LABORATORY AND NUMERICAL SIMULATIONS OF LIGHT NONAQUEOUS PHASE LIQUID (LNAPL) IN UNSATURATED ZONE

Samira Albati Kamaruddin*, Wan Nor Azmin Sulaiman, Mohamad Pauzi Zakaria and Norhan Abd Rahman

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Introduction

The contamination of hydrocarbons in soil and groundwater by fuels and industrial chemicals has become a problem of growing concern. The contaminated groundwater is not only unsafe for human and animal consumption but also not suitable for irrigation purposes. The leaking from underground storage tanks (USTs) and pipelines, hazardous waste sites and surface spills are the general sources of nonaqueous phase liquids (NAPLs). The NAPLs is a common term used in hydrogeology to describe the immiscible, separate liquids phase when in contact with water and/or air that occurred in subsurface environment. These liquids typically have different density and viscosity than water (Charbeneau, 2000). A NAPL with a density less than water is classified as light nonaqueous phase liquid (LNAPL), and a NAPL denser than water is classified as dense nonaqueous phase liquid (DNAPL).

The LNAPL passes through unsaturated soil and float on the surface of groundwater while DNAPL moves downward through the saturated soil to settle. The geologic configuration is the key to disposition of NAPLs in the subsurface. For LNAPL, its movement in the unsaturated zone is of primary importance because the bulk liquid does not penetrate the saturated zone. In contrast, the structure of both saturated and unsaturated regions have major impact on DNAPL disposition. Thus, very often the LNAPL laboratory experiments under controlled condition associated with numerical simulations are mainly focus in the unsaturated region.

Due to the toxic nature of the chemicals involved, it is often not feasible to conduct the experiment in the field. Thus, model as a device which represents an approximation of a field situation can be used to study the LNAPL transport in the subsurface. Three types of hydrogeological models are analytical, physical and numerical. Analytical models applied the mathematical representation of a physical system that is solved analytically depending on simplified assumptions. The solution is generally not applicable for the analysis of complicated real world problems. Physical or also called experimental models are suitable for that case and may give better understanding of phenomena but impossible to be used as prediction tools.

The numerical models are usually used to provide prediction of the system behavior under natural conditions or in response to management decisions. Prior to model prediction, the numerical models need to be validated and verified with experimental data in which data acquisition in the field is typically very expensive and complete data sets are usually sparse especially in tropical environment. In addition, current saturation imaging technique need an attempt of using photographic method instead of photonattenuation because the technique is experimentally demanding (Kechavarzi, Soga, & Illangasekare, 2005), limited to slow measurements and hazard of working with high energy sources related to the technique (Bob, Brooks, Mravik, & Wood, 2008).

In the laboratory, researchers as notified by Oostrom et al. (2006, 2007) have used various names for their physical aquifer model. The same terms as recommended by them will be used throughout this paper to avoid inconsistency and misinterpretation. The term flow cell is referred to the aquifer models whereas the built tank with sand packed is termed as sand tank. The experiments have been categorized into qualitative and quantitative infiltration and redistribution experiments. Both categories consist of conducted experiments with and without numerical modeling. In this research the data acquisition for saturation mapping in quantitative LNAPL experiments are important for numerical simulation. The existing LNAPL infiltration and redistribution experiments that applied numerical models include simple numerical model (Hochmuth & Sunada, 1985), ECLIPSE (Høst-Madsen and Høgh Jensen, 1992), IMPES (Van Geel & Sykes, 1997), ARMOS (Waddill & Parker, 1997), and STOMP (Oostrom, Hofstee, & Dane, 1997; Oostrom, Hofstee, & Wietsma, 2006; Simmons, McBride, Cary, & Lenhard, 1992; Wipfler, Ness, Breedveld, Marsman, & van der Zee, 2004).

Objective

This research is conducted with the objectives (1) to investigate the infiltration, redistribution and attenuation mechanism of LNAPL in an unsaturated zone based on two-dimensional (2-D) laboratory model; (2) to simulate a 2-D model of LNAPL migration using numerical code of MOFAT; and (3) to assess the prediction of LNAPL migration in the unsaturated zone under tropical condition. In brief, the main scope of this study covers LNAPL simulations in an unsaturated homogenous porous medium, which is limited to 2-D experimental and numerical study that considers three-phase fluids, namely water, NAPL and gas.

Research Methodology

Numerical simulation and laboratory experiment are the two main research works in this study as shown in Figure 1. The numerical model is developed based on theoretical study and experimental data. The model needs to be validated and verified prior to assessment of model prediction. Therefore, the precision in data acquisition begins with selection of porous media that considers the availability and inexpensive materials with good consistency and uniformity. In order to consider the tropical condition such as Malaysia the rainfall recharge process is included in the numerical and experimental models by providing the artificial rainfall based on the recorded average annual rainfall.

