Evaluation of Sharp Interface Approach in modeling of LNAPL spreading and migration on the water table

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ABSTRACT
When the light non-aqueous phase liquid reaches the water table it will migrate in the direction of ambient groundwater flow. One of the simple models used to predict spreading and migration of LNAPL is the well known Sharp Interface Approach proposed by Corapcioglu (1996). The objective of this study is to examine the adequacy of Sharp Interface Approach in modeling of LNAPL spreading and migration on the water table. Simulation of LNAPL spreading and migration was performed in an aquarium filled with sand and subjected to a constant hydraulic gradient of water flow. Spreading and migration of LNAPL was monitored over the study area. Numerical results obtained using finite difference approach were compared with the observed behavior to discuss the discrepancies. The results show that although there is some difference between the experimental and numerical results, they both show the same trend in LNAPL migration in direction of groundwater flow.

RÉSUMÉ
Lorsque la liquide Légère de phase non aqueuse arrive à la nappe phréatique, elle émigre dans la direction de l'écoulement ambiant d'eaux souterraines. Un des modèles simples employés pour prévoir la propagation et la migration de LNAPL est l'approche bien connue d'interface forte proposée par Corapcioglu (1996). L'objectif de cette étude est d'examiner l'adéquation de l'approche d'interface forte dans la modélisation de la propagation et de la migration de LNAPL sur la nappe phréatique. La simulation de la propagation et de la migration de LNAPL a été effectuée dans un aquarium rempli de sable et soumis au gradient hydraulique constant de l'écoulement d'eau. La propagation et la migration de LNAPL ont été surveillées. Des résultats numériques obtenus utilisant l'approche de différence finie ont été comparés au comportement observé pour discuter les anomalies. Les résultats montrent que bien qu'il y ait une certaine différence entre les résultats expérimentaux et numériques, tous les deux montrent la même tendance à la migration de LNAPL dans la direction de l'écoulement d'eaux souterraines.

1 INTRODUCTION

Among the most important organic sources causing both soil and water pollution is non-aqueous phase liquid, (NAPL). This kind of contamination occurs as a result of spill, tank leaks and improper disposal practices. Generally, NAPL is divided into two categories. First, the one which is lighter than water i.e. light non-aqueous phase liquid, (LNAPL) and the next which is denser than water i.e. dense non-aqueous phase liquid, (DNAPL). Once LNAPL introduced to the soil, it migrates downward under gravitational force through the unsaturated zone until it reaches the capillary fringe. Then, it forms a mound above capillary fringe. At this stage, it starts to spread laterally as it migrates over the groundwater in the direction of highest gradient.

A review of the literature shows that a number of numerical methods have been developed to explain the migration and fate of LNAPL flow above the water table. Since each method has its own assumptions the applicability of them must be checked by comparing the results from numerical solution with the data measured directly from laboratory test or field exploration.

According to Corapcioglu (1996), migration of NAPL such as gasoline and fuel oil can be modeled in four general groups: sharp interface models, immiscible phase flow models with capillary, inter-phase mass transfer models and compositional models. Each group makes certain assumptions to generate a governing set of equations. Among them, sharp interface models have been investigated by a number of researchers and several analytical, semi-analytical, and numerical solutions have been presented during the last decades. Although there are some limitations in the sharp interface models, such as neglect of capillary forces in comparison to pressure and gravity forces, they can function as screening or site assessment tools due to their relative simplicity (Corapcioglu, 1994).

The model studied in this paper was derived by Corapcioglu et al. in 1996. Corapcioglu et al. (1996) developed the sharp interface model presented by Corapcioglu (1994) to describe the LNAPL mound spreading and migration with ambient groundwater flow. Kim & Corapcioglu (2001) modified the model of corapcioglu et al. (1996) to handle the residual mass loss in pores due to capillary forces.

In this study, the modified equation by Kim (2001) was solved numerically for a simulated spill of LNAPL condition in the lab and then the numerical results were compared by the experimental measurements to find the adequacy of the model in forecasting the migration and fate of LNAPL on water table. In other words, the objective was to check suitability of sharp interface model for prediction of oil contaminant transport and evaluating its weak and strong points. For this purpose, an experimental aquarium was built to measure directly the necessary data on migration and transport of released LNAPL into the soil.

