The Dynamics of a moving boundary between immiscible fluids in a porous medium

John McCarvill

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THE DYNAMICS OF A MOVING BOUNDARY BETWEEN IMMISCIBLE FLUIDS IN A POROUS MEDIUM

BY
John McCarvill
A Thesis Submitted in Partial Fulfillment of the Requirements for the Degree of MASTER OF SCIENCE in MECHANICAL ENGINEERING

Approved By:
Prof. R. J. Hefner
Prof. Ali Ogut
Prof. J. S. Torok (Thesis Advisor)
Prof. Charles W. Harris (Department Head)

Department of Mechanical Engineering
College of Engineering
Rochester Institute of Technology
Rochester, New York
1991
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August 9, 1991

John R. McCarvill
DEDICATION

I would like to dedicate my thesis work to my father Roger McCarvill, my mother Donna McCarvill and my brother Roger McCarvill, Jr. in appreciation for all their love and support. This endless love and support allowed me to complete my college education with great success.

I couldn’t have done it without you guys.

Thanks!!!

John R. McCarvill
ABSTRACT

The analysis and simulation of the dynamics 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 is studied. The aforementioned scenario is simulated using a finite element based software, FIDAP. Analytical solutions developed in one dimension illustrate the concepts and serve as a benchmark for numerical solutions. The aim of computer simulation is to develop a model applicable to real situations, yet flexible enough for future adaptations to other problems with little modification.
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LIST OF SYMBOLS

\(a(t)\) - Interface position in piston-like displacement.

A - Arbitrary constant.

\(B^2\) - Constant of parameters.

C - Leak off coefficient.

c\(_i\) - Fluid compressibilities.

c\(_p\) - Specific heat at constant pressure.

c\(_{sp}\) - Species concentration.

\(\dot{c}\) - Inertia coefficient.

c' - Concentration of solute in source or sink.

\(\bar{c}\) - Average specific heat.

d - Average diameter of pore spaces.

\(D^*_{ij}\) - Coefficient of Dispersion.

\(f_i\) - Body force component per unit mass.

g - Gravitational constant.

h - Piezometric Head.

\(\Phi, \Phi_i\) - Formation permeability.

k - Counter variable.

K - Hydraulic Conductivity within Darcy's term.

L - Distance of direct path through medium bed.

\(L_e\) - Average distance traveled by fluid particle.

p, p\(_i\) - Fluid pressures.

q - Specific discharge.

q\(_s\) - Heat flux.

R - Chemical reaction rate.

\(R_e\) - Reynolds’ number.
LIST OF SYMBOLS
(CONTINUED)

s - Distance traveled by fluid.

s(t) - Freezing boundary.

t - Time variable.

t_f - Final time.

T - Temperature variable.

T_c - Low temperature value.

T_h - High temperature value.

T_r - Medium tortuosity.

u - Pressure gradient value of velocity.

U(x,t) - Ice temperature at any given time or location.

\|u\|^m - Magnitude of velocity.

V - Velocity of fluid.

V_b - Material bulk space.

V_s - Volume of solid.

V_v - Material void space.

V(t) - Inlet velocity at x=0.

VV - Region of porous media saturated with fluid.

VV_f - Volume occupied by the fluid.

VV_s - Volume of solid material.

W - Volumetric flow rate of source or sink per unit volume of porous material.

w - Water temp. at any given time or location.

x - Distance traveled by boundary location.

z - Height of fluid.
LIST OF SYMBOLS
(CONTINUED)

α - Variable satisfying the transcendental Freeze.

β - Volume expansion coefficient.

δ_{i,j} - Kronecker delta.

η - Arbitrary solution variable.

γ - Specific weight.

λ - Latent heat of fusion times density divided
    by coefficient of heat conduction.

μ, \overline{\mu} - Fluid dynamic viscosity.

ν - Fluid kinematic viscosity.

Ω - Domain of porous media.

Ω_f - Region occupied by fluid.

φ - Formation porosity.

ρ - Fluid density.

σ_{ij} - Stress tensor.

τ_{ij} - Deviatoric stress tensor.
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CHAPTER I

INTRODUCTION

People of the world today seem to be careless with respect to situations concerning the environment. The apparently uncontrolled technology arising from the Industrial Revolution has started an environmental and political trend in which the environment is being exploited and any concern for this exploitation is being unregulated. Both quantity and quality of air, water and land are important to the future of mankind. Today the federal government has the responsibility of coordinating an effective water pollution control program with all resources available. Pollution surveillance is one of these responsibilities. Policies reflecting these actions are still scarce [1]. It is only relatively recently that there has been a modest engineering trend toward a more serious concern about the environment.

The topic of concern here is groundwater. Groundwater is the major source of potable water that is located in fully-saturated strata of earth below the surface. Two important concepts of quantity and quality are inherent concerning groundwater. The amount of water (quantity) extracted from an underground source strata (aquifer) and the amount of contaminant added to the strata effects the water quality. An increase in water withdrawal enhances the accumulation of these contaminants. The same amount of contaminant remains as the
amount of water present decreases thus intensifying the amount of contaminant with respect to the amount of pure water.

The abuse of the earth's resources is worsening and soon will be an important concern to all. Today's industrial metabolism generates by-products at an alarming rate. These by-products directly interact with the earth. Water is the most important element needed to sustain life. Man can survive without food for several weeks, but death occurs within a few days from a lack of water.

There are endless uses for water. Agriculture, industry and domestic uses all consume different amounts. In the United States forty-seven percent of the ground water is used for agricultural purposes, forty-four percent of ground water is used for industrial purposes and the remaining nine percent is required for domestic usage. Figure 1 shows approximate division of use graphically.

![WATER USES IN THE U.S.](image-url)
In the past, technology was uncontrolled. All over the world men and women have used technology to gain short-term profits without any action against long-term contamination effects. The earth's groundwater supply is diminishing rapidly with population growth and the increased per-capita intake. The present distribution of available water reservoirs is ninety-four percent ocean, four percent inaccessible, one and one-half percent polar ice caps. The remaining one-half of a percent is fresh water available for use. This is illustrated in Figure 2.

![Water Reserves Diagram]

**FIGURE 2**

These statistics are even more staggering when one also considers the fact that most all of the usable water is subject to some sort of contaminant. The sources of contamination originate from agricultural, industrial, domestic and environmental sectors. A quote from The Poor Richard Almanacks
by Benjamin Franklin [2] reads, "When the well's dry, we know the worth of water." This statement may have to be altered such that it reads: "When the well's dry or rendered useless, we know the worth of water."

At one time it was thought that the earth could naturally filter out any type of pollutant introduced by man through the hydrologic cycle, or just through filtration [3]. The hydrologic cycle starts with evaporation of surface water into the atmosphere, due to the water being exposed to heat and sunlight. When this evaporation occurs, the sediments are left behind, and for a relatively short period the water is pure. This pure water reacts with tiny particulate matter such as fumes, salt, smoke, soot, dust and other gases, creating droplets and eventually forming clouds. The point is reached when the condensed droplets or crystals become too heavy to remain airborne and fall to the earth as precipitation. Upon arrival to the earth, some of the precipitation is absorbed by vegetation and transpired. Some remains on the surface, some percolates into the ground, and the balance will flow into streams toward lower ground and eventually to the sea.

Seepage into the earth will take place as the water enters the porous soil and slowly percolates through the permeable layers of earth, until it reaches the water table. Percolation is accomplished with the help of gravity and air pockets within the porous strata.

Upon the trek to the aquifer, the natural cycle (excluding evapo-transpiration) promotes sedimentation and filtration.
After all these years, the natural filtering of the earth alone can no longer handle the large amounts of contaminants still being added. The strata of soil, sand, gravel and stone trap some of the suspended contents and allow the water to continue on. This natural filter is dangerously clogged from contamination sources, such as hazardous industrial wastes, nuclear wastes, sewage, oil spills, leachate from landfills, agricultural chemicals and burning of fossil fuels. Consequently the water holds on to the impurities throughout the filtration cycle. Once the natural level of free groundwater is reached, the water flows as an underground stream (aquifer). A schematic representation of a typical underground cross section is depicted in Figure 3. For a list of principal sources of contamination see Appendix A.

FIGURE 3
A plot of the trend of the future groundwater pollution is shown in Figure 4. It is imperative that something be done to prevent this contamination process from continuing and to possibly correct previously contaminated zones.

(Adapted From [4])

Some possible ideas would be to implement on-site filtration systems, clean up present aquifers, choose the optimum yield of aquifers, as well as to use the abundant ocean water and process it. In an ecological context, filtration is
an important phenomenon. The basic components of a filtration system consist of fluid masses and a porous medium. There are various scenarios concerning porous media and fluids that interact with these media. Groundwater pollution (contamination) consists mainly of dissolved matter (transport of mass). This transport of mass assumption has since been questioned by a few researchers. Fried (1975, [5] pp. 17-27) cites some laboratory diffusion experiments in which the results of this experiment did not match theoretical expectations. Another researcher, Dagan (1982, [6]), noted that there is no reason to believe that the diffusion equation is at all applicable to contamination transport through porous media [7]. This concern relates to the hydrodynamic dispersion or miscible displacement-type transport. Concentration levels are dealt with by advection-diffusion equations (species equations shown later in the text) [8]. No matter what source of contamination one studies, there will always be a sharp interface present. The invading fluid in some cases does not mix with the resident stagnant fluid (immiscibility). The investigation of sharp fronts present in immiscible fluid approximations yields distance-versus-time information. 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 the another. This boundary of interaction is termed as the front or frontal
boundary. The front is most important 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 low potential energy. This energy is in the form of pressure or piezometric head, h, (potential and pressure energy). Simulation of contamination flow within the aquifer allows easy tracking of a contaminant. The simulation will also allow better approximation of displacement and concentration data for statistical analysis.

Another dominant motivating factor that entails frontal movement is the process of water injection for secondary recovery of trapped oil in existing reservoirs. Water is forced into a secondary well and pushes the oil to the producing well [9]. In a petroleum reservoir formation there is almost always a water-oil interface. The type of reservoir of concern is one without natural drive mechanisms. 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 occur in a low Reynolds' number situation \((\text{Re} \leq 10)\), well within the range of validity of Darcy's Law [3]. Contamination of groundwater and secondary oil recovery are examples of general problems involving the tracking of a moving boundary.

To date, the uncertainty of what is actually going on below the surface of the earth is still ambiguous and of major concern. Before the use of computer simulation, three main models were capable of studying flow of two liquids with an abrupt interface and examining hydrodynamic dispersion. These models were the Sand Box Model, the Hele-Shaw Parallel-plate Analog and the Electric Ion Analog. The Sand Box Model is just a physical reduced-scale representation of the porous medium domain. The Hele-Shaw Parallel-plate Analog is a viscous flow model, either vertical or horizontal in arrangement, that simulates the fluid interface. The Electric Ion Analog is a resistance-capacitance network that maps ion motion into fluid motion. Although these models are often quite correct, they are also time-consuming, restrictive and expensive. By developing and studying simulation techniques with the use of a computer, engineers will be able to maximize their abilities to quickly identify the source of the problem and determine an optimum course of action.

Many breakthroughs have been made in the study of pollution. Engineers are beginning to understand the importance of environmental monitoring and management. The
determination of potable water quality is now done with monitoring wells. Some current approaches to monitoring the contamination of an aquifer are statistical in nature. Local soil matrix properties are statistically averaged with respect to samples taken by monitoring wells. The flow characteristics are averaged to give an approximate value at a given location.

The ability to precisely model the subsurface layers of earth is quite difficult. There are many types of earth strata. Soil properties are always nonhomogeneous unless a location to be studied is small and well defined. The combination of having to determine the matrix properties and the amount of contaminant present creates a very uncertain situation. The Environmental Protection Agency uses a computer simulation called MULTIMED to analyze and predict aquifer movement and contamination. Other programs, such as Hydrologic Evaluation of Landfill Performance (HELP), are also used to assess the damage done to fresh water aquifers and the soil matrix they reside in [10]. Other computer uses include water records logging systems (WRLS) that provide a data base of local aquifer information. The latest monitoring techniques involve the use of fiber optics, well tapping, and methylene blue die tracking [11-13]. All of the popular programs developed today create a data base of information or simulate a local occurance of concentration. But most are just incapable of handling diplacement 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
investment are a finite difference scheme for tracer testing and the Method Of Characteristics (MOC) developed for U.S. Geological Survey use. The finite difference method takes information obtained by monitoring wells and predicts the fate of contamination concentration [12]. The MOC deals with solute transport and dispersion of the contamination [13].

By using the combination of the frontal boundary approximation and diffusion theories, models constructed will more closely resemble what is actually occurring below the surface.

The aim of this investigation hand is to develop a model simulation that is applicable to real situations, yet able to be extended to a realistic problem with little modification. Modeling will include finite element analysis methods to track the location of the contamination front. By re-running the same problem, advection-dispersion of the contamination concentration inclusive in the same simulation package will be extracted. This tracking technique may be applied to many similar situations to be addressed in the following chapters.

