CHAPTER 3
METHODOLOGY

3.1 U_DYSAC2 computer code

U_DYSAC2 finite element computer code is developed by Muraleetharan and Wei (1999a) for static and dynamic analysis of saturated and unsaturated porous media problems. Three-phase analysis (soil, water, and air) is used to explain the behavior of unsaturated porous media through the Theory of Mixtures with Interfaces (TMI; Muraleetharan and Wei 1999b, Wei 2001; Wei and Muraleetharan 2002a, 2002b). U_DYSAC2 is one of the newly developed computer codes to solve for many kinds of problems, for example: wave propagation, two- and three-phase flow and consolidation (deformation of the soil skeleton), and earthquake loading on an unsaturated soil embankment.

The finite element matrix equations used in U_DYSAC2 are shown in Appendix A.

3.2 Modification for U_DYSAC2

1. U_DYSAC2 governing equations were derived assuming the three phases are solid skeleton, pore water, and pore air. The governing equations are modified to replace the air phase with another liquid phase, NAPL.
2. U_DYSAC2 code used Brook & Corey (1964) equations to describe the relationships between saturation, capillary pressure, and relative permeability. These equations create numerical difficulties when solving purely flow problems due to the use of bubbling pressure in the equations, as explained in Chapter 2. van Genuchten (1980) equation is used instead in the modified version.
3. From preliminary tests using U_DYSAC2 to simulate flow problems it was discovered that setting boundary conditions in U_DYSAC2 is not suitable for purely flow problems. Boundary condition specifications are modified.

4. From preliminary tests using U_DYSAC2 to simulate NAPL transport problems, it was discovered that U_DYSAC2 did not represent gravity effects correctly in the NAPL phase. Gravity effects for the NAPL phase is implemented in the new code.

3.3 Validation procedure

To validate the modified computer code two sets of studies are conducted. The first one is a parametric study and the second one compares U_DYSAC2 predictions with experimental results.

3.3.1 Parametric study: This study is conducted to evaluate the effects of DNAPL density, DNAPL viscosity, and ground water flow on the DNAPL transport patterns. The results of this study are presented in the next chapter.

3.3.1.1 The effects of DNAPL density and viscosity on the transport pattern

The values of DNAPL density and viscosity used in the parametric study are shown in Table 3.1. The intrinsic permeability, K (L^2), is a function of density (ρ) and viscosity(μ) , as shown below:

$$K = \frac{k \times \rho g}{\mu} \quad \text{, so} \quad K \; \alpha \; \frac{1}{\mu} \text{ and } \rho$$

where, k = coefficient of permeability (LT^{-1}),

and g = gravitational acceleration.

3.3.1.2 The effect of water flow on contaminant transport pattern

It is very likely for spills involving DNAPL there will also be a natural groundwater flow in the subsurface. The effect of this groundwater flow on the DNAPL movement is qualitatively studied here.

Table 3.1: The values of fluid density and viscosity used in the parametric study

	ρ_w (kg/m^3)	ρ_N (kg/m^3)	μ_w (Pa.s)	μ_N (Pa.s)
Vary density				
Base case	1.00×10^3	1.63×10^3	1.00×10^{-3}	2.30×10^{-3}
Run 1	1.00×10^3	1.00×10^3	1.00×10^{-3}	2.30×10^{-3}
Run 2	1.00×10^3	1.30×10^3	1.00×10^{-3}	2.30×10^{-3}
Run 3	1.00×10^3	2.00×10^3	1.00×10^{-3}	2.30×10^{-3}
Vary viscosity				
Base case	1.00×10^3	1.63×10^3	1.00×10^{-3}	2.30×10^{-3}
Run 4	1.00×10^3	1.63×10^3	1.00×10^{-3}	0.70×10^{-3}
Run 5	1.00×10^3	1.63×10^3	1.00×10^{-3}	1.00×10^{-3}
Run 6	1.00×10^3	1.63×10^3	1.00×10^{-3}	1.50×10^{-3}
Run 7	1.00×10^3	1.63×10^3	1.00×10^{-3}	5.00×10^{-3}

3.3.2 Compare with experimental results: Two studies where enough physical properties for the porous media and the DNAPL used were reported are used to quantitatively validate U_DYSAC2.

3.3.2.1 Centrifuge study of low density high viscosity DNAPL in a saturated porous medium (Abu-Hassanein and Pantazidou 1998, Panntazidou et al. 2000)

This study showed the transport pattern for low density, high viscosity DNAPL by using a centrifuge to accelerate the experiments. DNAPL density used was closer to water density. This study showed that the distribution was stable and resulted in smaller contamination areas when compared to low viscosity and high density DNAPL.

3.3.2.2 DNAPL transport in a heterogeneous stratified soil stratum (Kueper and Frind 1991)

This study showed the transport pattern of tetrachloroethylene (PCE) in a heterogeneous saturated sand pack. The flow direction of DNAPL was affected by the heterogeneities of the soil stratum.