Finite Element Stimulation of Ground Water Contamination by Hydrocarbons

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TECHNICAL COMPLETION REPORT

Finite Element Simulation of Groundwater Contamination by Hydrocarbons.

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CHAPTER 1.
INTRODUCTION

Historically Groundwater has been considered safe for human consumption. Today, however, there is a growing apprehension that this resource is becoming dangerously contaminated by natural and man-made pollutants.

One of the main threats to groundwater resources is the widespread occurrence of leakage and spillage of organic materials such as petroleum products that occur during their transport, storage and disposal. In Rhode Island at least a dozen such occurrences were reported.

The infiltration and migration of a contaminant in the subsurface is a complex process. Knowledge about the contaminant's movement and distribution is necessary to evaluate the extent of contamination due to oil spills. As a means to better assess and control the problems of contamination, numerical models have been developed to simulate the process of flow of contaminant through porous media such as soil. However, due to different chemical properties of contaminants and varying geological aspects of contaminated site it is necessary to understand the applicability of each numerical model available. Some modifications may be needed in order to apply these models to a specific site.
The first detailed analysis of hydrocarbon contamination of groundwater was done by Van Dam (1967). He considered the contaminant and water as two immiscible fluid phases. He studied the stages of contaminant infiltration and included capillary pressure term in the fluid potential. On the other hand, Mull (1971) and Scheigg (1977) neglected the capillary pressure effect and analyzed hydrocarbon infiltration assuming the soil to be homogeneous and isotropic. An aerial two dimensional numerical model was developed by Hochmuth (1981) and Hochmuth and Sunada (1985). They considered lateral migration and assumed vertical equilibrium and the capillary pressure saturation as a step function. In 1985, Faust developed a mathematical model to simulate the simultaneous flow of water and a second immiscible fluid under saturated and unsaturated conditions of porous media. This model is based on a simplification of the conventional three phase flow equations where pressure gradient in the air is assumed to be negligible.

Many investigators proposed mathematical models describing the water soluble fraction of contaminant. Hoffman (1971), Fried et al., (1979) and Bastien et al., (1977) treated the contaminant phase as an immovable source of constant or varying strength. Most, however, model the transport of dissolved constituents in the absence of a non-aqueous organic phase (see for example, van Genuchten and Wierenga, (1976), Pinder (1973), Gray and Hoffman, (1983a and 1983b)). Recently the multiphase flow problem
has been formulated by using a volume averaging theory (Hassanzadeh and Gray, 1979a and 1979b). Their formulation starts with a mass balance at the microscopic level for each phase. Then using a volume averaging technique, macroscopic mass balance equations are developed for various phases. In this approach, more than one contaminant can be considered. This formulation is utilized by Abriola and Pinder (1985a and 1985b) to study the vertical migration of hydrocarbons from a surface spill.
CHAPTER 2.

STATEMENT OF THE PROBLEM

In order to get a clear view of the problem consider a hypothetical scenario of a petroleum spill as shown in fig. 1. Initially the oil migrates downward through the unsaturated zone due to gravity. As the oil migrates downwards, its volume reduces continuously. This is because oil displaces air from the voids and is retained as residue. If the unsaturated zone is sufficiently deep and the amount of the spill is relatively small, the oil may not reach the groundwater table. On the other hand, if the amount of spill is relatively large, some oil may reach the water table and may form a mound of oil as shown in fig. 2. In general this oil mound flows in horizontal direction as well as vertical direction. However, this vertical pressure gradient is small and consequently vertical flow can be neglected. In order to simplify mathematical analysis of this problem, the following assumptions are made.

i) The Dupuit-Forchheimer approximation holds, i.e. flow is strictly horizontal.

ii) The flow of each phase (oil, water) obeys Darcy’s law.

iii) The capillary pressure-saturation curve can be idealized as shown in fig. 3. This curve is assumed to be constant over the study area.
For the analysis of the flow, two nonlinear differential equations are to be dealt with, both for oil phase and water phase which are interdependent. So it can be easily seen that an iterative scheme has to be used to make both the oil head and water head match. The governing equations are written from the basic equation developed by Boussinesq for fluid flow in an unconfined aquifer which is

\[
\frac{\partial}{\partial x} \left( K \cdot Z \cdot \frac{\partial H}{\partial x} \right) + \frac{\partial}{\partial y} \left( K \cdot Z \cdot \frac{\partial H}{\partial y} \right) = S_y \frac{\partial z}{\partial t}
\]

(1)

where

\( K \) = hydraulic conductivity of the porous medium.
\( Z \) = vertical dimension of the fluid in the aquifer.
\( H \) = hydraulic or piezometric head.
\( S_y \) = apparent specific yield.

From equation (1) two separate equations for water phase and oil phase were written by McWhorter and Sunada in 1977 as

\[
\frac{\partial}{\partial x} \left( K_{x,o} \cdot (Z_1 - Z_2) \right) \frac{\partial H_o}{\partial x} + \frac{\partial}{\partial y} \left( K_{y,o} \cdot (Z_1 - Z_2) \right) \frac{\partial H_o}{\partial y} = S_{y,o} \frac{\partial (Z_1 - Z_2)}{\partial t} - Q_o
\]

(2)

and

\[
\frac{\partial}{\partial x} \left( K_{x,w} \cdot (Z_2) \right) \frac{\partial H_w}{\partial x} + \frac{\partial}{\partial y} \left( K_{y,w} \cdot (Z_2) \right) \frac{\partial H_w}{\partial y} = S_{y,w} \frac{\partial Z_2}{\partial t} - Q_w
\]

(3)
Even though $Z_1, Z_2, H_o, H_w$ are written separately they are mutually dependant. This makes the equations (2) and (3) coupled. The relationships are

$$H_o = Z_1 - \frac{(p_c)^a}{\rho_o g} \quad \text{and} \quad H_w = \frac{\rho_o}{\rho_w} H_o + \frac{\Delta p}{\rho_w} z_2 - \frac{(p_c)^o}{\rho_w g}.$$

$Q_o$ and $Q_w$ are the source/sink terms for the oil and water respectively. These equations are solved in space using Galerkin finite element technique. In the right hand side of Boussinesq’s equation it can be seen that time derivative is present because of which an implicit time integration scheme is used to solve the equations.
CHAPTER 3.
NUMERICAL SOLUTION

The nonlinear Boussinesq's equation for flow in an unconfined aquifer (McWhorter and Sunada, 1977) is shown in the previous section.

