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BORANG PENGESAHAN
LAPORAN AKHIR PENYELIDIKAN

TAJUK PROJEK : Numerical modelling of multiphase flow, heat flow and pollutant transport in deforming porous media for subsurface systems.

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CONTENTS

1.0 INTRODUCTION

Groundwater plays an important role in the development of the world water resources potential. Groundwater has to be protected from the increasing threat of subsurface contamination. Subsurface contamination can be caused by leakage from ponds and lagoons which are widely used as components of larger waste-disposal systems, pesticides from agricultural soils, industrial product leaking underground storage tanks and pipelines and surface spills. Until today, groundwater contamination becomes most popular aspects to discuss. The migration of NAPLs, process of dissolution, factor influences, effects and the techniques for remediation of groundwater contaminant was done in order to make sure that this source could be use in long terms. Due to these reasons, needed some alternative in order to simulate the groundwater system to get the results of the contaminant. Many researchers were involved to develop a model of groundwater contamination by numerical method.

The simulation of groundwater contamination by NAPLs such as organic solvent, petroleum hydrocarbon requires a solution of the multiphase flow equation in deforming porous medium. The multiphase flow namely gas, water and NAPL was developed for a fully coupled numerical model for subsurface system by Rahman (1998). . Many of this pollutant are slightly such water soluble and highly volatile fluids, which it may exist as non-aqueous phase liquid (NAPL). The remaining non-aqueous phase liquids may persist for long periods of time, slowly dissolving into the groundwater and moving in the water phase through advection and dispersion

A study of numerical modelling of multiphase flow, heat flow and pollutant transports are very important to describe the phenomena of contamination in soil especially by organic waste such as Dense Non-aqueous Phase Liquid (DNAPL). A numerical model needed in order to study the movement of organic pollutants in subsurface system. This simulation also developed for use in non-isothermal problems of gas migration landfill system and for organic vapor in unsaturated zone. In additional a fully coupled model of water flow and airflow incorporate pollutant transport in deformable porous media has been studied by Schrefler (1995) which does not consider the interphase mass transfer in the simulation model.

Furthermore, transport contaminant may cause by organic liquid where the density of the gas in contact with the liquid changed with respect to the ambient of soil gas. Simulating the transport of volatile organic compound may show the importance of including density-driven gas flow as a transport mechanism in the unsaturated zone. In contaminant gas migration, the overall porosity, air and water saturation level effects the rates of diffusion in porous media. The equations using are such water phase tortuosity (τ) , Henry's law, Galerkin Method and others. The simulating are performed for volatile organic compound and the physical properties of the model.

2.0 Statement of Problems

Main point of this analysis is based on theoretical and numerical model of multiphase flow, heat flow and pollutant transport in deforming porous media for subsurface system by Rahman (1998). The theoretical model, which will develop in this research, extends from his code that considers the combined phenomena of geomechanic and geoenvironmental engineering problems. The theoretical approach may be used to other practical applications because it is including the hydro-geo-mechanical behaviour in saturated or unsaturated porous media, infiltration process with interface mass transfer, hydrothermal-mechanical and non-isothermal problems.

Besides the numerical solution of the problems solved by finite element method for spatial discretisation and a finite difference algorithm for temporal discretisation. The prediction of multiphase flow and pollutant transport processes in unsaturated zone are related to some capabilities of the proposed model such as the hydraulic properties, heat transfer, fluid density, fluid viscosity and interface mass transfer.

3.0 Objective of study

The main objective of this study is to develop a model that describes the phenomena which govern the fully coupled multiphase flow, heat flow and pollutant transport in deforming porous media for organic vapor in unsaturated zone and gas migration in landfill system.

3.1 Scope of Study

The scope and limitation of this study can be divided by three :

1. The numerical modelling of multiphase immiscible flow (namely water, gas and NAPL) in deforming porous medium.
2. The simulation of multiphase flow and pollutant transport in deforming porous medium for subsurface system in unsatured zone.
3. The numerical simulator of two dimensional problems for non-isothermal multiphase flow and pollutant transport in deforming porous medium considering the retardation processes.

3.2 Methodology of Study

The numerical simulator will be develop in this study, take account of the flow of multiphase fluid phases in response to viscosity and can be used to model transport in one and two dimension. The flow of all multiphase fluids as well as the water and gas phase transport are included. Mechanism of inter-phase mass transfer include volatilization NAPL into the gas phase, dissolution of NAPL into the water phase and Henry is law partitioning of chemical component between the water and gas phase. Also heat transport may occur by advection of the fluid phases and conduction. Retardation process also must be considered to know the behavior of contaminants. The governing equations which describe the displacement of soil, multiphase fluid pressure, temperature and pollutant transport are coupled and the resulting non-linear saturation and relative permeability function are incorporated into a Galerkin finite element model that is used to simulate the migration of fluids in a deforming porous media.

4.0 Literature Review

Groundwater contamination is caused by variety of substances originating form many different activities. Most of them originate from man's use of water and others from undesirable constituents into the groundwater. Therefore groundwater forms the part of the natural water cycle which is present within underground strata called aquifers. Others major sources of groundwater pollution are sanitary landfills. Eventhough a landfill is covered with infiltration or rainfall but leachate may reach into groundwater table and will pollute the resource.

Most groundwater contamination arises form sources at the ground surface but landfill leachates, spills and non-point agricultural contaminants are all introduced at or near the surface before they enter the groundwater system. This is the case which contaminants move downward through the unsaturated soil moisture zone to the water table. The zone of unsaturated will determine the percentage of the mass of the contaminants migrates from the ground surface to the underlying groundwater.

When contaminants enter the subsurface, they become subject to a variety of physical, chemicals, and biological processes that operate beneath the ground. The design of an effective ground water cleanup system requires an understanding of these processes because they control the fate of the contaminants and the ease with which they can be extracted. For an example the trichloroethylene (TCE). Fate of contaminants depends on natural physical characteristic, chemical characteristic, biological characteristic and chemical properties of contaminants.

Besides, the geochemical processes in subsurface environments are includes the dissolution-precipitation, oxidation-reduction, sorption-desorption, ion exchange and complexation. Contaminants in ground water can be classify as volatile organic compound (VOC), toxic in organic compound, polycyclic aromatic hydrocarbons (PAH), Pesticides, Phthalates and Polychlorinated biphenyls (PCBs). The migration pathways, mobility, and persistence are different based on the types of contaminants. Types of contaminants also can be classified as inorganic compound and organic compound.

4.1 Volatile Organic Compound (VOC)

According to the definition used by WHO and the USEPA volatile organic compound (VOC's) are substances which contain carbon atoms and which have a minimum vapour pressure of 0.13 kPa at standard temperature and pressure (293K, 101 kPa) (D.Kotzias and C.Sparta). VOC can be classified as an organic waste. The polarity of the compound is the most important behavior of the compound in the soil which can determines the large part both the fate of a compound when it is brought into the soil. A non-polar compound in general is hydrophobic and it will show a relatively strong tendency to adsorb to the organic fraction of the soil phase of the soil or to volatilize. The sorption of polar compounds to the solid phase of the soil differs from the sorption of non-polar compound.

The distribution of VOC in air, water and soil is governed by the partition coefficient for air or water and soil or water via Henry's constant. Consequently, the equilibrium distribution helps to assess potential concentrations of VOC in the different environmental compartment. It also can be regarded as an important parameter to determine the behavior patterns of chemical compounds in the environment. Such as a Henry's law constant (H), it is a physical property of a chemical where the characterizing it is partitioning between the two phases in an air or water binary system at equilibrium. Henry constant are required to predict the behavior of organic compound in the environment such as to describe the movement of volatile pollutants from the air or water and to the air or water. Therefore Henry's law constant is a function of temperature for a particle gas solvent system.

Besides, there are two aspects of VOC behavior in the soil. Firstly is the partitioning of the VOCs over the different soil phases and secondly is a transport through the soil system. When the soil is in equilibrium the mass of a contaminant will be distributed over the three soil phases (namely solid, water and air) in a constant ration.

Transport of VOC in soil can take place in both water and air by convection and diffusion. Convection is the process by which the contaminant moves with the phase in which it present. In diffusion, the contaminant moves relative to the phase which it is present. But in the horizontal movement of water, can be result of the ground water at the

soil surface. A vertical flow in the downward direction may be the result of leaching. The convection of contaminants with the soil air phase takes place when the soil air moves as a result of a rising ground water level.

Diffusion of a certain compound in the water and air phase of the soil are determined by the concentration gradient, the diffusion coefficient and a number of soil specific properties. The velocity of diffusion in air is about 10^5 to 10^6 times higher than in water.

4.2 Flow in unsaturated zone

The driving force for groundwater was demonstrated to be the potential gradient where as the flows takes place for high to low potential, regarding to Darcy's law. The concepts for unsaturated flow are not as fully developed as for saturated flow because it is not easy to apply.

There are a few steps in order to develop a model. Firstly, identify the concept of the model called conceptual modelling then mathematical modelling and lastly the numerical solution or analytical solution. Normally, the conceptual model is usually express in words while the mathematical model based on the assumption consideration. The numerical solutions are the techniques how to solve the problem by using a computer program such as a finite element method, finite different method, boundary element, finite volume and others.

4.3 Conceptual model

The first important thing to develop a model is to understanding the conceptual of the model. Therefore, the conceptual model consists of a set of assumption that reduce the real problem and the real domain to simplified versions that are manageable but yield acceptable solutions in terms of the objectives of the model study. The assumptions of the model are relate to domain geometry, aquifer material properties, dimensionality or mode of flow, water properties, interface condition, choice of state variables, distribution of sources and sinks and boundary condition. All these assumptions are needed in order to simplify the problems.

The conceptual modelling also are include to define the important processes, interpret the true groundwater characteristics from the available data, define the basic data bases for model calibration and assessing appropriate system responses against which to validate the model performances.

5.0 Description of Model

In modelling process, the first thing is to identify the critical steps in modelling in order to define the problems, defining material properties, boundary properties, initial condition, calibaration and etc. After that is to analyze a geo-hydrologic problem. Boundary types also are most important role in order to identify the boundary such as boundary flux and seepage surface.

Groundwater modelling also can be called as stages in the development of a prediction model. It is consists a conceptual model, mathematical model, numerical model and computer code for running the program developed. In conceptual model, the input data requirements are the dimensions and geometry of system, initial and boundary condition, values of model parameters and natural and artification stresses. But for data to construct a conceptual model are flow and solute transport. The assumption of the model also must be valid.

But must be remember that numerical models are valuable thinking tools to help us understanding the system. Data for model input is sparse therefore there is a lot of uncertainty of the results. Capabilities of state-of –the –art models are often primitif compared to the analytical needs of current groundwater problems.

5.1 Mathematical model

Mathematical model is represent as a formulation for numerical solution by using finite element method. To develop a mathematical model, physical model must be finalized in order to incorporate all the essential aspects of the physics while making appropriate simplifying assumptions. The principles of the conservation of mass and energy are

employed to derive the governing differential equations for fluid (water, gas and NAPL), heat and pollutant transport in terms of seven primary variables; i.e U, P_w, P_g, P_n , T,C_w and C_g. (Rahman,1998).

The seven fully coupled partial differential equations as appendix such as multiphase flow equation, energy, pollutant transport and etc are done by N.A Rahman, extension of the study of the nonisothermal consolidation model develop by Lewis and Schrefler (1987).

Coupled heat and contamination transport in porous media is classically described by a set of conservation equations, which model the flow of fluid mass, energy and contaminant mass in a macroscopic continuum. These conservation equations are implicitly linked through the dependency of the fluid density, fluid viscosity and matrix porosity upon the fluid pressure, fluid temperature and contamination mass fraction.

Multiphase flow equations to show the fluid phase behavior has been describe by Lewis and Schrefler. The equation governing the behavior of three immiscible and incompressible fluids flowing in a deforming porous medium can be obtained by combining Darcy's linear flow law with the mass conservation balance for each of the flowing phases. In pollutant transport equations, the governing equation may be obtained by corporating the combined mass flux equation into the continuity equation for mass transport.

In general, mathematical model are consists of primary equations and constitutive equations. The primary mathematical equations which may used in this research consists of soil, water, mixture gas, pollutant transport, energy, heat transfer and contaminant gas migration equations. The development of these mathematical equations are based on the following assumptions:

1. multiphase fluid with or without mass transfer between phases
2. Isotropic, homogeneous and deformable porous media.
3. Nonisothermal systems
4. Pollutant can be either miscible or completely immiscible with the other fluids
5. Mechanical properties of the medium are not changed by the pollutant
6. Phase change can take place

7. The solid does not the chemically react with the other phases
8. The constitutive relationship for the solid phase is given in terms of the effective stress and an infinitersimal strain.

In this study, the solid phase is assumed to be a linear elastic skeleton, the liquid phase is considered to be pore water and NAPL and the gas phase binary mixture of vapor and dry air.

5.2 Finite Element model and Discretization

The finite element method based on Galerkin's weighted residual approach which implements shape functions to approximate the unknown variables.(Zienkiewicz et.al). Therefore the analytical solutions are incapable of dealing with the highly complex and non-linear governing equations. The approach employs two-dimensional, nine noded isoparemetric elements. The primary unknown variables in this study such as fluid pressure, temperatures, concentrations and displacements.

6.0 Model Example

The objectives of this example is can be divided by 3 chategories :

a) To evaluate the potential of groundwater contamination from residual saturation of VOC for 1 dimensional by using fortran 90 Power Station.
b) To show the important of density-driven gas flow as a transport mechanism in the unsaturated zone.
c) To describe the migration of contaminant gas with interphase mass transfer through soil in a deforming porous medium under non-isothermal condition.

6.1 Model Assumptions

The unsaturated porous medium is assumed to be homogeneous, isotropic and containing an uniform water saturation with a certain fraction of organic carbon. The theoretical for unsaturated soil for a multiphase system considered organic vapor, gas and soil matrix.

In this study, liquid phase is consider to be water containing VOC whilst gas phase is consider to be binary mixture of air and gas phase chemical. So in order to simulate organic liquid, the liquid organic phase (NAPL phase) is assumed to be immobile (K_m =0) as is the water phase. The densities of gases as well as liquid are general function of composition, pressure and temperature.

6.2 Analysis results

Figure 1.0 shows the finite element schematic diagram for spatial discretization of the model and Figure 3.0 shown the computed mass fraction of the organic component as a function of distance along the column at various times. In figures 3.0(a), (b) and (c), the simulation results of the mass fraction of Toluene, Carbon Tetrachloride and Trichloroethylene (TCE) are shown with the same soil permeability for each phase ($k = 1 \times 10^{-13}$). The difference between these figures is because of the saturated vapor density and Henry's constant for the organic phase. Whilst, figure 3.0(d) shows the results for the mass fraction for Toluene when Henry's coefficient, H = 0 (i.e no dissolved gas phase in the water phase). The results indicate that the mass fraction concentration increase after one hour when compared with the results in figure 3.0(a). The same result was found in Figure 4.0 and figure 5.0 where as it shows that the result's simulation of VOC for $k = 1.0 \times 10^{-15}$ and $k = 1.0 \times 10^{-9}$. The results in figure 5.0 indicate that some types of contaminant can't move down properly when permeability, k is less than 1×10^{-9}. These matter happen because of the behavior of contaminant itself and the distribution into the phases. Lastly, Figure 2.0 shows the profile of temperature throughout the soil column for gas Toluene and indicated that the temperature increase of the body is very slow as same as Carbon Tetrachloride in clay soil.

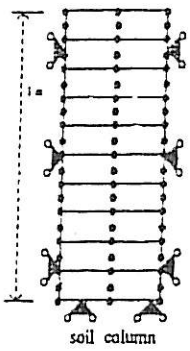


Figure 3.0: Finite element spatial and discretization

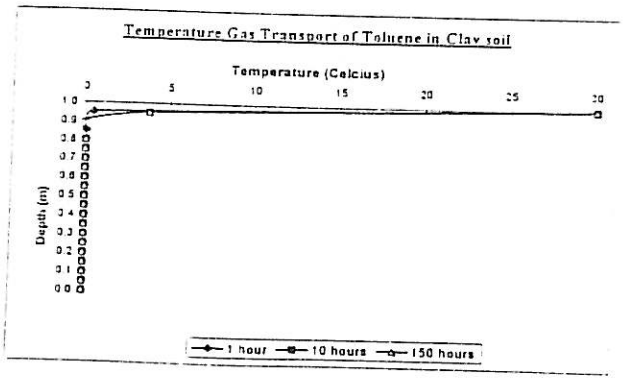


Figure 4.0: Temperature gas transport of Toluene in clay soil

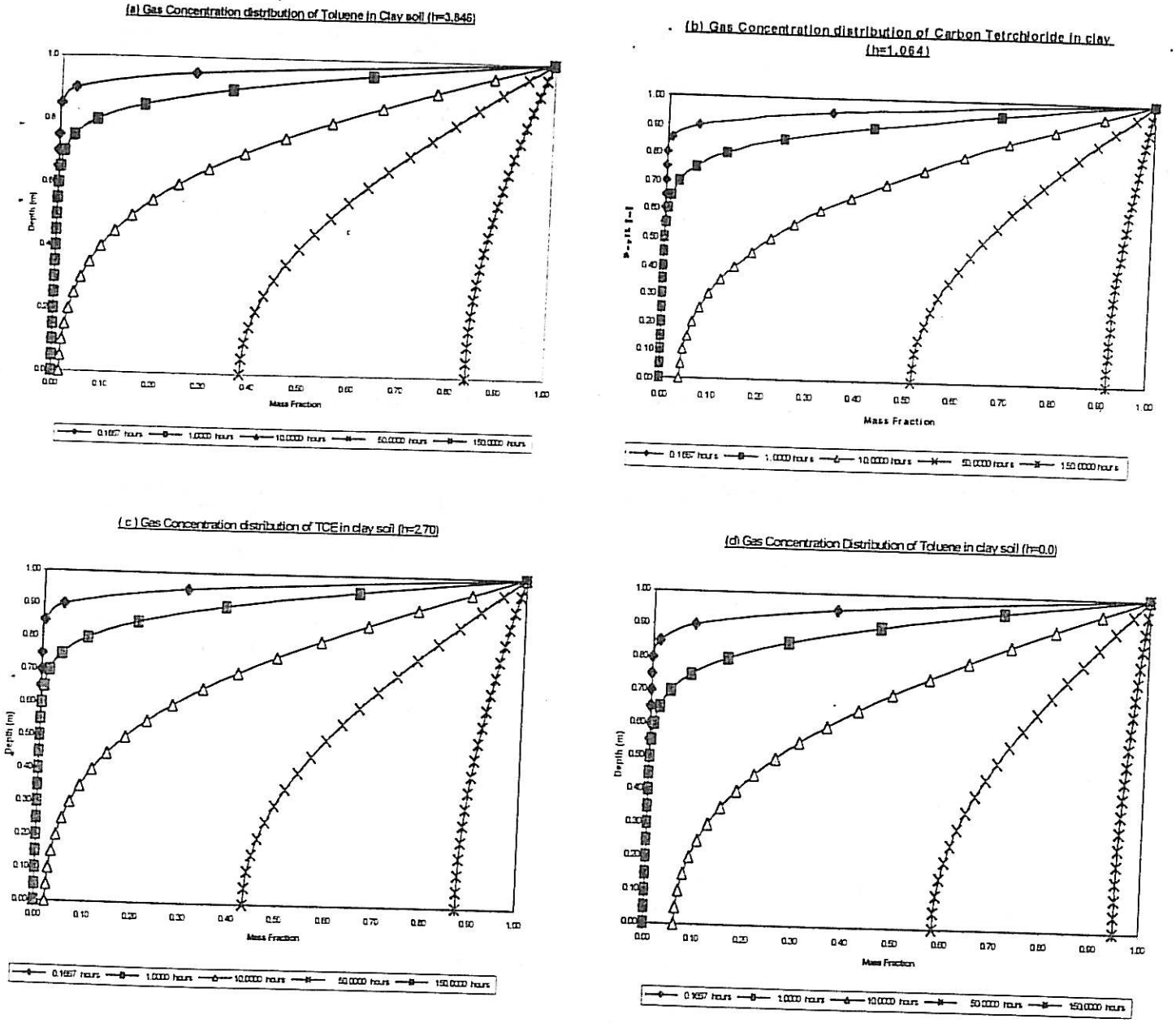
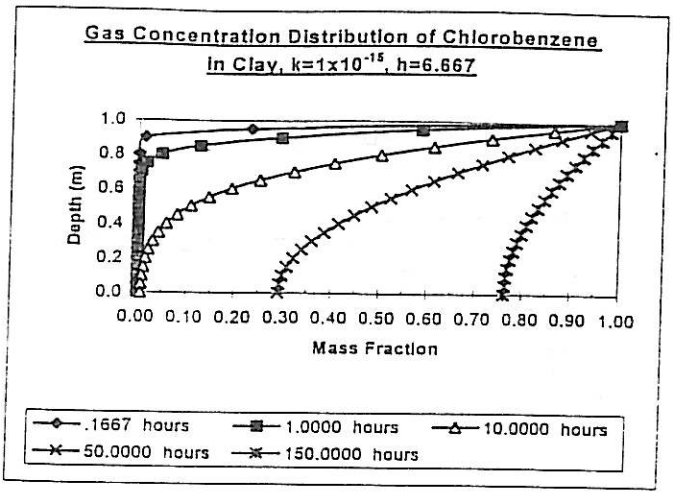
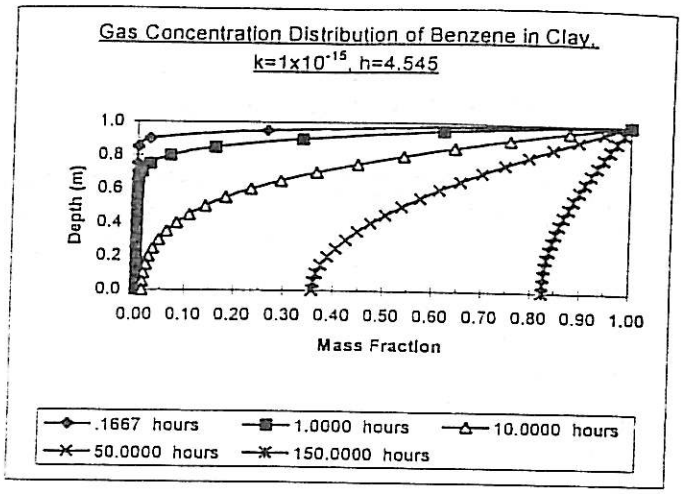
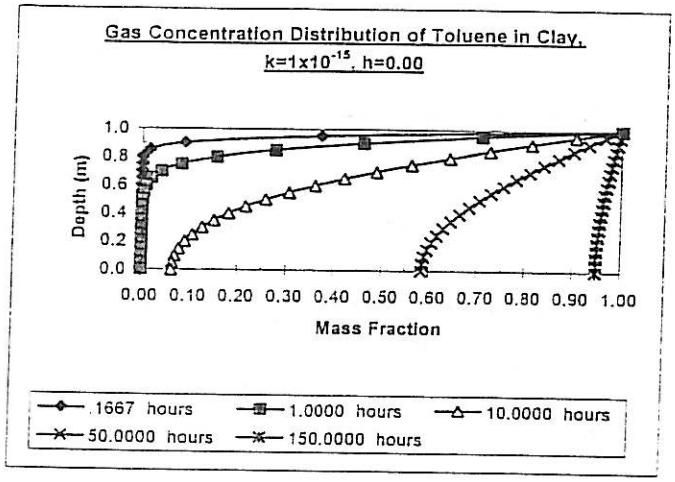
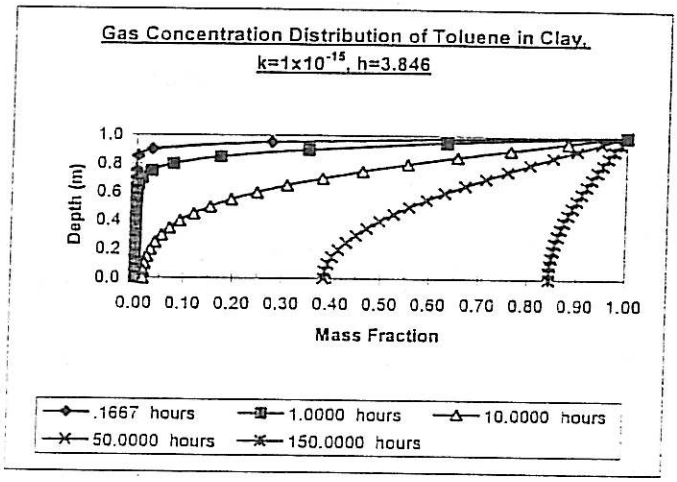


Figure 3.0: Results of Gas Concentration Distribution (a) Toluene , (b) Carbon Tetrachloride (c) TCE and (d) Toluene when h=0.0 in clay soil.









