

Rochester Institute of Technology

RIT Digital Institutional Repository

Theses

7-1-1997

Finite element modeling of a moving boundary problem

Chang Heub Lee

Follow this and additional works at: <https://repository.rit.edu/theses>

Recommended Citation

Lee, Chang Heub, "Finite element modeling of a moving boundary problem" (1997). Thesis. Rochester Institute of Technology. Accessed from

This Thesis is brought to you for free and open access by the RIT Libraries. For more information, please contact repository@rit.edu.

**Finite Element Modeling
of
A Moving Boundary Problem**
by

Chang Heub Lee

A Thesis Submitted In
Partial Fulfillment of the
Requirement for the
Master of Science
in
Mechanical Engineering

Approved by :

Professor _____
Josef S. Torok
Thesis Adviser

Professor _____
M. Scanlon

Professor _____
P. Venkataraman

Professor _____
Charles Haines
Department Head

DEPARTMENT OF MECHANICAL ENGINEERING
COLLEGE OF ENGINEERING
ROCHESTER INSTITUTE OF TECHNOLOGY

JULY 1997

Finite Element Modeling of A Moving Boundary Problem

I, Chang Heub Lee, hereby grant permission to the Wallace Library of the Rochester Institute of Technology to reproduce my thesis in whole for in part. Any reproduction will not be for commercial use or profit.

Date: July 22, 1997

Signature of Author: _____

DEDICATION

I would like to dedicate my thesis to my proud father Kyeong Jae Lee, my wise mother Yun Hee Park, my trustworthy brother Seong Ho Lee, in deep appreciation for all their love and support. This endless love and encouragement to allow me to complete my study at R.I.T.

To Dr. Josef S. Torok, my adviser, professor, mentor, and good friend, I express sincere and deepest gratitude and appreciation. Without him, I couldn't have done it.

I also thank all R.I.T. Mechanical Engineering Faculty members who have instilled me with vast knowledge and experience throughout my graduated study.

Finally, to myself Chang Heub Lee

“ Now it's real time for you to work in real world with real people and with your real knowledge. “

Finite Element Modeling of A Moving Boundary Problem

Abstract: The analysis and calculation of the finite element modeling of a moving boundary between immiscible fluids in a porous medium is presented. One fluid is introduced under prescribed inlet boundary conditions and the motion of the resulting interface boundary studied and calculated. The aforementioned scenario is calculated using a finite element program based on the software, MATLAB. Analytical solutions developed in one dimension illustrate the moving boundary movement and benchmark for numerical solutions. The aim of computer aided calculation is to develop and predict a model applicable to a real situation, yet flexible enough for future adaptation to other problems with little modification.

Table of Contents

List of Symbols.....	IV
List of Figures.....	V
1. Introduction.....	1
1.1 Background.....	1
1.2 Objective.....	6
2. The Theory of Fluid Flow In A Porous Medium.....	8
2.1 Introduction.....	8
2.2 Fluids.....	9
2.3 Porous Medium.....	10
2.4 Governing Equations.....	14
3. Finite Element Modeling Theory.....	21
3.1 Basic Finite Element Theory.....	21
3.2 Derivation of Finite Element Equations.....	31
4. Model Validation.....	40
4.1 Moving Boundary Problems.....	40
4.2 Finite Element Analysis Outline.....	41
4.3 Background On MATLAB.....	42
4.4 Re-scale Problem.....	46
4.5 Tests and Results.....	49

4.5-1 Case One.....	49
4.5-2 Case Two.....	51
4.5-3 Case Three.....	52
4.5-4 Case Four.....	53
5. Conclusion and Recommendation.....	54
6. Appendix.....	58
7. References.....	64

List of Symbols

A	Arbitrary constant.
C	Leak off coefficient
c_i	Fluid compressibility
c_p	Specific heat at constant pressure
c_v	Specific heat at constant volume
d	Average diameter of pore space
g	Gravitational constant
H	Piezometric head.
K	Formation permeability.
K	Hydraulic conductivity within Darcy's term.
L	Distant of direct path through medium bed.
L_e	Average distant traveled by fluid.
P	Fluid pressure
Q	Specific discharge.
R_e	Renold's number.
S	Distance traveled by fluid
S(t)	Location of boundary.
t	Time variable
T	Temperature variable
T_i	Medium tortuosity.
u	Pressure gradient value of velocity.
V	Velocity of fluid.
V_b	Material bulk space
V_s	Volume of solid
V_v	Material void space.
Z	Height of fluid.

List of Figures

Figure A : Interface between Two Immiscible Fluids.....	2
Figure B : Boundary Interaction of Two Fluid Interface.....	3
Figure C : Typical Porous Medium Saturated in Flow.....	11
Figure D : A Schematic Definition of Tortuosity.....	12
Figure E : A Phenomen, ‘ Fingering ‘	14
Figure F : Boundaries Denoted Two Different Areas Γ_1, Γ_2	26
Figure G : Discretization on the Domain Ω_e	31
Figure H : Local Domain on Ω_e	32
Figure I : Domain and Nodes.....	37
Figure J : Typical Type of Two Immiscible Fluids Movements.....	40
Figure K : Main Program Flow Chart.....	45
Figure L : Local Domain in Dimensionless Unit.....	46

Chapter 1

INTRODUCTION

1.1 Background

Moving boundary problems are characteristically found in geo-engineering systems that consist of fluid masses in a porous medium. The moving boundary of a system relates to how the system moves and allows one to predict the extent of the system at a certain time. With respect to fluid mechanics and soil mechanics, moving boundary problems are encountered in many applications. For example, groundwater pollution will be delayed or can be stopped if we can predict the movement of the moving boundary with proper calculation.

For years there have been many different studies of contamination. No matter what source of contamination one studies, there will always be a some type of interface present [16]. This is shown in **Figure A**.

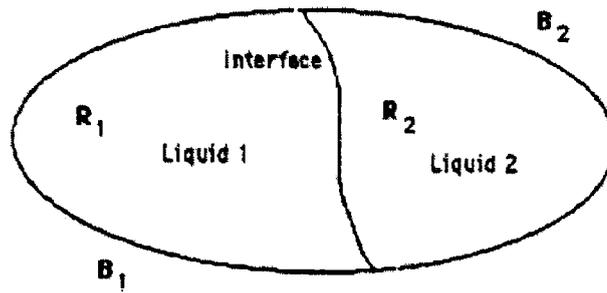


Figure A

The invading fluid in some cases does not mix with the resident stagnant fluid. This is known as immiscibility. In this case, a sharp interface is present. The investigation of sharp fronts present in immiscible fluid approximations becomes the focus system simulation. Concentration levels can then be studied for intensity. Location of this front enables one to identify where things are occurring and how to focus efforts of rectification.

When immiscible fluids flow through a porous medium, there is a boundary of interaction of one substance with another. **Figure B** shows a routine form of this boundary interaction procedure.

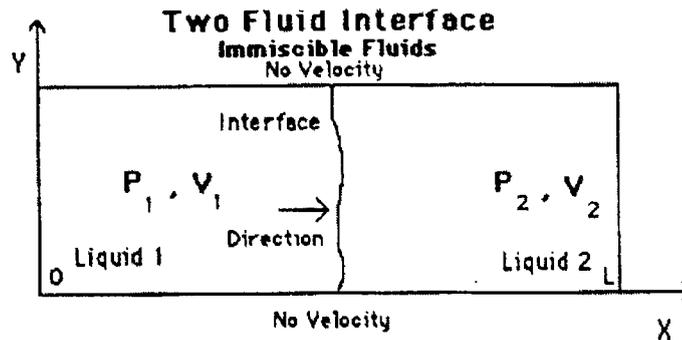


Figure B

This boundary is termed as the front or frontal boundary [2]. This boundary has two main important meanings. The first importance is due to the fact that it reflects the initial fluid interaction. This initial interaction will contain the bulk of the important flow information. By using this flow front information, solutions or alternative modes of action can be formulated in response to a given situation. Being able to forecast the reaction of infiltration of porous media will aid in the monitoring of contamination, clean-up operations, oil reservoir reserves, dam seepage and help predict a useful means of management for an effective plan of action.

A flow is created starting from a location of high potential energy and passing to a low potential energy. This energy is in the form of pressure or

piezometric head, or pressure differential, $h=\Delta P$. Another dominant factor that entails frontal movement is the process of water injection for a secondary recovery of trapped oil in existing reservoirs. Water is forced into a secondary well and pushes the oil to the producing well. In a petroleum reservoir formulation, there is almost always a water-oil interface [11]. The type of reservoir is one without a natural drive mechanism. This type of reservoir requires an input of energy supplied usually by the injection of a fluid. Injected water is introduced and permeates into the oil reservoir, forcing the oil out of the strata. These operations are termed pressure maintenance.

The aforementioned examples occurs in a low Reynolds' number situation ($R_e \leq 10$), well within the range of validity of Darcy's Law [4]. Contamination of groundwater and secondary oil recovery are examples of general problems involving the tracking of a moving boundary.

In practical situations, the uncertainty of what is actually going on below the surface of the earth is still ambiguous and a major concern. Many breakthroughs have been made in the study of pollution using soil mechanics and fluid mechanics. Engineers are beginning to understand the

importance of environmental monitoring and management. Nevertheless the ability to precisely model the subsurface layers of earth is quite difficult because there are many types of earth strata. Soil properties are always nonhomogeneous unless a location to be studied is small and well defined. All of the popular programs developed today create a database of information or simulate a local occurrence of concentration. However, most are just incapable of handling displacement and concentration of a contaminant over a given time period. The most useful programs to date that are capable of analyzing the scenario addressed in this investigation employ Finite Element Methods. These programs rely on information obtained by monitoring wells and predict the fate of the contamination concentration. By using the frontal boundary approximation, models constructed will more closely resemble what is actually occurring below the surface and help understand the pollution process [15].

The focus of this work is the development of a one-dimensional model that will be capable of studying the flow of two fluids with an abrupt interface and examining hydrodynamic dispersion.