DESCRIPTION OF PROBLEM

The objective of this research is to investigate two-dimensional Stokes flow of immiscible Newtonian fluids in a porous medium. This porous medium can have properties and
conditions that are similar to any given problem at hand. The porous medium will be considered stationary, homogeneous and saturated. The flow is considered isothermal and isotropic. The main focus of this investigation is the quantification of boundary interaction of one fluid substance with another. This problem is motivated by concerns relating to pollution of groundwater, dam seepage and the importance of secondary petroleum recovery, as explained previously. Such problems are inherently difficult, since the solution of the field equations are 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 serve as a reliability check before attempting analysis in higher dimensions. Coupled differential equations governing the movement of the boundary will be solved using ACSL to establish a benchmark [14]. Finite element analysis will be applied to different situations 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.
DESCRIPTION OF PHYSICAL CONCEPTS

Fluid flow in a porous medium is applicable in many fields of engineering. Those applications encompass movement of groundwater in an aquifer, fluids in filters, oil within its reservoir strata and even fluids in organic tissues, just to name a few. A fluid is a substance that will deform continuously under the presence of applied shear stresses. The underlying physics within this investigation involves the motion of a Newtonian fluid flowing through a porous medium. A Newtonian fluid is a continuum in which shear stress is directly proportional to the rate of deformation.

Below is an example relating porous media flow to a cotton cloth held tightly against a water hose. The outlet pressure in the hose forces water through the cloth voids and eventually out the other side. Initially the dry cloth is free of any water molecules, thus the cloth matrix contains cavities of air. Once the water is pushed through the cloth, the cloth is considered saturated with water and the once-empty cavities now contain water. A schematic representation is shown in Figure 5.

![Diagram of porous medium flow](image)
The important factors, when studying flow through porous media, are the physical characteristics of both the fluid and the medium in which the flow takes place. All fluids are made up of a collection of molecules. These molecules are in constant motion. To get around concentrating on each individual microscopic particle, the fluid will be treated macroscopically. Conceptualization of the fluid in this manner means to look at it as if it were an infinitely divisible substance or a continuum. Viewing a fluid as a continuum is the basis of classical fluid mechanics. Consequently, each of the fluid properties is assumed to have a point-wise average value in space. Therefore, quantities such as density, temperature, velocity, to name a few, are considered continuous functions of time and space [15].

The flow of a homogeneous, immiscible fluid through a porous material depends on basic fluid properties. The first property is the absolute viscosity, $\mu$, 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. Viscosity is a measure of the resistance of a fluid to shear deformation. Its magnitude is specified with respect to the viscosity of water [15]. The second property is the fluid's density, $\rho$. The definition of fluid density is the mass of the fluid per unit volume. 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:

\[ \rho = \rho (p,T) \]  

[14]

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 voids of varying sizes 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, \( \phi \) [16,17]:

\[ \phi = \frac{V_v}{V_b} = \frac{V_b - V_s}{V_b} \]  

[1.1]

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 [18].

Permeability, \( \kappa \), is a coefficient that expresses a given fluid's macroscopic effects due to the microscopic solid-fluid interaction within a porous medium. This internal hydrological property is independent of the fluid's viscosity [3].
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 6 shows a schematic definition of tortuosity.

![Figure 6](image)

**FIGURE 6**

Tortuosity is defined by the equation below:

$$T_t = \frac{L_e}{L} \quad [1.2]$$

The tortuosity value is greater than one, where the value one implies a direct path (i.e. unobstructed pipe, etc.)

Porosity, permeability, and tortuosity are material dependent. Most often these values can be determined by experimental methods, if they are not already tabulated [4]. These values are extremely difficult to determine for simulation purposes, for two main reasons. One reason being
the difficulty in simulating realistic material properties. The second reason being the complex nature inherent to solving the governing partial differential equations [19].

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 non-isotropic materials do. Yet another important feature of the matrix includes temperature effects. Isothermal processes assume no temperature effects.

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 occupying a porous medium is displaced by a less viscous fluid (such as oil and water). Fingering occurs when the fluid interface is unstable and disturbances appear in the shapes of fingers. These disturbances elongate with wave-like motions [20]. The FIDAP software recognizes the frontal boundary as a macroscopic, homogeneous occurrence. If this macroscopic wall was broken into sub-sections and studied, fingering could be identified. Fingering is depicted in Figure 7. Due to the macroscopic point of view taken in this investigation, this phenomenon will be neglected.

![Fig 7](Adapted From [16])

FIGURE 7 (Adapted From [16])
The solid-structured material matrix may or may not be well-suited for fluid transport. The material properties mentioned previously determine if the material is well-suited for fluid transport. Recall that the quantity, $\phi$, represents the ratio of the interconnected pore volume to the bulk volume of the medium. The higher the value of porosity, the better the material is suited for fluid flow. There are problems in which one may also have to take into account the elasticity of the medium. In the present analysis, the material is assumed to be inelastic.

Gravel or creviced rock are typical aquifer strata. Some cross sections of porous rock material are shown in Figure 8 (A-F).

![Image of cross sections](image.png)

**FIGURE 8 (Adapted From [16])**

A - Well-sorted sedimentary deposits (high porosity)
B - Poorly-sorted sedimentary deposits (low porosity)
C - Well-sorted sedimentary deposits, porous pebbles ($\phi$ high)
D - Well-sorted sedimentary deposits with interstices ($\phi$ low)
E - Porous rock by construction
F - Porous rock by fracturing
There is a wide range of porous materials. For simplicity, two situations are depicted in Figure 9. A favorable packing situation is shown in Figure 9a and an unfavorable packing is shown in Figure 9b.

FIGURE 9 (Adapted From [16])

The porous matrix interstices are either filled with gas (usually air) or are saturated with some fluid. This air or fluid is forced out when another gas or liquid is introduced under some pressure. When this other fluid is introduced, the frontal boundary approximation allows for a sharp or abrupt interface. It is important to note that aquifer velocity is usually assumed to be horizontal in nature [17].

Now let us address the situations concerning the compressibility of fluids. A compressible fluid has a density, $\rho$, that changes with respect to pressure and temperature, as stated before. If the function $\rho$ maintains a constant value, the fluid is then considered to be incompressible. In the
simulations where fluid interfaces are present, the fluids will both be considered incompressible.
CHAPTER II

MECHANICS OF FLUID FLOW

The mechanics of fluid flow depends on the available pressure gradient. The pressure gradient 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 an analytical model of the underlying physics, a few fundamental equations describing fluid transport phenomena in a porous medium must be developed.

The equations governing the physics take the form of partial differential equations. Neglecting inertial terms, the incompressible-flow Navier-Stokes equations of a liquid continuum in a gravitational field are

\[ \nabla (p + \rho gz) = \mu \nabla^2 V \]

\[ \text{div}(V) = 0 \]

Where \( z \), \( g \) 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.

The continuity equation, [3.1a], pertaining to an incompressible fluid within a solid, homogeneous, isotropic material matrix will be explained in detail later.

Low flow rate situations are termed laminar creeping flows. In these types of flows, the Navier-Stokes equations can be used. Equation [2.3] is the the governing equation for an incompressible fluid, known as the Navier-Stokes equation:

$$\rho \frac{D \vec{V}}{Dt} = \rho \vec{g} - \nabla p + \mu \nabla^2 \vec{V}$$

[2.3]

Fluids that display viscous or laminar character can be modeled using Darcy's law. For this 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

$$Re = \frac{\rho V d}{\mu}$$

[2.4]

As long as the Reynolds' number is within the range of 1 to 10, Darcy's law is also valid [15]. The diameter of the pore space
is defined in many different ways. It can be expressed in terms of permeability and porosity as

$$d \approx \sqrt{k}$$  \[2.5a\]

if one has a good approximation of permeability only. It can also be expressed as

$$d \approx \sqrt[3]{k/\phi}$$  \[2.5b\]

if a good approximation of both permeability and porosity exist.

Thus substitution into equation [2.4] results in

$$R_e \approx \frac{\rho V \sqrt{k}}{\mu}$$  \[2.6a\]

or

$$R_e \approx \frac{\rho V \sqrt{k/\phi}}{\mu}$$  \[2.6b\]

Depending on which approximation is used for d, that choice will dictate which $R_e$ to use. Equation 2.6b was used in the Reynolds' number calculations for the analysis. Using the
continuum approach, neglecting internal fluid friction and inertial effects, the average momentum balance reduces to a linear equation known as Darcy's law [3]. For an isotropic medium containing a homogeneous, incompressible fluid, Darcy's Law is stated as

$$\bar{q} = -K \frac{\partial h}{\partial s}$$  \hspace{1cm} [2.7]$$

where $\bar{q}$, $h$ and $s$ are the specific discharge, the piezometric head and the distance traveled by the fluid, respectively. Here hydraulic conductivity, $K$, is defined by

$$K = \frac{\kappa \gamma}{\mu} = \frac{\rho \kappa g}{\mu}$$  \hspace{1cm} [2.8]$$

The fluid velocities in the $x$ and $y$ directions are

$$V_x = -K \frac{\partial h}{\partial x}$$  \hspace{1cm} [2.9a]$$

$$V_y = -K \frac{\partial h}{\partial y}$$  \hspace{1cm} [2.9b]$$

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 as:

\[ u = -\frac{\kappa}{\mu} \left( \frac{dP}{dx} \right) \]  \[2.10\]

where \( u \) represents the fluid velocity.

**SIMILARITY SOLUTIONS FOR MOVING BOUNDARY PROBLEMS**

Solution by analogies is a convenient method of analyzing physically unrelated problems. A wide range of problems can be considered when implementing the parabolic partial differential equation of the form

\[ \frac{\partial^2 \Box}{\partial x^2} = B^2 \frac{\partial \Box}{\partial t} \]  \[2.11\]

in which: \( \Box \) \( \equiv \) Field Variable studied. \( B^2 \) \( \equiv \) Constant of parameters.
It is possible to correlate any situation, be it a moving interface driven by a pressure gradient or a melt interface driven by a temperature gradient. The field variable for the moving fluid interface would be, \( p \), and for the melt (freeze) boundary interface it would be \( T \). The coupling values lie within the \( B^2 \) term. For the fluid moving boundary, \( B^2 \) depends on \( c_i, \mu \) and \( \kappa \). The melt (freeze) boundary \( B^2 \) depends on \( \rho, c_p \) and \( \kappa \). Table 1 depicts the correlation more clearly. Simple changes of boundary conditions, initial conditions, material properties and fluid properties will yield an entirely different problem. Other alterations include changing the size and shape of the domain or modifying it in a specified location.

**TABLE 1**

<table>
<thead>
<tr>
<th>Pressure Driven Boundary</th>
<th>Temperature Driven Boundary</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Equation</strong></td>
<td></td>
</tr>
<tr>
<td>[ \frac{\partial^2 p}{\partial x^2} = B^2 \frac{\partial p}{\partial t} ]</td>
<td>[ \frac{\partial^2 T}{\partial x^2} = B^2 \frac{\partial T}{\partial t} ]</td>
</tr>
<tr>
<td><strong>Constant</strong></td>
<td></td>
</tr>
<tr>
<td>[ B^2 = \frac{\phi \mu c_i}{k_i} ]</td>
<td>[ B^2 = \frac{\rho c_p}{\kappa} ]</td>
</tr>
<tr>
<td><strong>Variables</strong></td>
<td></td>
</tr>
<tr>
<td>( \phi ) - porosity</td>
<td>( \rho ) - mass density</td>
</tr>
<tr>
<td>( \mu ) - dynamic viscosity</td>
<td>( c_p ) - specific heat</td>
</tr>
<tr>
<td>( c_i ) - compressibility</td>
<td>( \kappa ) - thermal cond.</td>
</tr>
<tr>
<td>( k ) - permeability</td>
<td></td>
</tr>
</tbody>
</table>
Moving boundary problems require a governing differential equation which must be solved within a domain that has varying spatial extent. One of the fundamental unknowns is the size of the domain. For some one-dimensional problems, the location of a free boundary may be determined by a similarity solution.

In one spatial dimension, locating the boundary of a domain of a system of differential equations involves the use of similarity solution methods. Numerical solution methods are necessary for problems in multiple space dimensions.

