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Project Summary

Approximate Multiphase Flow Modeling by Characteristic Methods

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The flow of petroleum hydrocarbons, organic solvents, and other liquids that are immiscible with water presents the nation with some of the most difficult subsurface remediation problems. One aspect of contaminant transport associated with releases of such liquids is transport as a water-immiscible liquid phase. Conventional finite element and finite difference models of multiphase flow may have extreme data and computational requirements. Sites with insufficient data or modeling for screening purposes may warrant using a simplified approach. In this document, approximate models of immiscible flow are presented for two- and three-phase flow. The approximations are constructed by representing the flow by hyperbolic equations which have method of characteristics solutions. This approximation has the additional benefit of being based on the fundamental wave behavior of the flow, which is revealed by the solutions of the models. An important result is that for three-phase flow, two flow regimes exist. The first is characterized by the displacement of one of the liquids into a bank which moves ahead of another liquid. The second is characterized by almost complete bypassing of a liquid by the other. The occurrence of the flow regimes is dependent on the organic liquid properties, soil type, and the initial amounts of the fluids present. Two-phase flows consisting of pulse applications of water result in overlapping simple waves and contact discontinuities. These models form the basis for future extension of the three-phase model to include pulse boundary conditions.

This Project Summary was developed by EPA's Robert S. Kerr Environmental Research Laboratory, Ada, OK, to announce key findings of the research project that is fully documented in a separate report of the same title (see Project Report ordering information at back).

Introduction

The focus of the research described in the full report is the transport of oily liquids within the subsurface. Subsurface contamination by oily wastes is recognized as a ubiquitous problem which presents some of the most challenging remediation difficulties. The three-phase flow of oily liquids in the unsaturated zone comprises one aspect of this problem. These fluids act as carriers for, or are themselves, hazardous organic chemicals. Motion of the organic liquid phase can enhance transport of hydrophobic organics by orders of magnitude over that occurring when water is the only mobile liquid.

Transport in the unsaturated zone is characterized by transient water flow caused by discrete rainfall events of varying intensity, duration, and inter-storm arrival time. Varying water fluxes play a central role in multiphase subsurface flow, as the rainfalls provide a driving force for the hydrologic inputs to the system. A focus of the research is the effect of transient flows in the water, organic, and air phases.

Since the governing equations for this problem are a system of coupled non-linear partial differential equations, numerical methods must be used for their solution. Existing complex models of multiphase flow can be CPU time-intensive, and their proper application is data-intensive. Numerical solution techniques sometimes introduce difficulties, since they are not approximation-error free. During the initial phase of site investigation, or for alternatives screening, a simplified approach is warranted, because data from typical RCRA and CERCLA sites is usually inadequate to justify a complex model. The approach that is taken is to represent the flow by a system of hyperbolic equations, which describe the wave behavior of the flow system. These equations can be solved by the method of characteristics. As will be shown, this technique results in models which have semi-analytic solutions. The latter are important because their analytic character allows rapid computation of many alternative scenarios. The models also have intrinsic value for checking numerical simulators. Most important, however, is the insight they provide into the fundamental character of the flow.

As stated above, the phases modeled are water, a water-immiscible organic liquid, and air. The term oleic liquid is used to indicate the organic liquid, usually such a liquid is called a NAPL (Non-Aqueous Phase Liquid). The word oleic is used because it means "oily" and carries the connotation of immiscibility with water. The terminology and the models presented herein are not restricted to petroleum based oleic liquids but also include organic solvents and other liquids.

The contents of the report are as follows: Section 2 contains a summary of the conclusions and recommendations. Section 3 describes the background and motivation for the work. Related models are briefly discussed. Section 4 reviews the multiphase, porous media, flow theory upon which the models are based. In Section 5 the classical and generalized method of characteristics solutions of hyperbolic equations is presented. The solution of a "Riemann problem" of mathematical physics is presented. The solution methodology is applied to one-dimensional, three-phase flow in soils. The fundamental character of the flow is shown through a series of illustrative examples. Since Riemann problems have restrictive boundary and initial conditions, the generalization to pulse boundary conditions is discussed in Section 6. Application of this theory is made to the infiltration of water subject to air phase resistance. A discussion of the results is presented in Section 7. These sections are summarized in the following pages.