1.2 Objectives

The primary objective of this investigation is to model and calculate the motion of a moving boundary of two immiscible Newtonian fluids in a porous medium using the Finite Element Method. Modeling will incorporate finite element analysis to track the location of the moving boundary front. The porous medium will be considered stationary, homogeneous and saturated. The flow is considered isothermal and isotropic [13].

The main focus of this investigation is the quantification of pressure along the time at the boundary interaction of one fluid substance with another. This study is motivated by a concern relating to pollution of groundwater, dam seepage and the importance of secondary petroleum recovery. Such problems are inherently difficult since the solution of the field equations is coupled with the determination of the location of an unknown moving boundary between the immiscible fluids.

Certain analytical solutions of the partial differential equations governing one-dimensional flow will first be developed. These will be served as a reliability check before attempting analysis in higher

dimensions. Coupled differential equations governing the movement of the boundary will be solved using the MATLAB based on the finite element method. Finite element analysis will be applied and used to a given situation as formulated in the following chapters.

The first step in modeling is to start with a conceptual model. The selection of a relevant domain and correct assumptions is crucial. Geometric boundaries, selection of porous material, fluid type, boundary conditions and initial conditions are all important. Before proceeding further, the description of the relevant physical concepts will be identified and addressed.

Chapter 2

THE THEORY OF FLUID FLOW IN A POROUS MEDIA

2.1 Introduction

The theory of fluid flow in a porous medium has found applications in various fields of engineering. It describes the movement of ground water in soil and porous rock, the seepage of water through earth fills and concrete dams and of fluids in filters, and the movement of oil and gas in oil fields. A fluid is a substance that will deform continuously under the presence of applied shear stresses [2]. The underlying physics within this investigation involves the motion of a Newtonian fluid. This represents a continuum in which shear stress is directly proportional to the rate of deformation. In a different case, gas is dissolved in the oil and is released where the pressure drops below the saturation value [13]. However, such two-phase fluids will not be treated here.

The mechanics of fluid flow depends on the pressure distribution in a fluid and its pressure gradient. The pressure gradient in a continuum results from surface forces per unit volume due to an applied pressure. Flow

occurs in the direction of high pressure to low pressure. In establishing the analytical model of the underlying physics, a few fundamental equations describing fluid transport phenomena in a porous medium must be developed.

2.2 Fluids

The continuum that will be considered in this investigation is a homogeneous, immiscible fluid. The resulting flow through a porous material depends on basic fluid properties. The first property is the absolute viscosity, μ , of the fluid. Absolute viscosity of a fluid is best explained by comparing how the fluid acts when a shear stress is applied on its surface in a plane parallel to the direction of motion [11]. Viscosity is the measure of the resistance of a fluid to shear deformation. Its magnitude is specified with respect to the viscosity of water [11]. The second property is the fluid's density, ρ . The definition of fluid density is the mass of the fluid per unit volume [11]. For an incompressible fluid, the density is constant. A compressible fluid, however, has a density that varies with pressure, p , and temperature, T , as described by the following equation of state [12]:

$$\rho = \rho (P, T) \quad (2.1)$$

also for a compressible liquid, we may set

$$\rho = \rho_0 e^{\beta(P-P_0)} \quad (2.2)$$

For most liquids, the compressibility β is a very small quantity of the order of 10^{-6} psi^{-1} . Hence, it is often possible to expand equation (2.2) in a Taylor series and to drop the higher terms [12]:

$$\rho = \rho_0 [1 + \beta(P - P_0)] \quad (2.3)$$

For a gas, we write

$$\rho = \rho_0 \left(\frac{P}{P_0} \right)^m \quad (2.4)$$

where m determines the thermodynamic character of the gas expansion :

$m=1$ corresponds to an isothermal expansion; $m = \gamma = C_p/C_v$ to an adiabatic expansion [4].

2.3 Porous Medium

A porous medium, such as sand or foam rubber, contains innumerable voids of varying sizes and shapes. These pores may be isolated from each other, or they may be interconnected to form a network of channels through which a fluid may flow. We are concerned only with the interconnected

part of the pore system, the effective pore space. Here is **Figure C** which shows typical porous medium saturated in the flow.

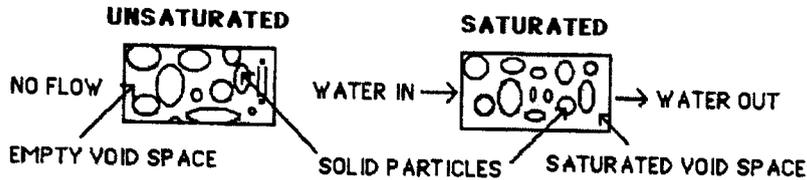


Figure C

Porous media naturally exist in many forms, for instance: sand soil, ceramics, foam rubber, cloth, bread and organic tissue, as well as other substances that contain innumerable void of varying size and shapes. These voids are interconnected, forming channels within the solid matrix of the porous domain. The ratio of the interconnected pore space to that of the total volume of the medium is the porosity, ϕ [4, 12]:

$$\phi = \frac{V_v}{V_b} = \frac{V_b - V_s}{V_b} \quad (2.5)$$

Here V_v , V_b and V_s are material void space, material bulk space and volume of solid, respectively. The porosity of a given material directly dictates how a resulting flow will develop.

Permeability, k , is a property that expresses a given fluid's macroscopic effects due to the microscopic solid-fluid interaction within a porous medium [4]. This internal hydrological property is independent of the fluid's viscosity. Permeability is simply a measure of the ability of a porous medium to transmit fluid through it. Another quantity that is important to a porous medium is its tortuosity, T_t . Tortuosity is the ratio of the average distance traveled by the fluid particle, L_e , to the direct path through the medium bed, L . **Figure D** shows a schematic definition of tortuosity.

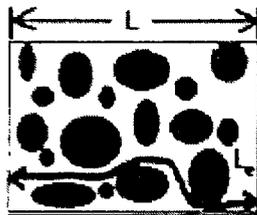


Figure D

Tortuosity is defined by the equation below [14]:

$$T_t = \frac{L_e}{L} \quad (2.6)$$

The tortuosity value is greater than one, where the value one implies a direct path.

Porosity, permeability, and tortuosity are material dependent. Most often these values can be determined by experimental methods, if they are not already tabulated. These values are extremely difficult to establish for computation purposes for two main reasons. One reason being the difficulty in simulating realistic material properties. The second reason is the complexity inherent to deriving models based on the governing partial differential equations.

An important feature of a porous matrix is its variation of properties with respect to direction. Isotropic materials display no variation in properties with respect to direction, whereas anisotropic materials do. Yet, another important feature of the matrix includes temperature effects. Isothermal processes assume no temperature effects [19].

Briefly considering the microscopic realm of immiscible fluids in a porous matrix, there is a peculiar local phenomenon at the interface. This phenomenon, known as ‘ fingering ‘, occurs when a viscous fluid, such as in

oil and water [5, 18]. Fingering occurs when the fluid interface is unstable and disturbances elongate with wave-like motions. Fingering is depicted in **Figure E**.

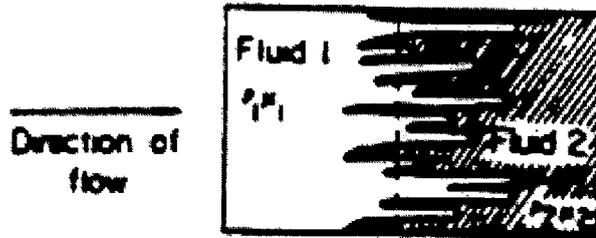


Figure E

The mode in this investigation assumes the frontal boundary as a macroscopic, homogeneous interface. If this macroscopic wall were broken into sub-sections and studied, fingering could be identified. Due to the macroscopic point of view taken in this investigation, this phenomenon will be neglected.

2.4 Governing Equations

The equations governing the physics take the form of partial differential equations. Neglecting inertial terms, the incompressible-flow

Navier-Stokes equation of a liquid continuum in a gravitational field is along with the continuity equation $div(\vec{V}) = 0$ [10, 17].

$$\nabla(P + \rho gz) = \mu \nabla^2 V \quad (2.7)$$

Of the equation (2.7), z , g and v are the height of the fluid, gravitational constant and the velocity of the fluid, respectively. These equations quantitatively describe the dynamic and kinematic relationships between the fluid, the flow medium, and the flow parameters at any given location.

Low flow rate situations are termed laminar creeping flows. In these types of flows, the Navier-stokes equation is [11]

$$\rho \frac{D\vec{v}}{Dt} = \rho \vec{g} - \nabla P + \mu \nabla^2 \vec{v} \quad (2.9)$$

Fluids in a porous medium that display a laminar character can be modeled using Darcy's law [4]. The rate of fluid flow at the moving boundary interface is also assumed to satisfy Darcy's law, which relates the flow rate to the pressure gradient. For the case of a Newtonian fluid, this relationship is linear. Thus, the motion of the moving boundary is governed by the pressure distribution within the reservoir. The existing fluid in the reservoir is assumed to be of finite extent, containing a slightly compressible Newtonian fluid. The incoming fluid and the reservoir fluid are assumed to

be immiscible, resulting in a piston-like displacement of the two fluids [3]. The location of the moving fluid-fluid interface, because unknown, as well as the rate at which it advances can be tracked after exact calculation of pressure distribution.

For the above governing relationship to be applicable, two conditions must be satisfied. The first condition requires that the porosity must be small in comparison with the other characteristic dimensions of the flow. The second condition requires that the Reynolds' number must be within the laminar regime. The Reynolds' number is defined as the dimensionless grouping.

$$R_e = \frac{\rho v d}{\mu} \quad (2.10)$$

As long as the Reynolds' number is within the range of 1 to 10, Darcy's law is also valid [4]. Flows in geological formations inherently have low Reynolds' numbers. The diameter of the pore space, d , is defined in many different ways. It can be expressed in terms of permeability and porosity as [9];

$$d \approx \sqrt{\frac{k}{\phi}} \quad (2.11)$$

if a good approximation of both permeability and porosity exist. It can also be expressed as [9];

$$d \approx \sqrt{k} \quad (2.12)$$

if one has a good approximation of permeability, only.