One simple example that can be considered is that of freezing water [22]. This type of problem is termed a Stefan problem, in which the boundary of the domain must be solved for in addition to solving the governing heat equations. Consider a tube of water at room temperature that has one end subjected to a heat sink (below freezing temperature). The water will freeze, starting at the end subjected to the cold temperature $T_c$. The frontal boundary of the freezing portion of the water will traverse the tube and eventually reach the opposite end. This type of problem is formulated and schematically represented in Figure 10.
Initially, $T_h > 0$ for $x > 0$ and $T_c$ is subsequently maintained for all time at $x = 0$. The position of the freezing boundary, $x = s(t)$, will be tracked as it moves into the fluid. The unknowns that are solved for are the temperature of the water, $w(x,t)$, the temperature of the ice, $U(x,t)$, and the location of the moving boundary, $x = s(t)$. The equations that govern the heat transfer are:

$$U_t = U_{xx}, \text{ for the domain } 0 < x < s(t), t \geq 0 \quad [2.12a]$$

Equation [2.12a] is true for a Stefan number of one, that is setting thermo-physical properties of water and ice equal. Also,

$$w_t = w_{xx}, \text{ for the domain } s(t) < x < \infty, t \geq 0 \quad [2.12b]$$

Next we apply the boundary condition for the ice temperature

$$U(0,t) = T_c \quad [2.12c]$$

and the initial condition for the water temperature

$$w(x,0) = T_h \quad [2.12d]$$

Further defining the necessary temperature interface conditions that exist at the freezing boundary to be zero

$$U(s(t),t) = 0 \quad [2.12e]$$

$$w(s(t),t) = 0 \quad [2.12f]$$
and representing the transfer of latent heat to create the ice by

\[ U_x(s(t),t) - w_x(s(t),t) = \lambda \ s'(t) \]  \hspace{1cm} [2.12g]

We can now apply similarity solution techniques. Lambda, \( \lambda \), represents the latent heat of fusion times the density divided by the coefficient of heat conduction.

Applying similarity methods to the above partial differential equation, we are able to solve for the interface displacement [22]. When a similarity solution is performed, the original number of independent variables in the partial differential equation is reduced by taking algebraic combinations of the independent variables. Therefore, for \( n \) original independent variables, a form of the partial differential equation is constructed such that it will not depend directly on all \( n \) variables. A similarity solution is assumed of the form:

\[ U(x,t) = f(\eta) = f\left(\frac{x}{\sqrt{t}}\right) \]  \hspace{1cm} [2.13a]

and

\[ w(x,t) = g(\eta) = g\left(\frac{x}{\sqrt{t}}\right) \]  \hspace{1cm} [2.13b]

The above forms are only possible when forcing equation [2.12g] to satisfy the conditions imposed by the similarity
representation

\[ s(t) = \alpha \sqrt{t} \]  \hspace{1cm} [2.13c]

Substitution of \( U(x,t) \), \( w(x,t) \) and \( s(t) \) into the differential equation yields the equivalent system of ordinary differential equations

\[ f''(\eta) + \frac{1}{2} \eta f'(\eta) = 0, \quad \text{for } 0 < \eta < a \]  \hspace{1cm} [2.13d]

\[ g''(\eta) + \frac{1}{2} \eta g'(\eta) = 0, \quad \text{for } a < \eta < \infty \]  \hspace{1cm} [2.13e]

along with the corresponding initial and boundary conditions

\[ f(0) = T_c, \]  \hspace{1cm} [2.13f]

\[ f(a) = 0, \]  \hspace{1cm} [2.13g]

\[ g(\infty) = T_h, \]  \hspace{1cm} [2.13h]

\[ g(a) = 0 \]  \hspace{1cm} [2.13i]

\[ f'(a) - g'(a) = \frac{\lambda a}{2} \]  \hspace{1cm} [2.13j]

The above ordinary differential equations may be solved by series methods to arrive at
\[ f(\eta) = T_c - T_h \frac{\text{erf}(\eta/2)}{\text{erfc}(\eta/2)} \] \[ \text{[2.13k]} \]

and

\[ g(\eta) = T_h \frac{\text{erf}(\eta/2)}{\text{erfc}(\eta/2)} \left[ \text{erf}(\frac{\eta}{2}) - \text{erf}(\frac{\eta}{2}) \right] \] \[ \text{[2.13l]} \]

Here \( \alpha \) satisfies the transcendental equation (necessary condition) for the freezing boundary

\[ \frac{T_h}{\text{erf}(\frac{\eta}{2})} + \frac{T_c}{\text{erfc}(\frac{\eta}{2})} = -\left( \frac{\Delta \sqrt{\pi}}{2} \right) \exp\left( \frac{a^2}{4} \right) \] \[ \text{[2.13m]} \]

Equations [2.13a] through [2.13m] are now the newly represented governing equations of the freeze problem to be solved. Once a solution is reached in terms of \( \alpha \) and \( \eta \), the solution to the original problem is easily obtained. As mentioned before, there are a variety of problems that can be studied. The melt situation is analogous to freezing. The only difference is the movement direction of the boundary. The movement follows the direction of the temperature gradient. Figure 11 shows the melt interface and its intrinsic direction. Another example of the formulation and solution of a moving boundary problem is from geophysics.
The following is a description of the piston-like displacement of two compressible fluids in a semi-infinite domain [23]. The problem formulation and solution follow for specified types of conditions.

The pressure in each domain is expressed as

\[ p_1(x,t) ; \quad x < a(t) \]
\[ p(x,t) = \begin{cases} 
  p_1(x,t) & ; \quad x < a(t) \\
  p_2(x,t) & ; \quad x > a(t) 
\end{cases} \]

where \( a(t) \) is the interface position. The representative diffusion equation, as explained in the previous section, is expressed as

\[ \frac{\partial^2 p_i}{\partial x^2} = \phi \mu_i c_i \frac{\partial p_i}{\partial t} \]  \[ 2.14a \]
The specific boundary and initial conditions to be considered are:

\[ p(0,t) = p_I \quad ; \quad t > 0 \quad [2.14b] \]

\[ p(x,0) = p_0 \quad ; \quad x \geq 0 \quad [2.14c] \]

and that \( \lim_{t \to \infty} p(x,t) = p_0 \) at any time \( t < \infty \). \quad [2.14d]

Equation [2.14b] specifies a constant input pressure, \( p_I \). The initial condition [2.14c] represents the minimum pressure, \( p_0 \), at any location along the \( x \)-direction. Finally, boundary condition [2.14d] shows as \( x \) gets extremely large, the pressure will equal the minimum pressure \( p_0 \).

Interface conditions at \( x = a(t) \):

Following from Darcy's Law

\[ \phi \frac{\partial a}{\partial t} = -\frac{x}{\mu_i} \frac{\partial p_i}{\partial x} \quad [2.14e] \]

For continuity of pressure, \( p_1 = p_2 \) at the interface \( x = a(t) \). \quad [2.14f]
Solution to equations [2.14a] through [2.14f] parallel the previous similarity solutions. The form of the solution is given over the respective domains by

\[ p_1(x,t) = A \text{erf} \left( \frac{x}{2\sqrt{\xi t}} \frac{1}{\phi \mu_1 c_1} \right) + p_f \quad [2.14g] \]

and

\[ p_2(x,t) = B \text{erfc} \left( \frac{x}{2\sqrt{\xi t}} \frac{1}{\phi \mu_2 c_2} \right) + p_s \quad [2.14h] \]

where

\[ \text{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-w^2} dw \quad [2.14i] \]

is known as the error function. The complementary error function is defined as

\[ \text{erfc}(z) = 1 - \text{erf}(z) \]

The constants A and B as well as the interface location a(t) are determined from equations [2.14e] and [2.14f]. By substituting equations [2.14g] and [2.14h] into equation [2.14f], the following necessary condition must be satisfied:
\[ A \text{ erf} \left( \frac{a}{2 \sqrt{\phi \mu_1 c_1}} \right) + p_f = B \text{ erfc} \left( \frac{a}{2 \sqrt{\phi \mu_2 c_2}} \right) + p_o \]  

[2.14j]

for specified selection of \( \mu_i \) and \( c_i \). Equation [2.14j] will hold true for all time if \( a(t) = \lambda \sqrt{t} \). This solution results in a constant interface pressure

\[ A \text{ erf} \left( \frac{\lambda}{2 \sqrt{\phi \mu_1 c_1}} \right) + \Delta p = B \text{ erfc} \left( \frac{\lambda}{2 \sqrt{\phi \mu_2 c_2}} \right) \]  

[2.14k]

where

\[ \Delta(p) = p_f - p_o, \]

For convenience, set

\[ \beta = \lambda \sqrt{\frac{\mu_1 \phi}{2 t \Delta(p)}} \]

Now we can combine equations [2.14e], [2.14g], [2.14h] and [2.14k] to obtain a single equation for \( \beta \).

\[ \sqrt{\frac{2}{\pi}} c_i \Delta(p) - \beta e^{\frac{1}{2} c_1 \Delta(p)} \beta^2 \text{ erf} \left( \frac{1}{2} c_i \Delta(p) \beta \right) = \]
\[
\sqrt{\frac{c_1\mu_2}{c_2\mu_1}} \beta e^{\frac{\mu_2}{2\mu_1} c_2 \Delta(p)} \beta^2 \text{erfc} \left( \sqrt{\frac{\mu_2 c_2 \Delta(p)}{2\mu_1}} \beta \right) \tag{2.141}
\]

For specific material and fluid properties, equation [2.141] can be solved for the constants A and B with known $\beta$. Using equations [2.14g] and [2.14h] the pressure profile can thus be determined.

With constant injection pressure, $p_f$, the fluid front location is now

\[
a(t) = \left( \frac{2t(p_f - poo)}{\phi \mu_i} \right)^{\frac{1}{2}} \sqrt{t} \tag{2.15a}
\]

and the necessary fluid inlet velocity is

\[
V(t) = \frac{C}{\sqrt{t}} \tag{2.15b}
\]

where

\[
C = \left( \frac{\phi \mu_i (p_f - poo)}{2\mu_i} \right)^{\frac{1}{2}} \tag{2.15c}
\]

The above derivation illustrates a similarity solution for the displacement of two compressible fluids in a porous medium.
Still another example is the interface between incompressible, immiscible fluids. One fluid exists in the medium at a pressure $p_2$ and a velocity $V_2$ and a second fluid is introduced at a pressure $p_1$ and a velocity of $V_1$. The interface is formed and moves in the general direction of the pressure gradient. Assuming $p_1 > p_2$, liquid 1 will be entering the domain of liquid 2. Frontal displacement occurs. For a schematic representation including boundary conditions, see Figure 12. Again the important information that one desires is the displacement of the interface as a function of time [23]. This situation will be simulated using FIDAP. All of the above scenarios are examples of situations for which computer simulation is necessary for modeling and analysis.
POROUS MEDIUM FLOW PROBLEMS

As stated before, a considerable number of problems in geotechnical engineering involve the movement of gases and/or liquids through porous media. A few examples were already mentioned. To get an understanding of how these fluids and media interact, we can implement computational methods to formulate and simulate certain phenomena.

The continuum formulation of the porous medium problem within the framework of finite element analysis (FEA) is based on the assumptions that the porous medium is homogeneous, isotropic and that the fluid and solid are in thermal equilibrium. In a domain of interest, Ω, there is a region $V_V$ containing a rigid porous material saturated with an incompressible fluid, as well as a region occupied entirely by fluid, $Ω_f$. The saturating fluid may be the same as or different from the flooding fluid. Letting $V_V f$ be the volume occupied by the fluid and $V_V$, the volume occupied by the solid, the entire region is symbolically expressed as

$$V_V = V_V f + V_V s,$$  \[2.16a\]

The porosity, $\phi$, of the porous medium is specified here by
\[ \phi = \frac{\nabla \cdot f}{\nabla \cdot} \] 

[2.16b]

The momentum, incompressibility and energy equations on a volume-averaged basis become:

**MOMENTUM:**

\[
\frac{\rho}{\phi} \frac{\partial u_i}{\partial t} + \left[ \frac{\rho c}{\sqrt{k_i}} \|u\|^m + \frac{\mu}{k_i} \right] \mu_i = -p_i + [\bar{\mu}(u_{i,j} + u_{j,i})] + \rho f_i
\]

[2.16c]

Setting \( \bar{\mu} \) and \( c \) equal to zero for Darcy's formulation yields

\[
\frac{\rho}{\phi} \frac{\partial u_i}{\partial t} + \frac{\mu}{k_i} \mu_i = -p_i + \rho f_i
\]

[2.16d]

**CONTINUITY:**

\[(\rho u_i)_i = 0\]

[2.16e]

**INCOMPRESSIBILITY:**
\[ u_{i,j} = 0 \]  \[ 2.16f \]

**ENERGY:**

\[
(\rho c_p) \frac{\partial T}{\partial t} + \rho c_p u_j T_{,j} = (\kappa T_{,i})_{,i} + \mu \phi + q, \]  \[ 2.16g \]

The next equation [2.16h] is termed the species equation. The species equation is often seen in mass diffusion problems. It is necessary to present the species equation to inform the reader of its importance in a contamination situation. This equation will be described in the Advection-Dispersion Section.

**SPECIES:**

\[
\rho \left( \frac{\partial c_{sp}}{\partial t} + u_j c_{sp, j} \right) = \left[ (\rho \alpha_m) c_{sp, j} \right] + q + R \]  \[ 2.16h \]

where \( \hat{c} \) is the inertial coefficient, \( ||u|| \) is the magnitude of the velocity, \( c_p \) is the specific heat at constant pressure, \( c_{sp} \)
is the species concentration, R is the chemical reaction rate and q, is the heat flux. The subscript ε indicates an effective property and is related to fluid and solid matrix properties by the assumed relations:

\[(\rho c_p)_\varepsilon = \phi c_p + (1 - \phi)(\rho c_p), \quad [2.16i]\]

\[\kappa_\varepsilon = \phi \kappa + (1 - \phi)\kappa, \quad [2.16j]\]

Effective properties are statistically determined by the most common occurrence of values for these properties. This means there is no simple correct value for any given property. Different situations yield different property values [24]. The above equations and concepts will be implemented in the various cases during simulation.