If the maximum saturation is assumed to be equal to the porosity, then for previously uncontaminated soil the apparent specific yield of oil \((S_{y,a})\) for oil entering soil is \(S_{y,a} = \theta (1 - S_{r,w})\). While for the oil draining from the soil, \(S_{y,a} = \theta (1 - S_{r,w} - S_{r,o})\) where \(\theta\) is the porosity, and \(S_{r,w}\) and \(S_{r,o}\) are the residual saturation in water and oil respectively. The value for water at all times is \(S_{y,w} = \theta (1 - S_{r,w})\).

The Galerkin residual finite element technique is used to solve the differential equation. The scheme is explained for oil phase. For water phase it is exactly similar except that the subscript 'o' which denotes oil should be substituted by 'w' which denotes water phase and vice versa. The governing partial differential equation for the oil phase is

\[
\frac{\partial}{\partial x} \left(K_{x,o}(\Delta z) \frac{\partial h_o}{\partial x} \right) + \frac{\partial}{\partial y} \left(K_{y,o}(\Delta z) \frac{\partial h_o}{\partial y} \right) = S_{y,o} \frac{\partial (\Delta z)}{\partial t} - Q_o \tag{4}
\]

where \(\Delta z = (Z_1 - Z_2)\) (see fig. 1.)
The finite element discretization is made for the head as

\[ H_0 = H_0' = \sum_{i=1}^{n} N_i(x,y) H_i(t) \]

\[ = [N] \{H\} \text{ (in matrix form)} \]

where

\( H_0' \) = the series approximation.

\( N_i \) = shape functions

\( H_i \) = head coefficients for the shape functions.

The series approaches the exact solution as \( n \) tends to infinity. By choosing appropriate shape functions the head coefficients \( H_i \) can be set to be the head values at the nodal points.

In the numerical model four different elements are available in the element library. The shape functions corresponding to the elements are given in appendix A. Substituting the approximation \( H_0' \) into equation (4) yields

\[ \frac{\partial}{\partial x} (K_{x,0} \frac{\partial H_0'}{\partial x}) + \frac{\partial}{\partial y} (K_{y,0}(\Delta z) \frac{\partial H_0'}{\partial y}) - S_{y,0} \frac{\partial (\Delta z)}{\partial t} + Q_0 = R \]

where \( R \) is the residual. When \( R \) becomes zero solution coincides with the exact one. \( R \) approaches zero as \( n \) tends to infinity. The best solution is the one in which \( R \) is minimized. Galerkin technique is used to minimize \( R \) by requiring \( m \) conditions of orthogonality of the function \( R \).
and the shape functions \( N_i, (i = 1,2,\ldots,m) \). Using the definition of orthogonal function we can write \( \int_A \nabla \cdot \mathbf{N}_i \, dx \, dy = 0 \)

or for the oil phase

\[ \int_A \left[ \frac{\partial}{\partial x} \left( K_{x,0} (\Delta z) \frac{\partial H}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_{y,0} (\Delta z) \frac{\partial H}{\partial y} \right) - S_y,0 \frac{\partial (\Delta z)}{\partial t} + Q_o \right] N_i \, dx \, dy = 0 \]  

where

\[ i = 1, 2, \ldots, m \]

In addition, \( H_0 \) must satisfy boundary and initial conditions. By using chain rule we can write

\[ \int_A N_i \left[ \frac{\partial}{\partial x} \left( K_{x,0} (\Delta z) \frac{\partial H}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_{y,0} (\Delta z) \frac{\partial H}{\partial y} \right) \right] \, dx \, dy = \]

\[ \int_A \left[ \frac{\partial}{\partial x} \left[ N_i (K_{x,0} (\Delta z) \frac{\partial H}{\partial x}) \right] + \frac{\partial}{\partial y} \left[ N_i (K_{y,0} (\Delta z) \frac{\partial H}{\partial y}) \right] \right] \, dx \, dy \]

\[- \int_A \left[ \frac{\partial N_i}{\partial x} \left( K_{x,0} (\Delta z) \frac{\partial H}{\partial x} \right) + \frac{\partial N_i}{\partial y} (K_{y,0} (\Delta z) \frac{\partial H}{\partial y}) \right] \, dx \, dy \]

Using Green's theorem we can write

\[ \int_A \left[ \frac{\partial}{\partial x} \left[ N_i (K_{x,0} (\Delta z) \frac{\partial H}{\partial x}) \right] + \frac{\partial}{\partial y} \left[ N_i (K_{y,0} (\Delta z) \frac{\partial H}{\partial y}) \right] \right] \, dx \, dy \]

\[ = \Phi \left[ -N_i (K_{y,0} (\Delta z) \frac{\partial H}{\partial y}) \right] \, dx + \left[ N_i (K_{x,0} (\Delta z) \frac{\partial H}{\partial x}) \right] \, dy \]

\[ \Phi \, N_i \left[ (K_{x,0} (\Delta z) \frac{\partial H}{\partial x}) \, n_x + (K_{y,0} (\Delta z) \frac{\partial H}{\partial y}) \, n_y \right] \, ds \]
where \( n_x \) and \( n_y \) are the direction cosines between the outward normal to the surface \( S \) and the \( x,y \) coordinates axes respectively. If we observe equation (8) the term

\[
\phi N_i \left[ (K_x, 0 (\Delta Z) \frac{\partial O}{\partial x}) n_x + (K_y, 0 (\Delta Z) \frac{\partial O}{\partial y}) n_y \right]
\]

is the flux across the boundary of the region \( S \) and is referred to as the natural boundary condition in variational calculus (Pinder, 1974). It can be expressed as \( \int_{S(N_S)_i} q \cdot ds \) where \( (N_S)_i \) are boundary shape functions.

