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Investigation of light non-aqueous phase liquid penetration in double-porosity using physical experiment and computer simulation

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Abstract. Groundwater resources benefits to human activity for developing country. Groundwater contamination is crucial, particularly due to the amount of leakage and spillage of hydrocarbon liquids such as light non-aqueous phase liquids (LNAPLs), resulting in contaminated the groundwater and unsafe for domestic and agriculture activities. Penetration of hydrocarbon liquids into groundwater can be seen through double-porosity soil. Therefore, this paper investigates the penetration of LNAPLs in double-porosity soil using computer modelling to calibrate and validate from physical experiment data. These computer modelling and physical experiment studies discuss the pattern and rate of LNAPL penetrations by employing PetraSim commercial software and digital image processing technique (DIPT) by using acrylic glass cylinder, mirror and Nikon D90 digital camera. The LNAPL volume of 70 ml and 150 ml were poured instantaneously onto the surface of soil sample for calibration and validation purposes. The penetration pattern in double-porosity were monitored and recorded using digital camera at pre-determine time intervals. The images were processed using Surfer software and Matlab routine to plot the LNAPL penetration pattern. PetraSim simulation was used to calibrate and validate the penetration of LNAPL through double-porosity soil with physical experiment data. As a result, the PetraSim results valid with the physical experiment results. The Nash-Sutcliffe efficiency results more than 0.50 with percentage of differences for calibration and validation are 1.34% and 5.47% between physical experiment and PetraSim simulation. As a conclusion, PetraSim simulation can be used for further investigation on LNAPL penetration through subsurface soil.

1. Introduction

Groundwater is the major source of water supply either for domestics, industrials or agricultures. This resource is increased tremendously due to civilization grew rapidly. Groundwater contaminations by petroleum hydrocarbon one of the critical issues in geo-environmental and these issues reducing the quality and quantity of groundwater as shown in figure 1 [1]. The contamination is not easily detected and caused serious problems, even more dangerous [2]. The contaminations would penetrate through the subsurface system (i.e., saturated and unsaturated zone) whereas the soil consists of double-porosity media [3]. Double-porosity media shows two specific scales of porosity medium and size of pore distribution that focussing on inter-aggregated pores and intra-aggregate pores in soil such as in agricultural and compacted soil [4, 5]. Characteristics of double-porosity medium can be re-created in one-dimensional infiltration of experiment test [6, 7]. Moreover, the researchers [8 – 15] have started immerge and contributed to deeper knowledge on physical laboratory in double-porosity soil's characteristic. The only feasible alternative is to construct a physical experiment and computer modelling simulation due to cost issue and time consuming rather than full-scale experiment. The constructed model can reasonably describe the behaviour of full-scale experiment system meanwhile the computer modelling simulation able to simulate the experimental parameter with boundary condition. Based on Agaoglu *et al.* [16], experiments involve non-invasive imaging techniques which used observation and characterization of systems for bigger precision. The groundwater modelling is used for prediction of fluid flow system in future such as management water resources, remediation and protection on quality and quantity of groundwater resources. Computer modelling is needed because original situation usually cannot be studied in laboratory scale physical models. Thus, in order to provide geo-environment sustainability, attention and focus towards liquid leakages in subsurface is needed. Therefore, this paper discusses the penetration rate of LNAPL through the double-porosity soil and validates the penetration rate by using PetraSim simulation.

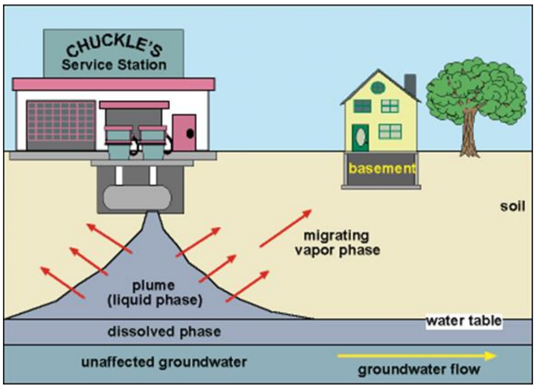


Figure 1. Leakage NAPL from underground storage gas station [17].