**ADVECTION-DISPERSION**

The advection-dispersion assumption of dealing with contamination is based on Fick's Second Law of Diffusion. As mentioned before, there has been some disagreement on the validity of this assumption. After sufficiently long periods of time, Fick's Second Law can be assumed to be applicable.
The governing equations are as follows:

**MASS FLUX DUE TO DISPERSION:**

\[
\frac{\partial}{\partial x_i} \left( D_{ij} \frac{\partial c_{sp}}{\partial x_i} \right)
\]  

[2.17a]

**ADVECTION-DISPERSION:**

\[
\frac{\partial}{\partial x_i} \left( D_{ij} \frac{\partial c_{sp}}{\partial x_i} \right) - \frac{\partial}{\partial x_i} \left( c_{sp} v_i \right) - \frac{c_{sp}' W}{\phi} + \sum_{k=1}^{t_f} R = \frac{\partial c_{sp}}{\partial t}
\]  

[2.17b]

Where \( D_{ij} \), \( c' \) and \( W \) are coefficient of dispersion, concentration of solute in a source or sink and volume flow rate of a source or sink per unit volume of a porous material. This assumption yields concentration-versus-time information when applied. The background mentioned here serves to inform the reader of the equations governing this type of solution.
FRONTAL APPROXIMATION (ABRUPT INTERFACE)

There is a transition zone between two immiscible liquids flowing simultaneously in a porous medium. This zone is usually quite narrow relative to the regions occupied by each liquid. These interfaces are important in the study of fluid injection for recovery of oil from an oil reservoir and in immiscible contamination situations. This front is also seen between miscible fluids, such as in the case of salt water intrusion or miscible contamination situations. The difference is that after a short period of time, the sharp boundary develops into a transition zone. Assuming this zone is quite small, miscible approximations are able to be modeled as well [17]. Figure 13 schematically shows the interface.

![Interface Between Two Immiscible Fluids](image)

**FIGURE 13**

Let $R_i$, denote some porous medium region occupied by its respective liquid, 1 or 2. Let $B$ denote external boundaries. In the case of a free surface, the upper boundary will be subjected to atmospheric pressure conditions.
CHAPTER III

MOVING BOUNDARY PROBLEMS

The formulation of a problem involving a moving boundary involves setting up a mesh that is capable of deforming. This is done by constructing a mesh with nodes located on a moving boundary, thus introducing additional degrees of freedom. 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. The free surface condition occurs when a liquid comes into contact with a gas, such as air. There is an interface between the liquid and gas. Problems that involve a free surface interface are not easily tractable, so approximate solutions are needed. Reliable quantitative predictions for contamination movement can be found using simulations based on knowledge acquired earlier, possibly by the data base already developed or from existing monitoring wells.
**FINITE ELEMENT ANALYSIS OUTLINE (FEA)**

The finite element technique 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.

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 the necessary condition $\delta I = 0$ over each element. Instead 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 PDE expressing the field variable.
2 - Put the PDE into variational form.
3 - Divide the physical domain into elements.
4 - Apply the B.C.’s.
5 - Solve in terms of the assumed basis functions.
6 - Set up local matrices.
7 - Assemble globally.
8 - Solve for unknowns.

For a more detailed explanation, refer to sources [26-32].
Background on FIDAP

Computer aided analysis can play a significant role in understanding a physical situation. Focusing on groundwater monitoring, computer analysis allows the engineer to perform simulations and parametric studies to determine the operating characteristics for prescribed situations. The overall benefit being improvement and shortening of the design process, problem variation capabilities and an understanding of the system's response in a given situation before prototype construction. The use of FIDAP was selected due to the program's ability to deal with porous medium flow and moving boundary problems. FIDAP, an acronym for Fluid Dynamics Analysis Package, uses the finite element method to simulate phenomena dealing with incompressible fluid flows.

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

Continuity Equation:
\[ \frac{\partial p}{\partial t} = \rho(u_i) \]  \hspace{1cm} [3.1a]

LINEAR MOMENTUM EQUATION:

\[ \rho \left[ \frac{\partial u_i}{\partial t} + u_i u_{i,j} \right] = \sigma_{i,j,j} + \rho f_i \]  \hspace{1cm} [3.1b]

ENERGY EQUATION:

\[ (\rho c_p) e \frac{\partial T}{\partial t} + \rho c_p u_j T_{,j} = (\kappa \varepsilon T_{,i})_{,j} + \mu \phi + q_j \]  \hspace{1cm} [3.1c]

The system of the generated differential equations is then solved by internal numerical techniques. The results of velocities, pressures and temperatures throughout the region of interest are then easily accessible through post-processing.

Simple steps are followed to generate a working file in FIDAP. These steps, as well as the above equations, are discussed in detail in the FIDAP user manual. A simple outline to the general problem is shown below:
1 - Generate mesh.
2 - Input physical properties.
3 - Input boundary and initial conditions.
4 - Specify the class of problem.
5 - Specify solution procedures.
6 - Governing partial differential equation transformation into algebraic equations.
7 - Solution of algebraic equations.
8 - Graphical output of field variables and derived output quantities.

In the above outline, sections 1 thru 5 are done within an input file generated by the user (pre-processing). Sections 6 thru 8 are done internally by the software and the output is done by user menu interaction (post-processing) [33].

**GENERIC MODEL**

Figure 14a shows a sketch of the computation domain that is used to approximate the conceptual model. The experimental time intervals is assumed to be 0.01 seconds for accuracy. The acquifer has an assumed horizontal background velocity which yields a Reynolds' number of no more than ten in order to accommodate for Darcy's Law.
The aquifer under consideration is assumed to be uncontaminated at the onset of the modeling. The particular case selected for analysis was a confined top and bottom aquifer. The contaminant (or tracer) is entering from the left, flowing toward the right. The initial interface location is at mid-distance on the x-axis for the horizontal problem and at mid-distance on the y-axis for the vertical problem.

The first case to be studied will be the simple steady-state and transient representation of a porous medium. The subsequent cases will focus more on the free surface capabilities of FIDAP.

The next case to be simulated on FIDAP will be the melt problem. This is established as a bench-mark check to be
compared to the analytical ACSL output of the similarity pressure problem. The cases following the bench-mark test will be two-fluid interface and advection-dispersion problems.

All problems will be run first in the steady-state case for development of a usable initial guess in the transient regime. Using this steady-state solution, the transient solution will be obtained by restarting the problem. A final run will be made to establish the relevant concentration information.

**FILE CONSTRUCTION AND CLASSIFICATION ON FIDAP**

Three fundamental problems have been modeled using FIDAP. These problems are classified as the melt interface tracking, two-fluid interface tracking and an advection-dispersion model. All three of these problems will be modeled on the same generated mesh configuration shown in Figure 14b. The number of elements and nodes can be altered at any time to further discretize the domain of interest. For the problem at hand, simplicity allows minimal mesh refinement to save on computer run-time. The differences in the files are the input conditions and element declarations corresponding to the particular problem of interest. To simulate and solve these problems effectively, the correct representation according to FIDAP is extremely important. Each simulation will be two-
dimensional and discretized with quadrilateral elements that have nine nodes each. The individual files will be explained in the following paragraphs.

For the melt interface problem, elements are declared as continuum for the liquid, solid for the frozen material and melt at the interface. Using the melt elements enables nodes along a string or line called a spine to move. The spine adds another degree of freedom to the node and thus allows displacement information to be obtained. The boundary conditions needed for this melt problem are high temperature, low temperature and a melt temperature. In selecting the high and low temperatures, a temperature gradient is defined. The material properties define the density and viscosity of the liquid. To arrive at a transient solution, one must first run a steady-state, fixed-node solution to obtain a reasonable initial guess. This steady-state solution is then read in and used to initiate the transient solution run.

For the two-fluid interface problem, elements for both fluids are continuum-type. Again, the use of spines is necessary to enable tracking of transient displacement information. The boundary condition selected for this file is an inlet velocity that dictates the Reynolds number of the flow. This velocity input inherently creates a pressure gradient. The fluid properties consist of viscosity and density. For the attempted runs, a non-dimensionalized solution was needed, due to the resulting small magnitudes of velocity. It is extremely important to do this correctly. For
additional instruction on nondimensionalization, see FIDAP General Information Manual [34]. The transient solution also requires a steady-state solution for a reasonable initial guess.

For the advection-dispersion problem file, elements are declared as species-type elements. Using the species declaration allows the mass transport (advection-dispersion) equations to be solved. Boundary conditions needed for this problem are inlet flux conditions. This will enable one species (fluid one) to enter the region of the other fluid, thus changing the concentration of each one. A converged solution will ultimately yield concentration information.

All of these input files (see Appendix E) are run through FIMESH and FIPREP, which are internal to the FIDAP software, ensuring correct pre-processing. Once a successfully created file is completed in FIPREP, a solution is generated by running the file through FIDAP. Many solution techniques are available in FIDAP. It is up to the user to select the one that converges most efficiently.

Once a solution has successfully converged, one uses the post-processor portion of the FIDAP software, FIPOST, to obtained output information. This output ranges from color contour plots of velocity vector, pressure, streamline, history of front displacement, history of diffusion and convergence plots. Other output is available as well, but the aforementioned information is of primary concern.
The initial model file deals with a porous rectangular block of material that has a fluid entering the top left corner and leaving the entire right side. The top, bottom and bottom left side maintain boundary conditions that do not allow flow (no x or y velocities). A schematic representation of the aforementioned problem is shown in Figure 15a. For the first run, the fluid was chosen to be water and the solid matrix having properties of sand. Both steady-state and transient runs were made with this file to obtain a solution that would establish reliability of the software and its transient capabilities. The steady-state solutions for velocity vectors, pressure contours and streamline contours are shown in Figures 15 b-d. The transient solutions for the same conditions are shown in Figures 16 a-c.
FIGURE 15d

Porous steady state flow model 1, velocity in left.

FIGURE 16a

Porous transient flow model 1, velocity in left.
The main objective of the next simulation is to analyze flows in a porous medium which contain a moving interface. Two immiscible liquids of different densities and viscosities will enter an empty block of porous material (cavity of earth), each with some initial velocity. The upper surface, will stay unexposed to the atmosphere. This is refered to as the fixed boundary case. Eventually a portion of the program is altered to allow a free surface to form between the upper liquid and the atmosphere. This is refered to as the free case. For every transient free-surface run on FIDAP, a steady-state fixed case must be solved for an initial guess at a solution. This problem is described in the FIDAP Examples Manual section entitled Merging Liquid Streams (see Appendix C) The output from the above programs are shown in Figures 17 a-d and Figures 18 a-e.

The output presented shows the fixed case in Figure 17. The plots a-d show mesh, velocity vector, pressure contour and streamline contour information, respectively. The output shows the free case in Figure 18. The plots a-e show deformed mesh, free surface, velocity vector, pressure contour and streamline contour information, respectively. These results show that free surface capabilities can be readily implemented.
TWO MERGING LIQUIDS WITH ONE EXTERNAL AND AN INTERIOR

SCREEN LIMITS
XMIN 0.000E+00
XMAX 0.250E+02
YMIN 0.000E+00
YMAX 0.405E+01

FIDAP 5.01
27-JUN-91
11:25:14
FIGURE 18b

TWO MERGING LIQUIDS WITH ONE EXTERNAL AND AN INTERIOR

FREE SURFACE PLOT

SCREEN LIMITS
XMIN 0.000E+00
XMAX 0.250E+02
YMIN -905E+01
YMAX 0.131E+02

FIDAP 5.01
27-JUN-91
11:24:08
TWO MERGING LIQUIDS WITH ONE EXTERNAL AND AN INTERIOR

VELOCITY VECTOR PLOT

SCALE FACTOR
0.50000E+02
MAX. VECTOR
0.16333E+01
PLOTTED AT NODE
358

SCREEN LIMITS
XMIN 0.00000E+00
XMAX 0.25000E+02
YMIN 0.00000E+00
YMAX 0.40500E+01

FIGURE 18c
TWO MERGING LIQUIDS WITH ONE EXTERNAL AND AN INTERIOR

PRESSURE CONTOUR PLOT

LEGEND
-- 0.6857E+00
-- 0.4794E+01
-- 0.8903E+01
-- 0.1301E+02
-- 0.1712E+02

MINIMUM
-0.13686E+01
MAXIMUM
0.39718E+02

SCREEN LIMITS
XMIN 0.000E+00
XMAX 0.250E+02
YMIN 0.000E+00
YMAX 0.405E+01

FIDAP 5.01
27-JUN-91
11:14:29
The next problem relates to the example in the FIDAP Examples Manual and is included for illustrative purposes. It deals with isothermal seepage in the vicinity of a water channel located in a region of saturated soil. The problem is assumed to be two-dimensional. For the description of the entire problem, see Appendix D. The output of the processed solution is shown schematically in the Figure 19 a-d. The plots in a-d show mesh, velocity vector, pressure contour and streamline information, respectively.
**FIDAP IMPLEMENTATION LOGIC**

A moving boundary problem with the two-fluid interface within a porous medium is the primary simulation model of interest. The distance that the interface moves with respect to time is the critical information desired. The only complication was the need to couple the porous media capabilities with the free surface capabilities. From research and information acquired through FIDAP manuals and the software support group, the initial problem was thought to be easily modeled. The porous medium, frontal boundary mapping problem was never before attempted on FIDAP. To develop the solution of a moving boundary problem in a porous medium, it is necessary to couple the porous potential of FIDAP with the free surface potential of FIDAP. In each individual capability there are many unknowns to be solved for. Combining both of these capabilities creates a situation with insufficient information needed to solve the equations. FIDAP can handle these separately. Again, due to the complexity of both the porous media field equations and free surface equations, it was discovered that it can not be simulated on FIDAP.

