technique allows the improvement of the existing numerical and semi-analytical calculation methods for both LNAPL and DNAPL mound spreading and migration with ambient groundwater flow in aquifer.

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