2. Physical experiment and computer modelling theory

Computer modelling was used to identify the validity of physical experiment result. Groundwater modelling can be used to simulate the penetration rate of LNAPL through the double-porosity, after calibration and validation have been done on computer modelling respect to results of physical experiment. In physical experiment, it is important to understand fluid flow in porous media structure. There are two types of soil structure; single porosity and double-porosity. Single porosity is defined as the whole structure of soil have a similar porosity scales, meanwhile the double-porosity is defined as the structure of soil with two different scales of porosity in the natural state [4]. According to Black [18], the first oil drilled was named Drake Discovery Well in Pennsylvania and double-porosity soil concept was found. The studies on fluid flow on double-porosity was conducted by Loke *et al.* [9], Rahman and Loke [10], Abd Rashid *et al.* [12], Abd Rashid *et al.* [13], Abd Rashid *et al.* [14], Abd Rashid *et al.* [15] and Loke *et al.* [19]. Based on the previous researchers [20 – 23] had revealed the penetration of NAPL can be investigated using digital image processing technique (DIPT) as a non-invasive method. According to Agaoglu *et al.* [16], non-invasive imaging methods are one of experimental with technologies to determine the NAPL saturation and pattern in subsurface system. The determination of NAPL saturation and pattern with different phases on laboratory studies using image processing technique are the cheaper, simple and powerful method [24 – 27].

Validation for physical experimental results was used using computer modelling. Computer modelling becomes more imperative especially in groundwater flow and transport including planning processes, government policy making and groundwater management [28 – 33]. It will help to understand the multiphase behaviour based on its mechanisms and procedures of groundwater system. Furthermore, the modelling help for engineering designs, regulations, screening and planning alternative policies improvement for cost-effective support in water resources protection and restoration studies [30, 34 – 37]. It is essential to analyse the contamination problem that incorporated with hydrologic parameters and overall the quantity of input data are needed from laboratory studies, field investigations and literature review. The determination of NAPL flow with different phases on numerical studies using multi-phase system on isothermal or non-isothermal condition in 1-Dimenisonal to 2-Dimensional with deformable structure of soil are the most researchers used in numerical studies [8, 22, 38, 39]. The best groundwater modelling for multiphase system with unsaturated condition is Tough2 computer modelling [40]. The Tough2 simulator [41] is widely used for the numerical simulation of many types of subsurface flow and transport problems, including modelling geothermal and other reservoirs.

3. Material and methods

This section discusses the materials and methodology adopted in this study. The flow chart of the research methodology is presented as shown in figure 2. The methodology will cover the soil investigation and preparation, digital image acquisition setup and procedure, and computer modelling. The penetration pattern of LNAPL in experimental and computer modelling are briefly discussed in the following subsequent sections.

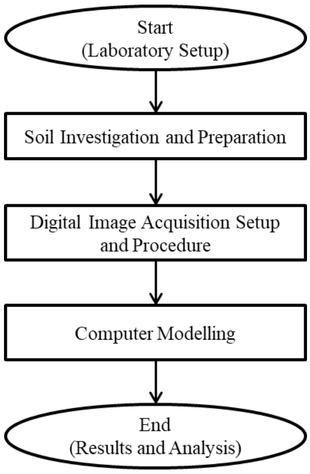


Figure 2. Research methodology flowchart.

3.1. Soil investigation and preparation

Laterite soil was collected at latitude 1º33´39´´N and longitude 103º38´44´´E at School of Electrical, Faculty of Engineering, Universiti Teknologi Malaysia, Skudai, Johor, Malaysia. The laterite soil was obtained about 1 meter below the ground surface to prevent from weathered soil and dried soil sample collected. The laboratory soil characteristics properties results were based on the British Standard BS1377-1:1990 and BS1377-2:1990. According to table 1, the natural moisture content, optimum moisture content, maximum dry density, liquid limit plastic limit, and plasticity index were 33.29% 31%, 30.97%, 1.20 Kg/m^3, 66.17%, and 32.88%, respectively.

Table 1. Laterite soil characteristics.

Characteristics	Value
Natural Moisture Content	31 %
Optimum Moisture Content	30.97 %
Maximum Dry Density	1.20 Kg/m^3
Liquid Limit	66.17 %
Plastic Limit	32.88 %
Plasticity Index	33.29 %
USCS Classification (Fine Fraction)	CH

The soil samples were prepared as double-porosity soil [7] as shown in figure 3. The dried laterite soil was mixed with 25% of water content and was kept in zip lock plastic bag at room conditions to prevent the evaporation of the moisture. The soil sample was kept with minimum of 24 hours for curing process. The soil sample that passed through the 2.36mm sieve was then placed in the acrylic glass cylinder. The soil sample in acrylic glass cylinder was compressed until it reached a height of 100mm using a simple compression machine. Figure 3 display double-porosity laterite soil from side and plan view. Figure 3 (a) shows the side view while figure 3 (b) shows the plan view of double-porosity soil. The soil sample shows the distinctive of laterite granules and the finer inter-aggregated pores. The distinctive of granules and finer-aggregated pores have a similar structure with previous researcher [11].