2 THEORETICAL FRAMWORK

The starting point to develop a governing equation is the mass balance equation of LNAPL phase in a porous medium. This equation can be expressed as follow:

$$\nabla.\rho_o q_o + \frac{\partial (\rho_o s_o n)}{\partial t} = 0 \qquad [1]$$

Where ρ_o is the density of the NAPL phase; q_o is the specific discharge of the NAPL phase; S_o and S_w are the degrees of phase saturations of LNAPL and water phases, respectively; t is the time; and n is the porosity. By employing sharp-interface assumptions and vertically averaging the NAPL phase mass balance equation, Corapcioglu et al. (1996) developed a mathematical model describing LNAPL transport on the water table.

$$\frac{k_{or} K_o L_o (\rho_w - \rho_o)}{n \rho_w (S_{oo} - S_{oun})} \nabla^2 L - \frac{q_w k_{or} K_o}{K_w n (S_{oo} - S_{oun})} \nabla L = \frac{\partial L}{\partial t} \pm \frac{Q_o}{n (S_{oo} - S_{oun})} \delta (x - \xi) \delta (y - \zeta) \qquad [2]$$

Where ρ_w is the density of water phase, K_o and K_w are the hydraulic conductivities of LNAPL phase and water phase respectively; k_{or} is the relative permeability of the NAPL phase; S_{oo} and S_{oun} are saturation degree of mobile NAPL and immobile NAPL respectively; L is the NAPL thickness on the water table; L_o is the reference thickness of the NAPL mound; q_w is the specific discharge of water; Q_o is the rate of NAPL leaking/pumping at point (ξ,ς); and δ denotes the Dirac delta function used to represent point sources; ∇ is the differential operator; x and y are the coordinate of any point in the study area.

3 EXPERIMENTAL MATERIALS AND METHODS

3.1 EXPERIMENTAL SET UP AND PROCEDURE

For the laboratory simulation of LNAPL spreading and migration on the water table, a three-dimensional aquarium 2000 mm long, 870 mm wide and 700 mm high was fabricated. The aquarium consisted of an aluminum plate at bottom and 10 mm glass as the surrounding walls supported by an aluminum frame.

The aquarium was divided into three compartments separated from one another by framed wire mesh (Figure.1). The end compartments served as upstream and downstream reservoirs for simulating the ambient groundwater flow across the soil medium placed in the middle compartment. Using this configuration, a differential head of 16 mm was imposed leading to a steady state water flow rate of 9.47 mLmin^{-1} through the soil.

The soil poured in the middle space was packed by manual compaction in three layers separately. To reach a uniform porosity a 100 mm × 100 mm wood tamper falling under its own weight from a distance of 100 mm above the soil was used. This created a porous medium with an average porosity 0.36. The height of the soil profile was around 350 mm with 150 mm above water table.

Prior to sand pouring, 24 perforated polyethylene pipes, 14 mm internal diameter, were installed at predetermined coordinates to monitor development of the oil profile in the soil (Figure .1).

As for injection of oil, a glass box 100 mm * 100 mm with 150 mm height was placed on the center line of aquarium at a distance of 250 mm from the upstream reservoir. The location of this box is shown in Figure 1 by a square at the intersections of axes 2 & E.

The aquarium was slowly filled with water from the bottom to minimize air pockets trapping in the subsurface and stratification. The water level was raised and lowered around the specified level of saturation a few times to minimize the accumulation of trapped air in the saturation zone as well as to let the soil settle before starting the test. The water was then drained to the desire water table level of 200 mm from base of aquarium providing a vadose zone height of 150 mm above the water table. Next, a hydraulic gradient of 0.01±0.003 was imposed across the entire soil profile.

The LNAPL spill was initiated after the water flow rate became steady. A total of 525 mL of oil was mixed with sand to prepare 15,000 cu. mm of contaminated soil. Then this amount of contaminated soil was poured into the glass box placed in the aquarium previously. At this stage the glass box was removed to let the oil migrate laterally on the surface of water table. The time was recorded and migration of oil was monitored. To monitor the migration and spreading of oil over the study area, the thickness of the oil in the observation wells was measured with an oil-water interface meter at different time internals.