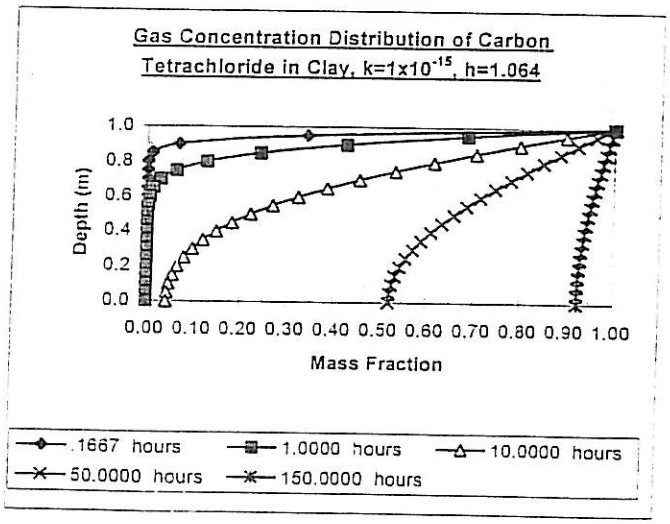


Figure 4.0: *Results of simulation for different transport mechanism of Volatile Organic Compounds in Clay soil. ($k = 1.0 \times 10^{-15}$)*

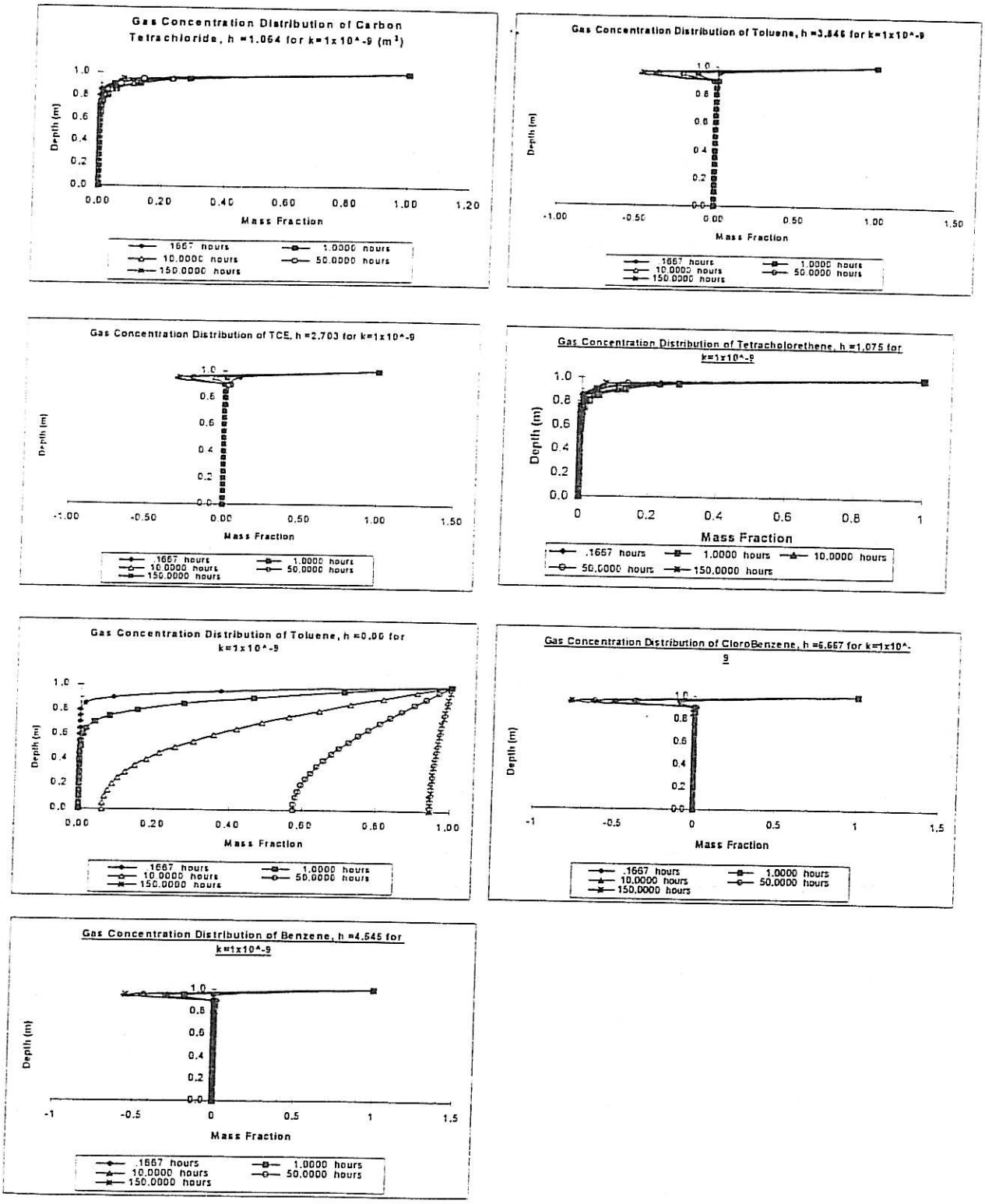


Figure 5.0: *Results of simulation for different transport mechanism of Volatile Organic Compounds in Clay soil. ($k = 1.0 \times 10^{-9}$)*

7.0 Expected Results and Conclusions

7.1 Expected Results

From this study, the benefits or expected results are:

1. Development of a fully coupled numerical model of multiphase flow, heat flow and pollutant transport in deforming porous media for subsurface media incorporating physical processes such as interphase mass transfer and density effects in the model.
2. This model can be use as a remediation program for subsurface contamination such as for dense non-aqueous liquid phase.
3. The results of outcome of the research can be publishing in the international and local Journal.

7.2 Conclusions

From the overview, we know that groundwater contaminant are very dangerous to ourselves especially if the soil consist the organic waste DNALP such as TCE, PCB, VOC and etc. From the previous research done by N.A Rahman titled the numerical modelling of multiphase flow, heat flow and pollutant transport in deforming porous media for subsurface system are indicate the behavior of NAPL such as LNAPL and also DNAPL. Most of the examples from his research consist one or two- phases problems. So, in order to investigate fully coupled three-phase flow in pollutant transport, we need to continue his study. Besides, the developed of numerical simulation also can use for non-isothermal multiphase flow and pollutant transport in deforming porous media. Additionally, adsorption and biodegradation reactions may be considered in future model development. So, as a conclusions that N.A Rahman's model can be use in future and need some additional modification in order to simulate the pollutant transport for non-isothermal conditions in unsaturated zone especially to simulate the contaminants of VOC.

Appendix 1

Numerical modelling of Volatile Organic Compounds in Vadoze Zone

Malaysian Science & Technology Congress 2000

16th - 18th October 2000

at:

Casuarina Royal Park Hotel, Ipoh

Paper titled:

NUMERICAL MODELLING OF VOLATILE ORGANIC COMPOUNDS IN VADOZE ZONE

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Johor, Malaysia.

Hensley, P.J and Savvidou C. (1993). **Modelling of coupled heat and contaminant transport in groundwater.** In K.U.Weyer (ed.), Proc. Int. Conf. On Subsurface Contamination by Immiscible Fluids: 149-158, Calgary, Canada, Rotterdam: Balkema.

Lujan, C.A. (1985). **Three-phase flow analysis of soil spills in partially water-saturated soil.** Ph.D thesis, Dep. Of Civ. Eng., Colo. State Univ., Fort Collins.

Metcalfe, D.E., and Furqahar, G.J. (1987). **Modeling gas migration through unsaturated soils from waste disposal sites.** Water, Air and Soil Pollutant, 32, 247-259.

Millington, R.J. and Quick, J.P. (1961). **Permeability of porous solids.** Trans. Faraday Soc., 57, 1200-1207.

Schrefler, B.A., Zhan, X. and Simoni, L. (1995). **A coupled model for waterflow, airflow and heat flow in deformable porous media.** Int. J. Numer. Methods Heat Fluid Flow, 5, 531-547.

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Thomas, H.R. and King, S.D. (1991). **Coupled temperature or capillary potential variations in unsaturated soil.** ASCE Journal of Engineering Mechanics, 117(11), 2475-2491.

Thomas, H.R. and He, Y. (1995). **Analysis of coupled heat, moisture and air transfer in a deformable unsaturated soil.** Geotechnique, 45,4,677-689.

may dominate the transport of contaminants in the gas phase. The dominant mechanism for the transport of volatile organic compounds is usually cited as molecular diffusion. However, recent research has shown that other factors including density and pressure gradients, multicomponent diffusion effects, rising and falling water tables and thermal gradient effects, may be important as well.

This paper presents a numerical model describing the migration of contaminant gas with interphase mass transfer through soil in a deforming porous medium under nonisothermal conditions. Previous studies (Falta et. al, 1989), (Metcalfe and Farquhar, 1979), (Findikakis and Leckie, 1979) and (Abriola et. al, 1992) did not apply thermal conditions in their model.

2.0 PHYSICAL MODEL

The physical model for multiphase flow in unsaturated flow can be describe as below:

a) The phase saturation sum to unity. This is the concept for completely water saturation.
b) Capillary pressure and temperature are function of saturation.
c) Relative permeability is a function of saturation.
d) The pressures are depends on density and viscosity.

Besides, the model considers the relationship between the hydraulic properties of the porous medium via saturation, relative permeability and capillary pressure. Where the distribution of the zones as a function of capillary pressure. The relative permeabilities for the water, k_{rw}, and gas, k_{rg} phases are calculated form capillary pressure value using the Brooke & Corey (1964) equations and relative permeability for NAPL, k_{rn} based on Lujan (1985).

In fluid density function, for non-isothermal case, the thermal effects on the rate of fluid accumulation in the mass conservation equation are considered. The density of gas can be expressed in terms of the ideal gas law (Schrefler et. al, 1995) whilst the NAPL phase density would be a function of composition as well as temperature and pressure (Hensley et. al, 1993). The solid density ρ_s and the pore liquid density ρ_α are assume to be pressure, temperature and contaminant concentration dependent (R.W Lewis and N.A Rahman).

Fluid density is taken to be linear function of pressure, temperature and contaminant concentration. For flow solubility organic contaminant requires the consideration of interphase mass transfer. Dissolution and volatilization of the NAPL phase are responsible for the input of the pollutant into the groundwater and soil gas, and gas water partitioning can significantly effect transport within these phases (Dorgaten and Tsang, 1992). The dissolution rate is controlled by C_{wm} which is equilibrium concentration of the organic matter in the water phase and controlled by a rate coefficient κ_{nw}.

Interphase mass transfer by dissolution and volatilization will generally be the dominating phase exchange in regions where a significant amount of the NAPL phase is present. Gas-water partitioning is mainly controlled by Henry's law with a constant value of H that express the relation between C_g and C_w at equilibrium, where $H = \frac{C_{gm}}{C_{wm}}$ and κ_{wg} is the mass transfer coefficient for gas-liquid partitioning between the water and gas phases.

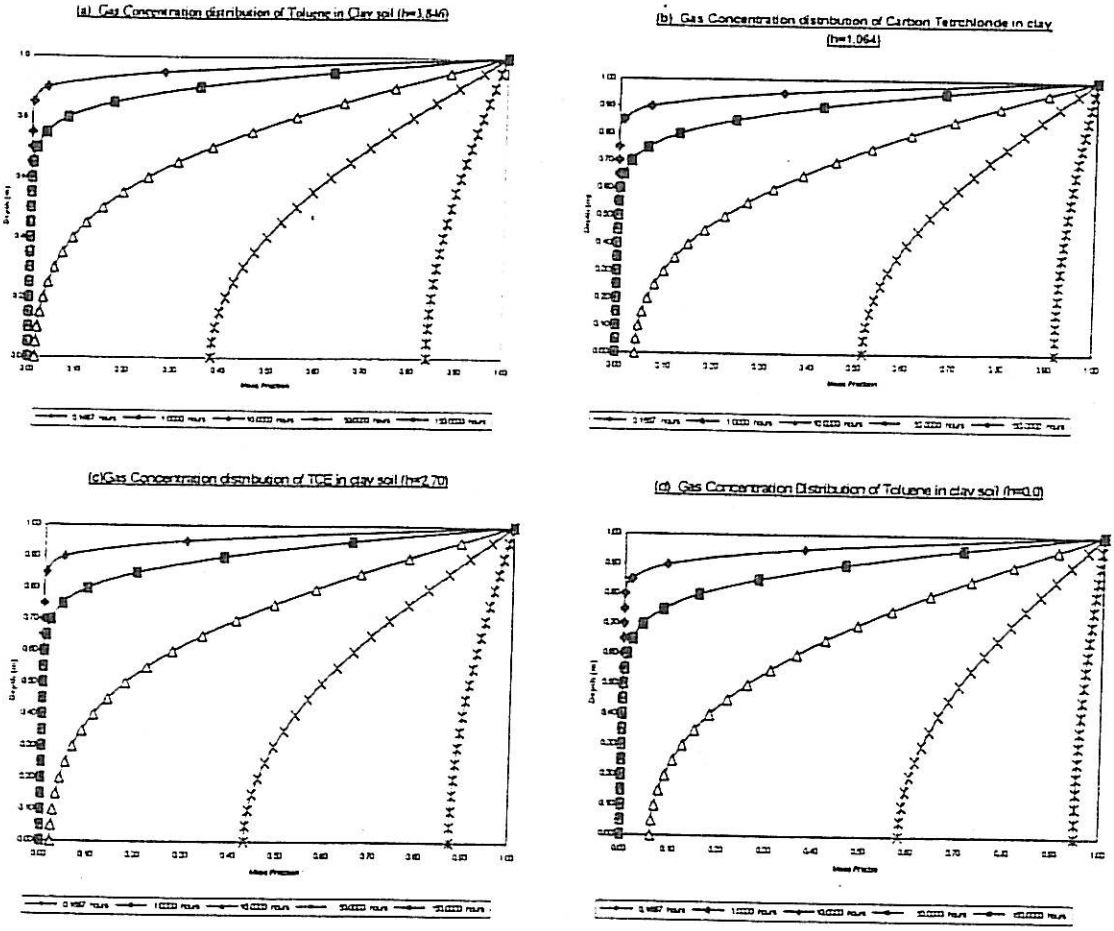

FIGURE 3.0: Results of simulation for different transport mechanism of Volatile Organic Compounds in Clay soil.

Figure 1.0 shows the finite element schematic diagram for spatial discretization of the model and Figure 3.0 shown the computed mass fraction of the organic component as a function of distance along the column at various times. In figures 3.0(a), (b) and (c), the simulation results of the mass fraction of Toluene, Carbon Tetrachloride and Trichloroethylene (TCE) are shown with the same soil permeability for each phase ($k = 1 \times 10^{-13}$). The difference between these figures is because of the saturated vapor density and Henry's constant for the organic phase. Whilst, figure 3.0(d) shows the results for the mass fraction for Toluene when Henry's coefficient, $H = 0$ (i.e no dissolved gas phase in the water phase). The results indicate that the mass fraction concentration increase after one hour when compared with the results in figure 3.0(a). Figure 2.0 shows the profile of temperature throughout the soil column for gas Carbon Tetrachloride and indicated that the temperature increase of the body is very slow.

5.0 NUMERICAL EXAMPLES

The unsaturated porous media is assumed to be homogeneous, isotropic and containing a uniform water saturation with a certain fraction of organic carbon. This model for nonisothermal with a surface temperature jump of 50°C above the reference temperature, T_{ref} of the column. The simulated domain is a 1 meter soil column. A constant source of the contaminant is introduced at the top surface of the column (concentration in water of 1 mg/l). The initial condition for temperature is $T = T_{ref}$ and the soil column was assumed to be unsaturated with an initial water saturation of 0.445. The initial pore water pressure was 420 KN/m^2 and the boundary pore water pressure was instantaneously changed to a value of −280 KN/m^2. The boundary condition are:

a) lateral surface $\mu_h = 0, q_w = q_g = 0$

b) top surface $P_w = 420$ KN/m^2, $P_g = P_{atm}$, $T = T_{ref} + 50$°C

c) bottom surface $\mu_v = 0, q_w = q_g = 0$

The material properties :

a)	Thermal conductivity	$\lambda_T = 1.15$ W/m°C
b)	Heat capacity	$c_{ps} = 1.25 \times 10^5$ J/Kg°C
c)	Thermal expansion coefficient	$\beta_s = 1.0x10^{-6}$ °C^{-1}
		$\beta_{Tw} = 2.1x10^{-4}$ °C^{-}

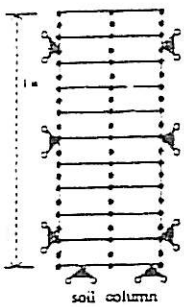

FIGURE 1.0: Finite element spatial Discretization

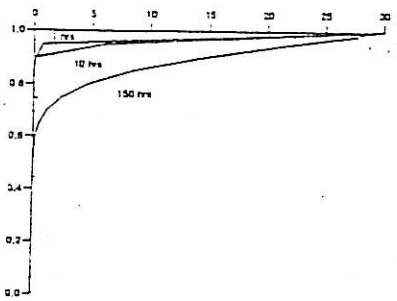

FIGURE 2.0: Temperature gas transport of Carbon Tetrachloride in clay soil

3.0 THEORETICAL FORMULATION

Unsaturated soil is a multiphase system comprising organic vapor, gas and the soil matrix. In this formulation the liquid phase is considered to be water containing volatile organic compounds whilst the gas phase is considered to be a binary mixture of air and a gas phase chemical. Both phases are assumed to flow through a deformable porous matrix. In order to develop a mathematical model of gas phase contaminant transport in a deforming porous medium, an approach is adopted which treats the fully coupled equations of equilibrium, flow of liquid water *(w), gas (g), heat (T)* and contaminant gas (C_{gi}).

To simulate organic liquid and transient density-driven flows, the present model, which simulates the coupled transport of a volatile organic compound in the liquid and gas phase, heat flow and the transport of gas was modified. Both the gas phase and the liquid water are mobile. The liquid organic phase (NAPL phase) is assumed to be immobile ($K_m = 0$) as is the water phase. Diffusion of the organic phase through the water phase and in the gas phase is considered, however the gas phase viscosity is assumed to be constant.

Densities of gases as well as liquids are general functions of composition, pressure and temperature. Of special interest for the present problem are the density changes within the gas phase, since they can get much greater than in the fluid phases, and thus may have a significant influence on flow and transport.

The equilibrium equation of the mathematical model consists of primary equation and constitutive equation. In primary equations, it's consists of soil equation, liquid-water equation, gas mixture equation, heat transfer equation and contaminant gas migration equation.

4.0 FINITE ELEMENT MODEL AND DISCRETIZATION

The finite element method based on Galerkin's weighted residual approach which implements shape functions to approximate the unknown variables. Therefore the analytical solutions are incapable of dealing with the highly complex and non-linear governing equations. In this Galerkin method, nine-noded quadrilateral elements and the respective associated shape function are used (Schrefler, 1995). Primary unknown variables in this study such as fluid pressure, temperatures, concentrations and displacements.

6.0 CONCLUSIONS

A numerical model describing the migration of contaminant gas with interphase mass tranfer through soil in a deforming porous medium under nonisothermal conditions has been presented. Nonlinear saturation and relative permeability functions are incorporated into a Galerkin finite element model. The governing equations, in terms of soil displacements, fluid pressures, temperature and concentrations are given in the form of coupled non-linear partial differential equations. The simulation of organic compounds in an unsaturated zone, showed the importance of interphase mass transfer in the contaminant gas. The results of this study indicate the density-driven gas flows in the unsaturated zone will occur during the evaporation and diffusion of volatile organic liquids. The magnitude of these flows is mainly a function of the organic liquid saturated vapor pressure, Henry's coefficient, molecular weight and gas phase permeability.