Research Scope

The specific motivation for this work is that previous attempts to model multiphase flow of contaminants by simplified methods are limited to plug flow or to kinematic conditions. Plug flow models require the assumption that the fluids occupy a fixed portion of the pore space. Kinematic models allow more realistic fluid distributions but are limited to gravity driven flows. As a result, an intense rainfall, high viscosity oleic phase, and/or low permeability soil may cause the model to break down. In the present work, the general approximate framework of the kinematic approach is retained, and extensions to overcome the model's limitations are sought. The models that are presented allow some dynamic phenomena to be included along with the kinematic or gravity phenomena.

Two types of solutions are presented. First is the solution to a classical problem of mathematical physics, called a Riemann problem. Mathematically, a Riemann problem is defined as a hyperbolic system of equations with constant injection and uniform initial conditions. Although this is of limited direct applicability to field problems, the solution of the Riemann problem is important for several reasons: Mathematically, there has been a great deal of work done on these solutions for systems other than those presented here. In the report, the application of this work to multiphase flow is explored. Second, the solutions of the Riemann problem reveal some of the fundamental character of the flow. Results are presented which illustrate several typical flow regimes for three-phase flows. Third, one-dimensional solutions of the Riemann problem form the basis for multi-dimensional front tracking models of petroleum reservoirs which may be adaptable for subsurface contaminant transport.

The second type of solution is for systems which can be represented by injection conditions which consist of discrete pulses. The model system for this application is the infiltration of water, subject to air phase resistance. The solution of this problem consists of an extension and generalization of the Riemann problem solution techniques. The solution which is presented is the first step in developing a model for a surface spill of an oleic contaminant, followed or preceded by a sequence of rainfall events.

Model Formulation

The three-phase flow model is based on the assumption that the medium is uniform and the flow is one-dimensional. Each phase has a residual or trapped saturation which remains constant. The relative permeabilities are described by equations that are based on the Burdine, and Brooks and Corey theories. All phase transport properties are assumed to remain constant. The model describes immiscible transport without interphase partitioning phenomena, or any sources/sinks in the domain of interest.

As indicated in Appendix 1 of the full report, the model neglects the gradients of the capillary pressure. One of the main effects of the capillary gradient is to smooth sharp fronts. Because of the way that the speed of the sharp front is determined, the mean displacement speed of the true smooth front matches that of the sharp front. Flow visualization experiments conducted at the Robert S. Kerr Environmental Research Laboratory and elsewhere suggest that infiltrating fronts indeed remain sharp for a variety of situations. This assumption is critical for eliminating the parabolic character of the phase conservation equations, so that the method of characteristics can be applied to this problem. Application of the method of characteristics reduces the system of n coupled partial differential equations to a system of 2n coupled ordinary differential equations. In general, the latter are easier to solve numerically than the former.

Two important caveats must be noted. First, a necessary condition for the existence of classical solutions is that the system remains hyperbolic throughout the solution domain. The condition for hyperbolicity is that the eigenvalues remain real and distinct throughout the solution domain. For the multiphase flow problem considered here, this is demonstrated in Section 5. Second, the classical solutions are guaranteed to exist only in the "small," i.e., in a small neighborhood of the initial data. Proper initial data does not prevent discontinuities from forming within the solution domain. At these discontinuities, the partial derivatives appearing in the conservation equations do not exist, so neither do the classical solutions. In order to overcome this difficulty, solutions which satisfy integral forms of the mass conservation equations are used. In the present work, these are used where the sharp fronts replace the true fronts. The classical and generalized solutions are patched together to construct the complete solution, which consists of regions with smooth saturation variation separated by sharp fronts.