Thus substitution into equation (2.10) results in [9];

$$R_e \approx \frac{\rho v \sqrt{k}}{\mu} \quad (2.13)$$

or

$$R_e \approx \frac{\rho v \sqrt{\frac{k}{\phi}}}{\mu} \quad (2.14)$$

Depending on which approximation is used for d , that choice will dictate which R_e to use. Equation (2.14) was used in the Reynolds' number calculation for the analysis. Using the continuum approach, neglecting internal fluid friction and inertial effects, the average momentum balance to a linear equation is known as Darcy's law [4]. For an isotropic medium containing a homogeneous, incompressible fluid, Darcy's law is stated as [9];

$$\vec{q} = -K \frac{\partial h}{\partial s} \quad (2.15)$$

where \vec{q} , h and s are the specific discharge, the piezometric head and the distance traveled in the field by the fluid, respectively. Here hydraulic conductivity, K , is defined by [13]

$$K = \frac{k\gamma}{\mu} = \frac{\rho kg}{\mu} \quad (2.16)$$

In a two-dimensional flow, the fluid velocities in the x and y directions are

$$v_x = -K \frac{\partial h}{\partial x} \quad (2.17)$$

$$v_y = -K \frac{\partial h}{\partial y} \quad (2.18)$$

In many instances, flow through a porous medium is linearly proportional to the applied pressure gradient and inversely proportional to the viscosity of the fluid. This is expressed for one-dimensional flow as :

$$v = -\frac{k}{\mu} \left(\frac{dp}{dx} \right) \quad (2.19)$$

where v represents the fluid velocity.

Another equation we consider is related to the piston-like displacement of compressible Newtonian fluids in porous media. The law

of conservation of mass and the Navier Stokes equations of classical fluid mechanics in general govern the motion of a viscous fluid [2].

The continuity equation for unsteady flow of a fluid with density ρ through a medium with porosity ϕ , based on material balance, is

$$\vec{\nabla} \cdot (\rho \vec{v}) + \phi \frac{\partial \rho}{\partial t} = 0 \quad (2.20)$$

where the superficial velocity \vec{v} is defined as the volume rate of flow per unit cross-sectional area of the solid plus fluid [4]. For the flow of a viscous fluid through a porous medium, the Navier Stokes Equations are replaced by Darcy's law, which for the case of a Newtonian fluid penetrating an isotropic porous medium has the form :

$$\vec{v} = -\frac{k}{\mu} (\vec{\nabla} p - \rho \vec{g}) \quad (2.21)$$

where k is the permeability of the invaded medium, μ and $\vec{\nabla} p$ are the viscosity and pressure gradients of the flow field and \vec{g} is the gravitational acceleration vector [11]. Substitution of the Darcy relation into the equation of continuity (2.20) results in :

$$\vec{\nabla} \cdot \left[\frac{\rho k}{\mu} (\vec{\nabla} p - \rho \vec{g}) \right] = \phi \frac{\partial \rho}{\partial t} \quad (2.22)$$

The pressure and density are assumed to be related by the conventional equation of state [2]:

$$\rho = \rho_0 \exp(cp) \quad (2.23)$$

which for the case of constant compressibility, c , leads to

$$\nabla \vec{p} = c_\rho \vec{\nabla}_\rho \quad (2.24)$$

In most petroleum reservoir applications, effects of gravity are ignored, as well as variations in the permeability of the surrounding medium and viscosity of the penetrating fluid. Consequently, equations (2.22) and (2.24) can be shown to give the governing differential equations for the pressure distribution

$$\nabla^2 p = \frac{\phi \mu c}{k} \frac{\partial p}{\partial t} \quad (2.25)$$

for a slightly compressible fluid ; that is, when

$$c \|\vec{\nabla} p\| \ll |\nabla^2 p| \quad (2.26)$$

when the fluid is incompressible, the diffusion equation (2.25) reduces to Laplace's equation [4]

$$\nabla^2 p = 0 \quad (2.27)$$

Chapter 3

FINITE ENEMENT MODELING THEORY

3.1 Basic Finite Element theory

The finite-element method is an approximation procedure for solving a differential equation of boundary and/or initial-value type in engineering and mathematical physics. The procedure employs the subdivision of the solution domain into many smaller regions of convenient shapes, such as triangles and quadrangles, and uses approximation theory to estimate the solution on each finite element. Suitably disposed coordinates are specified for each element, and the solution of the differential equation is approximately replaced using values of the dependent variables at these nodes.

Using a variation principle, or a weighted-residual method, the governing differential equations are then transformed into finite-element equations governing the (each) isolated element. These local equations are collected together to form a global system of ordinary differential or algebraic equations including proper accounting of boundary conditions.

The nodal values of the dependent variables are determined from the solution of this matrix equation system. We will look at a general idea of the finite element method ; then, with a couple of examples, we can find how the theory applies to real cases.

Finite element methods are based on the local application of variational principles. In a variational framework, a generalized solution to an operator equation is found by minimizing a giving functional. The advantage afforded by a variational formulation is that differentiability properties of solutions are relaxed. This is advantageous for solutions that are only piecewise smooth.

The term “ variational formulation “ is used contextually to mean the weak formulation, in which weak refers to the fact that a function satisfies a boundary value problem in a certain averaged sense [7, 8]. The differential equation is recast in an equivalent integral form by trading differentiation between a test function and the dependent variable. When the differential operator is symmetric, the weak formulation can be further posed as a minimization problem for a given functional, $I (u)$ [7]. From the calculus of variations, the minimizing function is the true solution of the differential

equation. An approximate solution will be expressed by a linear combination of appropriately chosen functions [15].

$$u = \sum_{j=1}^N C_j \Phi_j \quad (3.1)$$

The parameter C_j is determined such that the function u minimizes the function $I (u)$, i.e. u satisfies the weak formulation [7, 15].

In addition to satisfying a governing equation, the solution to a boundary value problem must admit specified values on the boundary of the domain. On the other hand, if the solution or its derivatives are specified initially (i.e. at a set time t), then it is referred to as an initial-value problem which is a combination of the above.

In order to appreciate the fundamental principles of the finite element method, one must understand the concepts of functional and variational operators. Consider the integral expression [15]:

$$I (u) = \int_a^b F(x, u, u') dx \quad (3.2)$$

where the integrand $F (x, u, u')$ is a given function of the three arguments x , u , and du/dx . The value of the integral depends primarily upon u , hence $I (u)$ is appropriate. The integral in Eq. (3.2) represents a scalar for any

given function $u(x)$. $I(u)$ is called a functional since it is a value defined by integrals whose arguments themselves are functions. Mathematically, a functional is an operator mapping u into a scalar $I(u)$.

A functional $I(u)$ is said to be linear in u if and only if the relation

$$I(\alpha u + \beta v) = \alpha I(u) + \beta I(v)$$

holds for all scalars α, β and functions u and v [7, 17]. A functional of two arguments, $B(u, v)$, is said to be bilinear if it is linear in each of its arguments u and v .

The integrand, $F = F(x, u, u')$, depends on the independent variable x and dependent variables u and u' . An infinitesimal change in u is called a variation in u and is denoted by δu . The operator δ will be referred to as the variational operator. The variation, δu of a function u , represents an admissible infinitesimal change in the function $u(x)$. If u is specified on some portion of the boundary, its variation there must be zero since the specified value cannot be varied. The homogeneous form of the boundary conditions on u must be satisfied by any variation of the function u . The variation δu is arbitrary elsewhere on the boundary [7].

Boundary conditions play an important role in the derivation of the approximation function. The variational formulation facilitates classification of boundary conditions into essential and natural boundary conditions. For details, see Reddy [7] Section 2.2.

In the following, the three basic steps in the variational formulation of boundary value problems are outlined. Consider the following differential equation in two dimensions, defined on some domain Ω . It is hypothesized that $F(x, u, u_x, u_y)$ is differentiable, so that

$$\frac{\partial F}{\partial u} - \frac{\partial}{\partial x} \left(\frac{\partial F}{\partial u_x} \right) - \frac{\partial}{\partial y} \left(\frac{\partial F}{\partial u_y} \right) = 0 \quad \text{within } \Omega \quad (3.3)$$

along with given boundary conditions [7].

$$\begin{aligned} \frac{\partial F}{\partial u_x} n_x + \frac{\partial F}{\partial u_y} n_y &= \hat{Q} \quad \text{on } \Gamma_1 \\ u &= u' \quad \text{on } \Gamma_2 \end{aligned} \quad (3.3)$$

That is, flux is specified on part of the boundary denoted Γ_1 and the value of the function is specified on the remaining Γ_2 . The following **Figure F** shows the boundaries denoted Γ_1 and Γ_2 .

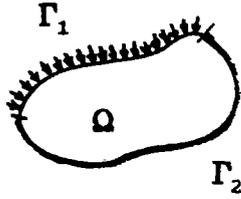


Figure F

The first step is to multiply Eq. (3.3) by a test function, v , and integrate the product over the domain Ω . That test function can be thought of as a variation in u (δu), which satisfies the homogeneous form of the boundary conditions on Γ_2 . v may otherwise be an arbitrary continuous function.

Since Eq. (3.3) is satisfied pointwise, one can integrate both sides over the domain to arrive at the weaker form Eq. (3.3),

$$0 = \int_{\Omega} v \left[\frac{\partial F}{\partial u} - \frac{\partial}{\partial x} \left(\frac{\partial F}{\partial u_x} \right) - \frac{\partial}{\partial y} \left(\frac{\partial F}{\partial u_y} \right) \right] dx dy \quad (3.4)$$

Note that the integral form still contains the same order of differentiation.

The second step involves the transfer of the differentiation from the dependent variable u to the test function v . It is desirable to transfer the partial derivatives with respect to x and y (u_x & u_y) to v so that only first

order differentiation is required of both u and v . This results in an equalization of smoothness for both u and v , and thus is a weaker continuity requirement on the solution u to the variation problem. In the process of transferring the differentiation, i.e. integration by parts, we obtain the natural boundary conditions. Eq. (3.4) is now expressed as

$$0 = \int_{\Omega} [V \frac{\partial F}{\partial u} + \frac{\partial v}{\partial x} \frac{\partial F}{\partial u_x} + \frac{\partial v}{\partial y} \frac{\partial F}{\partial u_y}] dx dy - \int_{\Gamma} V (\frac{\partial F}{\partial u_x} n_x + \frac{\partial F}{\partial u_y} n_y) ds$$

(3.5)

The coefficients of v in the second integral represent the natural boundary conditions [7].