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NUMERICAL MODELLING OF VOLATILE ORGANIC COMPOUNDS IN VADOZE ZONE

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ABSTRACT

In recent years, contamination of groundwater by industrial product especially Volatile Organic Compounds (VOC's) has become a problem of growing concern. In the locations where the depth of the water table is large and the amount of infiltration is small, gas phase chemical transport may be dominant process by which the groundwater becomes contaminated. In this study, a numerical model has been developed that describes the phenomena which govern fully coupled multiphase fluid flow, heat flow and pollutant transport (nonaqueous phase liquids) through soil in a deforming porous media for subsurface systems. The flow of all multiphase fluids, as well as the water and gas phase transport, are included. Mechanisms of interphase phase mass transfer include volatilization of NAPL into the gas phase, dissolution of NAPL into the water phase, and Herny is law partitioning of chemical component between the water and gas phase. Also heat transport may occur, by advection of the fluid phases and conduction. Nonlinear saturation and relative permeability functions are incorporated into a Galerkin finite element model, which is subsequently used to simulate multiphase immiscible fluid flow under unsaturated conditions in porous media. The governing partial differential equations, in terms of soil displacements, fluid pressures, concentrations and temperatures which are coupled and non-linear, are solved by the finite element method. The weighted residual finite element approach is employed to achieve spatial discretisation of the problem while temporal discretisation is achieved by a fully implicit scheme. Numerical implementation of the formulation is discussed and example problems are performed to demonstrate the model capability for geoenvironmental application.

Keywords: multiphase system, unsaturated zone, interphase mass transfer, pollutant transport, One dimensional and finite element.

1.0 INTRODUCTION

Understanding the mechanism of gas phase chemical transport is necessary in order to evaluate the potential of groundwater contamination form residual saturations of volatile organic compound, such as solvents and hydrocarbon fuels in the unsaturated zone and to interpret the results of soil gas surveys. The transport of contaminants in the gas phase may occur due to both advection and diffusion and is influenced by phase partitioning into the water and solid phases. Gas phase advection may result from gas pressure or gas density gradients.

As a organic liquids with high vapor pressures and molecular weights evaporate, the density of the gas in contact with the liquid changes with respect to the ambient soil gas. These density contrast results in an advective gas flow, the magnitude of which is dependent on the properties of the evaporating chemical and the porous medium. Under certain condition, this density-driven gas flow

Appendix 2

Numerical modelling of fully coupled multiphase flow in subsurface systems

Numerical Modelling of Fully Coupled Multiphase Flow in Subsurface Systems

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ABSTRACT

Subsurface flow is simulated through numerical solution of fluid mass balance equation, where the subsurface systems may be either saturated, or partly or completely unsaturated and a multiphase flow model, based on two-phase flow model of Brooks and Corey, is presented to express the dependence of saturation and relative permeability on the capillary pressure. A fully coupled finite element model has been developed which describes multiphase fluid flow through soil: namely gas, water and a nonaqueous phase liquids (NAPL) in a deforming porous media for subsurface systems. The governing partial differential equations, in term of soil displacements and fluid pressure, which are coupled and non-linear, are solved by the finite element method. Numerical implementation of the formulation are discussed and example are performed to demonstrate the model related to geomechanic and geoenvironmental problems.

INTRODUCTION

Groundwater contamination in the subsurface is not a new or emerging issue, which can be highly toxic at very low concentrations. It can cause a great damage to our environment and public low concentrations. In recent years, accident oils spill, leaking from underground storage tank (UST), pipeline and waste disposal site are getting more attention from various parties. There are very importance to improve the understanding of the mobilization, transport mechanism and fate of pollutant in the subsurface in checking the risk of public expose to the contaminants and in evaluating various remediation scenarious.

The simulation of groundwater contamination in subsurface systems by nonaqueous phase liquids (NAPLs), such as petroleum hydrocarbons and immiscible industrial chemicals, requires a solution of the multiphase flow equations for deforming porous medium. During the last decade, several numerical models of multiphase immiscible flow have been reported in the groundwater literature for evaluating NAPL contamination and remedial scenario [1]-[9]. Faust [1] presented a two-dimensional finite difference simulator for NAPL and water phase flow in a three phase (air, water, NAPL) system. In this model, it is assumed that the gas phase is at atmospheric and a separate mass balance equation for the air component is not included. The study was verified by comparisons with the Buckley Leverett solution for one-dimensional two-phase flow and with two-dimensional saturated unsaturated flow simulators. The capabilities of this simulator were extended to include three-dimensional Cartesian and two-dimensional cylindrical coordinate systems by Faust et. al [2].

A two-dimensional two-phase flow finite element code was reported by Osborne and Sykes[4]. This model simulates the flow of the NAPL and water phases in a system having no gas phase. The formulation is developed for a two-dimensional Cartesian coordinate system. The code was verified by comparison with a one-dimensional finite difference two-phase flow simulator developed by Little [10]. A two-dimensional finite element simulator for NAPL and water phase flow in three phase systems was developed by Kuppusamy et al [5]. As in the work of Faust[1], they assume that the gas phase is at constant pressure and do not calculate the gas phase flow field. The simulator uses a two-dimensional Cartesian coordinate system. The code was validated by comparisons with column laboratory experiments for water displacement by an NAPL. Kaluarachchi and Parker [6] present a similar two-dimensional Cartesian finite element model employing same assumptions as Faust [1] and Kuppusamy et. al [5]. In their study, they verified the model by comparison with the theoretical equilibrium distribution of a NAPL following the infiltration of a NAPL into a variably water saturated column. Panday et. al [9] presented three-phase numerical model for simulating the movement of NAPLs through porous media. The model formulations and numerical schemes are tested for highly nonlinear field conditions. Attention

is focused on situations involving one, two and three-dimensional flow through porous media.

While these models have found fairly wide application in simulating multiphase flow in shallow systems, coupling this problem with soil deformation, which is an important engineering problem has, to date, received very little attention. As far as soil deformation problem is concerned, Li and Zienkiewicz[11] studied the interaction of two-phase immiscible flow with the porous medium. The model was based on the mass conservation equation as a function of intrinsic phase velocities and the solid and liquid equilibrium equations for a unit element of porous medium. The equation is discretized using finite elements, with quadratic scheme for the time domain. A fully coupled model for both water flow and airflow in a deformable porous media has also been studied by Schrefler and Zhan[12]. The model has been extended by Schrefler et al [13] to incorporate immiscible pollutant transport problems, by solving subsets of the whole group of governing equations.

The main objective of this study is to develop a model that describes the flow of multiphase immiscible fluids in a deforming porous medium. This study presents the flow formulation and associated numerical techniques for a comprehensive model used for simulating multiphase problems. The governing equations describing the displacement of soil and multiphase fluid pressures are coupled and the nonlinear partial differential equations are solved by the finite element method. Nonlinear saturation and relative permeability functions are incorporated into a Galerkin finite element model that is used to simulate multiphase systems and subsurface migration of NAPL contaminants in porous media.

DESCRIPTION OF THE MODEL

The physical model on which the approach is the same as that used by Lujan[3] for three-phase flow analysis and by Lewis and Schrefler[15] for deforming multhiphase flow in porous media. Contaminant transport models for miscible components cannot describe the migration of an immiscible contaminant. The flow of an immiscible contaminant is controlled by its own flow potential, which depends on pressure, gravity and surface forces and is not necessarily similar to the groundwater flow potential [1]. In order to describe mathematically the flow of immiscible fluids through a porous medium, it is necessary to determine functional expressions that best define the relationship between the hydraulic properties of the porous medium, i.e., saturation, relative permeability and capillary pressure. The porous medium voids are assumed to be filled with water, gas and NAPL, and thus the sum of their saturation will be unity, i.e.

$$S_n + S_w + S_g = 1 \qquad (1)$$

where S is saturation of the fluid phase, n, w, g represented as NAPL, water and gas respectively. When more than one fluid exists in a porous medium, the pressure exerted by the fluids may be evaluated using the effective average pore pressure, $\bar{p}$, which is calculated from

$$\bar{p} = S_n P_n + S_w P_w + S_g P_g \qquad (2)$$

The water pressure (P_w), gas pressure (P_g) and NAPL pressure (P_n) are related through the capillary pressure and the three capillary pressure terms are defined as,

$$P_{cnw} = P_n - P_w, \qquad P_{cgn} = P_g - P_n,$$
$$\text{and} \quad P_{cgw} = P_g - P_w \qquad (3)$$

where, P_{cgw} is the capillary pressure between the gas and water phases, P_{cnw} is the capillary pressure between the NAPL and the water phase and P_{cgn} is the capillary pressure between the gas and NAPL phases. In general, for a multiphase system, the saturation of any of the three phases ($\alpha = w,g,n$) is a function of three capillary pressures relationships i.e., NAPL-water, gas-NAPL and gas-water respectively,

$$S_\alpha = f(P_{cgw}, P_{cnw}, P_{cgn}) \qquad (4)$$

The gas-water capillary pressure, expressed in terms of the other two capillary pressures yields the following,

$$P_{cgn} = P_{cgw} - P_{cnw} \qquad (5)$$

And we can rewrite equation (4) as

$$S_\alpha = f(P_{cgw}, P_{cnw}) \qquad (6)$$

The distribution of zones, as functions of capillary pressures, is defined as follows

I. Water only $[P_{cgw} \le P_{dgw},\ P_{cnw} \le P_{dnw}]$ $\qquad S_w = 1.0$

II. Water & gas $[P_{cgw} > P_{dgw}]$ $S_w = S_{max}[P_{dgw}/P_{cgw}]^\lambda + S_{rw}$
$S_g = 1 - S_w$

III. Water & NAPL $[P_{cnw} > P_{dnw}]$

$S_w = S_{max}[P_{dnw}/P_{cnw}]^\lambda + S_{rw}$ $\qquad S_n = 1 - S_w$

IV. Water, NAPL & gas $[P_{cnw} > P_{dnw},\ P_{cgn} > P_{dgn}]$
$S_g = 1 - S_w - S_n$

$S_w = S_{max}[P_{dnw}/P_{cnw}]^\lambda + S_{rw}$

$S_n = S_{max}([P_{dgn}/P_{cgn}]^\lambda - [P_{dnw}/P_{cnw}]^\lambda) + S_{rn}$

where

$S_{max} = 1 - S_{rw} - S_{rn} - S_{rg}$

and S_{rw} is the residual water saturation, S_{rg} is the residual saturation of the gas phase, S_{rn} is the residual saturation of the NAPL phase and λ is a pore size distribution index. Also, P_{dgw} is the displacement pressure for gas and water system, P_{dnw} is the displacement pressure for NAPL and water system and P_{dgn} is the displacement pressure for gas and NAPL system. Lujan[3] proposed expression for the relative permeability's when the effective saturation's are calculation from capillary pressures using the Brooks and Corey[16] equation as follows:

$$k_{rw} = S_{ew}^{(2+3\lambda)/\lambda}, \; k_{rg} = (1 - S_{te})^2(1 - S_{te}^{(2+3\lambda)/\lambda}) \quad (7)$$

$$k_{rn} = (S_{te} - S_{ew})^2(S_{te}^{(2+3\lambda)/\lambda} - S_{ew}^{(2+3\lambda)/\lambda}) \quad (8)$$

where,

$$S_{ew} = [S_w - S_{rw}] / S_{max} \text{ and}$$

$$S_{te} = [1 - S_g - S_{rw} - S_{rn}] / S_{max}$$

where S_{ew} is the effective water saturation and S_{te} is the total effective liquid saturation. In addition to the above constitutive relations, the equations of state are needed to determine the fluid densities as function of pressure. These equation are given as follows

$$\rho_w = \rho_w[1 - \beta_w(T - T_o) + 1/K_w(P_w - P_{wo})] \quad (9)$$

$$\rho_n = \rho_{no}[1 - \beta_n(T - T_o) + 1/K_w(P_n - P_{no})] \quad (10)$$

$$\rho_g = \rho_{go}P_gT_o/(P_{go}T) \quad (11)$$

where the subscript o indicates an initial steady state, β is the thermal expansion co-efficient of the fluid phase, ρ is the fluid density, K_w is the bulk modulus of the water phase, K_n is the bulk modulus of the NAPL phase and T is the absolute temperature.

MATHEMATICAL MODEL

In a multiphase flow model, the simultaneous flow of the fluid phases; water, NAPL and gas in a porous medium, depends primarily on the gravitational force and capillary pressures between the three fluids. The fluid pressures and displacement values are used as the primary dependent variables. The development of four fully coupled, partial differential equations, including the three immiscible fluid flow equations, along with the equilibrium equation is an extension of the one-phase consolidation model development by Lewis and Schrefler[15].

Equilibrium equation

A general equilibrium equation requires both the effective stress relationship and the constitutive law relating the effective stress to the strains of the solid skeleton. The effective stress relationship is given by

$$\sigma = \sigma' - mP \quad (12)$$

where σ' is the effective stress, m is $[1\ 1\ 0]^T$ and P is the fluid pressure. The nature of m implies that the fluids pressure only effects the normal stress components, and that the shear stress components are equal for the normal stress and the effective stress. The effective stress is utilized in the constitutive relationship for the soil. In incremental format, this takes the following form;

$$d\sigma' = D_T(d\varepsilon - d\varepsilon_c - d\varepsilon_p - d\varepsilon_o) \quad (13)$$

where $d\varepsilon$ represents the total strain of the skeleton, $d\varepsilon_c = Cdt$ is the creep strain, $d\varepsilon_p = m(dp/3K)$, represents the overall volumetric strain caused by uniform compression of the particles by the pressure of the pore fluid and ε_0 represents all strains not directly associated with stress changes. The tangential stiffness matrix D_T and the creep term C are dependent on the level of effective stress, and if strain effects are considered, also on the total strain of the skeleton ε. The equilibrium equation for the soil phase, relating the total stress to the body forces and boundary traction is derived using the principle of virtual work.

$$\int_\Omega \varepsilon^T d\sigma d\Omega - \int_\Omega \delta u^T b d\Omega - \int_{\hat{\Gamma}} \delta u^T t d\Gamma = 0 \quad (14)$$

Incorporation the concept of effective stress and the constitutive relationship into the equilibrium equation, and dividing by dt, the final general equation is given as

$$\int_\Omega \delta\varepsilon^T D_T \frac{\partial \varepsilon}{\partial t} d\Omega - \int_\Omega \delta\varepsilon^T m \frac{\partial \bar{p}}{\partial t} d\Omega + \int_\Omega \delta\varepsilon^T D_T m \frac{\partial \bar{p}}{\partial t}\frac{1}{3K_s} d\Omega$$
$$- \int_\Omega \delta\varepsilon^T D_T C d\Omega - \int_\Omega \delta\varepsilon^T D_T \frac{\partial \varepsilon_o}{\partial t} d\Omega - \int_\Omega \delta u^T \frac{\partial b}{\partial t} d\Omega -$$
$$\int_\Gamma \delta u^T \frac{\partial \hat{t}}{\partial t} d\Gamma = 0 \quad (15)$$

where t , K_s and b are the boundary traction factor, bulk modulus of the solid skeleton, and body force vector respectively. If one assumes that the soil matrix deformations are small and that the system is isothermal, the compression of the solid matrix will depend upon changes in fluid pressure and may be approximated by the use of linear elastic theory [17]. In all examples, a linear elastic material behaviour is assumed for soil deformation. On differentiating the effective average pore pressure from equation (2) with respect to time, we obtain

$$\frac{\partial \bar{p}}{\partial t} = S_n\frac{\partial P_n}{\partial t} + P_n\frac{\partial S_n}{\partial t} + S_w\frac{\partial P_w}{\partial t} + P_w\frac{\partial S_w}{\partial t} + S_g\frac{\partial P_g}{\partial t} + P_g\frac{\partial S_g}{\partial t} \quad (16)$$

The system of three nonlinear partial differential equations is also time dependent because of the term $\partial S_\alpha/\partial t$. In order to solve the system we need to rewrite this term as a function of pressure. Using the chain rule

$$\frac{\partial S_\alpha(P_{cnw}, P_{cgw})}{\partial t} = \frac{d S_\alpha}{dP_{cnw}}\frac{\partial P_{cnw}}{\partial t} + \frac{d S_\alpha}{dP_{cgw}}\frac{\partial P_{cgw}}{\partial t} \quad (17)$$

there, the equation (17) becomes

$$\frac{\partial S_\alpha}{\partial t} = \left(\frac{dS_\alpha}{dP_{cnw}}\right)\frac{\partial P_n}{\partial t} - \left(\frac{dS_\alpha}{dP_{cnw}} + \frac{dS_\alpha}{dP_{cgw}}\right)\frac{\partial P_w}{\partial t} + \left(\frac{dS_\alpha}{dP_{cgw}}\right)\frac{\partial P_g}{\partial t} \quad (18)$$

Finally, we have

$$\frac{\partial \bar{p}}{\partial t} = P_1\frac{\partial P_n}{\partial t} + P_2\frac{\partial P_g}{\partial t} + P_3\frac{\partial P_w}{\partial t} \quad (19)$$

where

$$P_1 = S_n + \frac{P_n dS_n}{dP_{cnw}} + \frac{P_w dS_w}{dP_{cnw}} + \frac{P_g dS_g}{dP_{cnw}}.$$

$$P_2 = S_g + \frac{P_n dS_n}{dP_{cgw}} + \frac{P_w dS_w}{dP_{cgw}} + \frac{P_g dS_g}{dP_{cgw}},$$

and

$$P_3 = S_w - P_n\left(\frac{dS_n}{dP_{cnw}} + \frac{dS_n}{dP_{cgw}}\right) - P_w\left(\frac{dS_w}{dP_{cnw}} + \frac{dS_w}{dP_{cgw}}\right) - P_g\left(\frac{dS_g}{dP_{cnw}} + \frac{dS_g}{dP_{cgw}}\right)$$

Three-phase flow equations

The fluid phase behaviour has been described by Lewis and Schrefler[15]. The equation governing the behaviour of three immiscible and incompressible fluids flowing in a deforming porous medium can be obtained by combining Darcy's linear flow law with a mass conservation balance for each of the flowing phases. Incorporating the formulation volume factors, B, and the relative permeability, into the continuity equations for each fluid phase α, gives

$$\nabla\left[\frac{Kk_{r\alpha}(S_\alpha)\rho_\alpha\nabla(P_\alpha + \rho_\alpha g h)}{\mu_\alpha B_\alpha(P_\alpha)}\right] = \text{rate of fluid accumulation} \quad (20)$$

The factors, which contribute to the rate of fluid accumulation of each flowing phase, are:

1. rate of change of total strain

(21)

2. rate of change of solid particle volume due to pressure change

(22)

3. rate of change fluid density

(23)

4. rate of change of saturation

(24)

5. change of solid particle size due to effective stresses changes $\partial\sigma'/\partial t$

(25)

where K is the absolute permeability matrix of the medium, μ is the dynamic viscosity of the fluid, g is the gravitational constant and h is the head above a given datum. On taking into account several factors that contribute to the rate of fluid accumulation, the general form of the continuity equation for each flowing phase may be expressed as follows:

$$-\nabla^T\left[\frac{Kk_{r\alpha}\rho_\alpha\nabla(P_\alpha + \rho_\alpha g h)}{\mu_\alpha B_\alpha}\right] + \frac{\partial\phi}{\partial t}\left(\frac{\rho_\alpha S_\alpha}{B_\alpha}\right) + \frac{\rho_\alpha S_\alpha}{B_\alpha}\left[\left(m^T - \frac{m^T D_T}{3K_s}\right)\frac{\partial\varepsilon}{\partial t} + \frac{m^T D_T C}{3K_s} + \left(\frac{(1-\phi)}{K_s} - \frac{m^T D_T m}{(3K_s)^2}\right)\left(P_1\frac{\partial P_n}{\partial t} + P_2\frac{\partial P_g}{\partial t} + P_3\frac{\partial P_w}{\partial t}\right)\right] + \rho_\alpha Q_\alpha = 0 \quad (26)$$

where Q_α represents external sinks or sources, kr_α is the relative permeability and ϕ is the porosity of a given phase. Equation (26) represents the general governing equations for multiphase incompressible fluid flow and isotropic soil in a deforming porous medium. The mobility terms in this equation are

strongly dependent on the unknowns, for example, the relative permeability depend on the fluid saturation. To solve the governing equations for the unknowns, u, P_w, P_g and P_n then knowledge of the constitutive parameters of the initial conditions and of the boundary conditions are required. The initial conditions specify the full displacement and pressures e.g.

$$u_i = u_i^o, \qquad P_\alpha = P_\alpha^o$$

The boundary conditions are specified as either prescribed values or fluxes,

$$u = u^b,$$

$$P_\alpha = P_\alpha^b, \quad q_\alpha = \frac{K k_{r\alpha} \rho_\alpha}{\mu_\alpha} \nabla (P_\alpha + \rho_\alpha g h) n$$

where b is the body force, q is the flux, o is the initial condition and n is the vector normal to the boundary.