Discontinuous solutions are notorious for being non-unique, and abundant examples of this behavior exist. Generalized entropy conditions (shock inequalities) are used to select physically realistic discontinuous solutions. Two types of discontinuous solutions are important for the report, k-shocks and contact discontinuities. By obeying the shock inequalities, a discontinuous solution is assured to be physically realistic and therefore the proper discontinuous solution. The shocks appearing in the solutions presented are shown to be proper k-shocks. The second type of shock is a contact discontinuity, for which the shock speed matches the characteristic speed on one side of the shock.

Numerical Solution Methods

Most of the model equations are reduced to ordinary differential equations by the application of the method of characteristics. Equations which do not have analytical solutions are solved by a Runge-Kutta-Fehlberg method. Fehlberg's methods have the advantage that they contain automatic step size control based on a specified truncation error tolerance. For this work, a third order method is used for the solution and an embedded fourth order method is used for the step size control. Discontinuous paths across the saturation space diverge from continuous paths when the latter are not straight. The equation governing this behavior is a single nonlinear algebraic equation; it is solved by a method which combines bisection, inverse quadratic interpolation, and the secant method. The routine automatically chooses the most appropriate technique.

Construction of Saturation Profiles

Solutions are constructed in two basic steps: First, an injection condition-plateau-initial condition route on the saturation composition space diagram (Figure 1) is determined. As explained in the report the solutions consist of two waves which may be continuous, continuous and terminate in a contact discontinuity, or discontinuous (k-shock). The wave associated with $\lambda 1$ (τηε smaller eigenvalue) is followed from the injection condition toward the plateau. This wave is called a λ_1-wave or slow wave, and is followed first, because with smaller eigenvalues this wave must be traversed before the faster wave (the λ_2-wave). At the plateau, the solution switches to the λ_2-wave to complete the route to the initial condition. The route determines the specific saturation compositions which exist in the solution. When discontinuities form, the route is adjusted as needed. The adjustment alters the saturation composition at the plateau and thus the wave speeds. When the routes are straight lines, the continuous and discontinuous routes are identical, and only one λ_2 route exists. In this example, the λ_1 routes are almost coincident. The second step is to determine the occurrence in space and time of the saturations along the route.