But in the numerical model only constant head boundaries and impermeable boundaries are used so the above term always equals to zero. Using this fact and the identity from equation (8) the governing equation (7) can be written as

\[
\iint_A \left[ \frac{\partial (N_i)}{\partial x} (K_x, 0 (\Delta Z) \frac{\partial O}{\partial x}) + \frac{\partial (N_i)}{\partial y} (K_y, 0 (\Delta Z) \frac{\partial O}{\partial y}) \right] \, dx \, dy \quad (9)
\]

\[
+ \iint_A N_i (S_y, 0 \frac{\partial (\Delta Z)}{\partial t}) \cdot \, dx \, dy - \iint_A N_i Q_o, i \, dx \, dy = 0
\]

where

\[ i = 1, 2, \ldots, m \]

But

\[ H_o' = [N] \{H_o\}, \quad \frac{\partial H_o'}{\partial x} = \frac{\partial [N]}{\partial x} \{H_o\} \]

and

\[ \frac{\partial H_o'}{\partial y} = \frac{\partial [N]}{\partial y} \{H_o\} \]
equation (9) becomes

\[
\iint_A \left[ \frac{\partial (N_i)}{\partial x} (K_{x,0} (\Delta Z)) + \frac{\partial (N_i)}{\partial y} (K_{y,0} (\Delta Z)) \right] (H_{o,i}) \, dx \, dy
\]

\[
+ \iint_A \left[ S_{y,0} \frac{\partial (\Delta Z)}{\partial t} \right] (H_{o,i}) \, dx \, dy
\]

\[
= \iint_A [N_i] \left[ S_{y,0} \frac{\partial (\Delta Z)}{\partial t} \right] (H_{o,i}) \, dx \, dy
\]

(10)

where \( i = 1, 2, \ldots, m \)

which written in matrix form

\[
\iint_A \left[ \begin{array}{c} \frac{\partial N_i}{\partial x} \\ \frac{\partial N_i}{\partial y} \end{array} \right] \left[ \begin{array}{ccc} K_{x,0} (\Delta Z) & 0 \\ 0 & K_{y,0} (\Delta Z) \end{array} \right] \left[ \begin{array}{c} \frac{\partial N_i}{\partial x} \\ \frac{\partial N_i}{\partial y} \end{array} \right] \{H_{o,i}\} \, dx \, dy
\]

\[
+ \iint_A [N_i] \left[ S_{y,0} \frac{\partial (\Delta Z)}{\partial t} \right] (H_{o,i}) \, dx \, dy
\]

(11)

where \( i = 1, 2, \ldots, m \)

and in element matrix form

\[
\iint_{A_e} \left[ N' \right]^T [K_0(\Delta Z)] [N'] \{H_o\} \, dx \, dy
\]

(12)

\[
+ \iint_{A_e} \left[ N \right]^T \left[ S_{y,0} \frac{\partial (\Delta Z)}{\partial t} \right] (H_{o,i}) \, dx \, dy
\]

(12)
where \[
\begin{bmatrix}
\frac{\partial N_1}{\partial x} & \frac{\partial N_2}{\partial x} & \cdots & \frac{\partial N_n}{\partial x} \\
\frac{\partial N_1}{\partial y} & \frac{\partial N_2}{\partial y} & \cdots & \frac{\partial N_n}{\partial y}
\end{bmatrix}
\]

and \(n\) is the number of nodal points per element.

The time derivative in the second term is evaluated as

\[
\frac{\partial (\Delta Z)}{\partial t} = \frac{\partial}{\partial t} (\bar{Z}_2 - \bar{Z}_1)
\]

(13)

\[
= \frac{\partial}{\partial t} \left( \frac{P_c}{\gamma_o} + \alpha_o H_w + \frac{\partial}{\partial t} \frac{P_c}{\gamma_o} \right) = (1 + \alpha_o) \frac{\partial H_o}{\partial t} - \alpha_w \frac{\partial H_w}{\partial t}
\]

where

\( (P_c)_o = \text{entry capillary pressure between air and oil} \)

\( (P_c)_w = \text{entry capillary pressure between oil and water} \)

\[
\alpha_o = \frac{\gamma_o}{\Delta Y}
\]

\[
\alpha_w = \frac{\gamma_w}{\Delta Y}
\]

\( \gamma_o = \text{unit weight of oil} \)

\( \gamma_w = \text{unit weight of water} \)

and

\( \Delta Y = \gamma_w - \gamma_o \)
Using the time integration scheme based on forward difference which is also called as fully implicit scheme the equation yields

\[ \iint [N']^T [K_o (\Delta Z)] [N'] \{H_o\} t \Delta t \, dx \, dy \]

\[ \frac{(1 - \omega_o)}{\Delta t} \iint_A [N]^T [S_{y,o}] [N] \{H_o\}_{t+\Delta t} - \{H_o\}_t \, dx \, dy \quad (14) \]

\[ - \frac{\alpha_w}{\Delta t} \iint_A [N]^T [S_{y,w}] [N] \{\Delta H_w\} \, dx \, dy - \iint_A [N]^T [Q_o] \, dx \, dy = 0 \]

which, written in symbolic form, is

\[ [S] \{\Delta H_o\}_{t+\Delta t} + \frac{[C]}{\Delta t} \{H_o\}_{t+\Delta t} - \{H_o\}_t - \{F\} = 0 \quad (15) \]

where \([S], [C], [F]\) are assembled matrices of all corresponding elemental matrices which, for the oil layer are

\[ (S)_{e,o} = \iint_{A_e} [N']^T \begin{bmatrix} K_{x,o} (z_1 - z_2) & 0 \\ 0 & K_{y,o} (z_1 - z_2) \end{bmatrix} [N'] \, dx \, dy \quad (16) \]

\[ [C]_{e,o} = (1 + \alpha_o) \iint_{A_e} [N]^T S_{y,o} [N] \, dx \, dy \quad (17) \]

\[ (F)_{e,o} = \iint_{A_e} [N]^T q_{r,o} \, dx \, dy + \{q_{p,o}\}_e \quad \]

\[ + \left[ \frac{\alpha_w}{\Delta t} \iint_{A_e} [N]^T S_{y,w} [N] \, dx \, dy \right] [\Delta H_w]_e \]
Rewriting the equation (15) for the convenience of computing gives

\[
\left( \frac{C}{\Delta t} + [S] \right) \{H_o\}_{t+\Delta t} = \left[ \frac{C}{\Delta t} \right] \{H_o\}_t + [F]
\]  
(19)