Two-dimensional laboratory model

Numerous laboratory model as reported by (Oostrom et al., 2007) are used as a guidance to select and fabricate the new sand tanks. The sand tanks are built based on represented flow cell to observe a migration of certain amount of LNAPL spills. The models are named according to the sequence of conducted experiments. Model A is an existing flow cell, whereas Model B is the new unit. The details of 2-D laboratory models are given in Table 1.

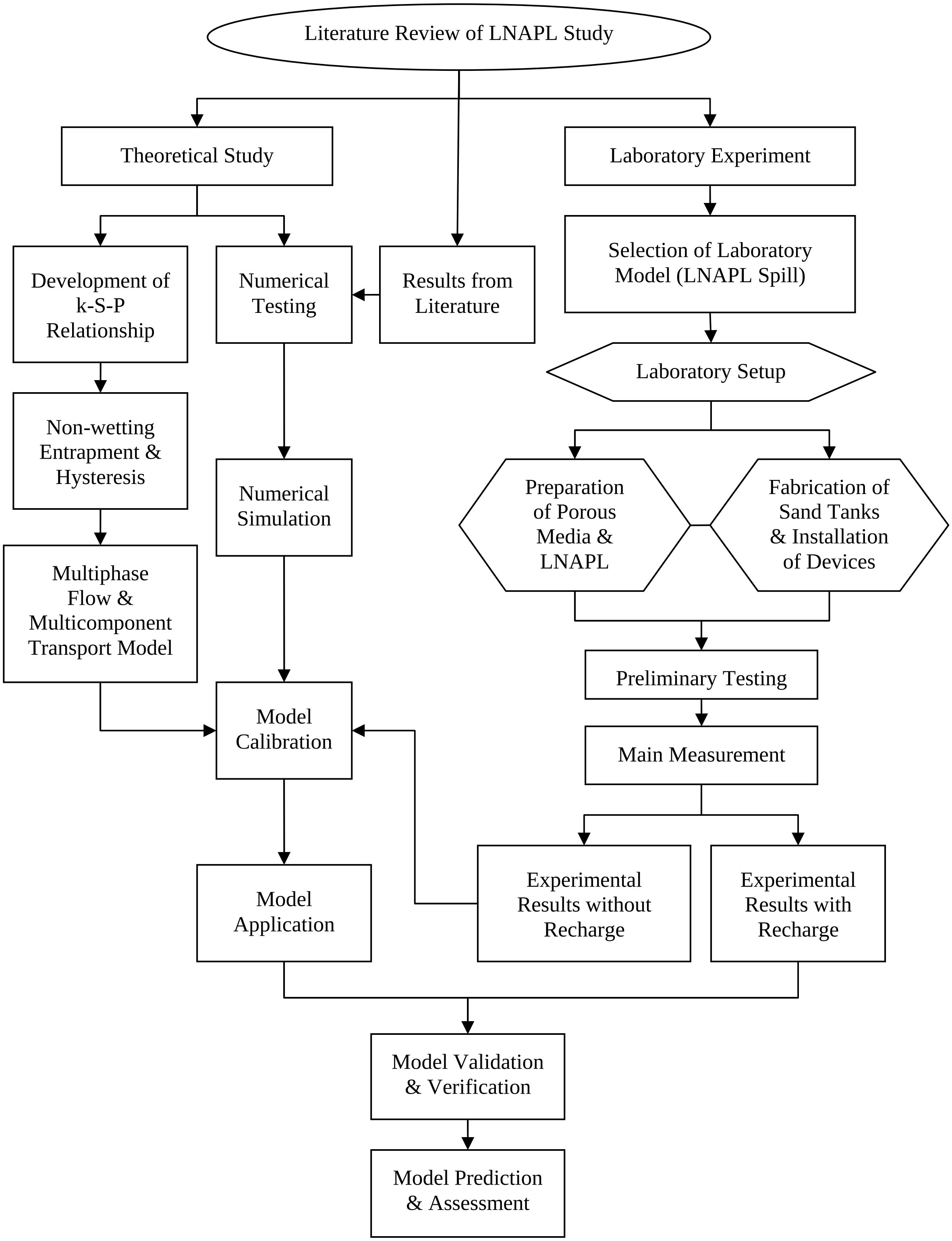

Figure 1. Flowchart of laboratory and numerical simulations of light nonaqueous phase liquid (LNAPL).