3.2 POROUS MEDIUM AND LNAPL PROPERTIES

The soil used was classified as well-graded sand (SW) according to the Unified Soil Classification System. The soil had a uniformity coefficient (D_{60}/D_{10}) of 1.54 with an effective grain size (D_{10}) of 0.55 mm and a medium grain size (D_{50}) of 3.4 mm. The permeability of the sand, measured directly through the aquarium outlet flow, was 7.6 mm sec^{-1}.

The NAPL source was crude oil with a density of 0.788 gr cm^{-3} and viscosity of 2.1167 cs.

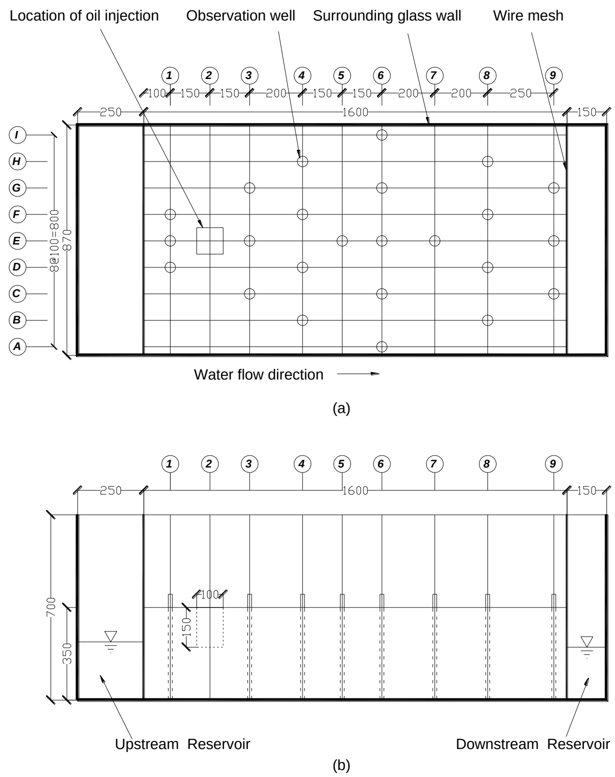


Figure 1. Schematic of pilot-scale aquarium, (a) Plan view, (b) Side view.

4 NUMERICAL MODELING

4.1 NUMERICAL SOLUTION

In order to evaluate the adequacy of the model, the experimental observations were compared with the numerical simulations. In this regard, the governing partial differential equation (Eq. 2) was solved numerically using the Hopscotch finite difference technique. Ansari (2005) used Hopscotch Method presented by Gourlay (1971) to solve the same governing equation. The main advantage of Hopscotch method is its unconditional stability.

A computer program was developed to solve the governing differential equation and obtain the numerical results from simulation of oil migration and its spreading on the water table. The program was capable of taking into account the residual mass loss which is left behind in the pores while the mound migrates on the groundwater surface.

Boundary conditions were defined as zero gradient of oil thickness on boundary nodes. Initial condition was imposed the NAPL thickness on the source nodes as well as groundwater flow velocity and its direction. For the solution, a grid spacing of 10 mm × 10 mm was adopted and positive X direction coincided with the ambient groundwater flow direction.

4.2 MODEL PARAMETERS

Parameters involved in the sharp interface model can be categorized as geotechnical, hydro-geological and leakage parameters (Ansari, 2005). Geotechnical parameters describe subsurface characteristic include porosity, degree of saturation of mobile LNAPL and residual degree of saturation of LNAPL. Hydro-geological parameters which deal with the multi phase flow of existing fluids in the porous medium include coefficient of permeability of water in the soil matrix, coefficient of permeability of LNAPL phase in the soil matrix, local groundwater flow direction and its velocity as well as the relative permeability of LNAPL phase.

Degree of saturation of the mobile oil and the residual oil degree of saturation was measured using the distillation extraction method by taking appropriate samples from the model soil at the end of test. The coefficient of permeability of the oil phase in the soil matrix was estimated using the measured coefficient of permeability of water and the relationship between hydraulic conductivity and intrinsic permeability. Relative permeability of the oil phase was estimated by using the equation presented by Parker and Lenhard (1987).

The input parameters used in the numerical modeling are given in Table 1.