Similar development for the water layer gives

\[
\left( \frac{[C]}{\Delta t} + [S] \right) \{H_w\}_{t+\Delta t} = \left[ \frac{[C]}{\Delta t} \right] \{H_w\}_t + [F]
\]  
(20)

with the elemental matrices as

\[
[S]_{e,w} = \iint_{A_e} \left[ N' \right]^T K_{x,w} (Z_2 - Z_0) \begin{bmatrix} 0 \\ 0 \\ K_{y,w} (Z_2 - Z_0) \end{bmatrix} [N'] \, dx \, dy
\]  
(21)

\[
[C]_{e,w} = a_w \iint_{A_e} \left[ N \right]^T s_{y,w} [N] \, dx \, dy
\]  
(22)

\[
[F]_{e,w} = \iint_{A_e} \left[ N \right]^T Q_{f,w} \, dx \, dy + \{Q_p\}_e + \frac{g_o}{\Delta t} \iint_{A_e} \left[ N \right]^T s_{y,o} [N] \, dx \, dy \{H_o\}_e
\]  
(23)
CHAPTER 4.

VERIFICATION OF THE NUMERICAL MODEL
AND NUMERICAL EXAMPLES

To verify the correctness of the model a problem is used for which analytical solution is available. The closed form solution for the problem used is developed by Hantush (1968). The theory of fresh water lenses developed by Hantush is based on the Dupuit-Forchheimer assumption and requires an isotropic media, a static and thick unconfined aquifer, no immobilization of either fluid (i.e. \( S_{r,0} = S_{r,w} = 0 \)). In Hochmuth's formulation oil replaces fresh water in the lense and the fresh water replaces saline water in the rest of the aquifer. All the assumptions made in the analytical solutions either were made in the development of the numerical model or can be incorporated in the input data. For further information on the exact form of the analytical solution refer to Hochmuth and Sunada (1985).
In the example chosen to verify the numerical model 160 cubic meters of oil is spilled over an area of 4 square meters over a period of 15 days. Since the soil is isotropic only one quadrant is considered and the plume profile along the radial direction is shown. The values for water and oil conductivities are same and the value used is 0.0125 centimeters per second. The values used for specific yield and density of oil are 0.3 and 0.8 grams per cubic centimeter respectively. The profiles of the plume are obtained after 4, 8, 16, 20 days(fig 13a-13d). The plume profile at the 16th day is compared against the analytical solution in fig 13-c. It can be seen that the results match excellently against the analytical solution.

More over, To demonstrate some of the important capabilities of the numerical model some examples are solved in this section.
Example 1: The problem investigated, basically, is a one dimensional flow problem (see fig.4) of contaminant through porous media. The flow is supposed to be taking place in a small plexiglass plume, 90 centimeter long, 4 centimeters wide and 40 centimeters tall. The porous media consists of 2.5 millimeters diameter spherical glass beads. This particular problem is studied because experimental investigation was done and the results were mentioned in Hochmuth (1981). But unfortunately the details given are not complete. So no comparisons were possible to calibrate the performance of the program. The properties of the porous media are given in table (1).

The contaminant is an oil mixture, consisting of 80% of soltrol 'c' and 20% of automatic transmission oil by volume. Soltrol 'c' is manufactured by the Phillips petroleum company and its stable properties make it useful in porous media studies. Since it is very clear, it is impossible to detect the oil/water interface visually. The automatic transmission fluid was added to make the interface distinct. The properties of the resulting fluid are given in table (2).
The numerical analysis is done for two data sets. For both the data sets the oil is recharged at the center of the plume and only half the plume is considered because of the symmetry. The initial water elevation is 20.5 centimeters.

For the first data set 18 six-noded triangular elements (parabolic shape functions) were used to solve the problem (see fig. 5.). The oil was recharged through the two center elements as an areal source at the rate of 40 cubic cms/min/sq. cms for a total time 4 min. For the time integration a total of 80 time steps are used with a time interval of 0.05 min. The interface elevations are shown in fig. 5a–5e at the times corresponding to 0.8 min., 1.6 min., 2.4 min., 3.2 min. and 4.0 min.

For the second data set 3 eight-noded elements were used to solve the problem (see fig. 6). The oil was recharged through the center element as an areal source at the rate of 4.0 cubic cms/min/sq. cms for a total time of 0.15 min. For the time integration a total number of 30 time steps are used with a time interval of 0.005 min. The interface elevations are shown in fig. 6a–6e at the times corresponding to 0.05 min., 0.075 min., 0.1 min., 0.125 min. and 0.15 min.

Example 2: In the second example, the soil parameters used are the same as those in example 1. This example demonstrates one of the important capabilities of the model, namely the variable recharging of the contaminants.
In this example, again there are two data sets. In both the data sets, the total amount of recharged contaminant is kept the same at 16 cubic cms. In the first data set, a discharge rate of 6 cubic cms per minute is used for the first 2 min and a discharge rate of 2 cubic cms per min is used for the next 2 minutes. The growth of the plume is shown in fig. (8a-8e). It is interesting to note that the final shapes of the plume in both cases match exactly with each other. That means the rate of discharge effects only the rate of growth of the plume. The final shape of plume is not affected by the rate of recharge as long as the total amount of recharge is the same.