The third step in the formulation consists of simplifying the boundary terms in Eq. (3.5) by applying the specified natural boundary conditions in the two boundary integrals over the subsets Γ_1 and Γ_2 .

$$0 = \int_{\Omega} [V \frac{\partial F}{\partial u} + \frac{\partial v}{\partial X} \frac{\partial F}{\partial u_x} + \frac{\partial v}{\partial y} \frac{\partial F}{\partial u_y}] dx dy - \int_{\Gamma_2} V (\frac{\partial F}{\partial u_x} n_x + \frac{\partial F}{\partial u_y} n_y) ds - \int_{\Gamma_1} V \hat{q} ds$$

(3.6)

The first boundary integral vanishes since v is specified ($\delta u = 0$) on Γ_2 .

The variational formulation thus results in a reduction of order as well as an automatic imposition of the natural boundary conditions [7, 17].

The weak form, Eq. (3.4), finally reduces to

$$0 = \int_{\Omega} \left[V \frac{\partial F}{\partial u} + \frac{\partial v}{\partial x} \frac{\partial F}{\partial u_x} + \frac{\partial v}{\partial y} \frac{\partial F}{\partial u_y} \right] dx dy - \int_{\Omega} V \hat{q} ds \quad (3.7)$$

The function u is said to be a weak solution of Eq. (3.3), if u satisfies Eq.

(3.7) for all appropriate test functions v . Eq. (3.7) can be more compactly stated in terms of bilinear functional $b(u, v)$ and a linear functional $l(v)$ as

$$B(v, u) = l(v)$$

for all admissible test functions v .

In Eq. (3.7),

$$B(v, u) = \int_{\Omega} \left[V \frac{\partial F}{\partial u} + \frac{\partial v}{\partial x} \frac{\partial F}{\partial u_x} + \frac{\partial v}{\partial y} \frac{\partial F}{\partial u_y} \right] dx dy$$

and

$$l(v) = \int_{\Omega} v dx dy + \int_{\Gamma_1} v \hat{q} ds \quad (3.8)$$

If the bilinear form $B(v, u)$ is symmetric, i.e. $B(v, u) = B(u, v)$, then the quadratic functional associated with the variational formulation is deduced as

$$I(u) = \frac{1}{2}B(u, u) - l(u). \quad (3.9)$$

Satisfying Eq. (3.9) is equivalent to minimizing $I(u)$. When the functional $I(u)$ is in this form, approximate method [5] may be used to minimize the functional.

An appropriate method for solution of the weak form, Eq. (3.7), is known as the Galerkin method. The solution u takes on the form

$$u_N = \sum_{j=1}^N c_j \Phi_j$$

in which Φ_j , the approximating basis functions, must satisfy the following conditions :

- 1) They must be well defined and nonzero as well as sufficiently differentiable as required by the bilinear form $B(\bullet, \bullet)$
- 2) Any set $\{ \Phi_i \} (i = 1, N)$ must be linearly independent
- 3) $\{ \Phi_i \} (i = 1, \infty)$ must be complete.

These conditions guarantee convergence to the solution. When defining the test function, knowledge of the anticipated solution as well as satisfaction of any essential or natural boundary conditions should be taken into account.

The Galerkin approximation is expressed as [7]

$$u_N = \sum_{j=1}^N c_j \Phi_j(X) \quad (3.10)$$

and the test function is correspondingly written as

$$V = \sum_{i=1}^m b_i \Phi_i \quad (3.11)$$

If the approximate solution Eq. (3.10) and the test function Eq. (3.11) is introduced into Eq. (3.8) and the test function Eq. (3.8), the problem is then reduced to find c_j , such that

$$B \left(u_N = \sum_{j=1}^N c_j \Phi_j(X), V_m = \sum_{i=1}^M b_i \Phi_i(X) \right) = F \left(\sum_{j=1}^M b_j \Phi_j \right) \quad (3.12)$$

for arbitrary constants b_j .

If $B(\bullet, \bullet)$ and $F(\bullet)$ are linear, an equivalent formulation is

$$\sum_{j=1}^N c_j B(\Phi_j, \Phi_i) = F(\Phi_i) \quad \text{for } i = 1, \dots, n \quad (3.13)$$

Eq. (3.13) represents a linear system of equation in the unknown coefficients c_j .

Alternatively, one can set

$$\int_{\Omega} (Au - f) v \Phi_j(x) d\Omega + B.C.'s\ Terms = 0$$

where A is a linear operator defining

$$Au = f$$

on the domain Ω .

3.2 Derivation of Finite Element Equation

In the Finite Element Method, for the one-dimensional problem we separate the given domain. **Figure G,H** shows the discretization

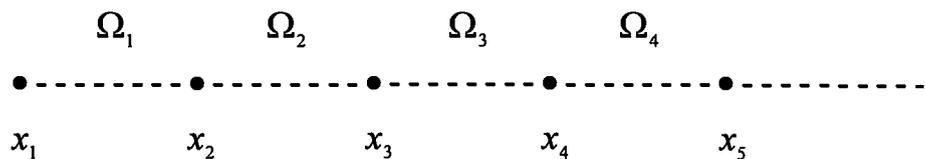


Figure G

On Ω_e :

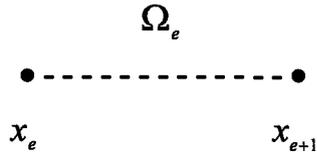


Figure H

The governing differential equation for the pressure distribution is equation (2.25) of chapter 2

$$\nabla^2 p = \frac{\phi\mu c}{k} \frac{\partial p}{\partial t} \quad (3.2a)$$

and, this can be rewritten as

$$\frac{\partial P}{\partial t} = \frac{k}{\phi\mu c} \frac{\partial^2 p}{\partial x^2} \quad (3.2b)$$

If we substitute $\frac{k}{\phi\mu c}$ as α , the resulting equation for the pressure

distribution will be

$$\frac{\partial P}{\partial t} = \alpha \frac{\partial^2 P}{\partial x^2} \quad (3.2c)$$

Based on variational principles, we construct the weak form of the differential equation

$$\int_{x_e}^{x_{e+1}} \left(-\alpha \frac{\partial^2 P}{\partial x^2} + \frac{\partial P}{\partial t} \right) \bullet v(x) dx = 0$$

$v(x)$ is a test function.

(3.2d)

Integrate by parts :

$$\begin{aligned} & \int_{x_e}^{x_{e+1}} \left(\alpha \frac{\partial P}{\partial x} \bullet \frac{dv}{dx} \bullet dx \right) + \int_{x_e}^{x_{e+1}} \frac{\partial P}{\partial t} \bullet v(x) dx \\ & - \alpha \frac{\partial P}{\partial x} \bullet v \Big|_{x_{e+1}} + \alpha \frac{\partial P}{\partial x} \bullet v \Big|_{x_e} = 0 \end{aligned}$$

(3.2e)

Set :

$$Q_e = Q_1^e = -\alpha \frac{\partial P}{\partial x} \Big|_{x=x_e}$$

$$Q_{e+1} = Q_2^e = \alpha \frac{\partial P}{\partial x} \Big|_{x=x_{e+1}}$$

(3.2f)

Therefore,

$$\begin{aligned} & \int_{x_e}^{x_{e+1}} \alpha \bullet \frac{\partial P}{\partial x} \bullet \frac{dv}{dx} dx + \int_{x_e}^{x_{e+1}} \frac{\partial P}{\partial t} \bullet v(x) \bullet dx \\ & = Q_{e+1} \bullet v(x_{e+1}) + Q_e \bullet v(x_e) \end{aligned}$$

(3.2g)

This is the weak form for each element, Ω_e .

For the second step, we assume the form of the approximate solution over a typical finite element. Now, on each element, set

$$P^e(x, t) = \sum_{j=1}^n u_j^e(t) \bullet \Psi_j^e(x)$$

Ψ_j are shape functions
 $u_j(t)$ are unknown coordinate functions

(3.2h)

then,

$$\frac{\partial P^e}{\partial x} = \sum_{j=1}^n u_j^e(t) \bullet \frac{d\Psi_j^e}{dx}$$

$$\frac{\partial P^e}{\partial t} = \sum_{j=1}^n \dot{u}_j^e(t) \bullet \Psi_j^e(x)$$

(3.2i)

Substitute

$$P = P^e$$

$$v(x) = \Psi_i^e(x), \quad i = 1, 2, \dots, n$$

(3.2j)

Previous equation can be changed as follow :

$$\int_{x_e}^{x_{e+1}} \alpha \bullet \frac{\partial P^e}{\partial x} \bullet \frac{d\Psi_i^e}{dx} dx + \int_{x_e}^{x_{e+1}} \frac{\partial P^e}{\partial t} \bullet \Psi_i^e(x) dx$$

$$= Q_{e+1} \bullet \Psi_i^e(x_{e+1}) + Q_e \bullet \Psi_i^e(x_e)$$

(3.2k)

for $i = 1, 2, \dots, n$

Further,

$$\begin{aligned}
\int_{x_e}^{x_{e+1}} \partial \bullet \left(\sum_{j=1}^n u_j^e \bullet \Psi_j^{e'} \right) \bullet \Psi_i^{e'} dx + \int_{x_e}^{x_{e+1}} \left(\sum_{j=1}^n \dot{u}_j^e \bullet \Psi_j^e \right) \bullet \Psi_i^e dx \\
= Q_e \bullet \Psi_i^e(x_e) + Q_{e+1} \bullet \Psi_i^e(x_{e+1})
\end{aligned}
\tag{3.21}$$