Table 1. Model input parameters

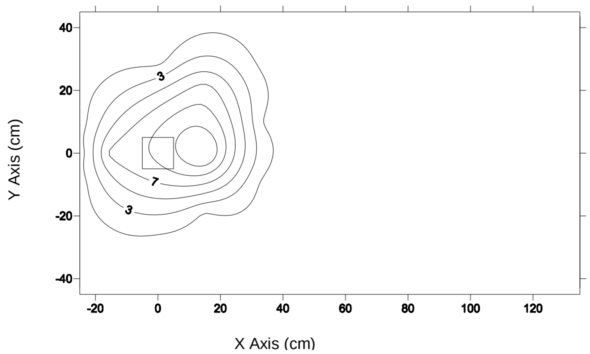
Parameters	*Symbol*	*Value*
Porosity	n	0.36
Darcy velocity (mm/min)	q_w	5.05
Hydraulic conductivity of water (mm/min)	K_w	459
Hydraulic conductivity of oil (mm/min)	K_o	157
NAPL saturation in NAPL lens	S_{oo}	0.64
Residual water saturation	S_{ow}	0.36
Residual NAPL saturation	S_{oun}	0.19
water density (kg/m^3)	ρ_w	995
NAPL density (kg/m^3)	ρ_o	788
NAPL relative permeability	k_{or}	0.77
NAPL source flow rate	Q_o	0
Radius of source (mm)	r	56.40

5 RESULTS AND DISCUSSION

5.1 EXPERIMENTAL RESULTS

The actual oil thickness was determined from the apparent thickness measured in the observation wells. To estimate actual oil thickness the equation developed by De Pastrovich et al. (1979) was used. Next, contour lines of oil thickness were drawn based on actual thickness assigned to the corresponding observation wells.

Ordinary “kriging”, mostly associated with the acronym BLUE (best linear unbiased estimator), which is a stochastic interpolation algorithm was implemented for the interpolation.



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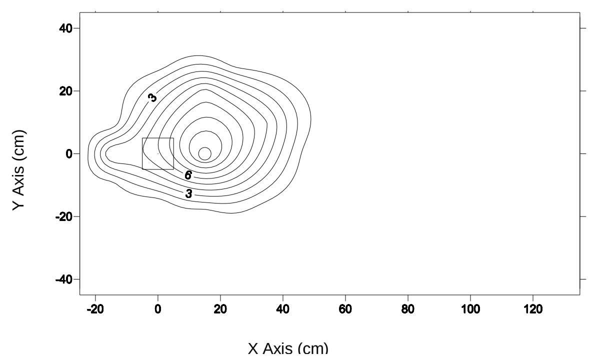

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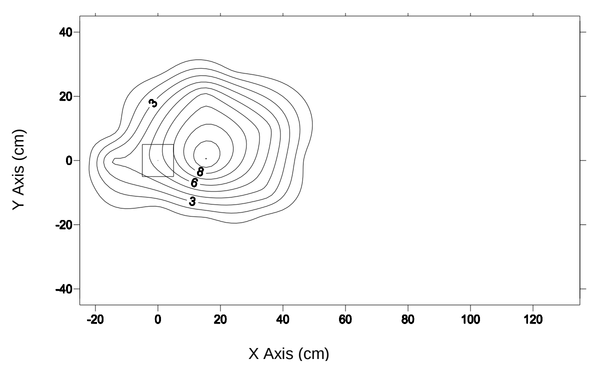

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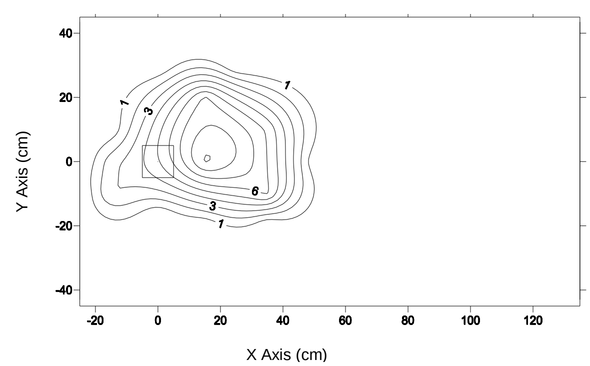

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Figure 2. Oil thickness contour lines at (a) 10 min, (b) 20 min, (c) 30 min, and (d) 40 min after releasing of oil for application of experimental (unit mm).