NUMERICAL MODEL

The finite element procedures, based on galerkin's weighted residual approach, is implemented as the numerical solution method, as analytical solutions are incapable of dealing with the highly complex and non-linear governing equations. Fluid pressures and displacement are taken as the primary unknown variables. Nine-noded element and the respective associated shape function are used. The approximation process is similar to that described by Schrefler et al[12]. The finite element discretization of the equilibrium and flow equations may now be expressed in terms of the nodal displacement, u, and nodal fluid pressures, i.e. P_n, P_w and P_g by using the Galerkin method. The unknowns are related to their nodal values by the following expression:

$$p = N^T P, \qquad \varepsilon = BU, \qquad u = N^T U \tag{27}$$

where N and B are the shape function and linear operator, respectively. Upon substitution of equation (27), we obtain the discretized form of equation (15) and (26) as follows;

$$\begin{bmatrix} A_{12} & A_{13} & A_{14} \\ A_{22} & A_{23} & A_{24} \\ A_{32} & A_{33} & A_{34} \\ A_{42} & A_{43} & A_{44} \end{bmatrix} \frac{d}{dt} \begin{bmatrix} U \\ P_w \\ P_g \\ P_n \end{bmatrix} +$$

$$\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & B_{26} & 0 & 0 \\ 0 & 0 & B_{37} & 0 \\ 0 & 0 & 0 & B_{48} \end{bmatrix} \begin{bmatrix} U \\ P_w \\ P_g \\ P_n \end{bmatrix} = \begin{bmatrix} A_{10} \\ A_{20} \\ A_{30} \\ A_{40} \end{bmatrix} \tag{28}$$

Equation (28) forms a coupled nonsymmetrical and nonlinear system of ordinary differential equation in time. A detailed explanation of the above coefficients are given in Reference (8) and (18). For convenience, equation (28) are written in the following form:

$$A\dot{x} + Bx = F \tag{29}$$

where $x = [u, P_w, P_g, P_n]$ and the matrices A, B, and F are obtained by inspection. The integration of the coupling terms A_{ij} and B_{ij} requires the use of a numerical technique. Here, however, the two-dimensional Simpson rule integration method is employed, involving 9 integration points. This method has an advantage when using with explicit time different technique, no need to assemble physically the global matrices and to solve the time step should be performed. The integration, using this method, is given by

$$\int F d_x d_y = \int F det[J] d\xi d\eta = \sum_{i=1}^{N} \alpha_i F_i (det[J])_i \tag{30}$$

where, N is the number of nodes in finite element grid and α is the weighting for Simpson rule integration using 9 integration points such as

$$\alpha = (1/9,\ 4/9,\ 1/9,\ 4/9, 16/9, 4/9, 1/9, 4/9, 1/9)$$

The coupling terms are evaluated for each element using this numerical technique, and the assembled into the global matrix. The format in the elemental matrices and the global matrix differs in the ordering of unknown variables. In the element matrices, the unknowns, x, are in the following order

$$x = [u_1 v_1 \ldots u_9 v_9\ P_{w1} \ldots p_{w9}\ P_{g1} \ldots P_{g9}\ P_{n1} \ldots P_{n9}]$$

In the global matrix, the unknowns, x, are in the following order

$$x = [u_1 v_1 P_{w1} P_{g1} P_{n1} \ldots u_N v_N P_{wN} P_{gN} P_{nN}]$$

Thus it is necessary to transform the coupling terms from the elemental matrices to the global matrix, when assembling the global matrix. Once the global matrix has been fully assembled, the partial differential equations have been transformed into first order ordinary differential equations. A linear variation of the unknown variables in times is assumed to approximate the first order time derivatives. The genaralised mid-points family of methods is employed to discretize the time derivatives, which yields the following recurrence scheme as

$$A\frac{(x^{n+1} - x^n)}{\Delta t} + B(\theta x^{n+1} + (1 - \theta) x^n) = \theta F^{n+1} + (1 - \theta) F^n \tag{31}$$

or,

$$x^{n+1} = \frac{1}{[A + \theta\Delta t B]}\left([A - (1-\theta)\Delta t B]x^n + \Delta t\,[\theta F^{n+1} + (1-\theta)F^n] \right) \quad (32)$$

where Δt is the time step length, x_{n+1} and xn are state vectors at time instants t_{n+1} and t_n and θ is a time weighting parameter, usually $0 \le \theta \le 1$. The matrices are evaluated at the time level $n + \theta$. The matrices are evaluated at the time level $n + \theta$. Because of the nonlinearities involved a solution scheme of the fixed points type is used within every time step. The convergence criteria implemented are based on a maximum change in the unknown variables between successive time steps.

The saturated state in equation (2) is detected by monitoring the sign of capillary pressure; when such a condition is reached the dry air conservation equation is dropped and gas pressure P_g is equal to the atmospheric pressure (switching' from partially saturated to fully saturated state equations, or vice versa). In practice, capillary and gas pressure oscillations usually arise when this switch is performed, so it is necessary to apply this procedure for slightly lower saturation value $S_w < 1$ (capillary pressure less than zero) which depends on the shape of saturation-capillary pressure relationship and the problem analyzed. These oscillations are possibly due to a sudden switch of element behaviour (these is a change in governing equations) in a part of the domain which in turn causes different convergence to solution in fully saturated and partially saturated zones of the domain and procedures oscillations in the Newton iteration procedure.

VALIDATION AND NUMERICAL EXAMPLES

In order to illustrate that the governing equations and constitutive relationships upon which the numerical model is based correctly, the numerical model is validated against fully and partially saturated elastic consolidation problem for which previous solutions are known and the examples are relevant to groundwater contamination problems.

For this purpose a one-dimensional, fully saturated, consolidation problem is solved and compared with a previous solution by Lewis and Schrefler[15]. A column of linear elastic material is $7m$ and $2m$ width and the pore pressure is equal to zero at the top surface (Figure 1). The top surface is the only drained boundary whilst the rest are assumed to be closed. The vertical displacements versus time of the top surface is shown in Figure 2(a) for the case of isothermal consolidation and a good agreement is observed when compared with the results of Lewis and Schrefler[15]. Obviously, the soil permeability $K_2 = 1 \times 10^{-11} m^2$ has a lower rate of settlement when compared with $K_1 = 4 \times 10^{-9} m^2$. The pore pressure versus time at several depths are shown in Figure 2(b).

Also, the code of multiphase immiscible flow is validated in partially saturated conditions based on a previous study by Schrefler et al [14]. Using the same boundary conditions as in Figure 1, a soil column was subjected to an external surface load of 1000 N/m^2 and with the soil permeability, $k = 0.46 \times 10^{-11}\ m^2$. The initial condition for pressures P_w and P_g depend on the initial saturation profiles. The boundary conditions and the other data of the porous medium were assumed to be the same as in Reference [14]. i.e,

Elastic modulus	$E = 6 \times 10^6\ N/m^2$
Poison's ratio	$\nu = 0.4$
Porosity	$\phi = 0.3$
Bulk modulus	$K_s = 0.14 \times 10^{10}\ N/m^2$
	$K_w = 0.43 \times 10^{13}\ N/m^2$
Viscosity	$\mu_w = 1.0 \times 10^{-3}\ N/m^2$
	$\mu_g = 1.0 \times 10^{-3}\ N/m^2$
P_{dgw}	$1.682 \times 10^3\ N/m^2$
λ	3.0
S_{rw}	0.2

Temporal discretizaton is performed with an initial step of 0.01 days and multiplied by 10 after repeating 10 steps until an elapsed time of i.e. 10 days the required time of time of the analysis. Figure 3 shows the comparison of vertical displacement versus time for selected depths. The results obtained using the developed code agree well when compared with those presented by Schrefler et al [14].

The example of soil column, 1m in height with a similar geometry and conditions of surface load in Figure 2 was applied. The domain was discretized in one dimension using a rectangular grid consisting of 10 elements and 63 nodes. A informs nodal spacing of 0.1m was used in the vertical direction. The soil column was assumed to be unsaturated with an initial water saturation of 0.52. The initial pore water boundary was – 280 kN/m^2 and the boundary pore water pressure was instantaneously changed to a value of – 420 kN/m^2 at the surface. The boundary Condition are a) lateral surdace $U_h = 0$, $q_w = q_g = 0$, b) top surface $P_w = -420\ kN/m^2$, $P_g = P_{atm}$ and c) bottom surface $U_v = 0$, $q_w = q_g = 0$. The parameters of the porous media are described as follows; $E = 0.6 \times 10^7\ N/m^2$, $\nu = 0.4$, $\phi = 0.3$, $K = 0.46 \times 10^{-11}\ m^2$, $K_s = 0.14 \times 10^{10}\ N/m^2$, $\rho_s = 2.0 \times 10^3\ kg/m^3$, $P_{dgw} = 225.0 \times 10^3\ N/m^2$, $\lambda = 3.0$ and $S_{rw} = 0.3966$. In Figure 4(a) the vertical displacements for selected points are

presented for the consolidation case. Figure 4(b) shows the distribution of water saturation versus time at different points within the column. Figure 5 shows the pore water pressure distribution throughout the soil layer due to a change in the pore water pressure at the boundary. The model describes the behaviour of unsaturated soil systems under environmental changes.

In order to study the spreading NAPL in a porous media system, the test example involves 1m in height of a vertical column with a soil permeability of 1.0 x $10^{-12} m^2$. The source boundary condition was set at 0.5 of the NAPL fluid saturation and a porosity of 0.40 was used through the column, initially completely saturated by water. The result is a displacement of the water from the column by the encroaching NAPL. The initial conditions are $P_w = P_n = P_{ref}$ and $U_v = U_h = 0$. The boundary conditions for the problem are:

a) Lateral surface $U_h = 0$, $q_w = q_n = 0$
b) Top surface $P_w = P_{ref} - P_{sw}$, $P_n = P_{ref} = 9810\ N/m^2$ or 1 meter of water and $P_{sw} = 0.5$ is the pressure to keep saturation 0.5
c) Bottom surface $U_v = U_h = 0$, $P_w = P_n = P_{ref}$

The material properties used are as follows:

Elastic modulus	$E = 5 \times 10^6\ N/m^2$
Poison's ratio	$\nu = 0.4$
Porosity	$\phi = 0.3$
Bulk modulus	$K_s = 1.0 \times 10^{12}\ N/m^2$
	$K_w = 0.43 \times 1013\ N/m^2$
P_{dgw}	$0.1784\ N/m^2$
λ	3.0
S_{rw}	0.2

The parameters chosen for the simulations were a NAPL density of 1461 kg/m^3 and a viscosity of 0.57 x $10^{-3}\ Ns/m^2$. The water phase was assigned a density of 1000 kg/m3 and a viscosity of 1.0 x $10^{-3}\ Ns/m^2$. The resulting profiles of vertical displacements and effective water saturation are shown in Figure 6(a) and (b) respectively for different time values. Similar behaviour was also reported by Schrefler et al [13].

Two-dimensional multiphase flow example which demonstrates the impact of an undetected leak of nonqueous phase liquid in a porous medium are presented. This problem was designed to study the migration of LNAPL (light nonaqueous phase liquids) from a continuous source at the soil surface. Figure 7.0 shows a schematic diagrams of the geometry for the simulated cross section and boundary conditions. The system is subjected to water infiltration at a rate of of 100 $kg/yr/m^2$. The LNAPL source, with a release rate of 900 kg/yr is located at the top left-hand edge. The assumption is that the pressures in the gas phase are negligible leads to two partial differential equations (P_w, P_n). The left and right-hand boundaries of the domain were treated as impermeable, and the bottom boundary was assigned constant-pressure conditions with $P_w = P_n = 101\ 325\ N/m^2$.

The simulation domain in Figure 8.0 presents 2 metre thick and 19.0 metre in length. The domain was discretized using a 2-D rectangular grid consisting of 40 elements and 187 nodes. Nodal spacing varied along the horizontal and vertical axis as shown in Figure 8.0. Value of the physical parameters used in the simulation are presented below,

Elastic modulus	$E = 10.0 \times 10^6\ N/m^2$
Poison's ratio	$\nu = 0.3$
Porosity	$\phi = 0.3$
Soil permeability	$K = 1.0 \times 10^{-12}\ m^2$
Water viscosity	$\mu_w = 1.0 \times 10^{-3}\ N/m^2$
LNAPL viscosity	$\mu_n = 1.0 \times 10^{-3}\ N/m^2$
Bulk modulus	$K_s = 6.1 \times 10^8\ N/m^2$
Density for LNAPL	$950.0\ kg/m^3$
P_{dgw}	$1.682 \times 10^3\ N/m^2$
S_{rw}	0.2
S_{rn}	0.02
λ	3.0

For a contaminating fluid less dense than water, the contaminant would be expected to pool in a zone near the water table. These conditions were observed in the results of the simulation. Figure 9.0 shows the initial water saturation in the model. The simulated saturation contours are shown in Figures 10.0 and 11.0, respectively. For the nonaqueous fluid, which is less dense than water, then the contaminant saturation are higher and do not extend nearly as for into the saturated zone. The lighter contaminants here also migrated further in a lateral direction. Figure 12.0 shows water saturation profile for LNAPL for t = 3.17 years.

CONCLUSION

A general formulation and solution procedure for multiphase immiscible flow in deforming porous material are presented. Nonlinear saturation and relative permeability functions are incorporated into a Galerkin finite element model. The governing equations in terms of the soil displacement and fluid pressure result in coupled, non-linear, partial differential equations. One and two-dimensional numerical simulations were performed for a homogenous porous media and indicate the behaviour of the soil properties and distribution of the contaminant after a fixed elapsed time.

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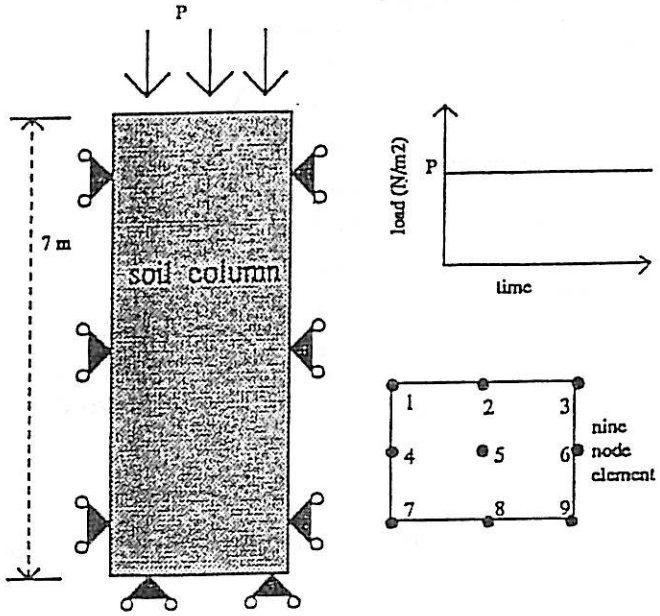
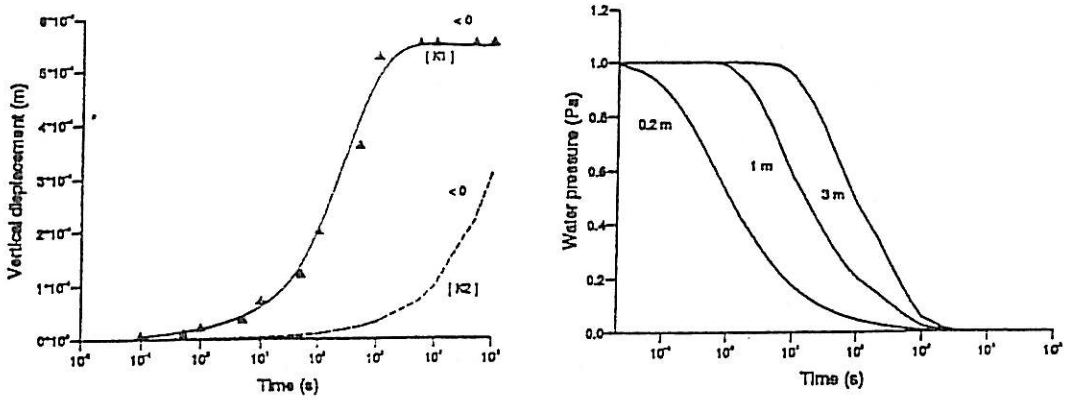


Figure 1: Soil column and finite element spatial discretization



(a) solid line-present code, triangle-Lewis & Schrefler (b)

Figure 2: Surface settlements(a) and water pressures(b) versus time for the one-dimensional saturated problem

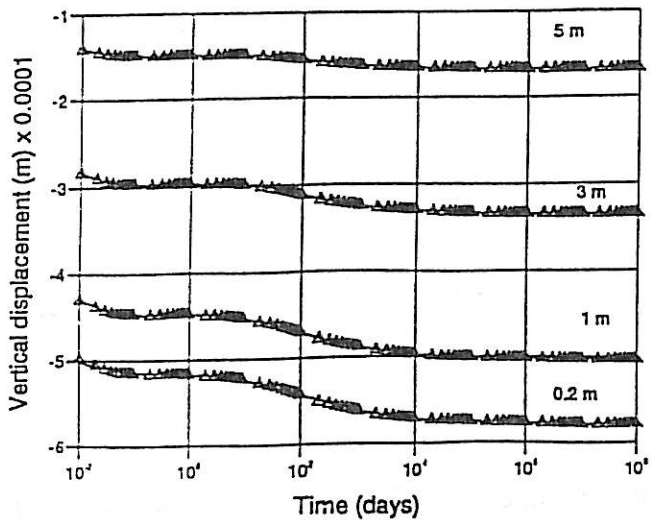
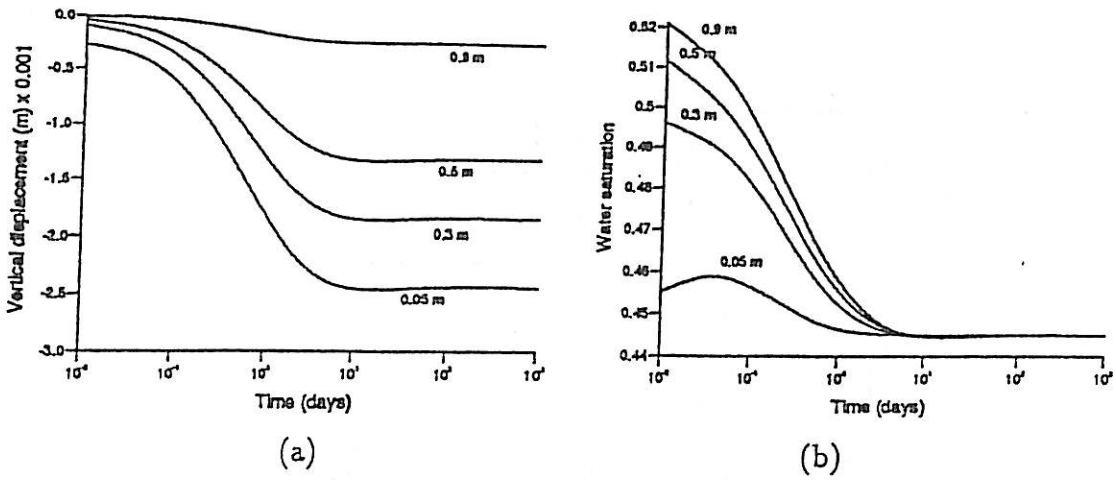


Figure 3: Profile of vertical displacement vs time (solid line-present code, triangle-Schrefler et al)



(a) (b)

Figure 4: Profile of vertical displacement(a) and water saturation(b) during consolidation

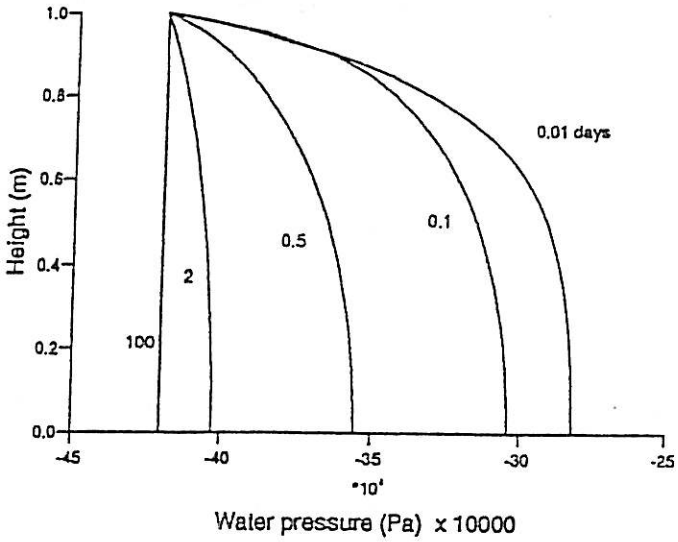
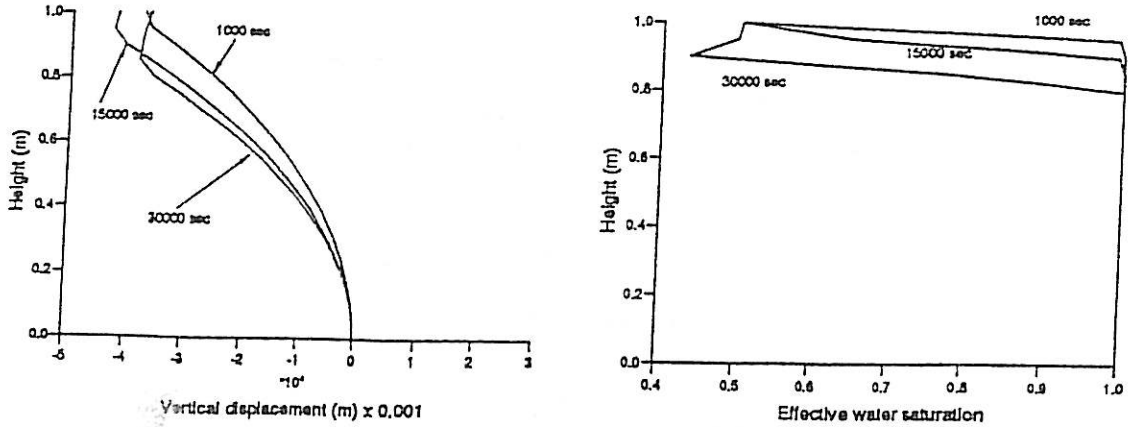


Figure 5: Pore water pressure distribution under consolidation



(a) (b)

Figure 6: Profile of vertical displacements(a) and water saturation(b) throughout soil column

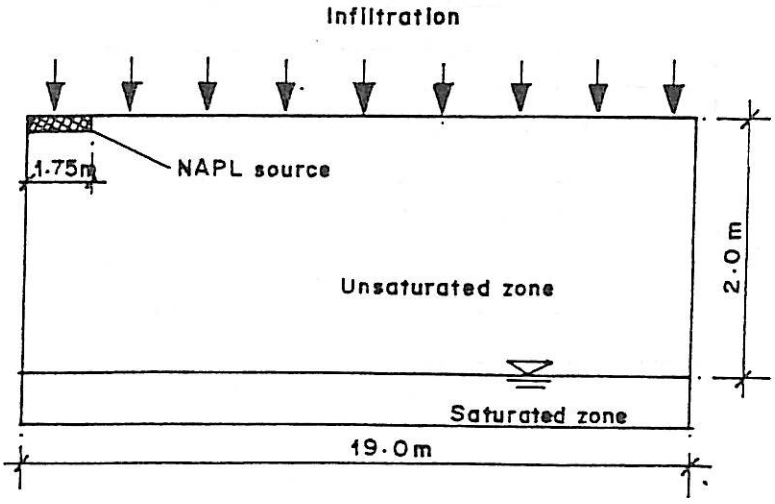


Figure 7: Schematic representation of boundary conditions and geometry for example application.