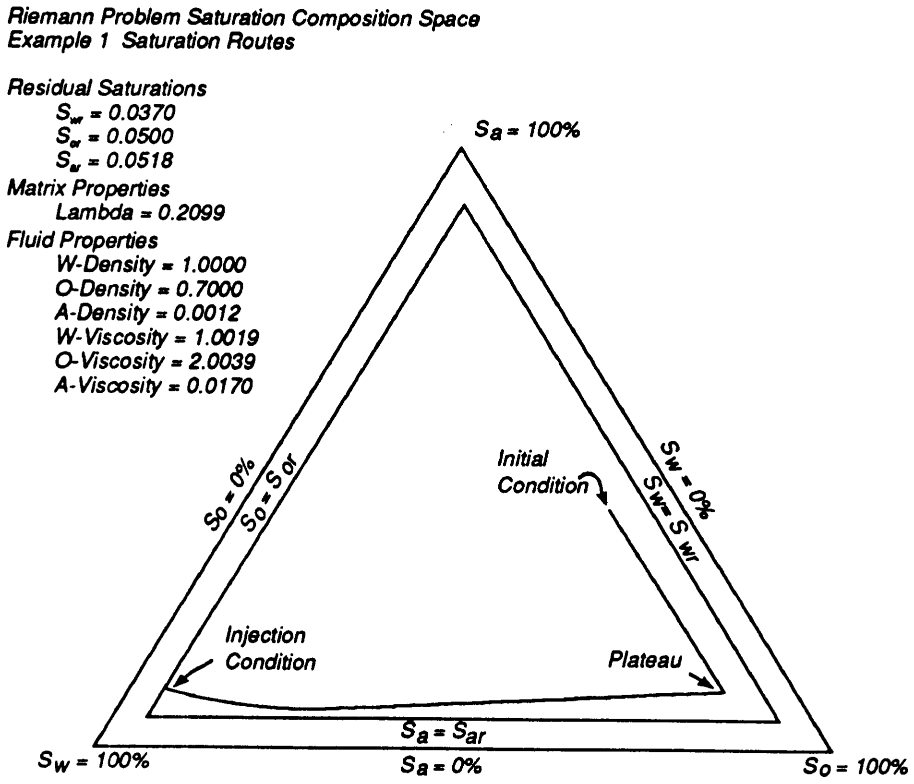

Figure 1. Example 1 saturation routes showing the continuous solution and the correction due to the discontinuities. In this case, the routes are nearly identical and not distinguishable on the figure.

Example 1 Oleic Liquid Bank Formation

In Example 1, water and air are injected into the soil with a total flux of 2.0 m/d, and a saturation composition of S = S (S_w, S_o, S_a) = S (0.8490, 0.0501, 0.1009), where S_w, S_o, and S_a are the percent of the pore space (saturation) filled by water, oleic liquid and air, respectively. The oleic liquid saturation at injection is slightly above residual (S_{or} = 0.0500), because the solution along the side of the inner triangle is degenerate. That is, the side is a two-phase region, with no path which enters the three-phase region. Also, the three-phase equations are singular along the edge and cannot be used.

A depth-time plot of the solution, which is called the base characteristic plane, is shown in Figure 2. Shown on the plot are the λ_1 - and λ_2-waves. In this case, the λ_1-wave has a continuous portion which is illustrated by the fan-shaped characteristic pattern. This wave is a λ_1-centered simple wave which terminates in a contact discontinuity. The λ_2-wave is discontinuous and is a 2-shock. The plateau emerges from the origin and expands with time because of the difference in speed between the contact discontinuity and the 2-shock. Ahead of the 2-shock is the initial condition; the location of the 2-shock corresponds to the maximum influence of the injection.

Figure 3 shows a depth-saturation profile for the solution at 24 hours after the beginning of the injection. Depth-saturation profiles complement the base characteristic plane as they show the fluid saturations at a given time in the solution. The water and total liquid saturation are plotted directly against the depth. The oleic liquid saturation is the difference between the total liquid and water saturations. Likewise, the air saturation is determined by subtracting the total liquid saturation from one. Recall that at the boundary (depth = 0), the oleic liquid is very near its residual saturation, and water and a small amount of air are injected. The general nature of this solution is that the injection at the surface causes the oleic liquid to be dis-

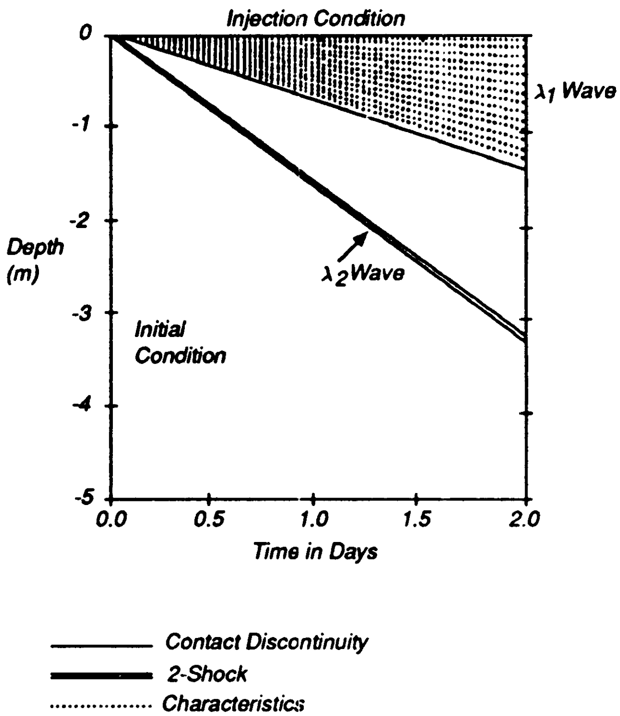

Figure 2. Example 1 base characteristic plane (depth-time plot of the solution). The solution consists of a centered simple wave, contact discontinuity, and 2-shock.