Table 1. Details of two-dimensional laboratory model

Model	Model A	Model B
Flow cell details		
Condition	Existing	New
Tank height (cm)	45	90
Flow cell height (cm)	36	84
Length (cm)	117	56
Width (cm)	10	5
Wall material	Acrylic	Perspex
Wall thickness (cm)	0.3	1.0
Sand properties		
Type of sand	Fine sand	Silica sand
Manufacturer	Local	Local
Porosity, ϕ	0.39	0.38
Mean size, D_{50}	0.13	0.32
Coefficient of uniformity, C_U	0.74	2.24
NAPL properties		
Type of NAPL	LNAPL	LNAPL
NAPL source	Toluene	Benzene
Manufacturer	J.T. Baker (9336-03)	Sigma-Aldrich (32212)
Amount (mL)	300	500
Density (g/m^3)	0.8669×10^6	0.88×10^6
Dye details		
Type of dye	Oil Red O	Oil Red O
Manufacturer	Sigma-Aldrich	Sigma-Aldrich
Amount (g)	1.5	0.04
Color	Red	Red

Fluid saturation measurement

An image analysis technique (IAT) as presented by Kechavarzi, Soga and Wiart (2000), is used to determine LNAPL, water and air saturation distribution. Using digital cameras and sand samples containing water, LNAPL and air, the optical density can be defined for the reflected luminous intensity. Image acquisition for both Model A and B experiments is conducted according to the initial condition of LNAPL spreads and then following the image acquisition schedule. Several images are taken during the first day of LNAPL injection followed by one image in the every following day until no changes in the contaminant migration has observed.

Fluid pressure measurement

The water and LNAPL pressures are measured with hydrophilic and hydrophobic tensiometers, respectively. The ceramic porous stones used for the LNAPL tensiometers are treated with chlorotrimethylsilane to render them hydrophobic. The tensiometers consisted of 1 bar pressure transducers connected via cylindrical brass tubing (30 mm long and 6 mm in diameter) to high nonwetting fluid entry pressure porous stones (10 mm long and 5 mm in diameter).

Expected experimental results

The typical experimental results are the shape and extent of NAPL saturation plumes, travel-time and-distance of 2-D NAPL flow and fluid-phase concentrations. With extension of these results the relationships of capillary pressure-saturation (*P*-*S*) and relative permeability-saturation (*k*-*S*) can be developed to find representation of the three-phase fluid relative permeability-saturation-pressure (*k*-*S*-*P*) relationship as a critical component of multifluid flow simulation (Schroth, Istok, Selker, Oostrom, & White, 1998).

Results & Discussion

Based on the recorded images obvious changes of shape and intensity of red colors were observed during the first day. While no great changes were observed in the next following days. The numerous recorded images would be used in the image processing to provide the image analysis data. A linear relationship between average optical density and fluid saturation will be developed at final stage of image analysis technique.

From the observation, the physical of sand tanks or flow cells may affect the experiment processes including the spread of LNAPL migration. For example insufficient wall thickness has resulted to the wall bending of Model A. The used of wall surface material (acrylic) has affected the image visualization and existing grids have created errors in image processing. The shorter flow cell of Model A has allowed less depth of penetration and no water drainage has considered in the model. The wider flow cell (10 cm) has increased the horizontal spread area of contaminant which is not appropriate for a 2-D model and has reduced the actual vertical migration. In order to obtain consistent and uniform sand packing, the pouring apparatus called hopper was used with special design to fit the open sand tank surface of Model B. The selected porous media also have been graded to fit the range of 0.1 to 0.6 mm.

Significance of Findings

Data acquisition of fluid saturations and pressures are the most essential in numerical model validation and verification. Without the transient pressure and saturation data, there would be insufficient constitutive relations for model prediction. Since the data acquisition of NAPL contamination are typically difficult and very expensive, it is recommended to improve laboratory techniques especially in NAPLs saturation imaging technique such as photographic methods. On top of that, enhanced numerical simulations is needed for a better future model predictions supported by high-end visualization of results. The future laboratory and numerical simulations should consider the present technologies involved in this field.

As more researchers preferred for non-destructive and non-intrusive techniques, the IAT provides an alternative with image acquisition using either a digital camera or video camera and the images processing software. The Image-Pro Plus® software (Media Cybernetics Inc.) and MATLAB® with up to date toolbox are the two available choices for that processing. Depending on the type of LNAPL source, MOFAT and STOMP are the most widely used codes for numerical simulations of the 2-D multiphase flow. The visualization of results for every simulation can be produced either using Surfer® or MATLAB®.

Previous simulation results indicate that the transport properties of individual non-inert components of an organic mixture play an important role in predicting the overall distribution of the contaminants in different phases. Simulation results also show that different locations of spill site may produce different shape and level of oil saturation contours which is subjected to the direction of the slope of water table (Samira, Sulaiman, Rahman, & Zakaria, 2009).

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