The next problems selected for simulation use FIDAP's porous potential and free surface potential, individually. The porous potential was shown in both the Isothermal Seepage flow problem and the block of earth example flow. The free surface potential was shown in the two-fluid interface and melt
problems.

Still another way that FIDAP can model the interface of fluids within porous media would be using the diffusion/mass-transport capabilities. This situation would ultimately yield concentration information as a function of time. Implementing FIDAP free surface capabilities and diffusion capabilities allow knowledge of location and concentration of contaminant as originally desired.

FIDAP takes a basic approach when dealing with moving boundary problems. This involves a deforming spatial mesh in which nodes located on a moving boundary are allowed to move such that they remain on the moving boundary. The location of the nodes on the boundary are determined by the additional degree of freedom added to the nodes on the interface. Coupling this simulation capability with a Newton-type iterative solution procedure results in simultaneous calculation of the position of the nodes on the moving boundary and the field variables at the new nodal location, once convergence is attained.

**FIDAP FREE SURFACE CAPABILITIES**

FIDAP has additional useful capabilities. One important aspect is its ability simulate two dimensional flow problems that involve moving or free boundaries of fluid-fluid or solid-
fluid type. There are several classes of these free boundary problems. The two that are of primary concern in this investigation are:

1 - Adjacent fluids with unknown shape and postition of the front.

2 - A solid-fluid phase change boundary whose position can be determined by the melting front information [23].

Both of these situations were modeled on FIDAP. The governing partial differential equations were discussed in previous sections.

**FIDAP/ACSL CORRELATION MELT OR PHASE CHANGE INTERFACE**

A melt interface problem is modeled on FIDAP for correlation purposes. This type of problem is often seen when studying crystal growth or melt casting. Correlating the melt interface problem with the fluid-fluid interface problem by matching the appropriate parameters, we will be able to apply similarity between the melt and fluid interface problem.

By applying appropriate conditions at the boundary surface between phases, the interface can be modeled and studied. The interface is assumed to be sharp between the liquid and solid phases of the material.

The modeling is done by taking a melting situation such as
melting ice. A temperature gradient is presented within the boundary conditions. A reliability check with ACSL was simultaneously done. The differential equation for a moving boundary, [2.14e] was used. The ACSL program iteratively solves this one-dimensional differential equation over the prescribed domain. Figures 20a and 20b schematically represent what is being done.

**Pressure Driven Problem**

![Pressure Driven Problem Diagram](image)

**Temperature Driven Problem**

![Temperature Driven Problem Diagram](image)
Defining first the field variable in the parabolic partial differential equation [2.11] as temperature for a melt problem and then a corresponding pressure value within the immiscible fluid interface problem correlation was possible. The following data was input into FIDAP and ACSL for comparison:

<table>
<thead>
<tr>
<th>FIDAP</th>
<th>ACSL</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature Gradient = 0.25</td>
<td>Pressure Gradient = 0.25</td>
</tr>
<tr>
<td>B² = 19.5</td>
<td>B² = 19.5 (A=-5.85)</td>
</tr>
</tbody>
</table>

The solution time intervals were first set for ten time-steps at a time increment of 0.01 seconds. Another file run was made with thirty time-steps. Figure 20 shows the mesh plot after construction on FIDAP. Plots obtained from FIDAP are shown in Figures 21 a and b again for ten and thirty time-steps respectively. Plots obtained on ACSL are shown in Figures 22 a and b for ten and thirty time-steps respectively. One can see the similarities in the results. Table 2 shows a comparison.
TABLE 2

<table>
<thead>
<tr>
<th>FIDAP RESULTS</th>
<th>ACSL RESULTS</th>
<th>% DEVIATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>Displacement</td>
<td></td>
<td></td>
</tr>
<tr>
<td>10 time-steps</td>
<td>0.06538</td>
<td>0.06238</td>
</tr>
<tr>
<td>30 time-steps</td>
<td>0.11758</td>
<td>0.117218</td>
</tr>
</tbody>
</table>

The above comparison of FIDAP solution values to ACSL solution values yields quite accurate results as stated previously. This check gives confidence in the FIDAP output. In addition, the rest of FIDAP's post processing output will supply other pertinent information. The rest of FIDAP's output for these two cases are shown in Figures 23 a-f and Figure 24 a-f for time-steps ten and thirty respectively. Both the output plots show free surface, velocity vector, pressure contour, streamline contour, temperature contour and convergence information.

In the free surface plots, Figures 23a and 24a, we see a displacement in the x-direction as expected. The velocity plots in Figures 23b and 24b show a minute clockwise circulation pattern developed by thermal convection currents. These velocities are quite small in magnitude and do not significantly effect our problem. Pressure plots in Figures 23c and 24c indicate a wall of high pressure at the fluid-solid interface as expected as well. The streamline plots, Figures 23d and 24d, again indicate the minute circulation due to thermal convection. Thermal plots in Figures 23e and 24e identify the high-low temperature interface at the water-ice
boundary. Finally, the convergence plots in Figures 23f and 24f illustrate a solution was arrived at quickly and efficiently.
**FIGURE 23a**

FREEZING BOUNDARY 10 TIME STEPS

FREE SURFACE PLOT

TIME STEPS

1 AND 10

SCREEN LIMITS

XMIN = 123E+00
XMAX = 213E+01
YMIN = 000E+00
YMAX = 200E+01

FIDAP 5.01
5 AUG 91

**FIGURE 23b**

FREEZING BOUNDARY 10 TIME STEPS

VELOCITY VECTOR PLOT

SCALE FACTOR

0 500E+02
MAX VECTOR PLOTTED

0 4132E-03
AT NODE 120

TIME = 0 100E-03
SCREEN LIMITS

XMIN = 123E+00
XMAX = 213E+01
YMIN = 000E+00
YMAX = 200E+01

FIDAP 5.01
5 AUG 91
INTERFACE BETWEEN TWO FLUIDS

The situation consisting of a sharp interface between two fluids can occur either when miscible or immiscible fluids are present. FIDAP can only model this free surface interface by assuming an immiscible situation. The next situations modeled on FIDAP approached the interface between two fluids under five different conditions. One file modeling horizontally moving fluids was solved using five transient time-steps. Another file, again modeling horizontally moving fluids was solved using twenty-five transient time-steps. Still another file modeling horizontal fluid movement was solved using twenty-five transient time-steps at a lower fluid viscosity. Modeling vertical fluid movement was done once with five time-steps and again with side flux for five time-steps. The output for these cases are shown in Figures 25 a-g, Figures 26 a-f, Figures 27 a-f, Figures 28 a-f and Figures 29 a-f. In Figure 25 a and b the history and deformed mesh are shown, respectively. The plots in Figure 25 c-g are the free surface, velocity vector, pressure contour, streamline contour and convergence information, respectively. The remaining plots of 26-29, a-f of each are history of displacement, free surface, velocity vector, pressure contour, streamline contour and convergence information, respectively.

Examining Figures 25a, 26a, 27a, 28a and 29a, we see that nodes residing on the fluid-fluid interface move in their
respective directions as expected. Figure 25b shows one example of how the mesh is deformed as a function of time with the use of the spines option. Figures 25c, 26b, 27b, 28b and 29b illustrate initial and final location of the free surface, as expected, for each example. Studying the velocity vector plots in Figures 25d, 26c, 27c, 28c and 29c allows one to identify the important velocity magnitude information that essentially governs the Reynolds number. In all cases we see the Reynolds number is within the Darcy's Law specification.

Moving on to the pressure plots in Figures 25e, 26d, 27d, 28d and 29d, the flow is shown to be undisturbed. The local low pressures indicated at the exit location of each plot when using the spine declaration are reasonable. The nodes at these locations are required to be stationary, thus a high pressure is indicated. The streamline plots in Figures 25f, 26e, 27e, 28e and 29e indicate again that there are no internal disturbances. Finally, the convergence plots in Figures 25g, 26f, 27f, 28f and 29f show a solution was quickly and efficiently obtained for each problem.
**FIGURE 25a**

**FIGURE 25b**
FIGURE 25c

TWO FLUID INTERFACE & TIME STEPS

FIGURE 25d

TWO FLUID INTERFACE & TIME STEPS

VELOCITY VECTOR PLOT

SCALE FACTOR 0.5000E+02
MAX VECTOR PLOTTED 0.1000E+02
AT NODE 441

TIME 0.500E-01
SCREEN LIMITS
XMIN = 1.00E+00
XMAX = 2.13E+01
YMIN = 0.000E+00
YMAX = 1.20E+01
RIDAP-91 5-AUG-91
FIGURE 26f

TWO FLUID INTERFACE 25 TIME-STEMS

CONVERGENCE HISTORY PLOT

REL ERROR VEL
O - COMBINED

TIME 0 1000-01

FIDAP 5 01 5-AUG-91

FIGURE 27a

TWO FLUID INTERFACE WITH LOW VISCOSITY

TIME HISTORY PLOT

A NODE 11.7
B NODE 221.X
C NODE 40.5

FIDAP 5 01 5-AUG-91
FIGURE 27b

TWO FLUID INTERFACE WITH LOW VISCOSITY

FREE SURFACE PLOT

TIME STEPS
1 AND 25

SCREEN LIMITS
XMIN = 0.000E+00
XMAX = 0.000E+00
YMIN = 0.000E+00
YMAX = 0.000E+00

FIDAP 5.01
5-AUG-91

FIGURE 27c

TWO FLUID INTERFACE WITH LOW VISCOSITY

VELOCITY VECTOR PLOT

SCALE FACTOR
0.000E+00

MAX VECTOR
PLOTTED
0.000E+00

NOD. 21

FIDAP 5.01
5-AUG-91
TWO FLUID INTERFACE WITH LOW VISCOSITY

CONVERGENCE HISTORY PLOT

RFI ERROR VFI
0 COMBINED

TIME 0 100E-01

FIDAP 5 01
5 AUG 91
An arbitrary viscosity was selected for both fluids. By changing the fluid property of viscosity, various cases can be conveniently simulated. Taking a look at the difference in the output when a lower viscosity of the saturated fluid is used, we see that the resulting boundary displacement is larger.

<table>
<thead>
<tr>
<th></th>
<th>High Viscosity</th>
<th>Low Viscosity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Displacement</td>
<td>0.41225</td>
<td>0.41304</td>
</tr>
</tbody>
</table>

This change in response was expected intuitively.

Selected problems that are presented were solely chosen for demonstration purposes. The capabilities of the modeling software with respect to the desired output has thus been sufficiently checked. However, the user must be experienced in the use of FIDAP software and know the physical problem at hand in order to model the situation.

The next simulation models are the vertical flow models as mentioned before.
FIGURE 29a

TRANSIENT VERT. BOUNDARY BETWEEN TWO FLUIDS

TIME HISTORY PLOT

A NODE 221.Y

FIDAP 5.01
26-JUN-91
12:17:32

FIGURE 29b

VERT. BOUNDARY BETWEEN TWO FLUIDS

FREE SURFACE PLOT

TIME STEPS
1 AND 5
VERT. BOUNDARY BETWEEN TWO FLUIDS

FIGURE 29d

VELOCITY VECTOR PLOT

SCALE FACTOR
0.5000E+02

MAX. VECTOR PLOTTED
0.3187E+01

AT NODE 1

PRESSURE CONTOUR PLOT

LEGEND

MINIMUM
-0.81063E+00
MAXIMUM
0.24422E+01
FIGURE 29e

VERT. BOUNDARY BETWEEN TWO FLUIDS

STREAMLINE CONTOUR PLOT

Legend:
- - 2.853E+00
- - 0.1147E+00
- - 0.5146E+00
- - 0.9146E+00
- - 0.1315E+01

Minimum
-0.48535E+00
Maximum
0.35146E+01

FIGURE 29f

TRANSIENT VERT. BOUNDARY BETWEEN TWO FLUIDS

CONVERGENCE HISTORY PLOT

REL. ERROR VEL
0 - COMBINED

Time 0.100E-01

FIDAP 5.01
27-JUN-91
09:26:41
ADVECTION-DISPERSION (SPECIES DIFFUSION)

FIDAP has the capability to model chemical concentration problems when there is a need for such information. This is done by declaring species elements that track the species concentration with respect to its initial zero concentration. A species element declaration instructs FIDAP to use the advection-dispersion equations during the solution process. These governing equations were presented in the prior text. The FIDAP output obtained is shown in Figures 30 a-f and Figures 31 a-f. The plots of each a-f represent history of species concentration, concentration contour, velocity vector, pressure contour, streamline contour and convergence information, respectively. One-dimensional problems are run prior to two-dimensional problems to illustrate individual capabilities. Two-dimensional examples were run to identify a more realistic situation.