placed into a bank moving ahead of the water front (CEFG on Figure 3). At this time, the water front is located at a depth of 0.73 meters (CD). The water saturation at the front remains constant at 0.7821. The oleic liquid displacement is not complete, as some of it is left behind the water front at saturations above residual (ABDE, the distance between A and B is the oleic liquid injection condition which is close to residual). The water saturation decreases from the injection (A) to the water front due to the oleic liquid that is bypassed (AD). The smooth variation in saturation above the water front corresponds to the λ_1-centered simple wave on Figure 2.

Most of the oleic liquid is displaced, however, into a bank moving ahead of the water front. In this example the oleic liquid bank is bounded above by the contact discontinuity and below by the 2-shock (Figure 2). The bank corresponds to the plateau in the saturation space where S = S(0.1000, 0.8034, 0.0966). The water saturation at the plateau equals the initial water saturation (S_w = 0.1000), because the λ_2-wave portion of the route is a straight line parallel to the water axis. The bank front (FG on Figure 3) moves faster than the water front (CD), and so the bank expands with time. The bank forms because the flux of the oleic liquid is high enough so that it can move ahead of the incoming water. The leading edge of the oleic liquid bank (FG) is discontinuous, because the λ_2 eigenvalues decrease from the plateau to the initial condition.

Example 2 Oleic Liquid Bypassing

Figure 4 shows the bypassing profile that is produced when the initial condition is S(0.5000, 0.1000, 0.4000), and the injection condition is the same as for Example 1. In essence, the effective conductivity of oleic liquid present initially is insufficient to match the speed of the incoming water. All of the oleic liquid is bypassed by the water. The base characteristic plane for Example 2 is shown in Figure 5. The λ_1-centered simple wave merges with the plateau before a discontinuity can form, so there is no contact discontinuity and no oleic liquid bank in this example. As in Example 1, the λ_2-wave is a 2-shock, the position of which determines the maximal influence of the injection. There is a slight discontinuity in oleic liquid saturation (0.1019 above vs. 0.1000 below) at this front (A). This small jump moves at the same speed as the water front.

More examples are presented in the report which illustrate the effects of oleic liquid properties, media properties (hydraulic conductivity and pore size distribution), gravity and the injection of the oleic liquid. In addition to developing the solution for one injection-initial condition pair, the equations can be solved for the entire suite of possible conditions. The report illustrates several full complete saturation composition spaces, showing all possible variations in saturations which are solutions of the classical Riemann problem. From these, general conclusions can be drawn concerning the displacement processes.

Generalization of Riemann Problem Solutions

Although solutions of Riemann problems provide much insight into fundamental fluid flow phenomena, the restrictive nature of their boundary and initial conditions limits their usefulness. In Section 6 of the report, the limitations on the boundary conditions are removed for the two-phase flow of air and water during infiltration. All of the principles involved also apply to three-phase flow problems. Two major issues are discussed: first is the determination of the total flux and second is the interaction of overlapping characteristic patterns.