(a) Side view (b) Plan view

Figure 3. Double-porosity laterite soil view.

3.2. Digital image acquisition setup and procedure

The physical experimental setup was developed to accomplish the objectives of this study effectively. Figure 4 displays the flowchart of physical experimental setup. Dimensions of 300mm high x 100mm outer and 94mm inner diameter designed for acrylic cylinder glass with a sealed base was used to execute the experiment. The experiment was first setup at 23ºC room temperature as shown in figure 5(a). The double-porosity laterite soil was prepared as mentioned in Section 3.1. Acrylic glass cylinder was used to store the circular soil for monitoring and measurement of LNAPL penetration through the whole area of circular soil. Gridlines of printed plane paper was sheathed onto the acrylic glass cylinder with gridlines 30mm x 30mm as shown in figure 5(b). The gridlines were used for DIPT to control the accuracy of measurement when reference image was taken. The calibration and validation were used 70 ml and 150 ml volume of LNAPL that poured instantaneously on top of soil sample.

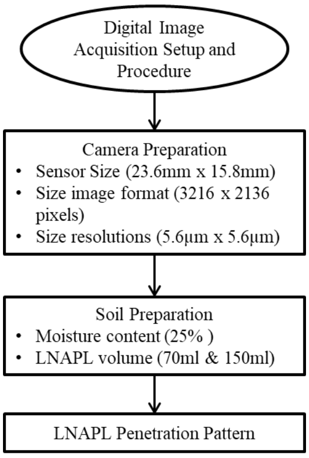
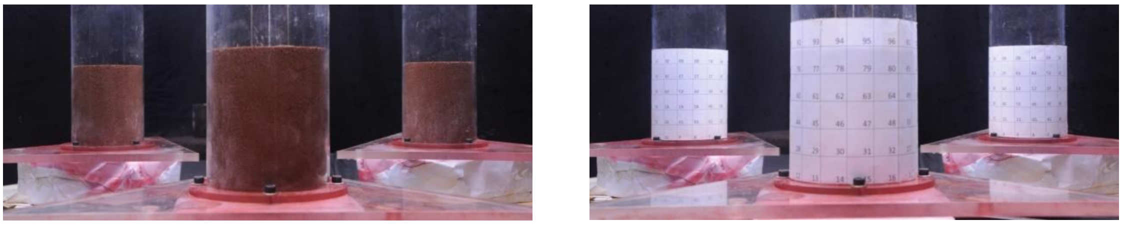


Figure 4. Physical Experimental setup flowchart.



(a) Physical experimental setup

(b) Gridlines sheathed for reference image taken

Figure 5. Physical Experimental setup for DIPT.

3.3. Computer modelling

Understanding remediation and penetration process of contaminant in groundwater system based on numerical modelling as a basic and fundamental knowledge has become an important tool due to developing of technologies [42]. PetraSim software was selected and in order to verify the calibration and validation on the physical experiments. This software allows everyone to understand the parameter and analysis of domain by automatically discretized the model grid or mesh in fully 3-D views [43]. Development of existing software in multiphase flow for TOUGH family code become more demanding and interesting especially in simulation coupled multiphase flow [44]. The rate of penetration for 70 ml LNAPL volume was selected to calibrate the PetraSim simulation and 150 ml LNAPL volume was selected to validate the physical experiment. Figure 6 shows the computer modelling flowchart analysis.

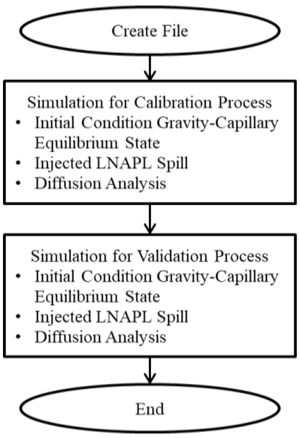


Figure 6. PetraSim simulation flowchart analysis.

4. Results and analysis

4.1. Physical experiment and PetraSim simulation penetration pattern of LNAPL through double-porosity soil results and analysis