As for the one-dimensional output, plots in Figures 30a-f relate to a situation where the contamination is moving in the horizontal direction. Figure 30a shows the time-history plot of the contamination concentration as seen by a centrally-located node on the initial boundary between the fluids. The species contour plot in Figure 30b illustrates the concentration increase graphically. Velocity, pressure and streamline plots in Figures 30c-e indicate an undisturbed situation in the flow field. The convergence plot in Figure
30f once again indicates a quick, efficient solution was obtained. The same description holds true for plots in Figures 31a-f. The only difference is that in these plots the contamination is moving in the vertical direction.
DIFFUSION OF CONTAMINANT, HORIZONTAL

FIGURE 30c

VELOCITY VECTOR PLOT

SCALE FACTOR 0.500E+02
MAX VECTOR PLOTTED 0 10500E+01
AT NODE 410

TIME 0 109E-01
SCREEN LIMITS
XMIN -129E-03
XMAX 0 213E+01
YMIN 0 000E+00
YMAX Pi 2Pi

FIDAP 5.01 5 AUG 91

FIGURE 30d

DIFFUSION OF CONTAMINANT, HORIZONTAL

PRESSURE CONTOUR PLOT

LEGEND

MINIMUM -6 36463E+04
MAXIMUM 0 74932E+08

TIME 0 109E-01
SCREEN LIMITS
XMIN -129E-03
XMAX 0 213E+01
YMIN 0 000E+00
YMAX Pi 2Pi

FIDAP 5.01 5 AUG 91
FIGURE 31a

DIFFUSION OF CONTAMINANT, VERTICAL

FIGURE 31b

DIFFUSION OF CONTAMINANT, VERTICAL

LEGEND

MINIMUM 0 159280E+00
MAXIMUM 0 06781E+00

SCREEN LIMITS

XMIN 0 0000+00
XMAX 0 2008+01
YMIN 0 0000+00
YMAX 0 2008+01
**FIGURE 31c**

**DIFFUSION OF CONTAMINANT, VERTICAL**

**VELOCITY VECTOR PLOT**

- **SCALE FACTOR**: 0.500E+02
- **MAX VECTOR PLOTTED**: 0.1050E+01
- **AT NODE**: 212

**TIME**: 0.100E-01

**SCREEN LIMITS**
- **XMIN**: 0.000E+00
- **XMAX**: 0.200E+00
- **YMIN**: 0.000E+00
- **YMAX**: 0.200E+00

**FTDAP 5 01 5-AUG-91**

**FIGURE 31d**

**DIFFUSION OF CONTAMINANT, VERTICAL**

**PRESSURE CONTOUR PLOT**

- **MINIMUM**: 0.059E+05
- **MAXIMUM**: 0.74082E+08

**TIME**: 0.100E-01

**SCREEN LIMITS**
- **XMIN**: 0.000E+00
- **XMAX**: 0.200E+00
- **YMIN**: 0.000E+00
- **YMAX**: 0.200E+00

**FTDAP 5 01 5-AUG-91**
The final problem modeled was chosen to illustrate a common occurrence of pollution. The example can be looked upon as a surface contamination situation or a sub-surface contamination situation. Surface pollution often takes the form of a contaminant pool or pit. First imagine the top line in Figure 32 as being the soil surface, which is a free surface. The main concern in this problem is the discharge that permeates into the soil below the source of contamination and eventually contaminates the fresh water aquifer. Next, Figure 32 may represent a chunk of soil at an arbitrary location below the soil surface. The main concern again is contamination permeating the soil, eventually reaching the water supply.

**FIGURE 32**
To model the above problems, a section of earth was constructed such that the upper left quadrant represented a contamination source. The permeabilities and porosities for materials A and B were set equivalent. The mesh configuration is illustrated in Figure 33a. The FIDAP output obtained is shown in Figure 33b-g. The plots of Figure 33b-g represent history of species concentration, concentration contour, velocity vector, pressure contour, streamline contour and convergence information, respectively. By changing the appropriate parameters in the FIDAP program, different cases of surface contamination can be modeled.

Observing the output in Figure 33, one can identify and assess what is occurring. The contaminant starts in the upper left corner of the mesh and permeates into both Material A and Material B, as expected. In this example, Material A and Material B are the same, thus the contamination concentration in each are quite close. For Material A, the concentration values are slightly higher due to gravitational effects.
FIGURE 33a

DIFFUSION OF CONTAMINANT. HORIZONTAL

FIGURE 33b

DIFFUSION OF CONTAMINANT. HORIZONTAL
FIGURE 33c

DIFFUSION OF CONTAMINANT, HORIZONTAL

FIGURE 33d

DIFFUSION OF CONTAMINANT, HORIZONTAL
FIGURE 33e

DIFFUSION OF CONTAMINANT. HORIZONTAL

FIGURE 33f

DIFFUSION OF CONTAMINANT. HORIZONTAL
FIGURE 33g

<table>
<thead>
<tr>
<th>ITERATION NO</th>
<th>NOFM</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 00000</td>
<td>0</td>
</tr>
<tr>
<td>2 00000</td>
<td>0</td>
</tr>
<tr>
<td>3 00000</td>
<td>0</td>
</tr>
<tr>
<td>4 00000</td>
<td>0</td>
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<td>5 00000</td>
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<tr>
<td>6 00000</td>
<td>0</td>
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<tr>
<td>7 00000</td>
<td>0</td>
</tr>
<tr>
<td>8 00000</td>
<td>0</td>
</tr>
<tr>
<td>9 00000</td>
<td>0</td>
</tr>
</tbody>
</table>

CONVERGENCE HISTORY PLOT

RFI ERROR VFI

1 COMBINED

TIME 0 1000E-01

FIDAP 5.01

5 AUG 91
Here, the same problem schematically shown in Figure 32 was solved using different values of material permeabilities and porosities. Selecting different material properties allows a situation such as sand and gravel to be modeled. Material A was set with a high porosity and permeability. Material B was set with a low porosity and permeability. Illustrations in Figure 34 a-g show the mesh with node numbers, history of concentration plot of one node on each material, species contour plot, velocity vector plot, pressure contour plot, streamline contour plot and convergence plot, respectively.

Viewing the output for this problem, we can see in Figure 34b, that nodal movement on the respective interfaces of Material A and Material B support the expectation that contamination will more readily flow into the high porosity and permeability material. The velocity plot in Figure 34d also supports this expectation by indicating a larger velocity value in the material with the higher porosity and permeability. The pressure plot in Figure 34e indicates a high pressure, or restrictive zone, occurring at the lower porosity material, again supporting reasonable expectations.
FIGURE 34a

DIFFUSION OF CONTAMINANT, HORIZONTAL

FIGURE 34b

DIFFUSION OF CONTAMINANT, DIFF PRT

TIME HISTORY PLOT

TIDAP 5 01
30-JUL-91
FIGURE 34g

DIFFUSION OF CONTAMINANT, HORIZONTAL

CONVERGENCE HISTORY PLOT

RFI ERROR VFI
0 - COMBINED

TIME 0 100E-01

FIDAP S 01
5 AUG 91
A similar problem was run setting Material A to a low porosity and permeability and Material B with a high porosity and permeability. Illustrations in Figure 35 a-f show history of concentration plot of one node on each material, species contour plot, velocity vector plot, pressure contour plot, streamline contour plot and convergence plot, respectively. Three additional plots in Figures 35g-i are included in this example to show concentration infiltration at initial, middle and final time-steps.

In both of the two-dimensional situations, it is shown that the material with the highest porosity and permeability has the greatest concentration increase of the contaminant. This response is expected from the physics. By modeling these situations, one can assess the importance of a computer simulation for groundwater contamination monitoring. Any specified boundary or initial conditions can be implemented quite easily by altering the input file.
FIGURE 35a

DIFFUSION OF CONTAMINANT, HORIZONTAL

FIGURE 35b

DIFFUSION OF CONTAMINANT, HORIZONTAL
FIGURE 35c

DIFFUSION OF CONTAMINANT, HORIZONTAL

VELOCITY VECTOR PLOT

SCALE FACTOR
0 1000E-03
MAX VECTOR PLOTTED
0 4145E-01
AT NODE 431

TIME 0 100E-01
SCREEN LIMITS
XMIN 0 666E-06
XMAX 0 208E+01
YMIN 0 840E-09
YMAX 0 200L+01

FIGURE 35d

DIFFUSION OF CONTAMINANT, HORIZONTAL

PRESSURE CONTOUR PLOT

LEGEND

MINIMUM 0 221E-08
MAXIMUM 0 24877E+08

TIME 0 100E-01
SCREEN LIMITS
XMIN 0 666E-06
XMAX 0 208E+01
YMIN 0 840E-09
YMAX 0 200L+01
FIGURE 35e

DIFFUSION OF CONTAMINANT. HORIZONTAL

STREAM TNP CONTOUR PLOT

LEGEND

I 1 78E+01
I 1 56E+01
I 1 33E+01
I 1 11E+01
I 89E+00
I 667E+00
I 444E+00
I 222E+00

MINIMUM
0 000000E+00
MAXIMUM
0 200000E+01

TIME 0 100E-01
SCREEN LIMITS
XMIN 0 200E-00
XMAX 0 200E-01
YMIN 0 200E-00
YMAX 0 200E-01
FIDAP 5 01
15 AUG 91

FIGURE 35f

DIFFUSION OF CONTAMINANT. DIFF POR

CONVERGENCE HISTORY PLOT

RFI ERROR VFI
0 - COMBINED

TIME 0 100E-01
FIDAP 5 01
15 AUG 91
CHAPTER IV

CONCLUSION AND RECOMMENDATIONS

The simulation results presented in the previous section reinforce the viability of using computer modeling in determining the characteristics and response of an aquifer subjected to contamination. The results were constructed from generic input that is common in most groundwater contamination situations. These results are helpful in determining the optimum management plan for containment and/or contamination clean-up.

A dynamic programming approach of modeling groundwater contamination has been illustrated. Full description and understanding of the physical and mathematical background of porous media flow was also presented. The similarity solutions presented are basically only applicable to one dimensional situations. The analytical solutions developed did however illustrate the concepts and serve as a benchmark for numerical solutions.

The importance of this type of environmentally-based problem goes far beyond the short term effects. With our current trend of pollution, every life-supporting resource of the earth will eventually be affected. Ultimately, occupants of the earth will suffer. Computer models are vital to the future of the earth's usable water supply and ultimately the
survival of mankind. A useful program has been identified and implemented here to illustrate current technological capabilities.

For the most part, fluid and soil information can be obtained from already existing monitoring wells and soil samples. This information can be input data for a full-scale model representation of a given set of conditions. The developed formulation methodology presents a cost-effective, accurate model that will support an optimal management plan for a groundwater contamination situation. The method has been illustrated on a fictitious block of earth, but with little modification and more computer space can be implemented on a real-life problem. FIDAP was found to be quite time and space intensive. The governing partial differential equations are very difficult to solve, even using numerical techniques. It is felt that with more computer storage space, FIDAP could handle a real-life occurrence. With even further manipulation, the model presented can be used in many similar situations.

It is important that future work be done to further develop the models under consideration. The first recommendation is that if this model was to be used frequently enough, request a special version of FIDAP to be programmed solely for groundwater analysis. This version should be capable of taking fluid and material parameter input and yield frontal displacement, contamination concentration and other useful output simultaneously. The system must also have sufficient computer storage space to compensate for the space
intensive run-time files and internally created FIDAP output files generated during each run. The second recommendation would be to select a real-life case to compare previously obtained information to program results. The third recommendation is to develop three-dimensional capabilities with the models. Yet another recommendation would be to include temperature effects in the simulation. The final recommendation is to develop a government policy which will supply research money for exploration of new technological tools useful in pollution management and control. Control of contamination will never be accomplished by people who are interested, but have no funds or resources at their disposal.

In summary, computer simulations are necessary in the development of a successful management scheme for groundwater contamination systems. The simulation process is a very useful tool, complementing the recent trend toward environmental engineering. Assumptions and important local information are constantly being updated to reflect recent occurrences. Optimization and feasibility studies can be performed prior to executing expensive, tedious management schemes. Simulations build confidence in the contamination flow characteristics, can reduce the number of monitoring wells and can control costs encountered during aquifer contamination studies. The time has come to implement our technological capabilities, in order to maintain control of pollution and thus save our planet from destruction.
REFERENCES


REFERENCES
(CONTINUED)

No.1, American Society of Civil Engineers Water Resources Planning and Management Division, NY, Mar./Apr. 1991.