Following the above mentioned strategy and with respect to the value of oil thickness in observation wells measured at 10, 20, 30, and 40 minutes from the start of the test, oil thickness contour lines of the LNAPL mound were drawn over the study area. Figure 2 shows the LNAPL thickness contour lines at these time intervals, respectively. From this figure, it is observed that migration and spreading of oil in the direction of water flow is more pronounced than in other directions. It can also be observed that the mound moves a little upstream the source as a result of spreading in the opposite direction of water flow.

The changes in thickness of oil in the observation wells located along the center line of the aquarium, i.e. axis E, can demonstrate migration of LNAPL along the direction of water flow. This profile is shown in Figure 3. From this figure, migration of the oil toward downstream is vividly obvious. Furthermore, as time passes by, the location of maximum oil thickness moves downstream and the value of maximum thickness reduce gradually.

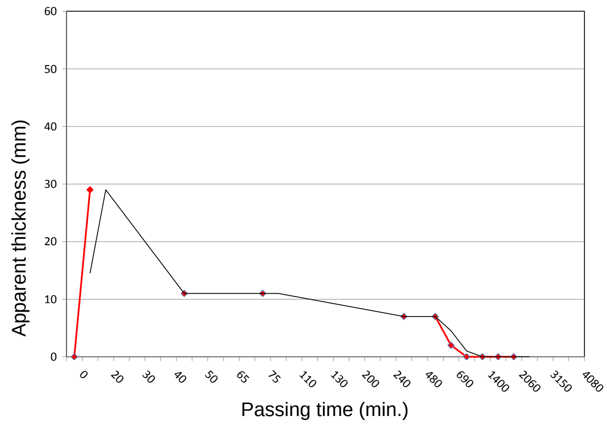
5.2 NUMERICAL RESULTS

For the sharp interface model stated previously, the parameters presented in Table 1 were used as input data for the numerical simulation.

Results of numerical solution at different times, 10, 20, 30 and 40 minutes after oil spill were calculated. Figure 4 illustrates oil mound profile along y=0 at different times. The contour line corresponding to L= 0.1 mm actual oil thickness at different times is shown in Figure 5. From Figures 4 and 5, it is observed that as time passed the mound moves in the direction of ambient flow of water. Furthermore, as the mound moves downstream the maximum thickness of oil decreases and the polluted area expands in such a way that the spread of oil in direction of ambient groundwater flow is more than the transverse direction. Moreover, Figure 4 shows spreading of the mound upstream of the source for the first few time steps which is in accord with the observed behaviour as shown previously in Figure 2.

5.3 COMPARISON OF NUMERICAL RESULTS WITH EXPERIMENTS

In order to compare effectively between experimental data and numerical solution, profiles of the oil mound obtained from numerical solution and experimental data were compared in a single graph for each time interval. Figure 6 shows the profiles of oil mound at time 10, 20, 30, and 40 minutes after oil spill. To draw the experimental profile of oil mound, a trend line was added to the experimental data representing the actual oil thickness. These experimental data obtained from the intersection of line y=0 with the contour lines in Figure 2. From Figure 6 it may be concluded that the location of maximum oil thickness obtained from numerical solution and experimental data is approximately the same for all time intervals studied. In other words, the model estimates the same movement of oil mound in the direction of groundwater flow as the experimental data. However, the actual oil thickness values obtained from experimental results are considerably higher than those obtained from the numerical simulation. It may be partly due to the inaccuracies inherent in the relationship used to convert the apparent oil thickness to the actual thickness.



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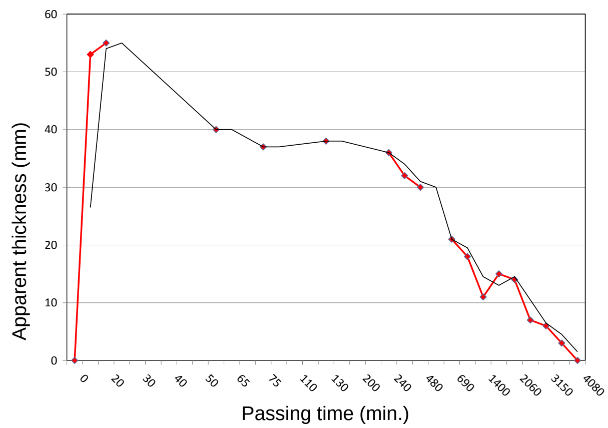