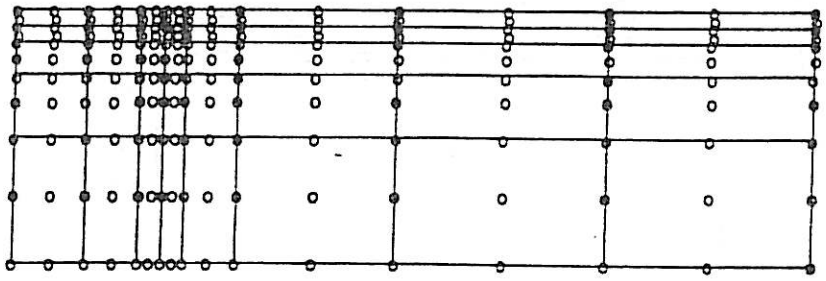


Figure 8: 2D mesh element.

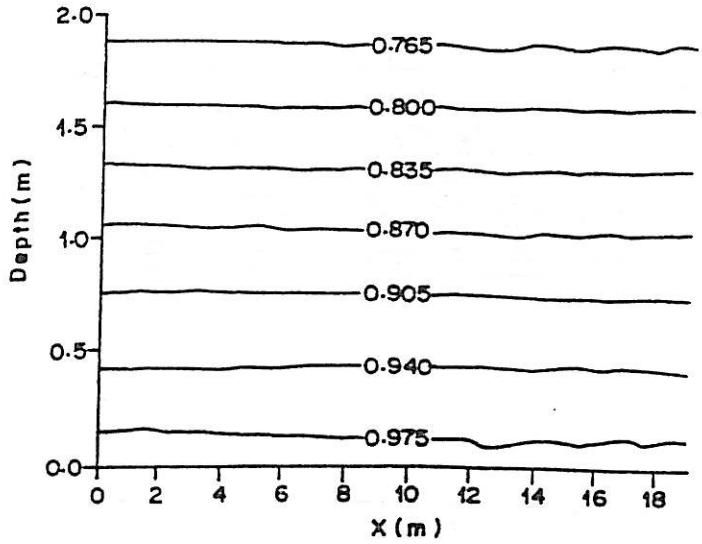


Figure 9: Initial water saturation (t = 0)

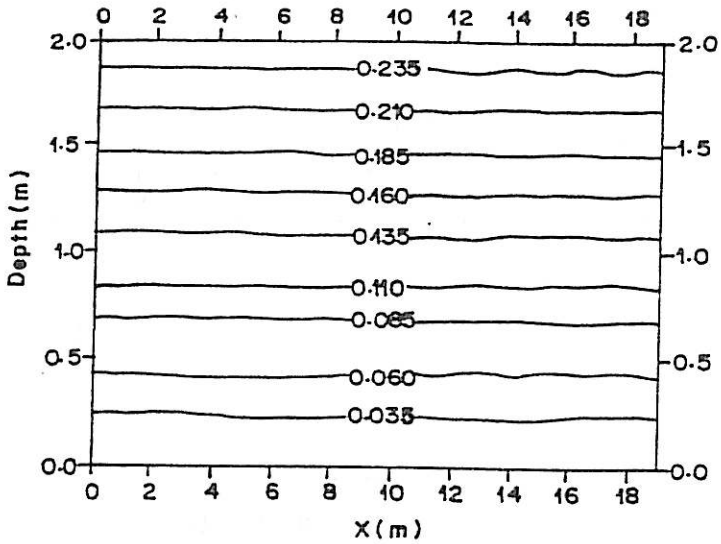


Figure 10: LNAPL saturation contours for cross-sectional simulation of NAPL migration (t = 1000 s)

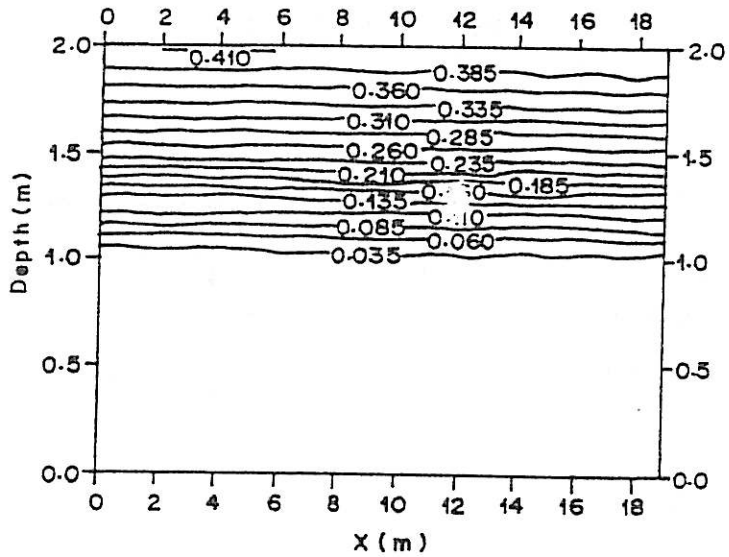


Figure 11: LNAPL saturation (t = 3.17 years)

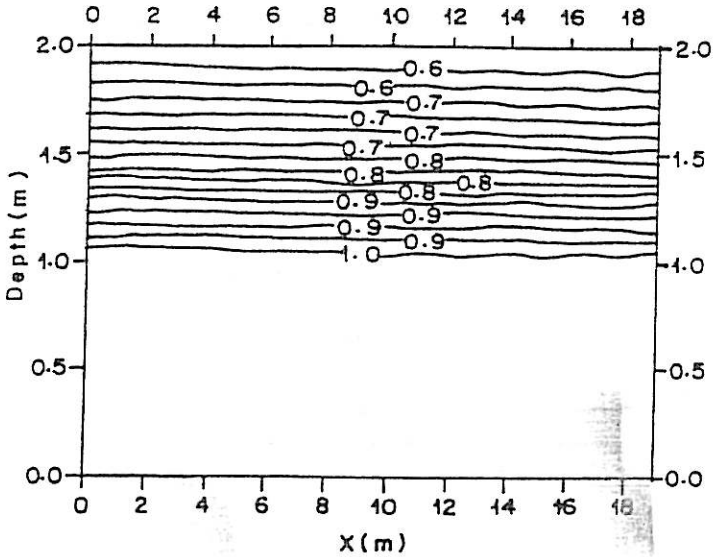


Figure 12: Water saturation (t = 3.17 years)

Appendix 3

Finite element modelling of multiphase immiscible flow in deforming porous media for subsurface systems

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COMPUTERS AND GEOTECHNICS

Finite element modelling of multiphase immiscible flow in deforming porous media for subsurface systems

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Abstract

A fully coupled numerical model has been developed which describes multiphase fluid flow through soil: namely gas, water and a nonaqueous phase liquid (NAPL) in a deforming porous media for subsurface systems. A multiphase flow model, based on the two-phase flow model of Brooks and Corey, is presented to express the dependence of saturation and relative permeability on the capillary pressure. Nonlinear saturation and relative permeability on the capillary pressure. Nonlinear saturation and relative permeability functions are incorporated into a Galerkin finite element model which is subsequently used to simulate multiphase immiscible fluid flow under saturated and unsaturated conditions in porous media. The governing partial differential equations, in terms of soil displacements and fluid pressures, which are coupled and non-linear, are solved by the finite element method. Numerical implementation of the formulation are discussed and example problems are performed to demonstrate the model and solution procedure.

1. Introduction

The simulation of groundwater contamination in subsurface systems by nonaqueous phase liquids (NAPLs), such as petroleum hydrocarbons and immiscible industrial chemicals, requires a solution of the multiphase flow equations for deforming porous media. During the last decade, several numerical models of multiphase immiscible flow have been reported in the groundwater literature for evaluating NAPL contamination and remedial scenarios [1–9]. Faust [1] presented a two-dimensional finite difference simulator for NAPL and water phase flow in a

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three phase (air, water, NAPL) system. In this model, it is assumed that the gas phase is at atmospheric pressure and a separate mass balance equation for the air component is not included. Since evaporation and transport of the organic chemical component in the gas phase is not considered in this simulation, a detailed treatment of the gas phase movement is probably not necessary under most conditions. The governing equations are discretized using a two-dimensional Cartesian coordinate system. The code was verified by comparisons with the Buckley Leverett solution for one-dimensional two-phase flow and with two-dimensional saturated unsaturated flow simulators. The capabilities of this simulator were extended to include three-dimensional Cartesian and two-dimensional cylindrical coordinate systems by Faust et al. [2].

A two-dimensional two-phase flow finite element code was reported by Osborne and Sykes [4]. This model simulates the flow of the NAPL and water phases in a system having no gas phase. The formulation is developed for a two-dimensional Cartesian coordinate system. The code was verified by comparison with a one-dimensional finite difference two-phase flow simulator developed by Little [10]. A two-dimensional finite element simulator for NAPL and water phase flow in three phase systems was developed by Kuppusamy et al. [5]. As in the work of Faust [1], they assume that the gas phase is at constant pressure and do not calculate the gas phase flow field. The simulator uses a two-dimensional Cartesian coordinate system. The code was validated by comparisons with column laboratory experiments for water displacement by an NAPL. Kaluarachchi and Parker [6] present a similar two-dimensional Cartesian finite element model employing same assumptions as Faust [1] and Kuppusamy et al. [5]. In their study, they verified the model by comparison with the theoretical equilibrium distribution of a NAPL following the infiltration of a NAPL into a variably water saturated column. Panday et al. [9] presented a three-phase numerical model for simulating the movement of NAPLs through porous media. The model formulations and numerical schemes are tested for highly non-linear field conditions. Attention is focused on situations involving one, two and three-dimensional flow through porous media.

While these models have found fairly wide application in simulating multiphase flow in shallow systems, coupling this problem with soil deformation, which is an important engineering problem has, to date, received very little attention. As far as soil deformation problems are concerned, Li and Zienkiewicz [11] studied the interaction of two-phase immiscible flow with the porous medium. The model was based on the mass conservation equation as a function of intrinsic phase velocities and the solid and liquid equilibrium equations for a unit element of porous medium. The equation is discretized using finite elements, with quadratic scheme for the time domain. A fully coupled model for both water flow and airflow in a deformable porous media has also been studied by Schrefler and Zhan [12]. The model has been extended by Schrefler et al. [13] to incorporate immiscible pollutant transport problems, by solving subsets of the whole group of governing equations.

The main objective of this study is to develop a model that describes the flow of multiphase immiscible fluids in a deforming porous medium. This study presents the flow formulation and associated numerical techniques for a comprehensive model

used for simulating multiphase problems. The governing equations describing the displacement of soil and multiphase fluid pressures are coupled and the nonlinear partial differential equations are solved by the finite element method. Nonlinear saturation and relative permeability functions are incorporated into a Galerkin finite element model that is used to simulate multiphase systems and subsurface migration of NAPL contaminants in porous media.

2. Description of the model

The physical model on which the approach is based is the same as that used by Lujan [3] for three-phase flow analysis and by Lewis and Schrefler [14] for deforming multiphase flow in porous media. Contaminant transport models for miscible components cannot describe the migration of an immiscible contaminant. The flow of an immiscible contaminant is controlled by its own flow potential, which depends on pressure, gravity and surface forces and is not necessarily similar to the groundwater flow potential [1]. In order to describe mathematically the flow of immiscible fluids through a porous medium, it is necessary to determine functional expressions that best define the relationship between the hydraulic properties of the porous medium, i.e. saturation, relative permeability and capillary pressure. The porous medium voids are assumed to be filled with water, gas and NAPL, and thus the sum of their saturation will be unity, i.e.

$$S_n + S_w + S_g = 1 \tag{1}$$

where S is saturation of the fluid phase, n, w, g represented as NAPL, water and gas respectively. When more than one fluid exists in a porous medium, the pressure exerted by the fluids may be evaluated using the effective average pore pressure, $\bar{p}$, which is calculated from

$$\bar{p} = S_n P_n + S_w P_w + S_g P_g \tag{2}$$

The water pressure (P_w), gas pressure (P_g) and NAPL pressure (P_n) are related through the capillary pressure and the three capillary pressure terms are defined as,

$$P_{cnw} = P_n - P_w,\ P_{cgn} = P_g - P_n,\ \text{and}\ P_{cgw} = P_g - P_w \tag{3}$$

where, P_{cgw} is the capillary pressure between the gas and water phases, P_{cnw} is the capillary pressure between the NAPL and the water phase and P_{cgn} is the capillary pressure between the gas and NAPL phases. In general, for a multiphase system, the saturation of any of the three phases ($\alpha = w, g, n$) is a function of three capillary pressures relationships i.e. NAPL–water, gas–NAPL and gas–water, respectively,

$$S_\alpha = f(P_{cgw}, P_{cnw}, P_{cgn}) \tag{4}$$

The gas-water capillary pressure, expressed in terms of the other two capillary pressures yields the following,

$$P_{cgn} = P_{cgw} - P_{cnw} \tag{5}$$

And we can rewrite Eq. (4) as

$$S_\alpha = f(P_{cgw}, P_{cnw}) \tag{6}$$

The distribution of zones, as functions of capillary pressures, is defined as follows:

I. Water only $[P_{cgw} \leqslant P_{dgw}, P_{cnw} \leqslant P_{dnw}]$ $\quad S_w = 1.0$

II. Water and gas $[P_{cgw} > P_{dgw}] S_w = S_{\max}[P_{dgw}/P_{cgw}]^\lambda + S_{rw}$ $\quad S_g = 1 - S_w$

III. Water and NAPL $[P_{cnw} > P_{dnw}]$, $P_{cgn} \leqslant P_{dgn}$

$$S_w = S_{\max}[P_{dnw}/P_{cnw}]^\lambda + S_{rw} \qquad S_n = 1 - S_w$$

IV. Water, NAPL and gas $[P_{cnw} > P_{dnw}, P_{cgn} > P_{dgn}]$ $\quad S_g = 1 - S_w - S_n$

$$S_w = S_{\max}[P_{dnw}/P_{cnw}]^\lambda + S_{rw} \qquad S_n = S_{\max}([P_{dgn}/P_{cgn}]^\lambda - [P_{dnw}/P_{cnw}]^\lambda) + S_{rn}$$

where,

$$S_{\max} = 1 - S_{rw} - S_{rn} - S_{rg}$$

and S_{rw} is the residual water saturation, S_{rg} is the residual saturation of the gas phase, S_{rn} is the residual saturation of the NAPL phase and λ is a pore size distribution index. Also, P_{dgw} is the displacement pressure for gas and water system, P_{dnw} is the displacement pressure for NAPL and water system and P_{dgn} is the displacement pressure for gas and NAPL system. Lujan [3] proposed expressions for the relative permeabilities when the effective saturations are calculated from capillary pressures using the Brooks and Corey [15] equations.

$$k_{rw} = S_{ew}^{(2+3\lambda)/\lambda}, k_{rg} = (1 - S_{te})^2(1 - S_{te}^{(2+\lambda)/\lambda}) \tag{7}$$

$$k_{rn} = (S_{te} - S_{ew})^2(S_{te}^{(2+\lambda)/\lambda} - S_{ew}^{(2+\lambda)/\lambda}) \tag{8}$$

where,

$$S_{ew} = [S_w - S_{rw}]/S_{\max} \text{ and } S_{te} = [1 - S_g - S_{rw} - S_{rn}]/S_{\max}$$

S_{ew} is the effective water saturation and S_{te} is the total effective liquid saturation. In addition to the above constitutive relations, the equations of state are needed to determine the fluid densities as functions of pressure. These equations are given as follows

$$\rho_w = \rho_{wo}[1 - \beta_w(T - T_o) + 1/K_w(P_w - P_{wo})] \tag{9}$$

$$\rho_n = \rho_{no}[1 - \beta_n(T - T_o) + 1/K_n(P_n - P_{no})] \tag{10}$$

$$\rho_g = \rho_{go}P_g T_o/(P_{go}T) \tag{11}$$

where the subscript o indicates an initial steady state, β is the thermal expansion coefficient of the fluid phase, ρ is the fluid density, K_w is the bulk modulus of the water phase, K_n is the bulk modulus of the NAPL phase and T is the absolute temperature.

3. Mathematical model

In a multiphase flow model, the simultaneous flow of the fluid phases; water, NAPL and gas in a porous medium, depends primarily on the gravitational force and capillary pressures between the three fluids. The fluid pressures and displacement values are used as the primary dependent variables. The development of four fully coupled, partial differential equations, including the three immiscible fluid flow equations, along with the equilibrium equation is an extension of the one-phase consolidation model development by Lewis and Schrefler [14]. Three conditions are assumed in the construction of the model:

(a) multiphase immiscible and incompressible fluid flow with no mass transfer between phases;
(b) isotropic, homogenous and deformable porous medium; and
(c) isothermal system.

3.1. Equilibrium equation

A general equilibrium equation requires both the effective stress relationship and the constitutive law relating the effective stress to the strains of the solid skeleton. The effective stress relationship is given by

$$\sigma = \sigma' - mP \tag{12}$$

where σ' is the effective stress, m is $[1\,1\,0]^T$ and P is the fluid pressure. The nature of m implies that the fluids pressure only effects the normal stress components, and that

the shear stress components are equal for the normal stress and the effective stress. The effective stress is utilized in the constitutive relationship for the soil. In incremental format, this takes the following form

$$d\sigma' = D_T(d\varepsilon - d\varepsilon_c - d\varepsilon_p - d\varepsilon_o) \tag{13}$$

where $d\varepsilon$ represents the total strain of the skeleton, $d\varepsilon_c = Cdt$ is the creep strain. $d\varepsilon_p = m(d_p/3K_s)$, represents the overall volumetric strain caused by uniform compression of the particles by the pressure of the pore fluid and ε_o represents all strains not directly associated with stress changes. The tangential stiffness matrix D_T and the creep term C are dependent on the level of effective stress, and if strain effects are considered, also on the total strain of the skeleton ε. The equilibrium equation for the soil phase, relating the total stress to the body forces and boundary traction is derived using the principle of virtual work.

$$\int_\Omega \delta\varepsilon^T d\sigma d\Omega - \int_\Omega \delta u^T d b d\Omega - \int_\Gamma \delta u^T d\hat{t} d\Gamma = 0 \tag{14}$$

Incorporation the concept of effective stress and the constitutive relationship into the equilibrium equation, and dividing by dt, the final general equation is given as

$$\begin{aligned} &\int_\Omega \delta\varepsilon^T D_T \frac{\partial\varepsilon}{\partial t} d\Omega - \int_\Omega \delta\varepsilon^T m \frac{\partial\bar{p}}{\partial t} d\Omega + \int_\Omega \delta\varepsilon^T D_T m \frac{\partial\bar{p}}{\partial t}\frac{1}{3K_s} d\Omega \\ &- \int_\Omega \delta\varepsilon^T D_T C d\Omega - \int_\Omega \delta\varepsilon^T D_T \frac{\partial\varepsilon_o}{\partial t} d\Omega - \int_\Omega \delta u^T \frac{\partial b}{\partial t} d\Omega - \int_\Gamma \delta u^T \frac{\partial\hat{t}}{\partial t} d\Gamma = 0 \end{aligned} \tag{15}$$

where K_s, $\hat{t}$ and b are the bulk modulus of the solid skeleton, boundary traction factor and body force vector respectively. If one assumes that the soil matrix deformations are small and that the system is isothermal, the compression of the solid matrix will depend upon changes in fluid pressure and may be approximated by the use of linear elastic theory [16]. In all examples, a linear elastic material behaviour is assumed for soil deformation. On differentiating the effective average pore pressure from Eq. (2) w.r.t time, we obtain,

$$\frac{\partial\bar{p}}{\partial t} = S_n\frac{\partial P_n}{\partial t} + P_n\frac{\partial S_n}{\partial t} + S_w\frac{\partial P_w}{\partial t} + P_w\frac{\partial S_w}{\partial t} + S_g\frac{\partial P_g}{\partial t} + P_g\frac{\partial S_g}{\partial t} \tag{16}$$

The system of three nonlinear partial differential equations is also time dependent because of the term $\partial S_\alpha/\partial t$. In order to solve the system we need to rewrite this term as a function of pressure. Using the chain rule,

$$\partial S_\alpha \frac{(P_{cnw}, P_{cgw})}{\partial t} = \frac{dS_\alpha}{dP_{cnw}} \frac{\partial P_{cnw}}{\partial t} + \frac{dS_\alpha}{dP_{cgw}} \frac{\partial P_{cgw}}{\partial t} \tag{17}$$

there, Eq. (17) becomes

$$\frac{\partial S_\alpha}{\partial t} = \left(\frac{\mathrm{d}S_\alpha}{\mathrm{d}P_{cnw}}\right) \frac{\partial P_n}{\partial t} - \left(\frac{\mathrm{d}S_\alpha}{\mathrm{d}P_{cnw}} + \frac{\mathrm{d}S_\alpha}{\mathrm{d}P_{cgw}}\right) \frac{\partial P_w}{\partial t} + \left(\frac{\mathrm{d}S_\alpha}{\mathrm{d}P_{cgw}}\right) \frac{\partial P_g}{\partial t} \tag{18}$$

Finally, we have

$$\frac{\partial \bar{p}}{\partial t} = P_1 \frac{\partial P_n}{\partial t} + P_2 \frac{\partial P_g}{\partial t} + P_3 \frac{\partial P_w}{\partial t} \tag{19}$$

where

$$P_1 = S_n + \frac{P_n \mathrm{d}S_n}{\mathrm{d}P_{cnw}} + \frac{P_w \mathrm{d}S_w}{\mathrm{d}P_{cnw}} + \frac{P_g \mathrm{d}S_g}{\mathrm{d}P_{cnw}}, \quad P_2 = S_g + \frac{P_n \mathrm{d}S_n}{\mathrm{d}P_{cgw}} + \frac{P_w \mathrm{d}S_w}{\mathrm{d}P_{cgw}} + \frac{P_g dS_g}{\mathrm{d}P_{cgw}}.$$

and

$$P_3 = S_w - P_n\left(\frac{\mathrm{d}S_n}{\mathrm{d}P_{cnw}} + \frac{\mathrm{d}S_n}{\mathrm{d}P_{cgw}}\right) - P_w\left(\frac{\mathrm{d}S_w}{\mathrm{d}P_{cnw}} + \frac{\mathrm{d}S_w}{\mathrm{d}P_{cgw}}\right) - P_g\left(\frac{\mathrm{d}S_g}{\mathrm{d}P_{cnw}} + \frac{\mathrm{d}S_g}{\mathrm{d}P_{cgw}}\right)$$