[25] Geophysics Study Committee, Studies In Geophysics, Groundwater Contamination, Geophysics Research Forum,
REFERENCES
(CONTINUED)


APPENDICIES
APPENDIX A
PRINCIPAL SOURCES OF CONTAMINATION

AGRICULTURAL
- Irrigation return flow
- Fertilizers
- Pesticide residues

MUNICIPAL AND INDUSTRIAL
- Surface disposal of solid wastes
- Surface disposal of liquid wastes
- Sewer leakage
- Leaky underground storage tanks
- Disposal wells
- Injection wells
- Mining activities
- Oilfield brines

Others
- Saline water intrusion
- Spills and surface discharges
- Septic tanks and cesspools
- Highway deicing
APPENDIX B
### Typical Porosity Values of Natural Sedimentary Materials

<table>
<thead>
<tr>
<th>Sedimentary Material</th>
<th>Porosity Value (percent)</th>
<th>Sedimentary Material</th>
<th>Porosity Value (percent)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Peat soil</td>
<td>60-80</td>
<td>Fine-to-medium mixed sand</td>
<td>30-35</td>
</tr>
<tr>
<td>Soils</td>
<td>50-60</td>
<td>Gravel</td>
<td>30-40</td>
</tr>
<tr>
<td>Clay</td>
<td>45-55</td>
<td>Gravel and sand</td>
<td>30-35</td>
</tr>
<tr>
<td>Silt</td>
<td>40-50</td>
<td>Sandstone</td>
<td>10-20</td>
</tr>
<tr>
<td>Medium-to-coarse mixed sand</td>
<td>35-40</td>
<td>Shale</td>
<td>1-10</td>
</tr>
<tr>
<td>Uniform sand</td>
<td>30-40</td>
<td>Limestone</td>
<td>1-10</td>
</tr>
</tbody>
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### Typical Values of Hydraulic Conductivity and Permeability

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<th>Permeant</th>
<th>Semipermeant</th>
<th>Impermeant</th>
</tr>
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<tbody>
<tr>
<td>A)</td>
<td>Aquifer</td>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td>B)</td>
<td>Soils</td>
<td>Clean gravel</td>
<td>Clean sand</td>
</tr>
<tr>
<td>C)</td>
<td>Rocks</td>
<td>Gravel</td>
<td>Coarse</td>
</tr>
<tr>
<td>D)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>E)</td>
<td></td>
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<td></td>
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<td>F)</td>
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<td></td>
</tr>
<tr>
<td>H)</td>
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<td></td>
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</table>

### Sieve no. and Size of opening (mm.)

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<th>Diameter (mm.)</th>
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<th>10&lt;sup&gt;-1&lt;/sup&gt;</th>
<th>10&lt;sup&gt;-2&lt;/sup&gt;</th>
<th>10&lt;sup&gt;-3&lt;/sup&gt;</th>
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<td>Sieve no</td>
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<td>10</td>
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<tr>
<td>Size of opening</td>
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<td>2.38</td>
<td>1.9</td>
<td>0.59</td>
<td>0.29</td>
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### M.I.T. & B.S. Classification

<table>
<thead>
<tr>
<th>Gravel</th>
<th>Sand</th>
<th>Silt</th>
<th>Clay</th>
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<tr>
<td>Coarse</td>
<td>Medium</td>
<td>Fine</td>
<td>Coarse</td>
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<tr>
<td>2</td>
<td>6.10&lt;sup&gt;-1&lt;/sup&gt;</td>
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<td>2.10&lt;sup&gt;-3&lt;/sup&gt;</td>
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### U.S. Dept. of Agriculture

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<table>
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<th>Sand</th>
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### Intern. Society of Soil Science

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## Dynamic Viscosity of Some Liquids (in centipoise)

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<th>20°C</th>
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</tr>
</thead>
<tbody>
<tr>
<td>Water</td>
<td>1.787</td>
<td>1.310</td>
<td>1.002</td>
<td>0.653</td>
<td>0.407</td>
</tr>
<tr>
<td>Benzene</td>
<td>0.902</td>
<td>0.759</td>
<td>0.649</td>
<td>0.492</td>
<td>0.351</td>
</tr>
<tr>
<td>Chloroform</td>
<td>0.700</td>
<td>0.626</td>
<td>0.564</td>
<td>0.465</td>
<td></td>
</tr>
<tr>
<td>Ethyl alcohol</td>
<td>0.177</td>
<td>0.145</td>
<td>0.119</td>
<td>0.827</td>
<td>0.504</td>
</tr>
<tr>
<td>Methyl alcohol</td>
<td>0.813</td>
<td>0.686</td>
<td>0.591</td>
<td>0.480</td>
<td></td>
</tr>
<tr>
<td>Ether</td>
<td>0.286</td>
<td>0.258</td>
<td>0.234</td>
<td>0.197</td>
<td></td>
</tr>
</tbody>
</table>
APPENDIX C
28. MERGING LIQUID STREAMS

28.1 Problem Description

The main purpose of this example is to illustrate the simulation of a flow which includes two distinct free surfaces. Two immiscible liquids of different viscosity flow down two ducts inclined at an angle to each other, which then merge into a single parallel-sided duct. An interface is formed between the two liquids, which do not mix. Further downstream the upper wall of the duct terminates and the streams emerge into the atmosphere. There are thus two free surfaces: the interface between the liquids, which begins at the junction of the ducts into a single duct, and the surface between the upper liquid and the atmosphere, which begins at the lip of the upper duct wall.

For the purposes of this simulation the liquids are taken to have the same density but different viscosities. The surface tension is zero at the interface between them, but is non-zero at the upper free surface.

28.2 Analysis

An initial mesh is designed assuming both interfaces to be flat and horizontal. A single family of spines is sufficient to cover the deformation of both the interfaces, since a spine may intersect more than a single free surface. The boundary conditions for the simulation and the mesh generated by FIMESH are shown in Figure 28.1.

The problem is solved in two stages. First the two interfaces are assumed to be fixed in position and the liquids are taken to have the same viscosity. This solution provides as initial estimate of the velocity field which is then used to restart the stipulated problem using the *ICNODE(VELOCITY,READ) Control card.

The FIPREP input file for the analysis is presented in Table 28.1.
MERGING LIQUID STREAMS

28.3 Results

Figure 28.2 shows the superposition of the initial mesh and the mesh configuration; this illustrates the extent of the distortion that took place in attaining the equilibrium state. Figure 28.3 is a contour plot of the pressure field and, in addition, clearly depicts the locations of the two free surfaces. As might have been expected, there is a distinct swelling effect for both liquids. Figure 28.4 shows the velocity field for the flow; the change from the parabolic distributions at the inflows is evident.

The FIPOST commands required to create these plots are summarized in Table 28.2.
Merging Liquid Streams

Figure 28.1: Boundary Conditions and Mesh for Liquid Streams
## Table 28.1: FIPREP Input File for Liquid Streams

*TITLE
TWO MERGING LIQUIDS WITH ONE EXTERNAL AND AN INTERIOR INTERFACE
*FIMESH(2-D. IMAX=7. JMAX=6)

<table>
<thead>
<tr>
<th>EXP</th>
<th>/1  2  3  4  5  6  7</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1  0  15 0  31 0  51</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>EXPJ</th>
<th>/1  2  3  4  5  6</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1  0  11 12 0  22</td>
</tr>
</tbody>
</table>

**POINT(CARTESIAN)**

1  1  1  1  0.10  0.
2  1  1  1  5.0  0.5
3  5  1  1  15.  0.5
4  7  1  1  25.0 0.5
5  7  3  1  25.0 1.5
6  3  3  1  5.0  1.5
7  1  3  1  0.0  0.99
8  1  4  1  0.0  2.01
9  3  4  1  5.0  1.5
10 7  4  1  25  1.5
11 7  6  1  25. 2.5
12 5  6  1  15. 2.5
13 3  6  1  5.0  2.5
14 1  6  1  0.10 3.0
15 5  4  1  15. 1.5
16 5  3  1  15. 1.5

**LINE**

1  2  5.  4
6  7  5.  3
8  9  5.  4
13 14 5.  3
14 8  3.  4
13 9  3.  4
2  3  3.  4
6  16 3.  4
9  15 3.  4
13 12 3.  4
3  4  5.  3
16 5  5.  3
15 10 5.  3
12 11 5.  3
3 16
4  5
10 11 2.  3
15 12 4.  3
MERGING LIQUID STREAMS

SURFACE
1 6
2 5
9 11
8 13

MERGE
9 15 6 16
15 10 16 5

ELEMENTS (QUADRILATERAL, NODES=9)
1 5
8 11

ELEMENTS (BOUNDARY, NODES=3)
11 13
5 6

BCNODE (COORDINATE)
5
6
11
13

BCNODE (UX)
1 2 0.
2 3 0.
3 4 0.
7 6 0.
8 9 0.
14 13 0.
13 12 0.
/11 12 0.

BCNODE (UY)
1 2 0.
2 3 0.
3 4 0.
4 5 0.
10 11 0.
6 7 0.
8 9 0.
12 13 0.
13 14 0.
/11 12 0.

BCNODE (UX, PARABOLIC)
1 7 1.49
8 14 1.49

BCNODE (UY, PARABOLIC)
1 7 1.49
8 14 -1.49

BCNODE (SURFACE)
12 13 1.
/11 13 1.
5 5 1.
9 9 1.
MERGING LIQUID STREAMS

NUMBER
2 1
SPINES
13 2 11 0.
END
*PROBLEM(NONLINEAR,STEADY,2-D,FREE)
/*PROBLEM(NONLINEAR,STEADY,2-D)
*PRESSURE(MIXED,DICNTINUOUS)
*EXECUTION(NEWJOB)
*SOLUTION(N.R.-20,VELCONV=.005,RESCONV=.005,ACCF=0.5)
*OPTIONS(STRESSDIVERGENCE)
*NODES(FIMESH)
*ICNODE(VELOCITY,READ)
/*VISCOSITY(SET=1,CONSTANT=.50)
/*VISCOSITY(SET=2,CONSTANT=.50)
/*VISCOSITY(SET=2,CONSTANT=.10)
*SURFACETENSION(SET=1,CONSTANT=0.,ANG1=0.,ANG2=180.)
*SURFACETENSION(SET=2,CONSTANT=2.,ANG1=0.,ANG2=180.)
*ELEMENTS(QUADRILATERAL,NODES=9,FIMESH,MVISC=2)
*ELEMENTS(QUADRILATERAL,NODES=9,FIMESH,MVISC=1)
*ELEMENTS(SURFACE,NODES=3,FIMESH,MSURF=2)
*ELEMENTS(SURFACE,NODES=3,FIMESH,MSURF=1)
*END
MERGING LIQUID STREAMS

Figure 28.2: MESH DEFORMATION FOR LIQUID STREAMS

Figure 28.3: PRESSURE CONTOUR PLOT FOR LIQUID STREAMS

Figure 28.4: VELOCITY VECTOR PLOT FOR LIQUID STREAMS
## MERGING LIQUID STREAMS

### Table 28.2: FIPOST Input Commands

<table>
<thead>
<tr>
<th>Command</th>
<th>Arguments</th>
</tr>
</thead>
<tbody>
<tr>
<td>DEVICE</td>
<td>2</td>
</tr>
<tr>
<td>SUPERIMPOSE</td>
<td></td>
</tr>
<tr>
<td>MESH</td>
<td>0</td>
</tr>
<tr>
<td>HEADING</td>
<td>2</td>
</tr>
<tr>
<td>FREE</td>
<td></td>
</tr>
<tr>
<td>SUPERIMPOSE</td>
<td></td>
</tr>
<tr>
<td>HEADING</td>
<td>1</td>
</tr>
<tr>
<td>VELOCITY</td>
<td>0</td>
</tr>
<tr>
<td>SUPERIMPOSE</td>
<td></td>
</tr>
<tr>
<td>HEADING</td>
<td>2</td>
</tr>
<tr>
<td>STREAMLINE</td>
<td>1, 2</td>
</tr>
<tr>
<td>HEADING</td>
<td>1</td>
</tr>
<tr>
<td>PRESSURE</td>
<td>0</td>
</tr>
<tr>
<td>SUPERIMPOSE</td>
<td></td>
</tr>
<tr>
<td>QUIT</td>
<td></td>
</tr>
</tbody>
</table>
APPENDIX D
14. ISOThERMAI SEEPAGE FLOW

14.1 Problem Description

This example considers the problem of isothermal seepage in the vicinity of a water channel located in a porous saturated soil. The problem is shown schematically in Figure 14.1. The problem is assumed to be two-dimensional.