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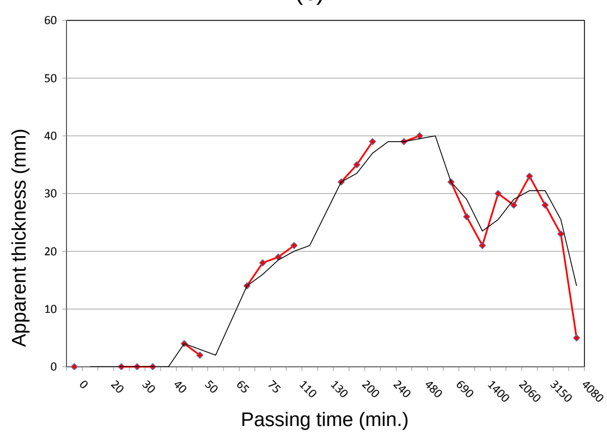

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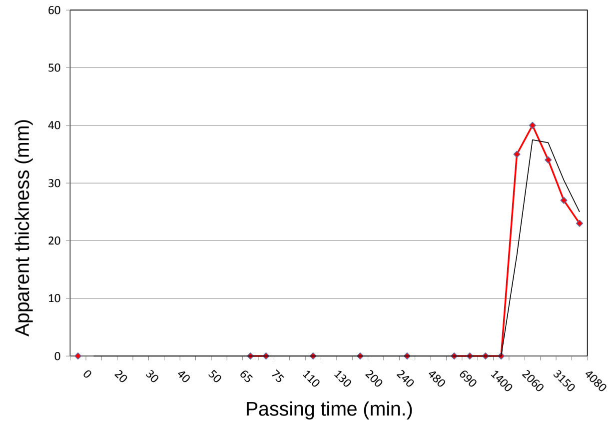

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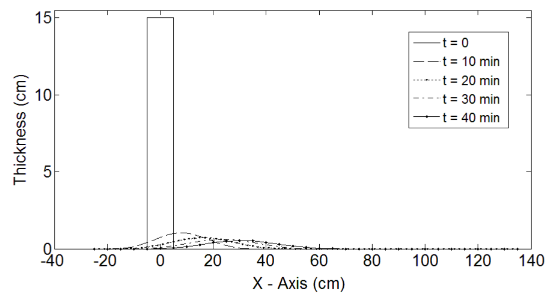
Figure 3. Representative difference in apparent oil thickness breakthrough curve at observation wells (a) 1-E, (b) 3-E, (c) 5-E, and (d) 6-E.



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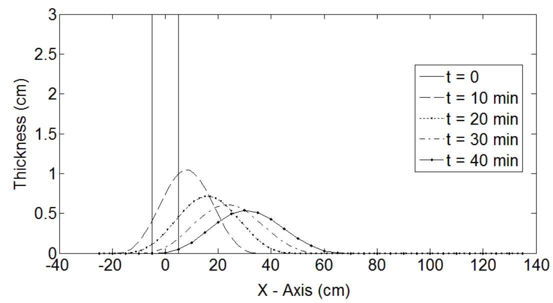

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Figure 4. (a) Spreading and migration of an initial rectangular oil mound profile along y=0 at different times, (b) profile of oil spreading and migration under magnification from part (a).

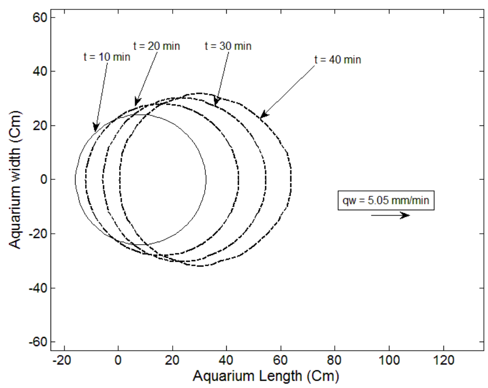
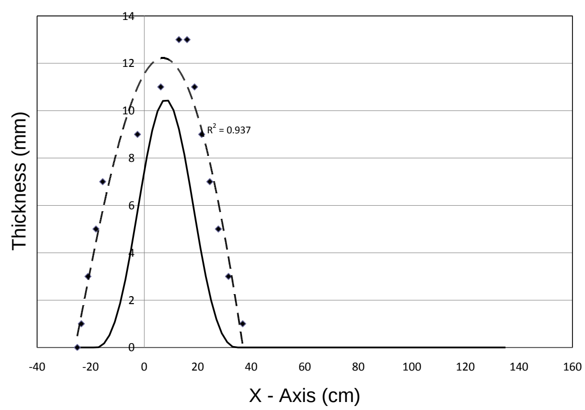


Figure 5. Contour lines of L=0.1 mm actual oil thickness at 10, 20, 30, and 40 minute after oil spill.