One reason why Riemann problem solutions become attractive is that there often can be found a single point in time and space where the total flux is known. Usually this is an injection condition, as was the case for the examples presented and in the classic Buckley-Leverett solution, where constant flux boundary conditions are applied. When the injection is not constant, then difficulty is encountered in determining the total flux; i.e., the total flux cannot be considered constant when a constant flux condition abruptly ends. After this occurs, there is zero flux of the injected fluid at the boundary; but the total flux clearly is not zero throughout the domain. A second case occurs when there is a constant rate rainfall at the boundary. The amount of water that can enter the profile is limited by the infiltration capacity of the soil, which is a function of the saturated hydraulic conductivity, relative permeability, antecedent water saturation, cumulative infiltration, and other factors. Thus, the water flux entering the profile varies with time, even when the precipita-

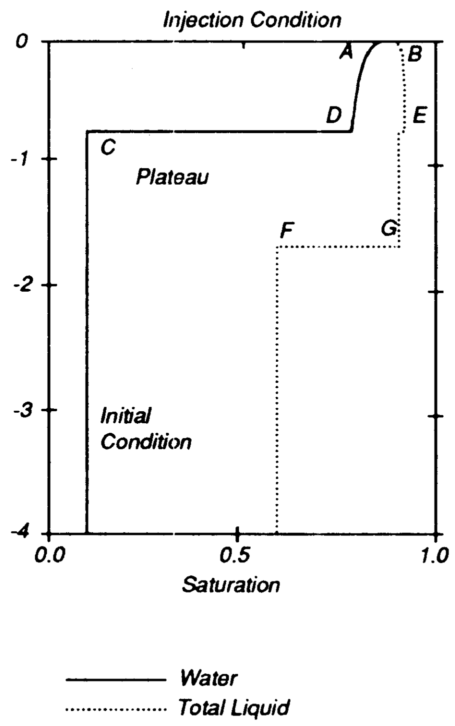

Figure 3. *Example 1 saturation profile at 24 hours showing fluid saturation versus depth of penetration. The oleic liquid is being displaced into a bank (CEFG) by the incoming water and air.*

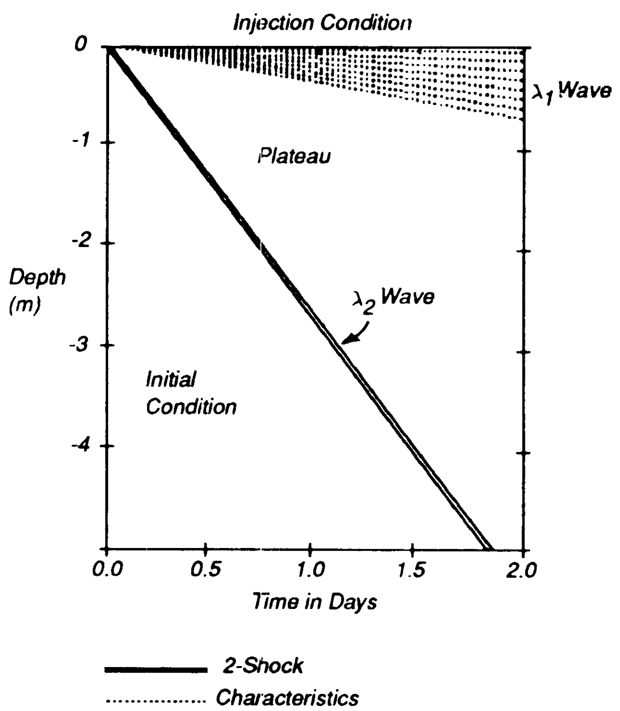

Figure 4. *Example 2 base characteristic plane (depth-time plot of the solution). The solution consists of a centered simple wave, and 2-shock.*

tion rate is constant. An expression for the water flux can be used to determine the total flux, assuming that at the surface the water flux equals the total flux. Although this is recognized as being only an assumption, it is expected that in most cases little error is introduced into the water flow. Integrating the Darcy's law equations results in an expression for the total flux which can be evaluated at any time in the solution. Because of the time variation in the total flux, the characteristics which previously were straight lines now curve. Thus, much additional complexity is introduced into the numerical implementation of the solution.

Discussion of Results

The application of characteristic methods to one-dimensional flow problems reveals the fundamental behavior of three-phase systems. Although the full governing equations are parabolic, the approximate hyperbolic equations which are solved in this report describe a fundamental portion of the flow phenomena. The efficiency that is achieved by simplifying the governing equations allows results to be developed which apply to any pair of injection and initial conditions for a given oleic phase and soil type. The semi-analytic nature of the solution is primarily responsible for the generation of these "universal" results. The following conclusions are drawn from the work.