14.2 Mesh Development and Boundary Conditions

The problem is assumed to be symmetric so that the finite element model is restricted to half of the problem geometry. The geometric and integer spaces for mesh generation using FIMESH are shown in Figures 14.3 and 14.4 respectively; the resultant mesh is shown in Figure 14.2. The boundary between the water channel and the soil is assumed to be permeable, i.e. flow normal to the boundary is allowed. A constant pressure (stress) boundary condition is applied at the surface of the soil. It is also assumed that the left-hand and bottom boundaries are placed far enough away that zero flow boundary conditions can be applied.

The viscosity is set to .01 so as to reduce the influence of the diffusion term in relation to the Darcy term in the momentum equation. The value of the a coefficient in the Darcy term is set to 100 to compensate for this viscosity value. Refer to Chapter 11, Section 11.10 of the FIPREP Users Manual, for a complete discussion of the interpretation of viscosity when simulating porous flows with FIDAP.

14.3 Results

The FIPREP input file for this problem is shown in Table 14.1. A two-dimensional, linear, steady-state analysis has been specified. The elements are specified to be porous using the POROUS keyword on the *ELEMENTS Control card. The BCFLUX Control card in FIMESH is used to specify a pressure boundary condition. Note that the corresponding *BCFLUX Control card in FIPREP could have similarly been used, however this would require the node numbers comprising the boundary to which the boundary condition is
ISOTHERMAL SEEPAGE FLOW

being applied. By specifying the boundary condition in FIMESH, this information is automatically generated. Similarly the necessary velocity boundary conditions are also set in the FIMESH input section. All these boundary conditions will be automatically integrated into the FIDAP input file by the FIMESH keywords on the *NODES and *ELEMENTS Control cards.

For this simulation, nine node quadratic elements and a mixed discontinuous pressure approximation have been employed. The results of the simulation are shown in two plots: the streamline contour plot (Figure 14.5) and the pressure contour plot (Figure 14.6). The seepage from the soil into the water channel is clearly seen from these plots.
ISOETHERMAL SEEPAGE FLOW

Figure 14.1: FLOW GEOMETRY AND BOUNDARY CONDITIONS

Figure 14.2: GENERATED MESH FROM FIMESH
ISOTHERMAL SEEPAGE FLOW

Figure 14.3: MESH DESCRIPTION IN GEOMETRIC SPACE

Figure 14.4: MESH DESCRIPTION IN LOGICAL (I,J) INTEGER SPACE
## ISOTHERMAL SEEPAGE FLOW

Table 14.1: FIPREP Input File for Seepage Flow

```
*TITLE
ISOTHERMAL SEEPAGE FLOW
*FIMESH(2-D, IMAX=23, JMAX=23)

EXPI
1 0 0 0 0 21 0 0 0 0 31 0 0 0 0 0 0 0 0 0 51

EXPJ
1 0 0 0 0 0 0 0 0 21 0 0 0 0 31 0 0 0 0 51

POINT
1 1 1 1 0 0
2 7 1 1 60 0
3 23 23 1 60 60
4 13 23 1 20 60
5 7 23 1 10 60
6 1 17 1 0 50
7 1 11 1 0 40
9 23 17 1 60 0
10 7 17 1 10 50
11 13 17 1 20 40
12 7 11 1 20 40

REFPOINT
8 1 23 1

LINE
1 2
9 3
6 7 3 3
10 12 3 3
10 11 3 3
5 4 3 3
6 10
10 5
7 1 4 3
12 2 4 3
11 9 4 3
4 3 4 3

SURFACE
1 10
10 3

MERGE
10 2 10 9

ELEMENTS(QUAD, NODES=9, ALL)

BCNODE(UX)
6 10
5 3
1 2
9 3
1 6
```
ISOTHERMAL SEEPAE FLOW

BCNODE(UY)
  10  5
  9  3
  1  2
  5  4
BCFLUX(Y,NODES=3)
  5  3 -196000
BCNODE(UX,FREE)
  10  10
BCNODE(UY,FREE)
  10  10
END
*PROBLEM(2-D)
*EXECUTION(NEWJOB)
*DENSITY(CONSTANT=1000.)
*PRESSURE(MIXED.DISCONTINUOUS)
*ICNODE(VELOCITY,STOKES)
*DATAPRINT(NORMAL,PAGE,NODES=3,ELEMENTS=1)
*POSTPROCESS
*NODES(FIMESH)
*ELEMENTS(POROUS,QUADRILATERAL,NODES=9,FIMESH,GLOBAL,MAPERM=1)
*VISCOSITY(CONSTANT=.01)
*PERMEABILITY(ACOEF,CONSTANT=100.,X=1.E-6,Y=3.E-6,POROSITY=.5)
*RENUMBER(PROFILE)
*END
ISOThERMAl SEEPEAGE FLOW

Figure 14.5: STREAMLINE CONTOUR PLOT

Figure 14.6: PRESSURE CONTOUR PLOT
APPENDIX E
PROGRAM MBP.csl "Tracking of Moving Boundary"

CONSTANT  
k = 1e-4, \( \mu = 1e-2 \), \( A = -5.85 \ldots \)
\( \phi = 0.07 \), \( c = 2.6 \ldots \)
\( \text{sic} = 0.0 \), \( \text{ttic} = 0.01 \), \( \text{TSTP} = 0.1 \)
\( \text{pf} = 0.25 \)

---COMMUNICATION INTERVAL IN SECS"

\( \text{CINTERVAL CINT} = 0.005 \)

\[ \omega = \sqrt{\frac{k}{(\phi \mu c)}} \]
\[ s = -(\frac{k}{\mu}) \times (A-pf) \times \exp(-s^2/(4\omega^2tt)) / \ldots \]
\[ \omega = \sqrt{3.14tt} \]
\[ \text{Termination condition} \]

END $"$ OF PROGRAM "$
DIFFUSION OF CONTAMINATION HORIZONTAL EXAMPLE

TITLE
DIFFUSION OF CONTAMINANT, HORIZONTAL
*FIMESH PORTION OF THE PROGRAM
*FIMESH(2-D, IMAX=5, JMAX=5)
/
EXPI(DELTA)
  1 0 10 0 10
/
EXPJ(DELTA)
  1 0 10 0 10
/
/SPATIAL LOCATIONS
POINT
/POINT# I J K X Y
  1  1  1  1 0  0
  2  3  1  1 1  0
  3  5  1  1 2  0
  4  5  3  1 2  1
  5  3  3  1 1  1
  6  1  3  1 0  1
  7  1  5  1 0  2
  8  3  5  1 1  2
  9  5  5  1 2  2
/
LINE
/POINT START FINISH
  1  2
  2  3
  6  5
  5  4
  7  8
  8  9
  1  6
  2  5
  3  4
  7  6
  8  5
  9  4
/
SURFACE
  1  9
/
ELEMENTS(QUADRILATERAL, NODES=9)
  6  8
  1  5
  2  9
/
BCNODES(UX)
  6  7  1.
/
BCNODES(UY)
  7  8  -1.
/
/BCNODES(VELO)
/
ICNODES(1SPECIES)
  6  8  1.
/BCFLUX(1SPECIES)
/ 2 3
/ 8 9
/
END

*PROBLEM(TRANSIENT, NONLINEAR, WEAKLY)
*TIMEINTEGRATION(BACKWARD, NSTEP=15, DT=.01, FIXED)
*PRESSURE(PENALTY=1E-9)
*EXECUTION(NEWJOB)
*SOLUTION(S.S.=10, VELCONV = 0.001, RESCONV = 0.001)
/*execution(datacheck)
*DENSITY(CONSTANT=1.0)
*VISCOSITY(CONSTANT=1.0)
*DIFFUSIVITY(CONSTANT=1.0)
*NODES(FIMESH)
*ELEMENTS(FLUID, QUADRILATERAL, NODES=9, FIMESH)
*ELEMENTS(POREOUS, QUADRILATERAL, NODES=9, FIMESH)
*ELEMENTS(POREOUS, QUADRILATERAL, NODES=9, FIMESH)
*PERMEABILITY(CONSTANT=100.,X=1.2E-6, Y=1.2E-6, POROSITY=0.5)
/*PERMEABILITY(CONSTANT=100., X=1.2E-6, Y=1.2E-6, POROSITY=0.5)
*END
FIDAP

/  
/DIFFUSION OF CONTAMINATION TWO MAT.
*TITLE
DIFFUSION OF CONTAMINANT, HORIZONTAL
/FIMESH PORTION OF THE PROGRAM
*FIMESH(2-D, IMAX=5, JMAX=5)
/
EXPI(DELTA)
  1 0 10 0 10
/
EXPJ(DELTA)
  1 0 10 0 10
/
/Spatial locations
POINT
/POINT# I  J  K  X  Y
  1  1 1 1 0  0
  2  3 1 1 1  0
  3  5 1 1 2  0
  4  5 3 1 2  1
  5  3 3 1 1  1
  6  1 3 1 0  1
  7  1 5 1 0  2
  8  3 5 1 1  2
  9  5 5 1 2  2
/
LINE
/POINT START FINISH
  1  2
  2  3
  6  5
  5  4
  7  8
  8  9
  1  6
  2  5
  3  4
  7  6
  8  5
  9  4
/
SURFACE
  1  9
/
ELEMENTS(QUADRILATERAL, NODES=9)
  6  8
  1  5
  2  9
/
BCNODES(UX)
  8  5  1.
/
BCNODES(UY)
  6  5 -1.
/
BCNODES(VELO)
  7  9
  1  3
ICNOD(1SPECIES)
  6  8  1.
1  5
2  9

BCFLUX(1SPECIES)
/  2  3
/  8  9
/
END

*PROBLEM(TRANSIENT, NONLINEAR, 1WEAKLY)
*TIMEINTEGRATION(BACKWARD, NSTEP=15, DT=.01, FIXED)
*PRESSURE(PENALTY=1E-9)
*EXECUTION(NEWJOB)
*SOLUTION(S.S.=10, VELCONV = 0.001, RESCONV = 0.001)
*/execution(datacheck)
*DENSITY(CONSTANT=1.0)
*VISCOSITY(CONSTANT=1.0)
*DIFFUSIVITY(CONSTANT=1.0)
*NODES(FIMESH)
*ELEMENTS(FLUID, QUADRILATERAL, NODES=9, FIMESH)
*ELEMENTS(POROUS, QUADRILATERAL, NODES=9, FIMESH, maperm=2)
*ELEMENTS(POROUS, QUADRILATERAL, NODES=9, FIMESH, maperm=3)
*PERMEABILITY(SET=2, CONSTANT=100., X=1.2E-6, Y=1.2E-6, POROSITY=0.5)
*PERMEABILITY(SET=3, CONSTANT=100., X=1.2E-5, Y=1.2E-5, POROSITY=0.2)
*END
/DIFFUSION OF CONTAMINATION TWO MAT.

*TITLE
DIFFUSION OF CONTAMINANT, diff. por.

*/FIMESH PORTION OF THE PROGRAM

*FIMESH(2-D, IMAX=5, JMAX=5)

/EXP(I)(DELTAS)
1 0 10 0 10

/EXP(J)(DELTAS)
1 0 10 0 10

/SPATIAL LOCATIONS

POINT

/POINT# I J K X Y
1 1 1 1 0 0
2 3 1 1 1 0
3 5 1 1 2 0
4 5 3 1 2 1
5 3 3 1 1 1
6 1 3 1 0 1
7 1 5 1 0 2
8 3 5 1 1 2
9 5 5 1 2 2

/ LINE

/POINT START FINISH
1 2
2 3
6 5
5 4
7 8
8 9
1 6
2 5
3 4
7 6
8 5
9 4

/ SURFACE

1 9

/ ELEMENTS(QUADRILATERAL, NODES=9)
6 8
1 5
2 9

/ BCNODES(UX)
8 5 1.

/ BCNODES(UY)
6 5 -1.

/ BCNODES(VEL0)
7 9
1 3

ICNODES(1SPECIES)
6 8 1.
1 5
2 9
/
/BCFLUX(ISPECIES)
/ 2 3
/ 8 9
/
END
/
*PROBLEM(TRANSIENT, NONLINEAR, 1WEAKLY)
*TIMEINTEGRATION(BACKWARD, NSTEP=15, DT=.01, FIXED)
*PRESSURE(PENALTY=1E-9)
*EXECUTION(NEWJOB)
*SOLUTION(S.S.=10, VELCONV = 0.001, RESCONV = 0.001)
/*execution(datacheck)
*DENSITY(CONSTANT=1.0)
*VISCOSITY(CONSTANT=1.0)
*DIFFUSIVITY(CONSTANT=1.0)
*NODES(FIMESH)
*ELEMENTS(FLUID, QUADRILATERAL, NODES=9, FIMESH)
*ELEMENTS(POROUS, QUADRILATERAL, NODES=9, FIMESH, maperm=2)
*ELEMENTS(POROUS, QUADRILATERAL, NODES=9, FIMESH, maperm=3)
*PERMEABILITY(SET=2, CONSTANT=100., X=1.2E-5, Y=1.2E-5, POROSITY=0.2)
*PERMEABILITY(SET=3, CONSTANT=100., X=1.2E-6, Y=1.2E-6, POROSITY=0.5)
*END