3.2. Three-phase flow equations

The fluid phase behaviour has been described by Lewis and Schrefler [14]. The equation governing the behaviour of three immiscible and incompressible fluids flowing in a deforming porous medium can be obtained by combining Darcy's linear flow law with a mass conservation balance for each of the flowing phases. Incorporating the formulation volume factors, B, and the relative permeabilities, into the continuity equations for each fluid phase α, gives

$$\nabla.\left[Kk_{r\alpha} \frac{(S_\alpha)\rho_\alpha}{\mu_\alpha B_\alpha(P_\alpha)} \nabla(P_\alpha + \rho_\alpha g h)\right] = \text{rate of fluid accumulation} \tag{20}$$

The factors, which contribute to the rate of fluid accumulation of each flowing phase, are:

1. rate of change of total strain

$$\frac{\partial \varepsilon_v}{\partial t} = m^T \frac{\partial \varepsilon}{\partial t} \tag{21}$$

2. rate of change of solid particle volume due to pressure change

$$\frac{(1-\phi)}{K_s}\frac{\partial \bar{p}}{\partial t} \tag{22}$$

3. rate of change fluid density

$$\phi S \frac{\partial}{\partial t}\frac{(1)}{B} \tag{23}$$

4. rate of change of saturation

$$\phi \frac{\rho}{B}\frac{\partial S}{\partial t} \tag{24}$$

5. change of solid particle size due to effective stresses changes $\partial\sigma'/\partial t$

$$-\frac{1}{3K_s} m^T \frac{\partial \sigma'}{\partial t} \tag{25}$$

where, K is the absolute permeability matrix of the medium, μ is the dynamic viscosity of the fluid, g is the gravitational constant and h is the head above a given datum. On taking into account several factors that contribute to the rate of fluid accumulation, the general form of the continuity equation for each flowing phase may be expressed as follow:

$$-\nabla^T\left[\frac{Kk_{r\alpha}\rho_\alpha}{\mu_\alpha B_\alpha}\nabla(P_\alpha+\rho_\alpha g h)\right]+\phi\frac{\partial}{\partial t}\left(\frac{\rho_\alpha S_\alpha}{B_\alpha}\right)+\frac{\rho_\alpha S_\alpha}{B_\alpha}\left[\left(m^T-\frac{m^T D_T}{3K_s}\right)\frac{\partial \varepsilon}{\partial t}\right.$$
$$\left.+\frac{m^T D_T C}{3K_s}+\left(\frac{(1-\phi)}{K_s}-\frac{m^T D_T m}{(3K_s)^2}\right)\left(P_1\frac{\partial P_u}{\partial t}+P_2\frac{\partial P_g}{\partial t}+P_3\frac{\partial P_w}{\partial t}\right)\right]+\rho_\alpha Q_\alpha=0 \tag{26}$$

where Q_α represents external sinks or sources, $k_{r\alpha}$ is the relative permeability and ϕ is the porosity of a given phase. Eq. (26) represents the general governing equations for multiphase incompressible fluid flow and isotropic soil in a deforming porous medium. The mobility terms in this equation are strongly dependent on the unknowns, for example, the relative permeability depends on the fluid saturation. To solve the governing equations for the unknowns, u, P_w, P_g and P_n knowledge of the constitutive parameters of the initial conditions and of the boundary conditions are required. The initial conditions specify the full displacement and pressures, e.g.

$$u_i = u_i^o, \qquad P_\alpha = P_\alpha^o$$

The boundary conditions are specified as either prescribed values or fluxes,

$$u = u^h, \qquad P_\alpha = P_\alpha^h, \qquad q_\alpha = -\frac{Kk_{r\alpha}}{\mu_\alpha}\rho_\alpha \nabla(P_\alpha + \rho_\alpha g h)n$$

where b is the body force, q is the flux, o is the initial condition and n is the vector normal to the boundary.

4. Numerical model

The finite element procedures, based on Galerkin's weighted residual approach, is implemented as the numerical solution method, as analytical solutions are incapable of dealing with the highly complex and non-linear governing equations. Fluid pressures and displacements are taken as the primary unknown variables. Nine-noded elements and the respective associated shape functions are used. The approximation process is similar to that described by Schrefler et al. [12]. The finite element discretization of the equilibrium and flow equations may now be expressed in terms of the nodal displacements, u, and nodal fluid pressures, i.e. P_n, P_w and P_g by using the Galerkin method. The unknowns are related to their nodal values by the following expression:

$$p = N^T P, \qquad \varepsilon = BU, \qquad u = N^T U \tag{27}$$

where N and B are the shape function and linear operator, respectively. Upon substitution of Eq. (27), we obtain the discretized form of Eqs. (15) and (26) as follows

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} & A_{14} \\ A_{21} & A_{22} & A_{23} & A_{24} \\ A_{31} & A_{32} & A_{33} & A_{34} \\ A_{41} & A_{42} & A_{43} & A_{44} \end{bmatrix} \frac{\mathrm{d}}{\mathrm{d}t} \begin{bmatrix} U \\ P_w \\ P_g \\ P_n \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & B_{26} & 0 & 0 \\ 0 & 0 & B_{37} & 0 \\ 0 & 0 & 0 & B_{48} \end{bmatrix} = \begin{bmatrix} A_{10} \\ A_{20} \\ A_{30} \\ A_{40} \end{bmatrix} \tag{28}$$

Eq. (28) forms a coupled nonsymmetrical and nonlinear system of ordinary differential equation in time. A detailed explanation of the above coefficients are given in Appendix I. For convenience, Eq. (28) is written in the following form:

$$A\dot{x} + Bx = F \tag{29}$$

where $x = [u, P_w, P_g, P_n]$ and the matrices A, B, and F are obtained by inspection. The integration of the coupling terms A_{ij} and B_{ij} requires the use of a numerical technique. Here, however, the two-dimensional Simpson rule integration method is

employed, involving nine integration points. This method has an advantage when used with an explicit time different technique. There is no need to physically assemble the global matrices and solve the time step. The integration, using this method, is given by

$$\int F \mathrm{d}_x \mathrm{d}_y = \int F \det[J] \mathrm{d}\xi d\eta = \sum_{i=1}^{N} \alpha_i F_i (\det[J])_i \tag{30}$$

where, N is the number of nodes in the finite element grid and α is the weighting for Simpson's rule integration using nine integration points such as,

$$\alpha = (1/9, 4/9, 1/9, 4/9, 16/9, 4/9, 1/9, 4/9, 1/9)$$

The coupling terms are evaluated for each element using this numerical technique, and then assembled into the global matrix. The format in the elemental matrices and the global matrix differs in the ordering of unknown variables. In the element matrices, the unknowns, x, are in the following order

$$x = [u_1 v_1 \ldots u_9 v_9 P_{w1} \ldots p_{w9} P_{g1} \ldots P_{g9} P_{n1} \ldots P_{n9}]$$

In the global matrix, the unknowns, x, are in the following order

$$x = [u_1 v_1 P_{w1} P_{g1} P_{n1} \ldots u_N v_N P_{wN} P_{gN} P_{nN}]$$

Thus it is necessary to transform the coupling terms from the elemental matrices to the global matrix, when assembling the global matrix. Once the global matrix has been fully assembled, the partial differential equations have been transformed into first order ordinary differential equations. A linear variation of the unknown variables in time is assumed to approximate the first order time derivatives. The generalised mid-point family of methods is employed to discretize the time derivatives, which yields the following recurrence scheme as,

$$A \frac{(x^{n+1} - x^n)}{\Delta t} + B(\theta x^{n+1} + (1-\theta)x^n) = (\theta F^{n+1} + (1-\theta)^{Fn} \tag{31}$$

or

$$x^{n+1} = \frac{1}{[A + \theta \Delta t B]} ([A - (1-\theta)\Delta t B] x^n + \Delta t [\theta F^{n+1} + (1-\theta) F^n]) \tag{32}$$

where Δt is the time step length, x_{n+1} and x_n are state vectors at time instants t_{n+1} and t_n and θ is a time weighting parameter, usually $0 \leqslant \theta \leqslant 1$. The matrices are evaluated at the time level $n+\theta$. Because of the nonlinearities involved a solution scheme of the fixed point type is used within every time step. The convergence criteria implemented are based on a maximum change in the unknown variables between successive time steps.

The saturated state in Eq. (2) is detected by monitoring the sign of capillary pressure; when such a condition is reached the dry air conservation equation is dropped and gas pressure P_g is equal to the atmospheric pressure (switching from partially saturated to fully saturated state equations, or vice versa). In practice, capillary and gas pressure oscillations usually arise when this switch is performed, so it is necessary to apply this procedure for a slightly lower saturation value $S_w < 1$ (capillary pressure less than zero) which depends on the shape of the saturation–capillary pressure relationship and the problem analyzed. These oscillations are possibly due to a sudden switch of element behaviour (these is a change in governing equations) in a part of the domain which in turn causes different convergence to solution in fully saturated and partially saturated zones of the domain and produces oscillations in the Newton iteration procedure.

5. Validation and numerical examples

In order to illustrate that the governing equations and constitutive relationships upon which the numerical model is based correctly, the numerical model is validated against fully and partially saturated elastic consolidation problems for which previous solutions are known and the examples are relevant to groundwater contamination problems.

For this purpose a one-dimensional, fully saturated, consolidation problem is solved and compared with a previous solution by Lewis and Schrefler [14]. A column of linear elastic material of 7 m depth and 2 m width and the pore pressure is equal to zero at the top surface (Fig. 1). The top surface is the only drained boundary whilst the rest are assumed to be closed. The vertical displacements versus time of the top surface is shown in Fig. 2(a) for the case of isothermal consolidation and a good agreement is observed when compared with the results of Lewis and Schrefler [14]. Obviously, the soil permeability $K_2 = 1 \times 10^{-11}$ m^2 has a lower rate of settlement when compared with $K_1 = 4 \times 10^{-9}$ m^2. The pore pressure versus time at several depths are shown in Fig. 2(b).

Also, the code of multiphase immiscible flow is validated in partially saturated conditions based on a previous study by Schrefler et al [17]. Using the same boundary conditions as in Fig. 1, a soil column was subjected to an external surface load of 1000 N/m^2 and with the soil permeability, $K = 0.46 \times 10^{-11}$ m^2. The initial condition for pressures P_w and P_g depend on the initial saturation profiles. The boundary conditions and the other data of the porous medium were assumed to be the same as in Ref. [17], i.e.

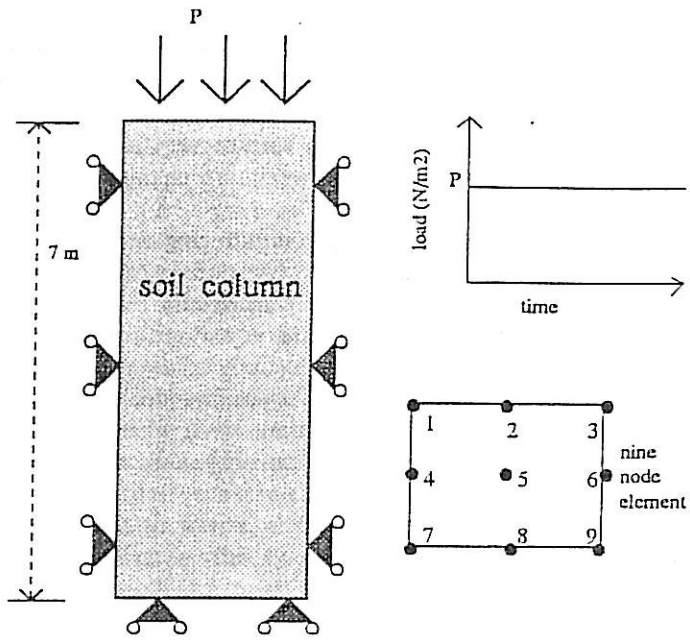

Fig. 1. Soil column and finite element spatial discretization.

Elastic modulus	$E = 6 \times 10^6$ N/m^2
Poison's ratio	$\nu = 0.4$
Porosity	$\phi = 0.3$
Bulk modulus	$K_s = 0.14 \times 10^{10}$ N/m^2
	$K_w = 0.43 \times 10^{13}$ N/m^2
Viscosity	$\mu_w = 1.0 \times 10^{-3}$ N/m^2
	$\mu_g = 1.0 \times 10^{-3}$ N/m^2
P_{dgw}	1.682×10^3 N/m^2
λ	3.0
S_{rw}	0.2

Temporal discretizaton is performed with an initial step of 0.01 days and multiplied by 10 after repeating 10 steps until an elapsed time of i.e. 10 days the required time of time of the analysis. Fig. 3 shows the comparison of vertical displacement vs time for selected depths. The results obtained using the developed code agree well when compared with those presented by Schrefler et al. [17].

The example of soil column, 1 m in height with a similar geometry and conditions of surface load in Fig. 2 was applied. The domain was discretized in one dimension using a rectangular grid consisting of 10 elements and 63 nodes. An uniform nodal spacing of 0.1 m was used in the vertical direction. The soil column was assumed to be unsaturated with an initial water saturation of 0.52. The initial pore water

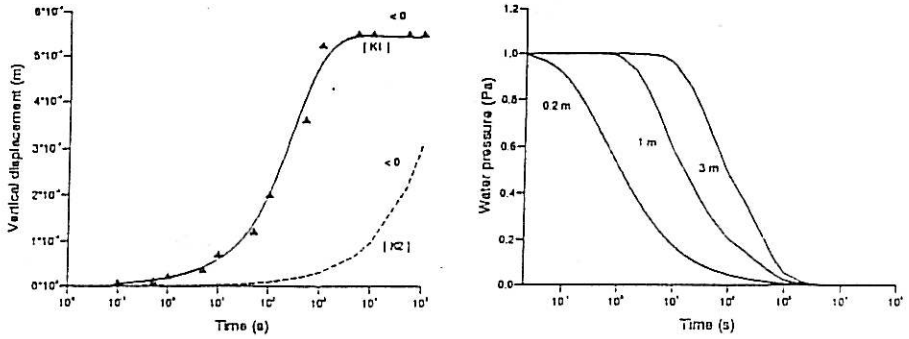

Fig. 2. (a) Surface settlement and (b) water pressures vs time for the one-dimensional saturated problem.

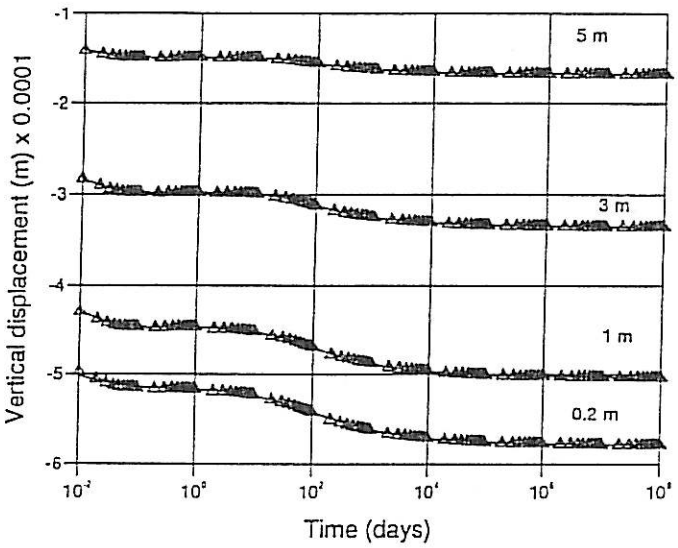

Fig. 3. Profile of vertical displacement vs time (solid line, present code, triangle: Schrefler et al. [17]).

pressure boundary was $-280\,\mathrm{kN/m^2}$ and the boundary pore water pressure was instantaneously changed to a value of $-420\,\mathrm{kN/m^2}$ at the surface. The boundary condition are (a) lateral surface $U_h = 0$, $q_w = q_g = 0$, (b) top surface $P_w = -420\,\mathrm{kN/m^2}$, $P_g = P_{atm}$ and (c) bottom surface $U_v = 0$, $q_w = q_g = 0$. The parameters of the porous media are described as follows; $E = 0.6 \times 10^7\,\mathrm{N/m^2}$, $\nu = 0.4$, $\phi = 0.3$, $K = 0.46 \times 10^{-11}\,\mathrm{m^2}$, $K_s = 0.14 \times 10^{10}\,\mathrm{N/m^2}$, $\rho_s = 2.0 \times 10^3\,\mathrm{kg/m^3}$, $P_{dgw} = 225.0 \times 10^3\,\mathrm{N/m^2}$, $\lambda = 3.0$ and $S_{rw} = 0.3966$. In Fig. 4(a) the vertical displacements for selected points are presented for the consolidation case. Fig. 4(b) shows the distribution of water saturation versus time at different points within the column. Fig. 5 shows the pore water pressure distribution throughout the soil layer

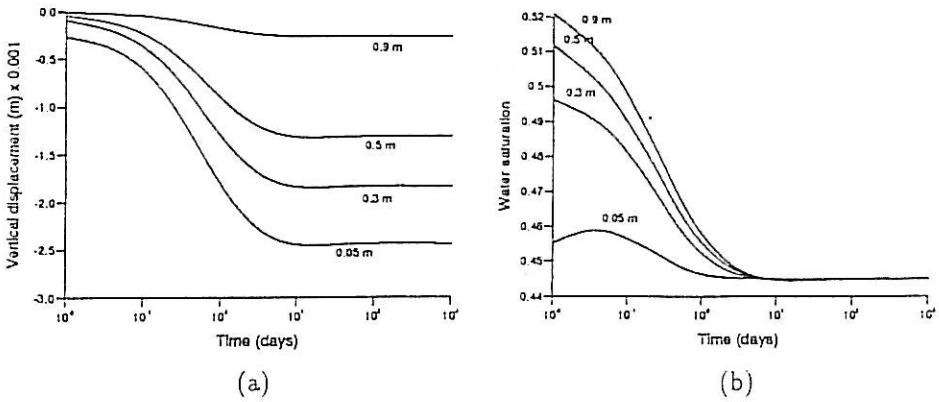

Fig. 4. Profile of (a) vertical displacement and (b) water saturation during consolidation.

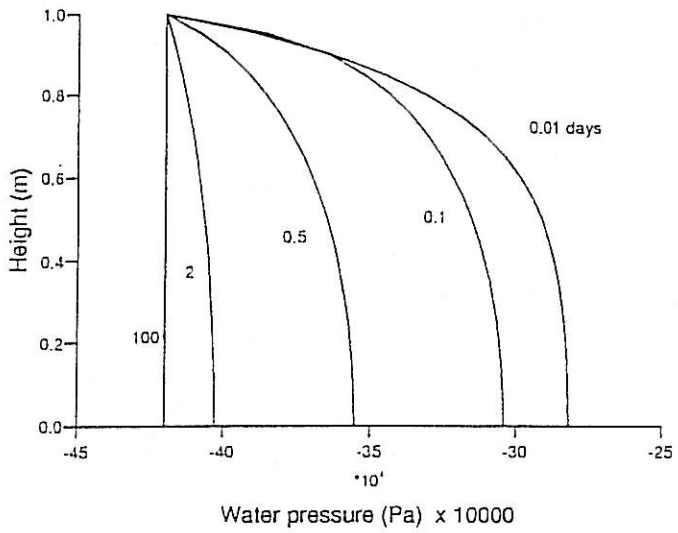

Fig. 5. Pore water pressure distribution under consolidation.

due to a change in the pore water pressure at the boundary. The model describes the behaviour of unsaturated soil systems under environmental changes.

In order to study the spreading NAPL in a porous media system, the test example involves 1 m in height of a vertical column with a soil permeability of $1.0\times10^{-12}\,\mathrm{m}^2$. The source boundary condition was set at 0.5 of the NAPL fluid saturation and a porosity of 0.40 was used through the column, initially completely saturated by water. The result is a displacement of the water from the column by the encroaching NAPL. The initial conditions are $P_w = P_n = P_{\mathrm{ref}}$ and $U_v = U_h = 0$. The boundary conditions for the problem are:

(a) Lateral surface $U_h = 0$, $q_w = q_n = 0$
(b) Top surface $P_w = P_{ref} - P_{sw}$, $P_n = P_{ref} = 9810\ \mathrm{N/m^2}$ or 1 m of water and $P_{sw} = 0.5$ is the pressure to keep saturation 0.5
(c) Bottom surface $U_v = U_h = 0$, $P_w = P_n = P_{ref}$

The material properties used are as follows:

Elastic modulus	$E = 5 \times 10^6\ \mathrm{N/m^2}$
Poison's ratio	$\nu = 0.4$
Porosity	$\phi = 0.3$
Bulk modulus	$K_s = 1.0 \times 10^{12}\ \mathrm{N/m^2}$
	$K_w = 0.43 \times 10^{13}\ \mathrm{N/m^2}$
P_{dgw}	$0.1784\ \mathrm{N/m^2}$
λ	3.0
S_{rw}	0.2

The parameters chosen for the simulations were a NAPL density of $1461\ \mathrm{kg/m^3}$ and a viscosity of $0.57 \times 10^{-3}\ \mathrm{Ns/m^2}$. The water phase was assigned a density of $1000\ \mathrm{kg/m^3}$ and a viscosity of $1.0 \times 10^{-3}\ \mathrm{Ns/m^2}$. The resulting profiles of vertical displacements and effective water saturation are shown in Fig. 6(a) and (b), respectively, for different time values. Similar behaviour was also reported by Schrefler et al. [13].

A two-dimensional multiphase flow example which demonstrates the impact of an undetected leak of nonqueous phase liquid in a porous medium is presented. This problem was designed to study the migration of LNAPL (light nonaqueous phase liquids) from a continuous source at the soil surface. Fig. 7 shows a schematic diagram of the geometry for the simulated cross section and boundary conditions. The system is subjected to water infiltration at a rate of $100\ \mathrm{kg/year/m^2}$. The LNAPL source, with a release rate of 900 kg/year is located at the top left-hand edge. The assumption is that the pressures in the gas phase are negligible leads to two partial differential equations (P_w, P_n). The left and right-hand boundaries of the domain

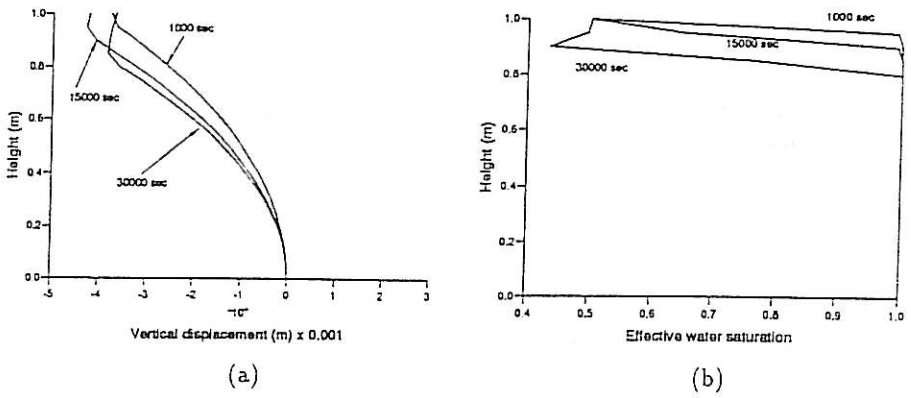

Fig. 6. Profile of (a) vertical displacement and (b) water saturation through-out soil column.

were treated as impermeable, and the bottom boundary was assigned constant-pressure conditions with $P_w = P_n = 101\,325\ \mathrm{N/m^2}$.