Re-write as

$$\begin{aligned}
\sum_{j=1}^n \left(\int_{x_e}^{x_{e+1}} \alpha \bullet \Psi_i^{e'} \bullet \Psi_j^{e'} \right) u_j^e + \sum_{j=1}^n \left(\int_{x_e}^{x_{e+1}} \Psi_i^e \bullet \Psi_j^e dx \right) \dot{u}_j^e \\
= Q_e \bullet \Psi_i^e(x_e) + Q_{e+1} \bullet \Psi_i^e(x_{e+1})
\end{aligned}
\tag{3.2m}$$

or

$$\begin{aligned}
\sum_{j=1}^n K_{ij}^e \bullet u_j^e + \sum_{j=1}^n M_{ij}^e \bullet \dot{u}_j^e = Q_e \bullet \Psi_i^e(x_e) + Q_{e+1} \bullet \Psi_i^{e+1}(x_{e+1}) \\
\text{for } i = 1, 2, \dots, n
\end{aligned}
\tag{3.2n}$$

where

$$\begin{aligned}
K_{ij}^e &= \alpha \int_{x_e}^{x_{e+1}} \Psi_i^{e'} \bullet \Psi_j^{e'} dx \\
M_{ij}^e &= \int_{x_e}^{x_{e+1}} \Psi_i^e \bullet \Psi_j^e dx
\end{aligned}
\tag{3.2o}$$

Now, it could be changed into matrix form

$$\begin{bmatrix} K_{ij}^e \end{bmatrix} \begin{bmatrix} u_1^e \\ u_2^e \\ \vdots \\ u_n^e \end{bmatrix} + \begin{bmatrix} M_{ij}^e \end{bmatrix} \begin{bmatrix} \dot{u}_1^e \\ \dot{u}_2^e \\ \vdots \\ \dot{u}_n^e \end{bmatrix} = \begin{bmatrix} Q_e \bullet \Psi_1^e(x_e) + Q_{e+1} \bullet \Psi_1^e(x_{e+1}) \\ Q_e \bullet \Psi_2^e(x_e) + Q_{e+1} \bullet \Psi_2^e(x_{e+1}) \\ \vdots \\ Q_e \bullet \Psi_n^e(x_e) + Q_{e+1} \bullet \Psi_n^e(x_{e+1}) \end{bmatrix}$$

(3.2p)

We will choose $\Psi_i^e(x)$ such that

$$\begin{aligned}
\Psi_i^e(x_e) &= 1 \text{ only if } i = 1, \text{ otherwise } \Psi_i^e(x_e) = 0 \\
\Psi_i^e(x_{e+1}) &= 1 \text{ only if } i = n, \text{ otherwise } \Psi_i^e(x_{e+1}) = 0
\end{aligned}$$

(3.2q)

For the equation (2-2p) we use the matrices of Reddy's Finite element [7]

$$\begin{aligned}
\begin{bmatrix} K_{ij}^e \end{bmatrix} &= \frac{\partial}{\partial h_e} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \\
\begin{bmatrix} M_{ij}^e \end{bmatrix} &= \frac{h_e}{6} \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}
\end{aligned}$$

(3.2r)

Before we go further, we will apply those matrices of the equation (3.2r) to an example of three element and four nodes. **Figure I** shows that the domain and nodes.

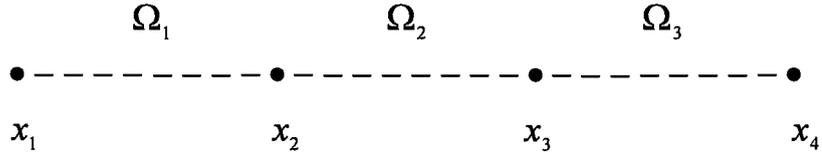


Figure I

Using the equation (3.2q), we can set the matrices for the equation of the problem of three elements and four nodes.

$$[K_{ij}^e] = \frac{1}{h} \begin{bmatrix} \alpha^1 & -\alpha^1 & 0 & 0 \\ -\alpha^1 & \alpha^1 + \alpha^2 & -\alpha^2 & 0 \\ 0 & -\alpha^2 & \alpha^2 + \alpha^3 & -\alpha^3 \\ 0 & 0 & -\alpha^3 & \alpha^3 \end{bmatrix}$$

$$[M_{ij}^e] = \frac{h}{6} \begin{bmatrix} 2 & 1 & 0 & 0 \\ 1 & 4 & 1 & 0 \\ 0 & 1 & 4 & 0 \\ 0 & 0 & 1 & 2 \end{bmatrix}$$

(3.2t)

Furthermore, we can also make the equation in the form of

$$[M]\{\dot{u}\} + [K]\{u\} = \{F\}$$

which is

$$\frac{1}{h} \begin{bmatrix} \alpha^1 & -\alpha^1 & 0 & 0 \\ -\alpha^1 & \alpha^1 + \alpha^2 & -\alpha^2 & 0 \\ 0 & -\alpha^2 & \alpha^2 + \alpha^3 & -\alpha^3 \\ 0 & 0 & -\alpha^3 & \alpha^3 \end{bmatrix} \begin{Bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{Bmatrix} +$$

$$\frac{h}{6} \begin{bmatrix} 2 & 1 & 0 & 0 \\ 1 & 4 & 1 & 0 \\ 0 & 1 & 4 & 0 \\ 0 & 0 & 1 & 2 \end{bmatrix} \begin{Bmatrix} \dot{u}_1 \\ \dot{u}_2 \\ \dot{u}_3 \\ \dot{u}_4 \end{Bmatrix} = \begin{Bmatrix} Q_1^1 \\ Q_2^1 + Q_1^2 \\ Q_2^2 + Q_1^3 \\ Q_2^3 \end{Bmatrix} \quad (3.2u)$$

This equation follows from the Flow Continuity so

$$Q_2^e + Q_1^{e+1} = 0$$

for all internal nodes. Thus, the equation (3.2u) will be

$$\frac{1}{h} \begin{bmatrix} \alpha^1 & -\alpha^1 & 0 & 0 \\ -\alpha^1 & \alpha^1 + \alpha^2 & -\alpha^2 & 0 \\ 0 & -\alpha^2 & \alpha^2 + \alpha^3 & -\alpha^3 \\ 0 & 0 & -\alpha^3 & \alpha^3 \end{bmatrix} \begin{Bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{Bmatrix} + \frac{h}{6} \begin{bmatrix} 2 & 1 & 0 & 0 \\ 1 & 4 & 1 & 0 \\ 0 & 1 & 4 & 0 \\ 0 & 0 & 1 & 2 \end{bmatrix} \begin{Bmatrix} \dot{u}_1 \\ \dot{u}_2 \\ \dot{u}_3 \\ \dot{u}_4 \end{Bmatrix} = \begin{Bmatrix} Q_1^1 \\ 0 \\ 0 \\ Q_2^3 \end{Bmatrix} \quad (3.2v)$$

In this investigation, the pressure distribution is the dependent variable. Therefore, we make the association

$$\begin{aligned}u_1 &= p_f(t) \\ \dot{u}_1 &= \dot{p}_f(t)\end{aligned}$$

(3.2w)

and subsequently solve for u_2, u_3, u_4 , the pressures at the remaining nodes.

Chapter 4

MODEL VALIDATION

4.1 Moving Boundary Problems

The formulation of a problem involving a moving boundary requires setting up a mesh that is capable of deforming. Constructing a mesh with nodes located on a moving boundary, thus introducing degrees of freedom, does this. A further modification of the problem entails the necessity to introduce additional boundary conditions to allow the determination of the moving boundary. There are many types of cases that can be constructed. The cases that are of interest in this investigation involve either a free surface boundary or an interface between two fluids. **Figure J** shows typical type of two immiscible fluids movement

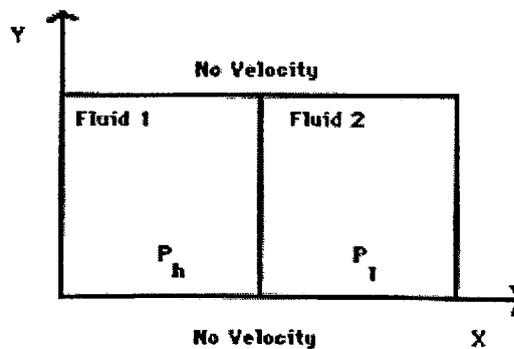


Figure J

The free surface condition occurs when a liquid comes into contact with a gas, such as air. However, the problems that involve a free surface interface are not easily tractable, so approximate solutions are needed.

Reliable numerical predictions for a contamination movement can be found using the finite element codes based on knowledge acquired earlier, by the database or existing monitoring data list.

4.2 Finite Element Analysis Outline

The finite element method entails the use of approximating interpolation functions associated with the partial differential equation. The variational method is applied piecewise over the domain to obtain a solution. Boundary conditions in the form of natural or essential are applied directly in the variational form.

As we mentioned in chapter three, the variational form is simply the weak formulation of the problem in which a quadratic functional $I(u)$ is to be minimized. This minimization yields Euler equations by invoking of solving the partial differential equation, the minimization problem leads to a system of equations which is solved directly.

The basic outline of this entire process is ;

1. Select the correct Partial Differential Equation expressing the field variable.
2. Put the PDE into variational form.
3. Divide the physical domain into elements.
4. Apply the Boundary Conditions.
5. Solve in terms of the assumed basis functions.
6. Set up local matrices.
7. Assemble globally.
8. Solve for unknowns.

4.3 Background on Matlab

Computer aided analysis can play a significant role in understanding a physical situation. Focusing on the boundary movement monitoring of two different fluids, computer analysis allows the engineer to approximate the location of the interface and parametric studies to determine the operating characteristics for prescribed situations involving two immiscible fluids. The overall benefit being prediction and preparation of the groundwater process or contamination progress, parameter variation sensitivities and an

understanding of the system's response in a given situation before prototype construction.

The use of MATLAB was selected due to the program's ability to deal with a large matrix calculation for the final finite element equations for the moving boundary problem in a porous medium. MATLAB, a well-known program in many engineering fields, will be used to implement. The finite element method to calculate the location of a boundary between two incompressible fluid flows as a function of time.