Example 3: In the third example an impermeable zone is introduced in order to simulate the presence of bed rock. The main purpose of this example is to demonstrate how the plume is affected by the presence of impermeable bed rock. The site chosen is circular and the impermeable zone is bounded by two concentric circles of radii 30 m and 60 m respectively. Conductivities of oil and water in other parts of the site is assumed to be 30 m/day. 400 cubic meters of oil is assumed to be spilled over a period of 2 days. The plume profiles are shown in fig. (17a-17c) correspond to times 15, 43, 72 hours respectively. Since the plume cannot penetrate the impermeable zone it gets adjusted in the permeable zone itself. This example also demonstrates the capability of the model to simulate impermeable bed rock.
Example 4: In the final numerical example some parametric studies are shown. In the study done for the thesis work conductivities are shown to affect the shape of the plume profile. In order to demonstrate this the radius of the front of the final plume profile is plotted as a function of the conductivities. In all cases the oil and water conductivities are kept same. In fig. 18a, conductivities in both x and y directions are the same (isotropic). In the second case (fig. 18b) anisotropy is introduced by keeping the conductivities in y direction at 1 cm/sec but varying the conductivities in x direction. The properties of porous media are given in table (1) and (2), respectively. In all the examples the amount of oil recharged is 16 cubic centimeters.
CHAPTER 5.

NUMERICAL SIMULATION OF CLEAN-UP OF CONTAMINATED GROUNDWATER BY PUMPING

Even though extensive work is done to understand the contamination process the clean-up process has not received much attention. In this chapter the numerical model is made use of to simulate the clean-up operation of contaminated groundwater by pumping this contaminant out. Some of the shortcomings that can be faced during the pumping is shown by means of simulating a suitable problem.

The problem chosen is numerical simulation of cleaning the spilled oil over a homogeneous, isotropic circular site. The porosity of soil is 0.32. The conductivities of oil and water are chosen to be the same for simplicity as 10.8 meters per day. Since the site chosen is a homogenous, isotropic circular region only a quadrant need be modelled. The plume profiles are shown along the radial line starting from the center. The oil spilled at the rate of 42.67 cubic meters per day over a period of 15 days. In reality conductivities of oil and water are not equal. The fact that they are chosen to be the same will not affect the conclusions made in this section.

Now if the oil is pumped out at a very high rate, only the oil which is directly under the point of pumping is removed whereas the oil in the other parts still remains in the same position. Very soon only the water starts getting pumped out instead of oil. This happens because of the
insufficient time available for part of the oil which is not directly beneath the point of pumping to migrate towards the point of pumping. This is demonstrated in the first example, in which oil is pumped out at a very high rate of 160 cubic meters per day from 20th day onwards. By 30th day only water gets pumped out instead of oil. This is demonstrated in fig. 14a-14c.

There are two ways to avoid this from happening. One of the ways is to pump in discrete fashion that is to pump for some time then stop pumping to give time for the plume to settle down and then start pumping again. This is one case in which numerical model can be helpful to determine the times of pumping and stopping. This is demonstrated in the next part of the simulation. The oil is pumped out at the same rate of 160 cubic meters per day from the 20th day but stopped at the 25th day for 10 days and then again started on the 35th day continued till the 45th day. The plume profiles on 25, 30, 35, 40, 45 days are shown in fig. 15a-15e respectively.

The most efficient way is to pump continuously at an optimum rate giving enough time for the plume to settle while pumping is still in process. The numerical model can be of immense help in determining the optimum pumping rate. This is demonstrated in the concluding part of the simulation. The oil is pumped out at a rate of 16 cubic meters per day starting from the 15th day till the 60th day. The plume profiles at the 10, 30, 60 days are shown in fig. 16a-16c respectively.
This computer model can be used to simulate flow of any two immiscible fluids through porous media. The porous media can have different porosities in x and y directions. The injection of contaminant can be through a nodal source or an elemental source. The rate of recharging can be varied through different time increments. The conductivities can be different in x and y directions. Another important feature which the computer model is capable of simulating is that for a given existing plume, the model can predict the plume profile after certain amount of time.
The solution scheme used in present work is more or less the same as the one used by Hochmuth and Sunada (1985). They mentioned some difficulties that were encountered during their work. Their initial runs had an initial condition of no oil thickness. The injection of oil caused the heads in the oil face at the nodes of recharging to be so high after the first time step that the oil/water interface elevation was lower than the bottom of the plume. This forced them to resort to a trial and error calibration procedure to come up with the initial conditions which would prevent the oil head from attaining high values. However they could not avoid the slug like response nevertheless absent in their experimental investigations. They also mentioned that a better agreement could probably be achieved either by taking smaller time steps or by trial and error calibration of initial conditions. They did not study this problem further. The above mentioned shortcoming also limits the usage of their model to very simple problems. Most of the real life problems involve complex geometry and boundary conditions. It is therefore imperative that the above mentioned slug like response be completely eliminated in order to apply the model to general and realistic problems.
The author studied the recommendations made by Hochmuth and Sunada and came to the following conclusions. Using smaller time steps did not prove to be very effective in eliminating the slug like response even though it did reduce the response by a small margin. It was concluded that eliminating the slug like response would necessitate very small time steps which in turn would require a large amount of computer time and make the usage of the model prohibitively expensive and impractical. It is practically impossible to come up with the initial conditions by trial and error calibration procedure which would reasonably eliminate the slug like response.

The solution procedure that has been suggested completely eliminates the slug like response and makes the usage of the model simple. In the model developed by Hochmuth and Sunada the initial conditions were to be given in terms of values for heads. The relationship between heads and interface elevation were

$$H_0 = z_1 - \frac{(p_c)^a}{\rho_0 g}$$  \hspace{1cm} (24)

$$H_w = \frac{\rho_0}{\rho_w} H_0 + \frac{\Delta \rho}{\rho_0} z_2 - \frac{(p_c)^0}{\rho_w g}.$$  \hspace{1cm} (25)

All the terms are explained in chapter 3. It is easily realized that by resorting to a trial and error calibration it is practically impossible to come up with values for heads which give rise to continual interface elevations ($Z_1$ and $Z_2$). In the present model the initial
conditions are given in terms of interface elevations from which heads are calculated using the above mentioned relations. The slug like response mentioned by Hochmuth and Sunada is mainly a result of highly irregular initial interface elevations which resulted from the initial head values given in Reference (12). It has also been observed in the present work that the effect of the sum of the capillary pressures and on the elevation of the plume is not as much as it was mentioned by Hochmuth and Sunada in their work (1985). This may be an outcome of the slug like response observed in reference (12).