For systems with constant injection conditions and uniform initial conditions (Riemann problems), flow occurs in two regimes. When the injection consists mostly of water, mobile oleic liquids (organic liquids or so-called NAPLs) are displaced into "banks" or are bypassed. The banks move ahead of, and are driven by, the incoming water. The bypassing profile is characterized by the water moving past the oleic liquid, without causing it to be displaced into the profile. The occurrence of the regimes is determined by the oleic liquid properties, media properties, and the initial amount of all fluids present. Although the type of boundary condition used in these solutions is not what is expected in the field, mathematically, it causes the hyperbolic problem to be a Riemann problem, for which there exists a large body of precise mathematical results. The flow regimes which exist in these solutions are believed to be fundamental for those expected from the solution of the hyperbolic system with general initial and boundary conditions.

The dependency of the results on the initial condition suggests that for cases where the oleic liquid has drained to a low saturation in the upper part of the soil profile, incoming rainfall will likely bypass the oleic liquid. Near the surface, this condition is likely to occur when a rainfall follows the end of an oleic liquid release by several hours. The oleic liquid has enough time to begin draining from the surface, so the incoming water experiences oleic liquid saturations which are low. Thus the bypassing regime is likely to be favored.

For systems with injections of mostly oleic liquid, the dominant flow regime is water bypassing. This conclusion confirms the intuition that the oleic liquid, which occupies a mid-range of the pore space due to its wetting behavior, does not displace water from the small pores. Preferential wetting causes the water to be too tightly held to the media to be easily displaced by a non-wetting liquid. Thus spills of oleic liquid to soil profiles, which contain water at the so-called field capacity, are likely to bypass the pre-existing water.

In all cases, the behavior of the oleic liquid is dependent on its properties (density and viscosity) relative to those of water. As the oleic liquid becomes more mobile, water injections favor the bank formation regime somewhat, because the oleic liquid is of high enough mobility to match the speed of the incoming water. The character of the results, however, always reflects preferential wetting as indicated in the conclusion stated above. Thus, in the example presented, the bypassing regime was only slightly larger for the higher mobility TCE case than the lower mobility oil, because of preferential wetting.

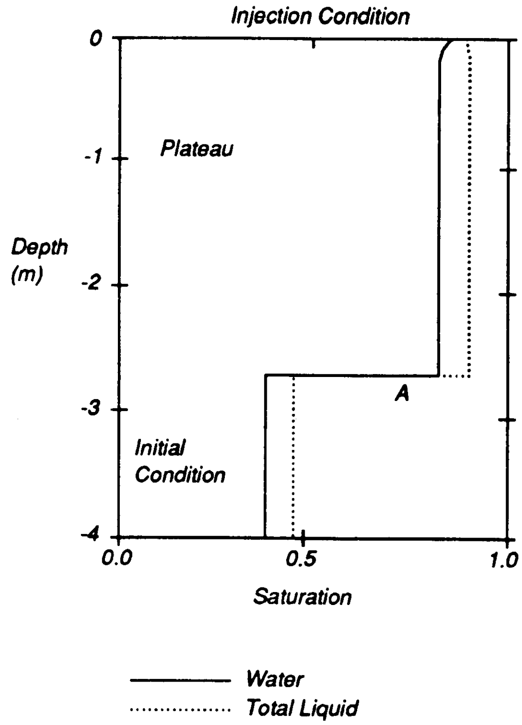

Figure 5 *Example 2 bypassing profile showing fluid saturation versus depth. The incoming water and air.bypasses the oleic liquid.*

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The complete report, entitled "Approximate Multiphase Flow Modeling by Characteristic Methods," (Order No. PB91-190959/AS; Cost: $23.00, subject to change) will be available only from:

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