In the finite element method the flow region is subdivided into a number of small regions called elements. The partial differential equations that govern the flow region as a whole region are replaced element-wise by ordinary differential equations. The original partial differential equations of a fluid flow are derived from the basic physical principles of conservation of mass, linear momentum, energy and species [4, 6] . These general equations are shown below [11];

CONTINUITY EQUATION

$$\frac{\partial \rho}{\partial t} = \rho(u_i)$$

LINEAR MOMENTUM EQUATION

$$\rho \left[\frac{\partial u_i}{\partial t} + u_i u_{i,j} \right] = \sigma_{i,j,j} + \sigma f_i$$

ENERGY EQUATION

$$\left(\rho c_p \right)_e \frac{\partial T}{\partial t} + \rho c_p u_j T_{,j} = \left(k_e T_{,i} \right)_{,i} + \mu \phi + Q_s$$

The system of the generated differential equation is then solved by implemented numerical techniques such as Runge-Kutta. The results of location of the boundary movement and time for each interface are easily accessible through post-processing.

Simple steps are followed to generate a working file in MATLAB. These steps, as well as the above equations, are discussed in detail in the MATLAB manual [19]. A simple program outline to calculate this moving boundary problem is shown below ;

1. Put the incoming pressure and differential value.
2. Input physical properties.
3. Generate mesh and put the size of the mesh.

4. Run the Runge method program.
5. Solution of algebraic equations.
6. Graphical output of derived output quantities.

In the above outline, sections 1 thru 3 are done within an input data calculated by the user (pre-processing). Sections 4 thru 6 are done internally by the MATLAB software.

The sequence of the program used in this research, **Figure K**, is below ;

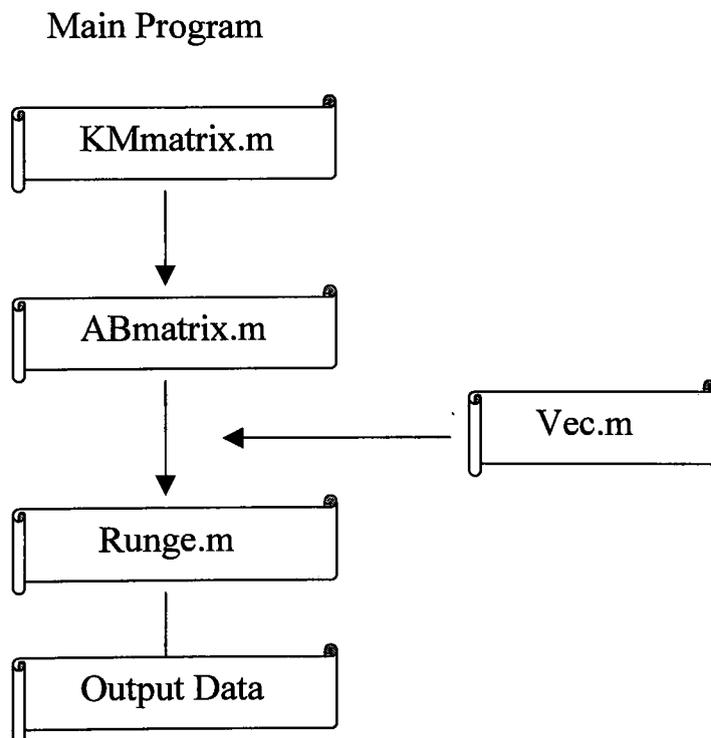


Figure K

4.4 Re-scale Problem

To actual calculation, we recast the equations (3.2a) and (3.2b).

From the equation (3.2a)

$$\nabla^2 p = \frac{\phi\mu c}{k} \frac{\partial p}{\partial t}$$

$$\frac{\partial^2 p}{\partial \chi^2} = \frac{\phi\mu c}{k} \frac{\partial p}{\partial t}$$

For the dimensionless distance, we can change

$$\frac{\partial^2 p}{\partial \xi^2} = \frac{\phi\mu c}{k} \frac{\partial p}{\partial t} \quad (4.1)$$

Figure L shows this



Figure L

and we let

$$\chi = \frac{\xi}{L} \quad (4.2)$$

$$\xi = L\chi \quad (4.3)$$

therefore

$$\frac{\partial}{\partial \chi} = L \frac{\partial}{\partial \xi} \quad (4.4)$$

$$\frac{\partial}{\partial \xi} = \frac{1}{L} \frac{\partial}{\partial \chi} \quad (4.5)$$

the equation (4.1) can be rewritten as

$$\frac{\partial^2 p}{\partial \chi^2} = \frac{L^2 \phi \mu c}{k} \frac{\partial p}{\partial t}$$

or

$$\frac{\partial p}{\partial t} = \frac{k}{L^2 \phi \mu c} \frac{\partial^2 p}{\partial \chi^2} \quad (4.6)$$

If we substitute $\frac{k}{L^2 \phi \mu c}$ as α , the resulting equation for the pressure

distribution will be

$$\frac{\partial p}{\partial t} = \alpha \frac{\partial^2 p}{\partial \chi^2} \quad (4.7)$$

For the actual calculation of α , we use the values given below :

$$k = 100 \text{ md} = 100 \cdot (10^{-15} \text{ m}^2)$$

$$= 10^{-13} \text{ m}^2$$

$$c = 10^{-9} \frac{\text{m} \cdot \text{s}^2}{\text{kg}}$$

$$\mu = 10^{-3} \frac{\text{kg}}{\text{m} \cdot \text{s}}$$

and

$$\begin{aligned}\alpha &= \frac{k}{L^2 \phi \mu c} = \frac{k}{L^2 \phi \cdot 10^{-12}} \cdot \frac{1}{\text{sec}} \\ &= \frac{10^{-13}}{L^2 \phi \cdot 10^{-12}} \cdot \frac{m}{\text{sec}} \\ &= \frac{10^{-1}}{\phi L^2} \cdot \frac{m^2}{\text{sec}}\end{aligned}$$

then

$$\begin{aligned}\text{sec} &= \frac{1}{60} m \\ \frac{1}{\text{sec}} &= \frac{60}{\text{min}}\end{aligned}$$

Therefore

$$\begin{aligned}\frac{k}{L^2 \phi \mu c} &= \frac{6}{L^2 \phi} \cdot \frac{m^2}{\text{min}} \\ &= \frac{360}{L^2 \phi} \cdot \frac{m^2}{\text{hr}}\end{aligned}$$

and with $L \approx 10^3 m$

$$\begin{aligned}\frac{k}{L^2 \phi \mu c} &= \frac{360}{10^6 \cdot \phi} \cdot \frac{1}{\text{hr}} \\ &= \frac{0.00036}{\phi} \cdot \frac{1}{\text{hr}}\end{aligned}$$

so, we have

$$\alpha = \frac{0.00036}{\phi} = 0.0007$$

if we consider the variation of the value of ϕ , we will have typical values of α in the range :

$$0.0001 \leq \alpha_1, \alpha_2 \leq 0.001 \quad (1 / hr)$$

Another constant of the main program in the MATLAB that we need to know is β . From the literature[16], we found

$$\beta \cong 0.01(m^2 \cdot hr / kg)$$

4.5 Tests and Results

4.5-1 Case One

We set the number of the elements and points as five and six for every each case. For case one, we choose the constants below