The simulation domain in Fig. 7 presents 2 m thick and 19.0 m in length. The domain was discretized using a 2-D rectangular grid consisting of 40 elements and 187 nodes. Nodal spacing varied along the horizontal and vertical axis as shown in Fig. 8. Value of the physical parameters used in the simulation are presented below.

Elastic modulus	$E = 10.0 \times 10^6\ \mathrm{N/m^2}$
Poison's ratio	$\nu = 0.3$
Porosity	$\phi = 0.3$
Soil permeability	$K = 1.0 \times 10^{-12}\ \mathrm{m^2}$
Water viscosity	$\mu_w = 1.0 \times 10^{-3}\ \mathrm{Ns/m^2}$
LNAPL viscosity	$\mu_n = 1.0 \times 10^{-3}\ \mathrm{Ns/m^2}$
Bulk modulus	$K_s = 6.1 \times 10^8\ \mathrm{N/m^2}$

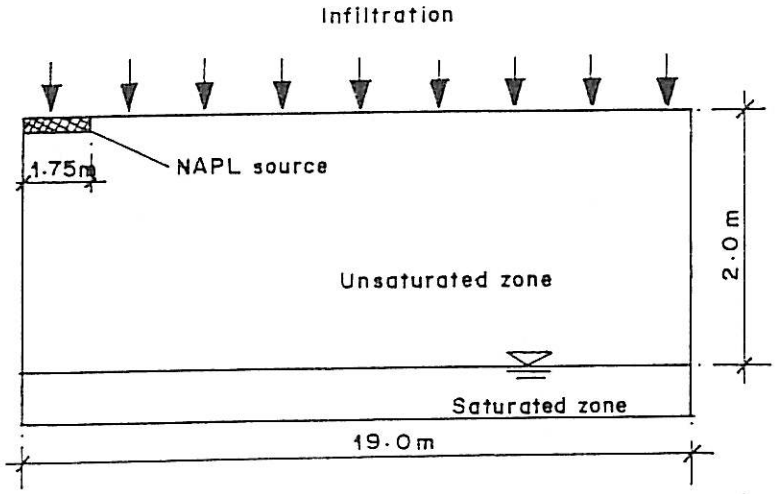

Fig. 7. Schematic representations of boundary conditions and geometry, for example application.

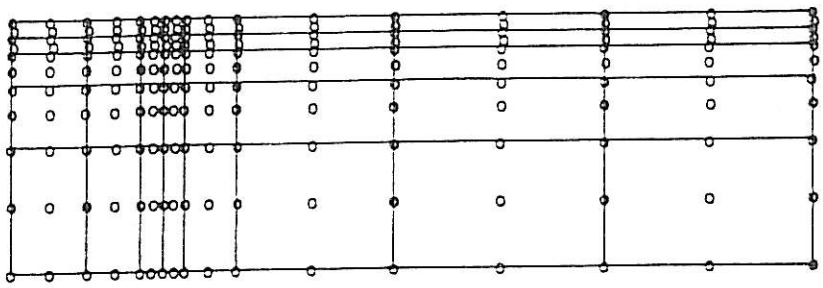

Fig. 8. 2-D mesh element.

Density for LNAPL	950.0 kg/m^3
P_{dgw}	1.682×10^3 N/m^2
S_{rw}	0.2
S_{rn}	0.02
λ	3.0

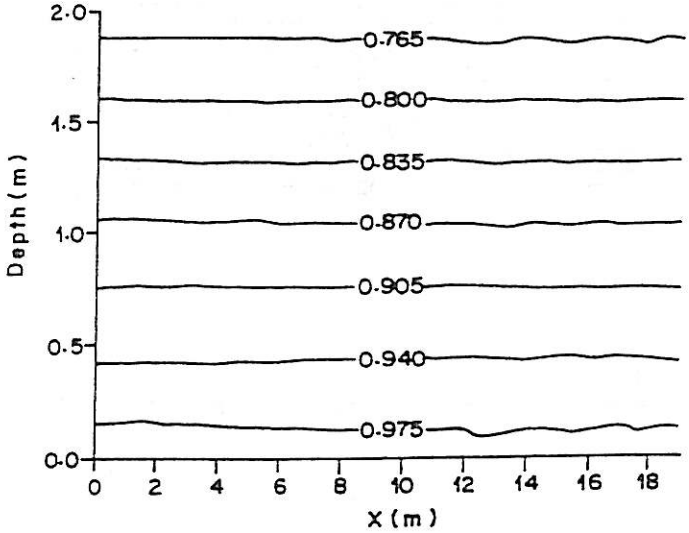

Fig. 9. Initial water saturation ($t = 0$).

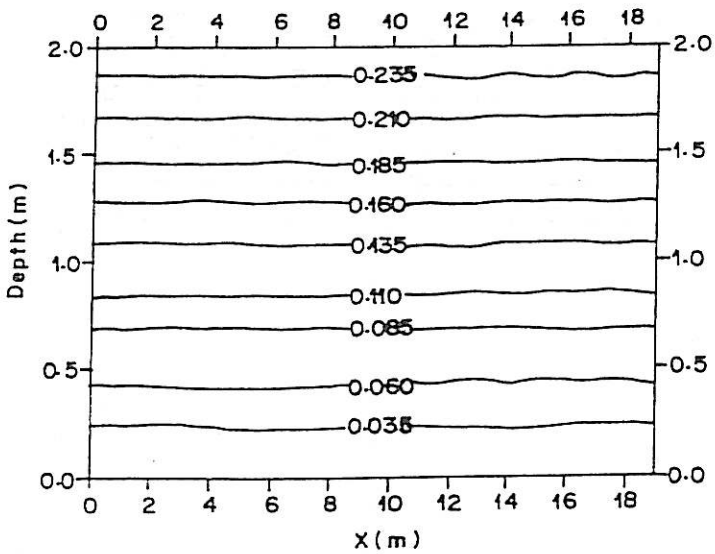

Fig. 10. LNAPL saturation contours for cross-sectional simulation of NAPL migration ($t = 1000$ s).

For a contaminating fluid less dense than water, the contaminant would be expected to pool in a zone near the water table. These conditions were observed in the results of the simulation. Fig. 9 shows the initial water saturation in the model. The simulated saturation contours are shown in Figs. 10 and 11, respectively. For

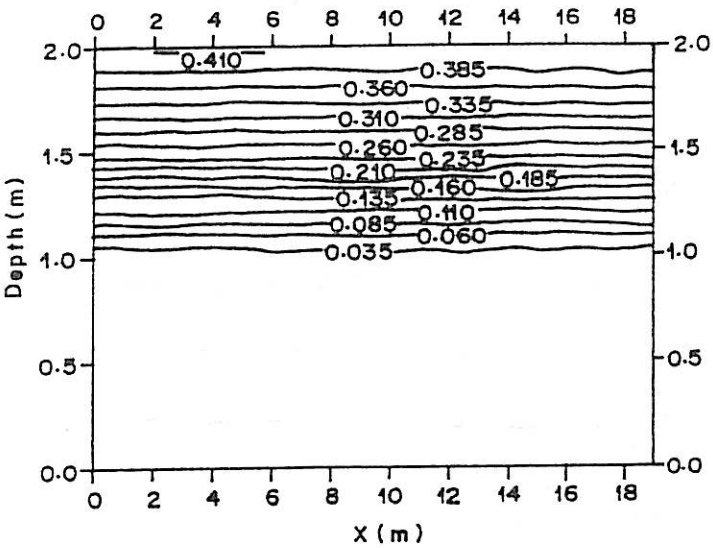

Fig. 11. LNAPL saturation (t = 3.17 years).

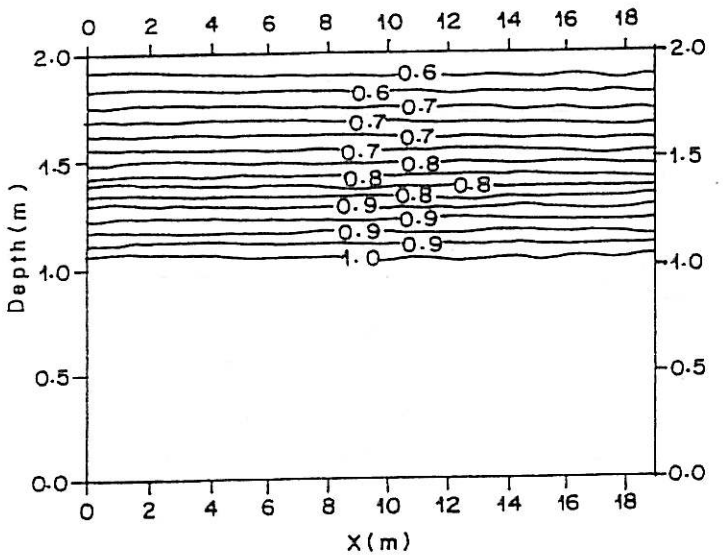

Fig. 12. Water saturation (t = 3.17 years).

the nonaqueous fluid, which is less dense than water, then the contaminant saturation are higher and do not extend nearly as far into the saturated zone. The lighter contaminants here also migrated further in a lateral direction. Fig. 12 shows the water saturation profile for LNAPL for $t = 3.17$ years.

6. Conclusions

A general formulation and solution procedure for multiphase immiscible flow in deforming porous material are presented. Nonlinear saturation and relative permeability functions are incorporated into a Galerkin finite element model. The governing equations in terms of the soil displacement and fluid pressure result in coupled, non-linear, partial differential equations. One and two-dimensional numerical simulations were performed for a homogenous porous media and indicate the behaviour of the soil properties and distribution of the contaminant after a fixed elapsed time.

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Appendix

$$A_{11} = \int_{\Omega} B^T D_T B \mathrm{d}\Omega$$

$$A_{12} = \int_{\Omega} \left[B^T D_T \frac{m}{3K_s} - B^T m \right] \left[S_w - P_n \left(\frac{\mathrm{d}S_n}{\mathrm{d}P_{cnw}} + \frac{\mathrm{d}S_n}{\mathrm{d}P_{cgw}} \right) - P_w \left(\frac{\mathrm{d}S_w}{\mathrm{d}P_{cnw}} + \frac{\mathrm{d}S_w}{\mathrm{d}P_{cgw}} \right) - P_g \left(\frac{\mathrm{d}S_g}{\mathrm{d}P_{cnw}} + \frac{\mathrm{d}S_g}{\mathrm{d}P_{cgw}} \right) \right] N^T \mathrm{d}\Omega$$

$$A_{13} = \int_{\Omega} \left[B^T D_T \frac{m}{3K_s} - B^T m \right] \left[S_g + P_n \left(\frac{\mathrm{d}S_n}{\mathrm{d}P_{cgw}} \right) + P_w \left(\frac{\mathrm{d}S_w}{\mathrm{d}P_{cgw}} \right) + P_g \left(\frac{\mathrm{d}S_g}{\mathrm{d}P_{cgw}} \right) \right] N^T \mathrm{d}\Omega$$

$$A_{14} = \int_{\Omega}\left[B^T D_T \frac{m}{3K_s} - B^T m\right]\left[S_n + P_n\left(\frac{\mathrm{d}S_n}{\mathrm{d}P_{cnw}}\right) + P_w\left(\frac{\mathrm{d}S_w}{\mathrm{d}P_{cnw}}\right) + P_g\left(\frac{\mathrm{d}S_w}{\mathrm{d}P_{cnw}}\right)\right]N^T \mathrm{d}\Omega$$

$$A_{10} = \int_{\Omega} B^T D_T C \mathrm{d}\Omega + \int_{\Omega} B^T D_T \frac{\partial \varepsilon_v}{\partial t}\mathrm{d}\Omega + \int_{\Omega} N\frac{\partial b}{\partial t}\mathrm{d}\Omega + \int_{\Gamma} N\frac{\partial \hat{t}}{\partial t}\mathrm{d}\Gamma$$

$$A_{21} = \int_{\Omega} N\frac{\rho_w S_w}{B_w}\left[m^T - \frac{m^T D_T}{3K_s}\right]B\mathrm{d}\Omega$$

$$A_{22} = \int_{\Omega} N\left[-\frac{\phi\rho_w}{B_w}\left(\frac{\mathrm{d}S_w}{\mathrm{d}P_{cnw}} + \frac{\mathrm{d}S_w}{\mathrm{d}P_{cgw}}\right) + \phi\frac{S_w}{B_w}\left(\frac{\mathrm{d}\rho_w}{\mathrm{d}P_w}\right) + \phi\rho_w S_w \frac{\mathrm{d}}{\mathrm{d}P_w}\left(\frac{1}{B_w}\right) + \rho_w\frac{S_w}{B_w}\left(\frac{(1-\phi)}{K_s} - \frac{m^T D_T m}{(3K_s)^2}\right)\left(S_w - P_n\left(\frac{\mathrm{d}S_n}{\mathrm{d}P_{cnw}} + \frac{\mathrm{d}S_n}{\mathrm{d}P_{cgw}}\right) - P_w\left(\frac{\mathrm{d}S_w}{\mathrm{d}P_{cnw}} + \frac{\mathrm{d}S_w}{\mathrm{d}P_{cgw}}\right) - P_g\left(\frac{\mathrm{d}S_g}{\mathrm{d}P_{cnw}} + \frac{\mathrm{d}S_g}{\mathrm{d}P_{cgw}}\right)\right)\right]N^T \mathrm{d}\Omega$$

$$A_{23} = \int_{\Omega} N\left[\frac{\phi\rho_w}{B_w}\left(\frac{\mathrm{d}S_w}{\mathrm{d}P_{cgw}}\right) + \rho_w\frac{S_w}{B_w}\left(\frac{(1-\phi)}{K_s} - \frac{m^T D_T m}{(3K_s)^2}\right)\left(S_g + P_n\left(\frac{\mathrm{d}S_n}{\mathrm{d}P_{cgw}}\right) + P_w\left(\frac{\mathrm{d}S_w}{\mathrm{d}P_{cgw}}\right) + P_g\left(\frac{\mathrm{d}S_g}{\mathrm{d}P_{cgw}}\right)\right)\right]N^T \mathrm{d}\Omega$$

$$A_{24} = \int_{\Omega} N\left[\frac{\phi\rho_w}{B_w}\left(\frac{\mathrm{d}S_w}{\mathrm{d}P_{cgw}}\right) + \rho_w\frac{S_w}{B_w}\left(\frac{(1-\phi)}{K_s} - \frac{m^T D_T m}{(3Ks)^2}\right)\left(S_n + P_n\left(\frac{\mathrm{d}S_n}{\mathrm{d}P_{cnw}}\right) + P_w\left(\frac{\mathrm{d}S_w}{\mathrm{d}P_{cnw}}\right) + P_g\left(\frac{\mathrm{d}S_g}{\mathrm{d}P_{cnw}}\right)\right)\right]N^T \mathrm{d}\Omega$$

$$B_{26} = \int_{\Omega} (\nabla N^T)^T \frac{K_{rw}\rho_w}{\mu_w B_w}\nabla N^T \mathrm{d}\Omega$$

$$A_{20} = \int_{\Omega} -(\nabla N^T)^T \frac{K k_{rw} \rho_w}{\mu_w B_w} \nabla(\rho_w g h) \mathrm{d}\Omega - \int_{\Gamma} N \frac{q_w}{B_w} \mathrm{d}\Gamma$$
$$- \int_{\Omega} N \rho_w \frac{S_w}{B_w} \left(\frac{m^T D_T C}{3K_s} \right) \mathrm{d}\Omega - \rho_w Q_w$$

$$A_{31} = \int_{\Omega} N \frac{\rho_g S_g}{B_g} \left[m^T - \frac{m^T D_T}{3K_s} \right] B \mathrm{d}\Omega$$

$$A_{32} = \int_{\Omega} N \Bigg[- \frac{\phi \rho_g}{B_g} \left(\frac{\mathrm{d}S_g}{\mathrm{d}P_{cnw}} + \frac{\mathrm{d}S_g}{\mathrm{d}P_{cgw}} \right) + \rho_g \frac{S_g}{B_g} \left(\frac{(1-\phi)}{K_s} - \frac{m^T D_T m}{(3K_s)^2} \right)$$
$$\left(S_w - P_n \left(\frac{\mathrm{d}S_n}{\mathrm{d}P_{cnw}} + \frac{\mathrm{d}S_n}{\mathrm{d}P_{cgw}} \right) - P_w \left(\frac{\mathrm{d}S_w}{\mathrm{d}P_{cnw}} + \frac{\mathrm{d}S_w}{\mathrm{d}P_{cgw}} \right) \right.$$
$$\left. - P_g \left(\frac{\mathrm{d}S_g}{\mathrm{d}P_{cnw}} + \frac{\mathrm{d}S_g}{\mathrm{d}P_{cgw}} \right) \right) \Bigg] N^T \mathrm{d}\Omega$$

$$A_{33} = \int_{\Omega} N \Bigg[\frac{\phi \rho_g}{B_g} \left(\frac{\mathrm{d}S_g}{\mathrm{d}P_{cgw}} \right) + \phi \frac{S_g}{B_g} \left(\frac{\mathrm{d}\rho_g}{\mathrm{d}P_g} \right) + \phi \rho_g S_g \frac{\mathrm{d}}{\mathrm{d}P_g} \left(\frac{1}{B_g} \right)$$
$$+ \rho_g \frac{S_g}{B_g} \left(\frac{(1-\phi)}{K_s} - \frac{m^T D_T m}{(3K_s)^2} \right) \left(S_g + P_n \left(\frac{\mathrm{d}S_n}{\mathrm{d}P_{cgw}} \right) + P_w \left(\frac{\mathrm{d}S_w}{\mathrm{d}P_{cgw}} \right) \right.$$
$$\left. + P_g \left(\frac{\mathrm{d}S_g}{\mathrm{d}P_{cgw}} \right) \right) \Bigg] N^T \mathrm{d}\Omega$$

$$A_{34} = \int_{\Omega} N \Bigg[\frac{\phi \rho_g}{B_g} \left(\frac{\mathrm{d}S_g}{\mathrm{d}P_{cgw}} \right) + \rho_g \frac{S_g}{B_g} \left(\frac{(1-\phi)}{K_s} - \frac{m^T D_T m}{(3K_s)^2} \right) \left(S_n + P_n \left(\frac{\mathrm{d}S_n}{\mathrm{d}P_{cnw}} \right) \right.$$
$$\left. + P_w \left(\frac{\mathrm{d}S_w}{\mathrm{d}P_{cnw}} \right) + P_g \left(\frac{\mathrm{d}S_g}{\mathrm{d}P_{cnw}} \right) \right) \Bigg] N^T \mathrm{d}\Omega$$

$$B_{37} = \int_{\Omega} (\nabla N^T)^T \frac{K k_{rg} \rho_g}{\mu_g B_g} \nabla N^T \mathrm{d}\Omega$$

$$A_{30} = \int_{\Omega} -(\nabla N^T)^T \frac{Kk_{rg}\rho_g}{\mu_g B_g} \nabla(\rho_g g h) \mathrm{d}\Omega - \int_{\Gamma} N \frac{q_g}{B_g} \mathrm{d}\Gamma - \int_{\Omega} N \rho_g \frac{S_g}{B_g} \left(\frac{m^T D_T C}{3K_s} \right) \mathrm{d}\Omega - \rho_g Q_g$$

$$A_{41} = \int_{\Omega} N \frac{\rho_n S_n}{B_n} \left[m^T - \frac{m^T D_T}{3K_s} \right] B \mathrm{d}\Omega$$

$$A_{42} = \int_{\Omega} N \left[-\frac{\phi \rho_n}{B_n} \left(\frac{\mathrm{d}S_n}{\mathrm{d}P_{cnw}} + \frac{\mathrm{d}S_n}{\mathrm{d}P_{cgw}} \right) + \rho_n \frac{S_n}{B_n} \left(\frac{(1-\phi)}{K_s} - \frac{m^T D_T m}{(3K_s)^2} \right) \left(S_w - P_n \left(\frac{\mathrm{d}S_n}{\mathrm{d}P_{cnw}} + \frac{\mathrm{d}S_n}{\mathrm{d}P_{cgw}} \right) - P_w \left(\frac{\mathrm{d}S_w}{\mathrm{d}P_{cnw}} + \frac{\mathrm{d}S_w}{\mathrm{d}P_{cgw}} \right) - P_g \left(\frac{\mathrm{d}S_g}{\mathrm{d}P_{cnw}} + \frac{\mathrm{d}S_g}{\mathrm{d}P_{cgw}} \right) \right) \right] N^T \mathrm{d}\Omega$$

$$A_{43} = \int_{\Omega} N \left[\frac{\phi \rho_n}{B_n} \left(\frac{\mathrm{d}S_n}{\mathrm{d}P_{cgw}} \right) + \rho_n \frac{S_n}{B_n} \left(\frac{(1-\phi)}{K_s} - \frac{m^T D_T m}{(3K_s)^2} \right) \left(S_g + P_n \left(\frac{\mathrm{d}S_n}{\mathrm{d}P_{cgw}} \right) + P_w \left(\frac{\mathrm{d}S_w}{\mathrm{d}P_{cgw}} \right) + P_g \left(\frac{\mathrm{d}S_g}{\mathrm{d}P_{cgw}} \right) \right) \right] N^T \mathrm{d}\Omega$$

$$A_{44} = \int_{\Omega} N \left[\frac{\phi \rho_n}{B_n} \left(\frac{\mathrm{d}S_n}{\mathrm{d}P_{cgw}} \right) + \phi \frac{S_n}{B_n} \left(\frac{\mathrm{d}\rho_n}{\mathrm{d}P_n} \right) + \phi \rho_n S_n \frac{\mathrm{d}}{\mathrm{d}P_n} \left(\frac{1}{B_n} \right) + \rho_g \frac{S_g}{B_g} \left(\frac{(1-\phi)}{K_s} - \frac{m^T D_T m}{(3K_s)^2} \right) \left(S_n + P_n \left(\frac{\mathrm{d}S_n}{\mathrm{d}P_{cnw}} \right) + P_w \left(\frac{\mathrm{d}S_w}{\mathrm{d}P_{cnw}} \right) + P_g \left(\frac{\mathrm{d}S_g}{\mathrm{d}P_{cnw}} \right) \right) \right] N^T \mathrm{d}\Omega$$

$$B_{48} = \int_{\Omega} (\nabla N^T)^T \frac{Kk_{rn}\rho_n}{\mu_n B_n} \nabla N^T \mathrm{d}\Omega$$

$$A_{40} = \int_{\Omega} -(\nabla N^T)^T \frac{Kk_{rn}\rho_n}{\mu_n B_n} \nabla(\rho_n g h) \mathrm{d}\Omega - \int_{\Gamma} N \frac{q_n}{B_n} \mathrm{d}\Gamma - \int_{\Omega} N \rho_n \frac{S_n}{B_n} \left(\frac{m^T D_T C}{3K_s} \right) \mathrm{d}\Omega - \rho_n Q_n$$

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Appendix 4

Finite element modelling of geo-mechanics and geoenvironmental engineering for subsurface systems

PROCEEDINGS OF THE ASIAN CONFERENCE ON UNSATURATED SOILS
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Finite element modelling of geomechanics and geoenvironmental engineering for subsurface systems

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ABSTRACT: This paper describes numerical simulation study of geomechanics and groundwater contamination. The problem of coupled multiphase flow, heat and contaminant transport in a subsurface system is important in environmental engineering. For this purpose, the main objective of this study was to develop a finite element model that describes the flow of multiphase fluids, together with coupled contaminant transport in a deforming porous medium for both isothermal and nonisothermal problems. The multiphase flow model of Brooks and Corey, which express the dependence of saturation and relative permeability on capillary pressure, is presented to simulate subsurface flow and pollutant transport in the system. Subsurface flow is simulated through numerical solution of fluid mass balance equation, where the subsurface system may be either saturated, or party or completely unsaturated. The governing partial differential equation, in term of soil displacement, fluid pressure, energy balance and concentrations are fully coupled and behave non linearly but can be solved by the finite element method. Numerical implementation of the formulation is discussed and examples related to subsurface problems are used to demonstrate the model.