According to Loke [11], the flow of dyed LNAPL was consistently penetrated downward toward double-porosity soil. It is observed, the pattern of LNAPL were horizontal x-axis line through the soil sample as the double-porosity soil was homogenous as shown in figure 7; experiment 1 (a) and experiment 1 (b), respectively. The circular soil column is unfolded to a flat 2D pattern plot, indicated the x-axis represents the column circumference and the y-axis is the depth of soil. The creation of pattern plotting were selected and used due to reddish soils' colour and red dyed toluene affect the contour plot analysis. In experiment 1 (a), pattern plot at 3, 45, 90 and 116 seconds, were selected for 150 ml LNAPL volume and for experiment 1 (b), the selected pattern plot at 3, 30, 45, 430 seconds for 70 ml LNAPL volume. It is observed that the dyed LNAPL penetration took 116 seconds minutes and 430 seconds to reach the bottom of soil sample for experiments 1 (a) and 1 (b). Penetration of LNAPL penetration through acrylic glass cylinder in experiment 1(a) was faster than experiment 1(b) due to amount of LNAPL volume poured on top of double-porosity soil. Capillary pressure affects the LNAPL penetration to seeping through the double-porosity soil. The capillary pressure onto double-porosity soil increased when the amount of LNAPL volume increased [11, 22, 45]. It is observed that the LNAPL has penetrated roughly more than half of the soil sample depth within 30 seconds.

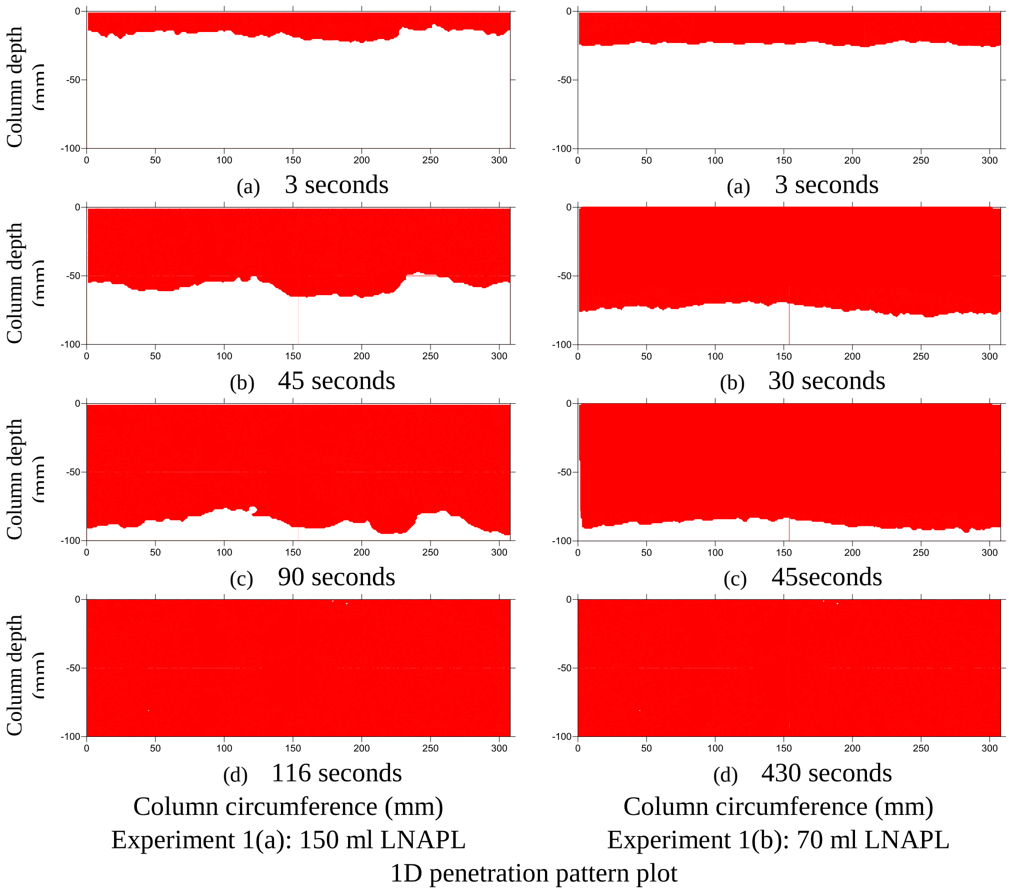


Figure 7. Penetration pattern of LNAPL through double-porosity soil for 150 ml LNAPL volume; Experiment 1(a) and 70 ml LNAPL volume; Experiment 1(b).

The LNAPL flow fully penetrated through the double-porosity laterite soil until to the bottom of soil sample for both physical experimental and PetraSim simulation. Based on the Nash-Sutcliffe efficiency for calibration and validation, the results are 0.84 and 0.51 which are more than 0.50 indicates as good calibration and validation [46, 47]. According to table 2, the differences percentage for experimental and computer simulation is less than 10%. The PetraSim software were calibrated and validated using 70 ml and 150 LNAPL volume of physical experiments that penetrated through the double-porosity soil. Calibration percentage differences between physical and PetraSim software is 1.34% meanwhile validation percentage differences is 5.47%; the percentage differences still in range; good and acceptable [48]. As results, the difference between the physical experiment and PetraSim software are quite negligible and accepted which shows that there is design conformity as presented in the calibration and validation curve as shown in figure 8 and figure 9. Based on table 2, it presents the comparison of results between calibration and validation of physical experiment and PetraSim software. Therefore, it is significant to justify the penetrations of LNAPL through the double-porosity laterite soil at field site for long term remediation and protection in order to check if the LNAPL would travel faster or slower.