$$P_f = 100(\text{Pa})$$

$$P_f \text{ dot} = 0$$

$$\beta = 0.01(m^2 \cdot hr / kg)$$

$$\alpha_1 = 0.0003(1 / hr)$$

$$\alpha_2 = 0.0006(1 / hr)$$

where

P_f is Incoming fluid pressure

$P_f \text{ dot}$ is differential value of P_f

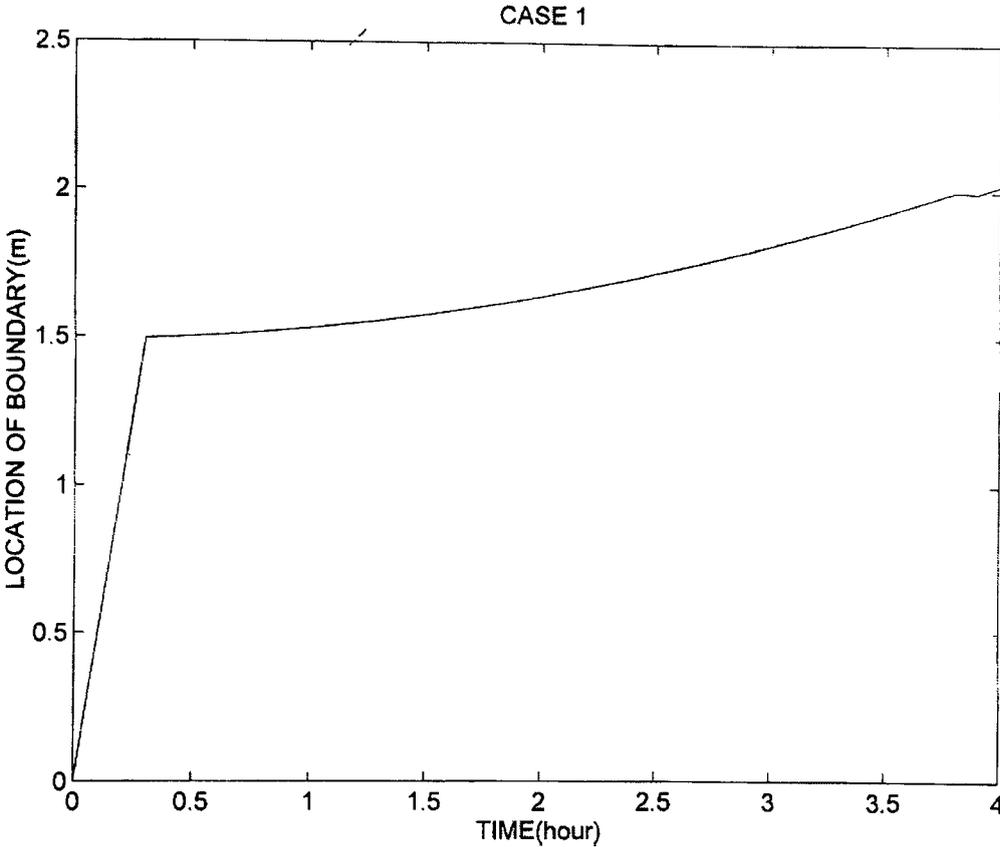
β is constant of S

S is the location of boundary or interface

α_1 is constant of incoming fluid

α_2 is constant of second fluid

and the result is given in **Plot 1**



Plot 1

4.5-2 Case Two

Case two has the constants below

$$P_f = 100(\text{Pa})$$

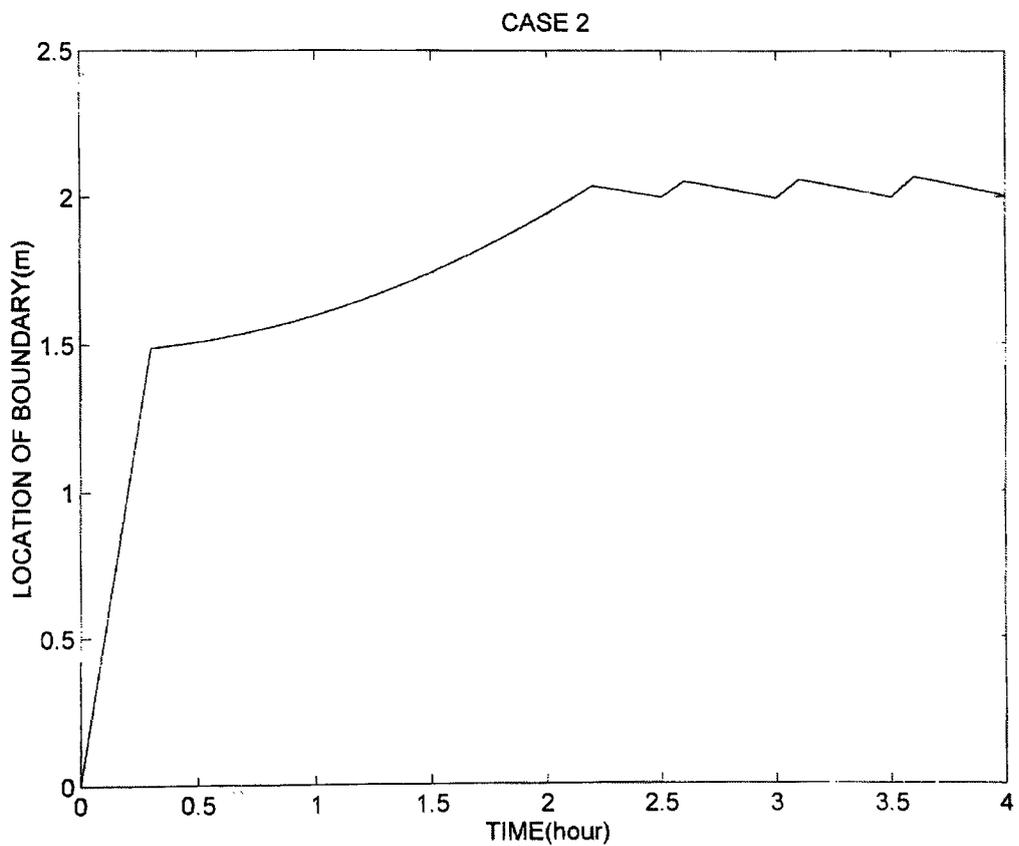
$$P_{dot} = 0$$

$$\beta = 0.01(\text{m}^2 \cdot \text{hr} / \text{kg})$$

$$\alpha_1 = 0.0009(1 / \text{hr})$$

$$\alpha_2 = 0.0001(1 / \text{hr})$$

and the result is shown in **Plot 2**



Plot 2

4.5-3 Case Three

Case three choose the constants below

$$P_f = 100(\text{Pa})$$

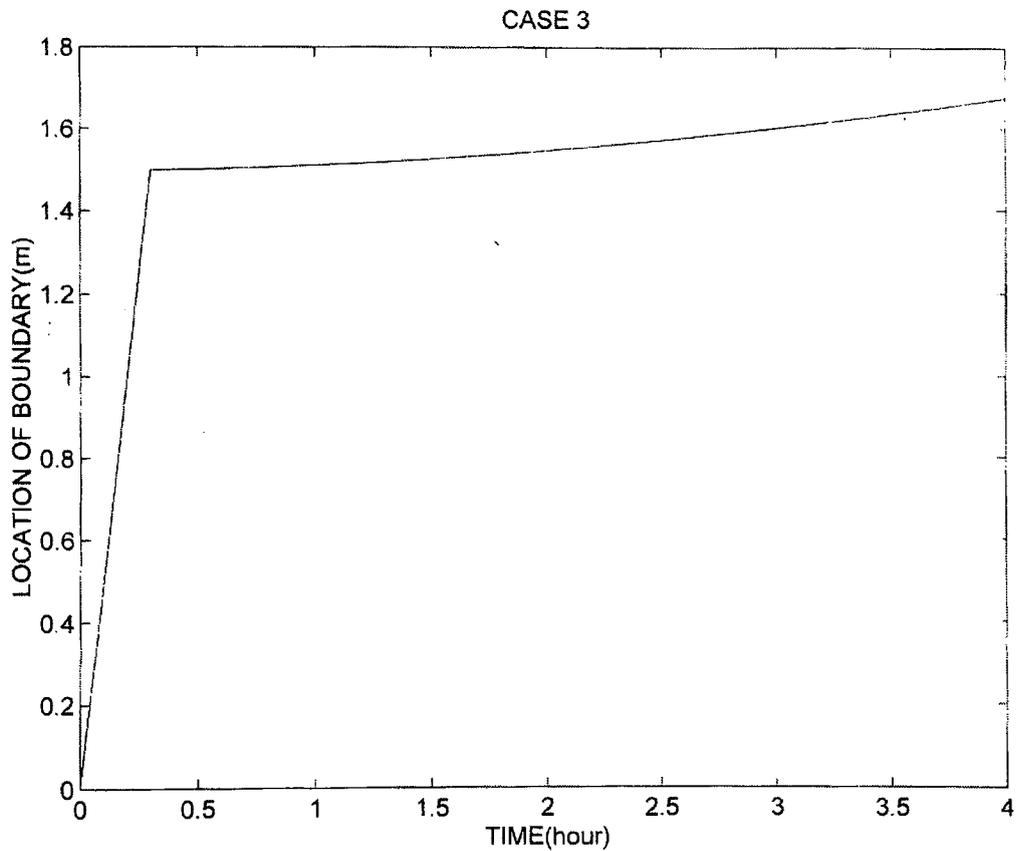
$$P_{\dot{}} = 0$$

$$\beta = 0.01(\text{m}^2 \cdot \text{hr} / \text{kg})$$

$$\alpha_1 = 0.0001(1 / \text{hr})$$

$$\alpha_2 = 0.001(1 / \text{hr})$$

and the result is given in **Plot 3**



Plot 3

4.5-4 Case Four

Case four choose the constants below

$$P_f = 100(\text{Pa})$$

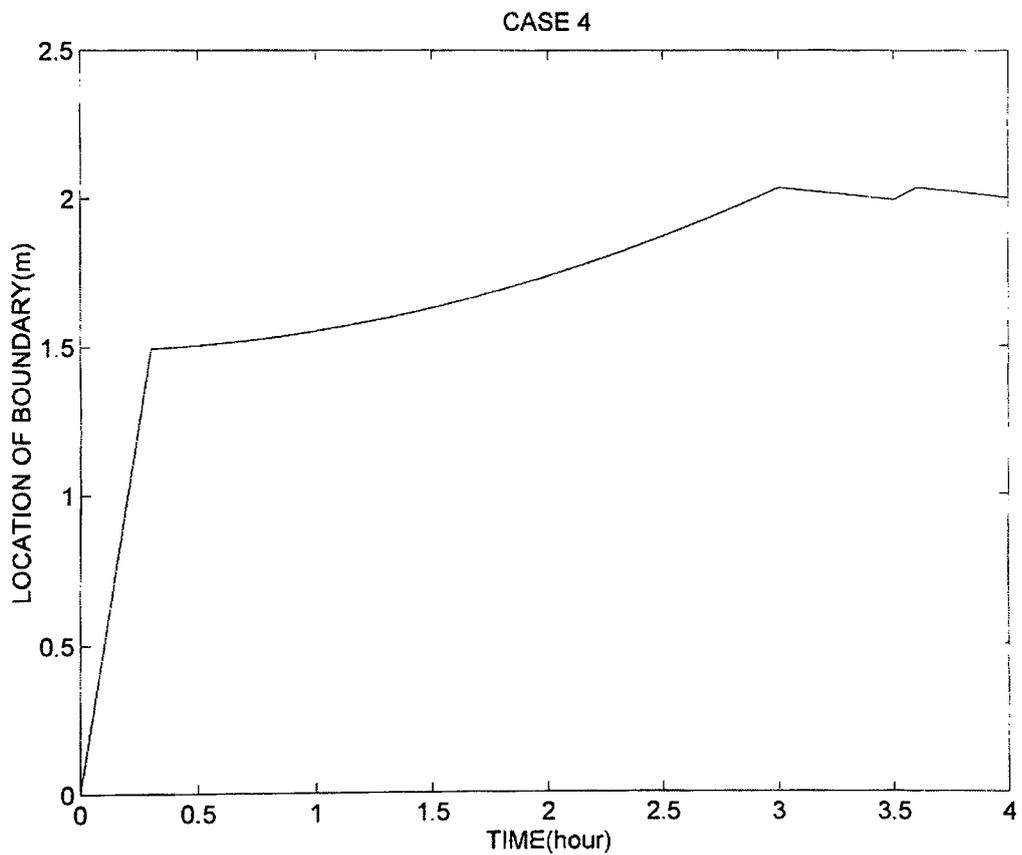
$$P_{\dot{}} = 0$$

$$\beta = 0.01(\text{m}^2 \cdot \text{hr} / \text{kg})$$

$$\alpha_1 = 0.0005(1 / \text{hr})$$

$$\alpha_2 = 0.0005(1 / \text{hr})$$

and the result is given in **Plot 4**



Plot 4

Chapter 5

RESULTS AND CONCLUSION

A one-dimensional moving boundary problem has been mathematically formulated. These types of problems occur in freeze-thaw situations and primarily in geo-engineering. The motivation for this investigation is based on the mechanics of two immiscible fluids in a porous medium. An invading fluid is pumped into a formation with the objective of increasing the pressure gradient in the resident fluid. The ultimate concern is enhanced oil recovery.