1 INTRODUCTION

The simulation of groundwater contamination in subsurface systems by nonaqueous phase liquids, such as petroleum hydrocarbons and immiscible industrial chemicals, requires a solution of the multiphase flow equations for deforming porous media. The spill and leakage of organic chemical into the global environment have resulted in widespread contamination of subsurface systems. Many of these pollutants are slightly water- soluble and highly volatile fluids (NAPLs). In the unsaturated zone, residual NAPL, as well as NAPL dissolved in the water phase, may also volatilize into the soil gas phase.

The remaining nonagueous phase liquids may persist for long periods of time, slowly dissolving into the groundwater and moving in the water phase via advection and dispersion processes. Several numerical models have been developed in order to study the movement of organic pollutants in subsurface systems and a few of the reported simulators consider interphase mass transfer of one or more NAPL components to the gas and water phase but assume that the NAPL is immobilized in the unsaturated zone (Baehr and Corapcioglu 1987 and Abd. Rahman and Lewis 1997).

Recently, a nonisothermal model has been developed by Falta et al. (1992), Adenekan et al. (1993) and Panday et al. (1995) for examining nonaqueous phase liquid contamination and remedial scenarios (i.e. stream injection). Fully coupled models for water flow, airflow and heat flow in deformable porous media have been studied by Schrefler et al. (1995) and Thomas and He (1995) which do not consider interphase mass transfer or other limitation (i.e. fluid density is assumed to be function of pressure, temperature and contaminant) in the simulation model for pollutant transport behavior.

The problem of coupled multiphase flow (namely gas, water and nonaqueous phase liquids), heat and contaminant transport in a subsurface system is important in environmental engineering. At present, there exists a critical need for the physical observation of coupled transport phenomena in porous media. These observations are required both as an aid to our understanding of coupled process and to evaluated current predictive methods for such phenomena. For this purpose, the main objective of

this study was to develop a finite element model that describes the flow of multiphase fluids, together with coupled contaminant transport, in a deforming porous medium for both isothermal and nonisothermal problems. The flow of all multiphase fluids, as well as the water gas phase transport, are included.

The governing equations which describe the displacement of soil, multiphase fluid pressures, temperature and pollutant transport are coupled and the resulting non- linear partial differential equation are solved by the finite element method. Non- linear saturation and relative permeability functions are incorporated into a partially water saturated porous media. The physical model and model description of the study based on the reference by Lewis et. al. (1998), Abd. Rahman and Lewis (1997, 1999) and Abd. Rahman (1998).

2 MATHEMATICAL MODEL

Contaminant transport models for miscible components cannot describe the migration of an immiscible contaminant. The flow of an immiscible contaminant is controlled by its own flow potential, which depends on pressure, gravity and surface forces and is not necessarily similar to the groundwater flow potential. In order to describe mathematically the flow of immiscible fluids through a porous medium, it is necessary to determine functional expressions that best define the relationship between the hydraulic properties of the porous medium, i.e. saturation, relative permeability and capillary pressure.

A mathematical model of the physical processes occuring in multiphase flow with heat and pollutant transport and soil deformation is given in this section, to present the mathematical model as a formulation suitable for numerical solution by the finite element method. The principles of the conservation of mass and energy are employed to derive the governing differential equation for fluid (water, gas and NAPL), heat and pollutant transport in terms of seven primary variables; i.e. U, P_w, P_g, P_n, T, C_w and C_g.

These conservation equations are implicitly linked through the dependency of the fluid density, fluid viscosity and matrix porosity upon the fluid pressure, fluid temperature and contamination mass fraction. In a multiphase, water, NAPL and gas in a porous medium, depends primarily on the gravitational force and the capillary pressures between the multiphase fluids.

The seven, fully coupled, partial differential equation i.e the multiphase fluid flow equations and the equilibrium equation are an extension of the study of the model developed by Lewis and Schrefler (1998), Schrefler (1995), Abd. Rahman and Lewis et al. (1999). Nonisothermal deforming porous medium are modelled by utilizing the equilibrium equation together with the governing equation of heat, fluid flow and pollutant transport through such a porous medium.

1) Equilibrium equation

$$\int_\Omega \delta\varepsilon^T D_T \frac{\partial\varepsilon}{\partial t} d\Omega - \int_\Omega \delta\varepsilon^T m \frac{\partial\overline{p}}{\partial t} d\Omega + \int_\Omega \delta\varepsilon^{TS} D_T m \frac{\partial\overline{p1}}{\partial t 3K_s} d\Omega - \int_\Omega \delta\varepsilon^T D_T C d\Omega - \int_\Omega \delta\varepsilon^T D_T m \frac{\partial T\beta_s}{\partial t 3} d\Omega - \int_\Omega \delta\varepsilon^T D_T \frac{\partial\varepsilon_a}{\partial t} d\Omega - \int_\Omega \delta u^T \frac{\partial b}{\partial t} d\Omega - \int_\Gamma \delta u^T \frac{\partial s}{\partial t} d\Gamma = 0 \quad (1)$$

2) Multiphase flow equation

$$-\nabla^T\left[\frac{Kk_{r\alpha\alpha}}{\mu_\alpha B_\alpha}\nabla(P_\alpha + \rho_\alpha gh)\right] + \rho_\alpha \frac{S_\alpha}{B_\alpha}\left[\left(m^T - \frac{m^T D_T}{3K_s}\right)\frac{\partial\varepsilon}{\partial t} + \frac{m^T D_T C}{3K_s} + \left(\frac{(1-\phi)}{K_s} - \frac{m^T D_T m}{(3K_s)^2}\right)\frac{\partial\overline{p}}{\partial t} + \left\{-(1-\phi)\beta_s + \frac{m^T D_T m}{3K_s}\frac{\beta_s}{3}\right\}\frac{\partial T}{\partial t}\right] \times \phi\frac{\partial}{\partial t}\left(\frac{\rho_\alpha S_\alpha}{B_\alpha}\right) + P_\alpha Q_\alpha + \Gamma_\alpha = 0 \quad (2)$$

3) Pollutant transport equation

$$\frac{\partial}{\partial t}(\phi S_g C_g) - \nabla.(V_g C_g) - \nabla.(\phi S_g D_{ig}\nabla C_g) - \overline{C}_g Q_g + \Gamma_g = 0 \quad (3)$$

4) Energy transport equation

$$\frac{\partial}{\partial t}[(1-\phi)\rho_s C_{ps} + \phi\rho_w S_w c_{pw} + \phi\rho_g S_g c_{pg} + \phi\rho_n S_n c_{pn}]T + \rho_w S_w c_{pw} V_w.\nabla T + \rho_g S_g c_{pg} V_g.\nabla T + \rho_n S_n c_{pn} V_n.\nabla T = \nabla.(\lambda_T \nabla T) + (1-\phi)\rho_s Q_s + \phi\rho_w S_w Q_w + \phi\rho_g S_g Q_g + \phi\rho_n S_n Q_n] \quad (4)$$

where, α represents the water(w (n) phase and Γ_α is the interpl Detailed notation can be found in and Abd. Rahman (1998).

3 FINITE ELEMENT DISCRETIZATION

Due to complexity of the theore the mathematical model, nume methods are required to achie solution of the governing differe finite element method, based on residual approach (Abd. Rahma discretization of the governin implemented as the numeric because analytical solutions are with the highly complex and n equations. The approach ado employs two- dimensional, nine element. Fluid pressures, ter trations and displacements are unknown variables.

3.1 *Numerical Formulation*

The procedure used is based on residual method, which implem to approximate the known simulations carried out , there freedom viz, u, P_g, P_w, Pn, Cw approximated as

$$x = N^T X$$

where N^T is the transpose of t X is the nodal value of the nine- noded elements and th the equations in the mathema be expressed in terms of the no v, nodal fluid pressures, i.e. temperature , T and the nodal and Cg using the Galerkin's of the governing equations is Galerkin's procedure of weig involving second spatial deriv by means of Gauss's theorem are then approximated in spa element techniques, and expr nodal variables.

The analysis of a mode degree of freedom field probl form, the discretized for equations are written in the fo

hase fluid flow equations and
ion are an extension of the
developed by Lewis and
efler (1995), Abd. Rahman
). Nonisothermal deforming
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$$\varepsilon^T m \frac{\partial p}{\partial t} d\Omega + \int_\Omega \delta\varepsilon^T D_T C d\Omega - \int_\Omega \delta\varepsilon^T D_T \frac{\partial \varepsilon_o}{\partial t} d\Omega - \frac{s}{t} d\Gamma = 0 \quad (1)$$

tion

$$\rho_\alpha gh)] + \frac{\partial \varepsilon}{\partial t} + \frac{{}^T D_T m}{K_s)^2}) \frac{\partial p}{\partial t} + \frac{\beta_s}{3}\} \frac{\partial T}{\partial t}] \times \Gamma_\alpha = 0 \quad (2)$$

ation

$$\Gamma_\theta = 0 \quad (3)$$

on

$$_w + \phi\rho_g S_g c_{pg} \; .\nabla T + \; _n.\nabla T = \nabla.(\lambda_T \nabla T) \quad (4)$$

where, α represents the water(w), gas(g) and NAPL (n) phase and Γ_α is the interphase mass transfer. Detailed notation can be found in Lewis et. al (1998) and Abd. Rahman (1998).

3 FINITE ELEMENT MODEL AND DISCRETIZATION

Due to complexity of the theoretical formulation in the mathematical model, numerical approximation methods are required to achieve the simultaneous solution of the governing differential equations. The finite element method, based on Galerkin's weighted residual approach (Abd. Rahman, 1998), is used for discretization of the governing equations and is implemented as the numerical solution method because analytical solutions are incapable of dealing with the highly complex and non- linear governing equations. The approach adopted in this study employs two- dimensional, nine noded isoparametric element. Fluid pressures, temperatures, concentrations and displacements are taken as the primary unknown variables.

3.1 Numerical Formulation

The procedure used is based on Galerkin's weighted residual method, which implements shape functions to approximate the known variables. In the simulations carried out , there are seven degrees of freedom viz, u, P_g, P_w, Pn, Cw, C_g and T which are approximated as

$$x = N^T X \quad (5)$$

where N^T is the transpose of the shape function and X is the nodal value of the variable. In this case nine- noded elements and the associated shape of the equations in the mathematical model, may now be expressed in terms of the nodal displacements , u, v, nodal fluid pressures, i.e. P_n, P_w, and P_g, nodal temperature , T and the nodal concentrations. i.e. Cw and Cg using the Galerkin's method. Discretization of the governing equations is obtained by applying Galerkin's procedure of weighted residuals. Terms involving second spatial derivatives are transformed by means of Gauss's theorem. The field variables are then approximated in space as is usual in finite element techniques, and expressed in terms of their nodal variables.

The analysis of a model deals with a seven degree of freedom field problem. Written in a matrix form, the discretized forms of mathematical equations are written in the following form:

$$A\bar{x} + Bx = F \quad (6)$$

Where x = [u, P_w, P_g, P_n, T, C_w, C_g] and the matrices A, B and F are obtained by inspection . Equation (6) is the final form of the governing equations where displacements, fluid pressures, temperature and concentrations are the primary unknowns. This equation forms a fully coupled nonsymmetrical and highly non-linear system of ordinary differential equations in time and is solved by an implicit scheme with the time weighting parameter set to one. In an implicit scheme, since the entire non-linear coefficient is dependent on the unknowns, iterative procedures are usually performed within each time step to obtain the final solution.

The coupling terms are evaluated for each element using this numerical technique and then assembled into the global matrix. The format in the elemental matrices and the global matrix differs in the ordering of unknown variables. Thus it is necessary to transform the coupling terms from the elemental matrices to the global matrix, when assembling the global matrix. Once the global matrix has been fully assembled, the partial differential equations have been transformed into first order ordinary differential equations. A linear variation of the unknown variables in time is assumed to approximate the first order time derivatives. The generalised mid- point family of methods is employed to discretize the time derivatives, which yields the following recurrence scheme,

$$x^{n+1} = \frac{1}{[A + \theta\Delta t B]} \times \left([A - (1-\theta)\Delta t B]x^n + \Delta t\left[\theta F^{n+1} + (1-\theta)F^n\right]\right) \quad (7)$$

For coupled heat, fluid flow and pollutant transport in deforming porous media, the discretization is accomplished through a fully implicit finite difference scheme. A linear variation of the unknown variables in time is assumed to be a good approximation for the first order time derivative. The generalized mid-point family of methods is employed to discretize the time derivatives. Because of the non-linearity involved, a solution scheme of the fixed-point type is used within every time step. The convergence criteria implemented are based on a maximum change in the unknown variables between successive time step.

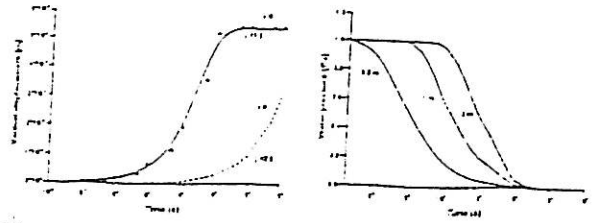

Figure 1. (a) Surface settlement and (b) water pressures vs. time for the one-dimensional saturated problem

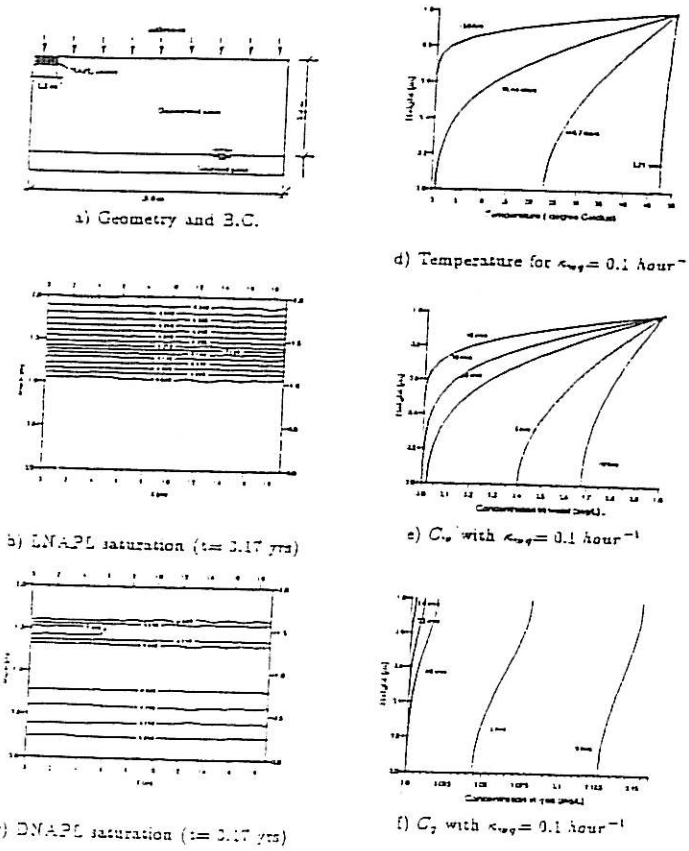

Figure 2. Pollutant Transport Examples

4 NUMERICAL EXAMPLES

Several analyses have been carried out in order to study the present model for isothermal and heat transfer affected to multiphase fluids flow and pollutant transport in deforming porous media. For this purpose a one dimensional, fully saturated, consolidation problem is solved and compared with a previous solution by Lewis and Schrefler (1987). A column of linear elastic material is 7 m height and 2 m wide and the pore pressure is equal to zero at the top surface. The top surface is the only drained boundary whilst the rest are assumed to be closed. The vertical displacement vs. time of the top surface is shown in Figure 1 (a) for the case of isothermal consolidation, and good agreement is observed when compared with the results of Lewis and Schrefler (1987). Obviously, the soil permeability $K_2 = 1x10^{-11}m^2$ has a lower rate of settlement when compared with $K_1=4x10^{-9}m^2$. The pore pressure vs. time at several depths shown in Figure 1 (b).

The first example demonstrates the impact of an

undected leak of non-aq
porous medium for an isot
was designed to study the
a continuous source at th
are considered: one in wh
has a density greater than
contaminant has a density
schematic diagram showi
simulated cross section a
presented in Figure 2 (a). T
water infiltration at a ra
NAPL source, with a rele
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that the pressure in the gas
leads to two partial differ
The left and right-hand b
were treated as imperm
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with Pw = 101325 Pa an
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and 19.0 metre in length.

The domain was di
rectangular grid consisting
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For an immiscible fluid w
water, gravity effect co
dominant. As a conse
downward migration of the
unsaturated zone and belo
take place. For a contamina
water, the contaminant wo
zone near the water table
observed in the result of s
c).

The second example is
elastic material, 1 metre
transport of a small amour
at the top of the soil colu
saturation of 0.445 and wi
jump of 50 °C above the
of the column. The initial
420 kN/m² and the bound
was instantaneously cha
-280 kN/m² at the surface
temperature distribution ve
times and it can be seen
required to achieve th
boundary condition valu
column. Figure 2(e,f) s
concentration profile in the
interphase mass transfer
The results indicate th
coefficients have a sign
immobilized NAPL.

undected leak of non-aqueous phase liquid in a porous medium for an isothermal case. This problem was designed to study the migration of NAPL, from a continuous source at the soil surface. Two cases are considered: one in which the contaminant phase has a density greater than water, and one which the contaminant has a density less than that of water. A schematic diagram showing the geometry of the simulated cross section and boundary condition is presented in Figure 2 (a). The system is subjected to water infiltration at a rate of 100 kg/yr/m^2. The NAPL source, with a release rate of 900 kg/yr, is located at the top left hand edge. The assumption is that the pressure in the gas phase are negligible and leads to two partial differential equations (Pw,Pn). The left and right-hand boundaries of the domain were treated as impermeable, and the bottom boundary was assigned constant-pressure conditions with Pw = 101325 Pa and Pn = 101325 Pa. The simulation domain in Figure 2 (a) is 2 metre thick and 19.0 metre in length.

The domain was discretized using a 2-D rectangular grid consisting of 40 elements and 187 nodes. As was noted, two base cases were simulated. For an immiscible fluid with a density greater than water, gravity effect could be expected to be dominant. As a consequence, an anticipated downward migration of the contaminant in both the unsaturated zone and below the water table, would take place. For a contaminating fluid less dense than water, the contaminant would be expected to pool in zone near the water table. These conditions were observed in the result of simulation in Figure 2 (b, c).

The second example is for a soil column of linear elastic material, 1 metre in height, simulates the transport of a small amount of pollutant introduced at the top of the soil column with an initial water saturation of 0.445 and with a surface temperature jump of 50 °C above the reference temperature, T_{ref} of the column. The initial pore water pressure was 420 kN/m^2 and the boundary pore water pressure was instantaneously changed to a value of -280 kN/m^2 at the surface. Figure 2 (d) shows the temperature distribution versus height for different times and it can be seen that a longer time is required to achieve the surface temperature boundary condition value throughout the soil column. Figure 2(e,f) show the corresponding concentration profile in the water and gas phase with interphase mass transfer values equal to 0.1 /hour. The results indicate that the mass transfer coefficients have a significant influence on the immobilized NAPL.

5 CONCLUSIONS

The investigation of the formulation of fully coupled multiphase flow (namely, water, gas and NAPL), heat flow and pollutant transport in deforming porous media is the main concern of this study. The mathematical formulation and numerical model have been tested for accuracy, stability and the ability to simulate different condition where u, P_g, P_w, Pn, Cw, C_g and T are the primary unknowns in the example.

Result of the multiphase flow example show the behaviour of NAPL infiltration in the model where the dominant gravity effect in a DNAPL situation is a downward migration of the pollutant and for LNAPL a horizontal spreading and flotation on the water table. For immobilized NAPL, the results show the usefulness of the present model in deforming porous media, including the mass transfer process and density effect for a nonisothermal model of pollutant transport.

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