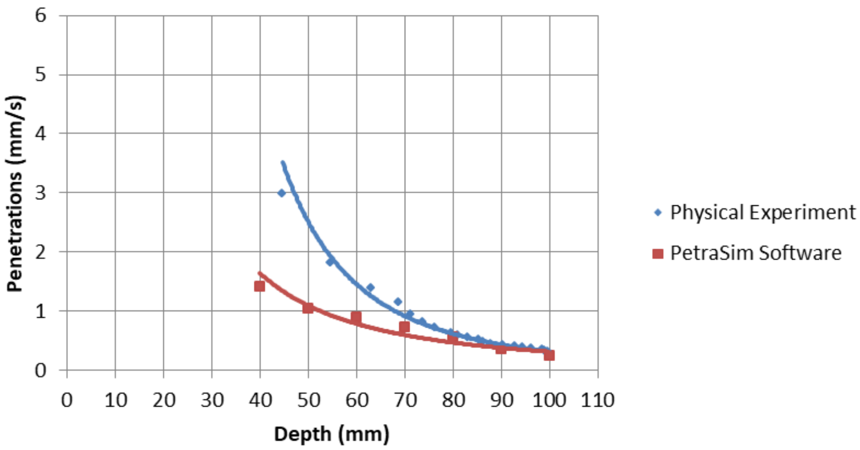


Figure 8. Calibration graph for PetraSim software respect to physical experiment using 70 ml LNAPL volume penetration rate.

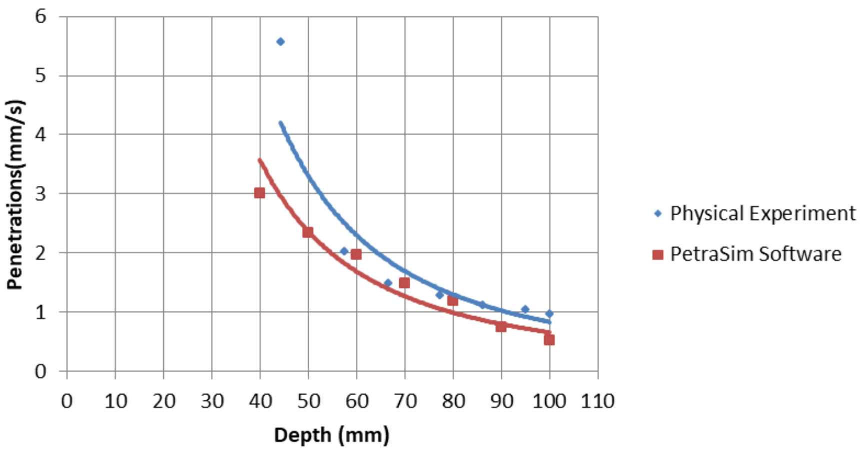


Figure 9. Validation graph for PetraSim software respect to physical experiment using 150 ml LNAPL volume penetration rate.

Table 2. Calibration and Validation of Penetration for Physical Experiment and PetraSim.

Parameter	Physical Experiment	PetraSim Software	Percentage Difference (%)
25% moisture content; 70 ml LNAPL volume; (mm/s); Calibration	0.74	0.75	1.34
25% moisture content; 150 ml LNAPL volume; (mm/s); Validation	1.69	1.60	5.47

5. Conclusion

In conclusion, the LNAPL penetrate faster in double-porosity soil with bigger volume LNAPL compared to lesser LNAPL volume. The rate of penetration was 1.69 mm/s and 0.74 mm/s for experiment 1 (a) ; 150 ml and experiment 1 (b); 70 ml, respectively. The penetration rate is influenced by the capillary pressure on surface of soil due to amount of LNAPL volume used. Increasing of capillary pressure was affected by the increasing of LNAPL amount that poured on top of soil surface. Furthermore, the physical experiment was calibrated and validated using PetraSim software. The calibration and validation display the Nash-Sutcliffe efficiency are 0.84 and 0.51 with percentage different of physical experiment and PetraSim software are 1.34% and 5.47%, respectively. PetraSim software is compatible and easy to be used for further investigation on remediation and protection of groundwater quality from contaminants (i.e. leakage or spillage of petrol tank), and prediction for long term environmental issues.

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