The element library of the present model consists of four different types of elements. They are 3 nodded linear triangular element, 6 nodded quadratic triangular element, 4 nodded isoparametric quadrilateral element and 8 nodded isoparametric quadrilateral element. In the work done by the author it was observed that the results converge to the exact solution rapidly for all the elements. So the advantage of using higher order shape functions is very minimal. A reason for this would be that the plume shapes do not involve complexities like singularities and rapid change of slopes and curvatures.

The reason for choosing fully implicit time integration scheme over explicit scheme, like central difference time integration is that the implicit scheme is unconditionally stable and it is preferred because the user need not concern about the stability problems. Another reason for not
choosing an explicit scheme is that it requires the matrices of two previous time intervals to be stored along with the present one where as the usage of implicit scheme requires the storage of one previous time interval along with the present matrices.

In the study done by Hochmuth and Sunada they had to use very small time steps in order to prevent the slug like response. In the present model it is possible to use reasonably big time steps without affecting the results since the slug like response is eliminated completely. But the convergence study with respect to the time steps was not done in the present research.
Fig. 1  Interface Elevations for Flow Equations.
(after Hochmuth, 1981)

Fig. 2  Lateral Migration of Oil, Initial Stage (After Van Dam, 1967)
Fig. 3  Idealized Capillary Pressure-Saturation Curve.
(after Hochmuth, 1981)

Fig. 4  Mesh Layout for Investigation.  (after Hochmuth, 1981)
AIR/OIL AND OIL/WATER INTERFACES AT CS A--A

LEGEND

--- AIR/OIL INTERFACE
--- OIL/WATER INTERFACE

Fig. 5a Plume Profile for the First Data Set of Example 1. at Time = 0.8 min.
Fig. 3.6: Plume profile for the first data set of Example 1, at Time 2, 3, 4, 5, 6, 7.
Fig. 5c  Plume Profile for the First Data Set of Example 1, at Time = 2.4 min.
Fig. 5d  Plume Profile for the First Data Set of Example 1, at Time = 3.2 min.
AIR/OIL AND OIL/WATER INTERFACES AT CS A-A

LEGEND

--- AIR/OIL INTERFACE

--- OIL/WATER INTERFACE

INTERFACE ELEVATIONS

HORIZONTAL DISTANCE

Fig. 5e Plume Profile for the First Data Set of Example 1, at Time = 4.0 min.
AIR/OIL AND OIL/WATER INTERFACES AT CS A-A

LEGEND

--- AIR/OIL INTERFACE

--- OIL/WATER INTERFACE

Fig. 6a Plume Profile for the Second Data Set of Example 1, at Time = 0.05 min.
Fig. 6b  Plume Profile for the Second Data Set of Example 1. at Time = 0.075 min.
AIR/OIL AND OIL/WATER INTERFACES AT CS A–A

LEGEND
- AIR/OIL INTERFACE
--- OIL/WATER INTERFACE

Fig. 6c Plume Profile for the Second Data Set of Example 1. at Time = 0.1 min.
Fig. 6d Plume Profile for the Second Data Set of Example 1, at Time = 0.125 min.
AIR/OIL AND OIL/WATER INTERFACES AT CS A--A

LEGEND
— AIR/OIL INTERFACE
---- OIL/WATER INTERFACE

INTERFACE ELEVATIONS

0.0 4.5 9.0 13.5 18.0 22.5 27.0 31.5 36.0 40.5 45.0

HORIZONTAL DISTANCE

Fig. 6e Plume Profile for the Second Data Set of Example 1, at Time = 0.15 min.
Fig. 7a Plume Profile for the First Data Set of Example 2, at Time = 1.6 min.
AIR/OIL AND OIL/WATER INTERFACES AT CS A-A

LEGEND

--- AIR/OIL INTERFACE
--- OIL/WATER INTERFACE

Fig. 7b  Plume Profile for the First Data Set of Example 2 at Time = 3.2 min.
Fig. 7c  Plume Profile for the First Data Set of Example 2. at Time = 4.8 min.
AIR/OIL AND OIL/WATER INTERFACES AT CS A–A

LEGEND

--- AIR/OIL INTERFACE

--- OIL/WATER INTERFACE

Fig. 7d Plume Profile for the First Data Set of Example 2, at Time = 6.4 min.
AIR/OIL AND OIL/WATER INTERFACES AT CS A-A

LEGEND
--- AIR/OIL INTERFACE
--- OIL/WATER INTERFACE

HORIZONTAL DISTANCE

INTERFACE ELEVATIONS

0.0 4.5 9.0 13.5 18.0 22.5 27.0 31.5 36.0 40.5 45.0

Fig. 7e Final Plume Profile for the First Data Set of Example 2
Fig. 3a Plume Profile for the Second Data Set of Example 2. at Time = 1.6 min.
Fig. 3b Plume Profile for the Second Data Set of Example 2 at Time = 3.2 min.
Fig. 8c  Plume Profile for the Second Data Set of Example 2, at Time = 4.3 min.
Fig. 8d Plume Profile for the Second Data Set of Example 2, at Time = 6.4 min.
AIR/OIL AND OIL/WATER INTERFACES AT CS A-A

LEGEND
- - AIR/OIL INTERFACE
----- OIL/WATER INTERFACE

Fig. 3e Final Plume Profile for the Second Data Set of Example 2.
Shape functions for three node triangle

Triangular element in $\xi - \eta$ phase

Graphical example of shape functions

Node 1($N_1$)

Node 3($N_3$)

Fig. 9 Three-Node Triangular Element (after Hochmuth, 1981)
Triangular element in $\xi - \eta$ phase

\[
\begin{align*}
N_1 &= (2\xi-1)(\xi) \\
N_2 &= 4(\xi)(\eta) \\
N_3 &= (2\eta-1)(\eta) \\
N_4 &= -4(\eta+\xi-1)(\eta) \\
N_5 &= (\eta+\xi-1)(2\eta+2\xi-1) \\
N_6 &= -4\xi(\eta+\xi-1)
\end{align*}
\]