The geological formation was modeled as a finite one-dimensional continuum. It was assumed to be homogeneous. The domain of the problem was discretized into linear finite elements. The governing equations were established locally, on each element. Thereby, the properties of two different fluids could be incorporated on an element-by-element basis.

Since the fluids were assumed to be immiscible, a well-defined boundary between the two fluids was postulated. The fluid properties on each side of the boundary were different. The primary unknowns in the problem are the pressure distributions in the fluids. The solution of the problem necessitates knowing the location of the boundary at any given instant of time. However, displacement of the boundary depends on the pressure distribution of the fluids.

The boundary motion was assumed to be governed by Darcy's law. At each time step, the governing diffusion equations were solved simultaneously with differential equation for the boundary. Based on a finite element formulation, the partial differential equations were put in semi-discrete form, maintaining a continuous time variable.

For convenience, ten elements were used, leading to unknown pressures at ten nodes. Recall that the boundary pressure is specified. The time advance equations resulted in a coupled system of ten ordinary differential equations. These were numerically integrated using a fourth-order Runge-Kutta method incorporated in the program.

At each time step, a check is made to determine which element contains the boundary at any given time. This is needed to calculate the element matrices, which depend on the local fluid properties. Hence the pressure distributions and boundary location are updated at each time step. The program is completely automated, prompting the user for all information.

In the numerical simulations, the parameters chosen were based on typical geo-engineering fluids and soil formations. Ten elements were used to keep computation times moderate. Although the program in principle will allow any number of elements, the properties of the porous medium were not varied. Simulations were run using different combinations of fluid properties. The significant variable being fluid viscosity. The pressure at the boundary node was held constant. The program, however, can handle variable input pressure.

The results look quite reasonable. The graphs of boundary location versus time invariably end up as monotone increasing, with decreasing slope. These agree with experimental evidence and results based on more

sophisticated modeling. Some of the curves are not smooth. These irregularities occur because of errors in inverting large matrices

The objective of this investigation has been met. Namely, to formulate the moving boundary problem and to show the feasibility of constructing a simple, but practical finite element model. A high-level language such as MATLAB allows one to write more efficient and shorter programs, than if one were to use FORTRAN. Simple numerical models lead to better insight and understanding of the fundamental aspects of complicated problems. Basic models can also be used to help calibrate and debug much more sophisticated programs.

As recommendation for further work, perhaps the individual subroutines of the main program could be modified. Any changes should incorporate more accurate numerical techniques. In addition, better stability would be achieved if the mesh were to be refined near the moving boundary. This would result in a deforming mesh, with a denser distribution of nodes moving with the boundary. Such refinements would yield smoother and more accurate results.

APPENDIX

1. MATLAB Program 1 : ABmatrix Program.

```
% PROGRAM ab.m
%
% This Program calculates the global A and B coefficient matrices
%
% Remove the first row and columns
%
A=BigK(2:Numpts,2:Numpts);
B=BigM(2:Numpts,2:Numpts);
%
%
% Compute the inverse of matrix B :
%
invB=inv(B);
C=invB*A;
%
```

2. MATLAB Program 2 : KMmatrix Program.

```
% PROGRAM    km.m
%
% This Program calculates the global K and M matrices
%
%
%
vec1=alf2*ones(1,Numelts);
vec2=-alf2*ones(1,Numelts);

%%
kk=1;
while kk < count
vec1(kk+1)=alf1;
vec1(kk)=alf1;
vec2(kk)=-alf1;
kk=kk+1;
end
%
vec3=zeros(1,Numpts);
%
vec3(1)=vec1(1);
for jj=2:Numelts
vec3(jj)=vec1(jj)-vec2(jj);
end
vec3(Numpts)=alf2;
%%
% Calculate the matrix K
BigK=diag(vec3,0)+diag(vec2,1)+diag(vec2,1)';
%
vvv=ones(1,Numelts);
dg=2*[vvv,0]+2*[0,vvv];
%
% Calculate the matrix M
BigM=diag(dg,0)+diag(vvv,1)+diag(vvv,1)';
%
```

3. MATLAB Program 3 : Main Program.

```
% PROGRAM main.m
% This Program execute all sub-program including calculation and
% graphing
%
% Numelts=input(' Type the number of elements : ' )
Numpts=Numelts+1
h=1/Numelts
h2=h*h;
% DEFINE THE CONSTANTS
%
alf1=input(' Please type the value of alpha one : ' )
alf2=input(' Please type the value of alpha two : ' )
%
t=0.
Tfinal=input(' Select final the time value tf : ' )
deltaT=input(' Select the time step delta t : ' )
tvals=fix(Tfinal/deltaT)+1
%
% INITIALIZE THE VALUES
%
count=1;
u0=zeros(1,Numelts)';
p=[pf , u0]';
u=u0;
n=1;
s=zeros(1,tvals);
%
while t <= Tfinal
%
%
KMmtrx
%
Abmtrx
%
VEC
%
% INTEGRATE
```

```

t=t+deltaT;
runge
p=[pf, u]';
%
% CALCULATE BOUNDARY LOCATION
s(n+1)=s(n)-deltaT*beta*((p(count+1)-p(count))/h);
count=fix(s(n+1))+1;
n=n+1;
%
%
end
%
% Plot out s(t) with respect to t
%
number=max([n,tvals]);
times=deltaT*( 1:(number) - ones(1,number) )
%
plot(times,s)

```

4. MATLAB Program 4 : Runge-Kutta Program.

```
% PROGRAM Runge.m
%
% h2 is " h squared "
%
k1=deltaT*(-(6*C*u)/h2+invB*VECT);
k2=deltaT*(-(6*C*(u+k1/2))/h2+invB*VECT);
k3=deltaT*(-(6*C*(u+k2/2))/h2+invB*VECT);
k4=deltaT*(-(6*C*(u+k3))/h2+invB*VECT);
%
u=u+(k1+2*k2+2*k3+k4)/6;
%
```

5. MATLAB Program 5 : Vector Program.

```
% PROGRAM   Vec.m
%
% This Program calculates the Right Hand Side Vector -
%
% pf and pfdot must be given !!
%
VECT= [ (6*alf1*pf)/h2 - pfdot, zeros(1,Numelts-1) ]';
%
%
```

REFERENCES

- [1] **Cecil, Lawrence K.**, Water-1970, 107 Volume 67, Chemical Engineering Progress Symposium Series, American Institute of Chemical Engineering, NY, 1971.
- [2] **Bear, Jacob and Verruijt, D.**, Modeling Groundwater Flow and Pollution, Reidel Publishing Company, Dordrecht, Holland, 1987.
- [3] **Torok, J.S., Dean R. H. and Advani, S.H.**, ‘ An Exact Solution for Piston-Like Leak-Off of Compressible Fluids ‘, ASME Journal of Energy Resources Technology, Vol. 106, 1984.
- [4] **Aronofsky, J. S., Ph. D.**, Fluid Mechanics Flow Through Porous Media.
- [5] **McTernab William F. and Kaplan, Edward**, Risk Assessment for Groundwater Pollution Control, American Society of Civil Engineering, NY, 1990.
- [6] **Aubrecht, Gordon**, Energy, Merrill Publishing Company, 1989.
- [7] **Reddy, J. N.**, An Introduction to the Finite Element Method, Mcgraw-Hill, Inc., 1976.
- [8] **Strang, William Gilbert and Fix, George, J.**, An Analysis of the

- Finite Element Method, Prentice-Hall, Englewood Cliffs, NJ, 1986.
- [9] **Fluid Dynamics International, Inc.**, FIDAP General Information Manual, Illinois, 1990.
- [10] **Zillinger, Daniel**, Handbook of Differential Equations, Academic Press, Boston, 1989.
- [11] **Fluid Dynamics International, Inc.**, Fluid in A Porous Medium Theoretical Research, Illinois, 1990.
- [12] **Li, Wen-Hsiung**, Differential Equations of Hydraulic Transients, Dispersion, and Groundwater Flow; Mathematical Methods in Water Resources, Prentices-Hall, Englewood Cliffs, NJ, 1990
- [13] **Torok, J. S.**, ‘ Mathematical Modeling and Analysis of Mechanisms Associated with the Propagation of Hydraulically Induced Fractures in Poro-Elastic Media ‘, Ph. D. Dissertation, The Ohio State University, 1985.
- [14] **Phillips, O. M.**, Flow and reactions in Permeable Rocks, Cambridge University Press, NY, 1991.
- [15] **Rao, S. S.**, The Finite element Method in Engineering: Second Edition, Pergamon Press Inc., NY 1989.
- [16] **Geophysics Study Committee**, Studies In Geophysics, Groundwater Contamination, Geophysics Research Forum,

Commission on Physical Sciences, Mathematical and Resources,
National Academy Press, 1984.

- [17] **Akin, J. E.**, Finite Element Analysis for Undergraduates, Academic Press Inc., Orlando, FRA. 1986.
- [18] **Hadak, Paul F. and Loaiciga, Hugo A.**, ‘ Mass Transport Modeling In Contaminated Buried-Valley Aquifer ‘, Vol.117 No.1 American Society of Civil Engineers Water Resources Planning and Management Division, NY, March/April 1991.
- [19] **John McCarvill**, ‘ The Dynamics of A Moving Boundary Between Immiscible Fluids In A Porous Medium ‘, Master Dissertation, Rochester Institute of Technology, 1991.
- [20] **The Math Work Inc.**, MATLAB, Version 4 User’s Guide, Prentice-Hall, Englewood Cliffs, NJ, 1995.