1. SUMMARY AND CONCLUSION

The Sharp Interface model represented by Corapcioglu (1996) was solved numerically and compared with oil mound migration and spreading observed in the laboratory to evaluate the adequacy of the model. The governing advection-dispersive transport equation was solved by the finite difference method using Hopscoth procedure. Experimental data obtained directly from the measured oil thickness in the observation wells over the study area were used to calibrate the model.



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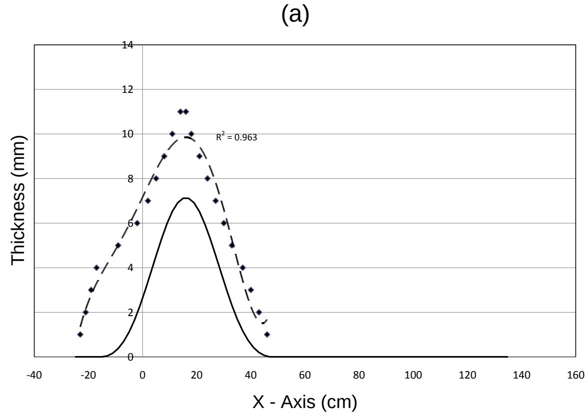

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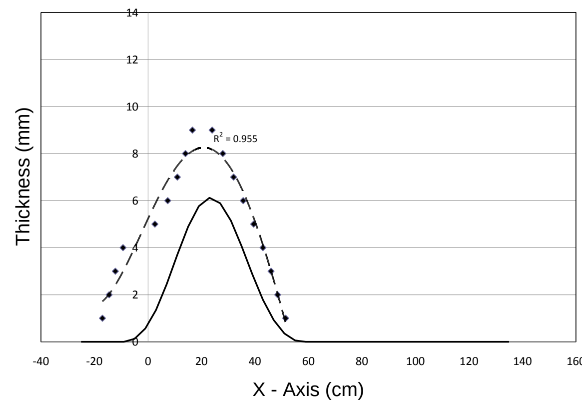

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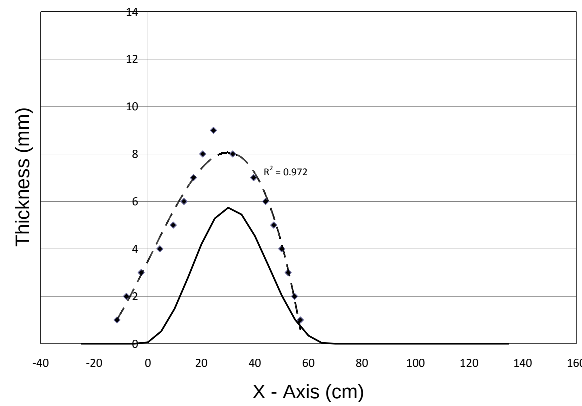

(d)

Figure 6. Oil mound profile obtains from experimental data and numerical solution of model at (a) 10 min., (b) 20 min., (c) 30 min., and (d) 40 min. after oil spill.

The comparison between the experimental data with the numerical results indicates the followings:

- The LNAPL thickness predicted by the model is smaller compared to the measured values. This may be attributed to the approximations involved in converting the apparent oil thickness in the wells to the actual thickness in the soil as well as by other assumptions inherent in the model itself.
- The LNAPL migration (movement with time) is reasonably predicted using the sharp interface model.
- The model was also capable of simulating the spreading of oil mound upstream of the source as observed in the experiments.

For the above mentioned points, it can be concluded that the sharp interface model may serve as a useful tool to predict spatial migration of oil mounds but it must be used with caution for estimating the variation of oil mound volume with time.

ACKNOWLEDGMENTS

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