Shape functions for 6-node triangle

Graphical example of shape functions

Fig. 10 Six-Node Triangular Element (After Thompson, 1980)
Fig. 11 Four-Node Two-Dimensional Element.  
(after K. J. Bathe)

(a) Four to 9 variable-number-nodes two-dimensional element

Include only if node $i$ is defined

\[
\begin{array}{cccccccc}
  h_1 = & \frac{1}{2}(1 + r)(1 + s) & -\frac{1}{2}h_3 & -\frac{1}{2}h_5 & -\frac{1}{2}h_7 & -\frac{1}{2}h_9 \\
  h_2 = & \frac{1}{2}(1 - r)(1 + s) & -\frac{1}{2}h_3 & -\frac{1}{2}h_5 & -\frac{1}{2}h_7 & -\frac{1}{2}h_9 \\
  h_3 = & \frac{1}{2}(1 - r)(1 - s) & -\frac{1}{2}h_3 & -\frac{1}{2}h_5 & -\frac{1}{2}h_7 & -\frac{1}{2}h_9 \\
  h_4 = & \frac{1}{2}(1 + r)(1 - s) & -\frac{1}{2}h_3 & -\frac{1}{2}h_5 & -\frac{1}{2}h_7 & -\frac{1}{2}h_9 \\
  h_5 = & \frac{1}{2}(1 - r^2)(1 + s) & -\frac{1}{2}h_3 & -\frac{1}{2}h_5 & -\frac{1}{2}h_7 & -\frac{1}{2}h_9 \\
  h_6 = & \frac{1}{2}(1 - s^2)(1 - r) & -\frac{1}{2}h_3 & -\frac{1}{2}h_5 & -\frac{1}{2}h_7 & -\frac{1}{2}h_9 \\
  h_7 = & \frac{1}{2}(1 - r^2)(1 - s) & -\frac{1}{2}h_3 & -\frac{1}{2}h_5 & -\frac{1}{2}h_7 & -\frac{1}{2}h_9 \\
  h_8 = & \frac{1}{2}(1 - s^2)(1 + r) & -\frac{1}{2}h_3 & -\frac{1}{2}h_5 & -\frac{1}{2}h_7 & -\frac{1}{2}h_9 \\
  h_9 = & \frac{1}{2}(1 - r^2)(1 - s^2) & -\frac{1}{2}h_3 & -\frac{1}{2}h_5 & -\frac{1}{2}h_7 & -\frac{1}{2}h_9 \\
\end{array}
\]

(b) Interpolation functions

Fig. 12 Interpolation Functions of Four to Nine Variable-Number-Nodes Two-Dimensional Element.  (after K. J. Bathe)
Fig. 13a. Plume profile on the 4th day for the verification problem.
Fig. 13b. Plume profile on the 8th day for the verification problem
Fig. 13c. Plume profile on the 16th day for the verification problem
AIR/OIL AND OIL/WATER INTERFACES

LEGEND

--- AIR/OIL INTERFACE

--- OIL/WATER INTERFACE

Fig. 13d. Plume profile on the 20th day for the verification problem.
Fig. 14a. Plume profile on the 10th day for the first example in chapter 8.
Fig. 14b. Plume profile on the 20th day for the first example in chapter 8.
Fig. 14c. Plume profile on the 30th day for the first example in chapter 8.
Fig. 15a. Plume profile on the 25th day for the second example in chapter 8.
Fig. 15b. Plume profile on the 30th day for the second example in chapter 8.
Fig. 15c. Plume profile on the 35th day for the second example in chapter 8.
Fig. 15d. Plume profile on the 40th day for the second example in chapter 8.
Fig. 15e. Plume profile on the 45 day for the second example in chapter 8.
Fig. 16a. Plume profile on the 10th day for the third example in chapter 8.
Fig. 16b. Plume profile on the 30th day for the third example in chapter 8.
Fig. 16c. Plume profile on the 60th day for the third example in chapter 8.
Fig. 17a. Plume profile after 15 hours for the numerical example
Fig. 17b. Plume profile after 43 hours for the numerical example.
Fig 17c. Plume profile after 72 hours for the numerical example 3
HYDRAULIC CONDUCTIVITIES

Fig 18a.

HYDRAULIC CONDUCTIVITY IN X DIRECTION

Fig. 18b.
### Table (1)

<table>
<thead>
<tr>
<th>Type</th>
<th>$K_W$ (cm/sec)</th>
<th>$\phi_e$</th>
<th>Grain Size</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Glass Beads</td>
<td>5.066</td>
<td>0.32</td>
<td>2.5 mm</td>
<td>Industrial glass beads type v-11</td>
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</tbody>
</table>

### Table (2)

<table>
<thead>
<tr>
<th>Ko (cm/min)</th>
<th>$(p_o)^a_w$ (dy/cm)</th>
<th>$\gamma_0$ (dy/cm$^3$)</th>
<th>$\gamma_w$ (dy/cm$^3$)</th>
<th>$S_{Y,0}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>10.5</td>
<td>980</td>
<td>980</td>
<td>768</td>
<td>0.05</td>
</tr>
</tbody>
</table>
BIBLIOGRAPHY


Appendix A

The shape functions of different elements that are available in the element library of the model:

1) 3 noded triangular element:

The coordinate system is transformed in order to make a general triangle at right angle (fig. 9). Shape functions that are being shown are written in the convenient coordinate system

\( N_1: \xi \)

\( N_2: \eta \)

\( N_3: 1-\xi-\eta \)

2) 6 noded triangular element:

The transformed coordinate system is shown in fig. 10. Shape functions written in transformed coordinate system are

\( N_1 = (2\xi - 1)\xi \)

\( N_4 = -4(\eta + \xi - 1)\eta \)

\( N_2 = 4\xi\eta \)

\( N_5 = (\eta + \xi - 1)(2\eta + 2\xi - 1) \)

\( N_3 = (2\eta - 1)\eta \)

\( N_6 = -4\xi(\eta + \xi - 1) \)
3) 4 noded quadrilateral element:

The transformed coordinate system is shown in fig. 11.
Shape functions written in transformed coordinate system are

\[ N_1 = \frac{1}{4} (1+\xi) (1+\eta) \]
\[ N_2 = \frac{1}{4} (1-\xi) (1+\eta) \]
\[ N_3 = \frac{1}{4} (1-\xi) (1-\eta) \]
\[ N_4 = \frac{1}{4} (1+\xi) (1-\eta) \]

4) 8 noded quadrilateral element:

The transformed coordinate system is shown in fig. 12.
Shape functions written in transformed coordinate system are

\[ n_1 = \frac{1}{4} \left[ (1+\xi) (1+\eta) - (1-\xi^2) (1+\eta) - (1+\xi) (1-\eta^2) \right] \]
\[ n_2 = \frac{1}{4} \left[ (1-\xi) (1+\eta) - (1-\xi^2) (1+\eta) - (1-\xi) (1-\eta^2) \right] \]
\[ n_3 = \frac{1}{4} \left[ (1-\eta) (1-\xi) - (1-\xi^2) (1-\eta^2) - (1-\xi^2) (1-\eta) \right] \]
\[ n_4 = \frac{1}{4} \left[ (1+\xi) (1-\eta) - (1-\xi^2) (1-\eta) - (1+\xi) (1-\eta^2) \right] \]
APPENDIX B

Notes on Galerkin residual finite element technique

The method of weighted residuals is a technique for obtaining approximate solutions to linear and nonlinear partial differential equations. It has nothing to do with the finite element method other than offering another means with which to formulate the finite element equations.

Applying the method of weighted residuals involves basically two steps. The first is to assume the general functional behaviour of the dependent field variable in some way so as to approximately satisfy the given differential equation and boundary conditions. Substitution of this approximation into the original differential equation and boundary conditions then results in some error called residual. The residual is required to vanish in some average sense over the entire solution domain.

The second step is to solve the equations resulting from the first step and thereby specialize the general functional form to particular function, which then becomes the approximate solution sought.

To be more specific we shall consider a typical problem. Suppose that we want to find an approximate functional representation for a field variable $u$ governed by the differential equation
\[ L(u) = f \tag{B.1} \]
in the domain \( D \) bounded by the surface \( S \).

The function \( f \) is a known function of the independent variables, and we assume that proper boundary conditions are prescribed on \( S \). The method of weighted residual is applied in two steps as follows.

First the unknown exact solution \( u \) is approximated by \( u' \), where either functional behaviour of \( u' \) is completely specified in terms of unknown parameters, or the functional dependence on all but one of the independent variables is left unspecified. Thus the dependent variable is approximated by

\[ u \approx u' = \sum_{i=1}^{m} N_i C_i \tag{B.2} \]

Where the \( N_i \) are the assumed functions and the \( C_i \) are either the unknown parameters or unknown functions of one of the independent variables. The upper limit on the assumption, \( m \), is the number of unknowns \( C_i \). The \( m \) functions \( N_i \) are usually chosen to satisfy the global boundary conditions.

When \( u' \) is substituted in equation (B.1) it is unlikely that the equation will be satisfied.
that is \( L(u') - f = 0 \) \hspace{1cm} (B.3)

in fact \( L(u') - f = R \)

Where \( R \) is the residual or error that results from approximating \( u \) by \( u' \). The method of weighted residuals seeks to determine the \( m \) unknowns \( C_i \) in such a way that the error \( R \) over the entire solution is small. This is accomplished by forming a weighted average of the error and specifying that weighted average vanish over the solution domain. Hence we choose \( m \) linearly independent weighting functions \( W_i \) and then insist that

\[
\int_D [L(u') - f] W_i \, dD = \int_D R W_i \, dD = 0, \quad i = 1, 2, \ldots, m
\]

then \( R \) is approximately equal to zero in some sense.

The form of the error distribution principle expressed in equation (B.4) depends on our choice for the weighting functions. Once we specify the weighting functions, equation (B.4) represent a set of \( m \) equations, either algebraic equations or ordinary differential equations to be solved for the \( C_i \). The second step, then, is to solve the equations (B.4) for the \( C_i \) and hence obtain an approximate representation of the unknown field variable \( u \) via equation (B.3). There are many linear problems and some nonlinear problems for which it can be shown that if \( m \) tends
to infinity then \( u' \) tends to \( u \).

We have a variety of weighted residual techniques because of the broad choice of weighting functions or error distribution principles that can be used. The error distribution principle most often used to derive finite element equation is known as the Galerkin criterion, or the Galerkin's method. According to the Bubnov – Galerkin method, weighting functions are chosen to be the same as the approximating functions used to represent \( u \), that is, \( W_i = N_i \) for \( i = 1, 2, \ldots, m \). When the weighting functions \( W_i = N_i \) the approach is called Petrov – Galerkin method.

Galerkin's method requires that

\[
\int_{D} \left[ L(u') - f \right] N_i \, dD = 0, \quad i = 1, 2, \ldots, m \quad (B.5)
\]

In the preceding discussion we assume that we are dealing with the entire solution domain. However, because equation (B.1) holds for any point in the solution domain, it also holds for any collection of points defining an arbitrary subdomain or element of the whole domain. For this reason we may focus our attention on an individual element and define a local approximation analogous to equation (B.2) and valid for only one element at a time. Now the familiar finite element representations of a field variable become available. The functions \( N_i \) are recognized as the interpolation functions \( N_i \) defined over the element, and the \( C_i \) are the undermined parameters, which may be the
nodal values of the field variable or its derivatives. Then from the Galerkin's method we can write the equations governing the behaviour of an element as

\[ \int_{\Omega} [L(u) - f] N_i \, d\Omega = 0, \quad i = 1, 2, \ldots, r \]

where as before the superscript \( (e) \) restricts the range to one element, and

\[ u^{(e)} = [N^{(e)}] \{u\} \]

\[ f^{(e)} = \text{forcing function defined over element \( (e) \)} \]

\[ r = \text{number of unknown parameters assigned to an element} \]