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Vertical Integration of Three-Phase Flow Equations for Analysis of Light Hydrocarbon Plume Movement

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Abstract. A mathematical model is derived for areal flow of water and light hydrocarbon in the presence of gas at atmospheric pressure. Vertical integration of the governing three-dimensional, three-phase flow equations is performed under the assumption of local vertical equilibrium to reduce the dimensionality of the problem to two orthogonal horizontal directions. Independent variables in the coupled water and hydrocarbon areal flow equations are specified as the elevation of zero gauge hydrocarbon pressure (air-oil table) and the elevation of zero gauge water pressure (air-water table). Constitutive relations required in the areal flow model are vertically integrated fluid saturations and vertically integrated fluid conductivities as functions of air-oil and air-water table elevations. Closed-form expressions for the vertically integrated constitutive relations are derived based on a three-phase extension of the Brooks–Corey saturation-capillary pressure function. Closed-form Brooks–Corey relations are compared with numerically computed analogs based on the Van Genuchten retention function. Close agreement between the two constitutive models is observed except at low oil volumes when the Brooks–Corey model predicts lower oil volumes and transmissivities owing to the assumption of a distinct fluid entry pressure. Nonlinearity in the vertically integrated constitutive relations is much less severe than in the unintegrated relations. Reduction in dimensionality combined with diminished nonlinearity, makes the vertically integrated water and hydrocarbon model an efficient formulation for analyzing field-scale problems involving hydrocarbon spreading or recovery under conditions for which the vertical equilibrium assumption is expected to be a satisfactory approximation.

Key words. Multiphase flow, vertical equilibrium model, immiscible flow.

1. Introduction

Groundwater contamination due to surface spills or subsurface leakage of hydrocarbon fuels, organic solvents, and other immiscible organic liquids is a widespread problem. Numerical models for phase-separated hydrocarbon migration in the vadose zone and groundwater have been presented recently by various researchers. Most analyses have been restricted to consideration of two-dimensional domains involving a vertical slice through unsaturated and/or saturated zones (Abriola and Pinder, 1985; Faust, 1985; Huyakorn and Pinder, 1978; Osborne and Sykes, 1986, Kuppusamy *et al.*, 1987; Kaluarachchi and Parker, 1988). While theoretically instructive, such models have limited applicability for the analysis of many field problems which involve complex geometry and boundary conditions. Fully three-dimensional multiphase-flow models have been discussed recently by Falta and Javandel (1987) and Faust (1988). However, the high computational cost of using such codes imposes severe restrictions on their practical utility.

An alternative modeling approach which has been widely employed in petroleum reservoir engineering involves vertical integration of the governing flow equations under the assumption of near-equilibrium conditions in the vertical direction, thus reducing the numerical dimensionality as well as the severity of the problem nonlinearity (Martin, 1968; Rosenzweig *et al.*, 1986; Aziz and Setari, 1979). Theoretical aspects of vertical averaging for multiphase-flow problems have been discussed by Gray (1975). The problem of hydrocarbon spreading from leaking underground storage tanks has been analyzed by various researchers using areal flow models for the special case of step-function saturation-capillary pressure relations. Analytical solutions which ignore water flow (Greulich and Kaergaard, 1984) and numerical models for coupled water and hydrocarbon flow (Hochmuth and Sunada, 1985) have been reported.

The objective of this paper is to derive a mathematical model for areal flow of water and light hydrocarbon by vertical integration of the governing three-dimensional, three-phase flow equations under the assumption of local vertical equilibrium. Closed-form expressions for vertically integrated fluid volumes and transmissivities are developed based on a three-phase extension of the Brooks–Corey saturation-capillary pressure function.

2. Vertical Integration of Governing Equations

2.1. GENERAL THREE-DMENSIONAL FLOW EQUATIONS

We wish to consider the problem of flow in a three-fluid phase porous media system with air, water, and a nonaqueous phase liquid, which we will refer to subsequently simply as 'oil'. Equations of motion for the two liquid phases may be written in tensor notation as

$$q_{w_i} = -\mathbf{K}_{w_{ij}}\left(\frac{\partial h_w}{\partial x_j} + \mathbf{u}_j\right), \tag{1a}$$

$$q_{o_i} = -\mathbf{K}_{o_{ij}}\left(\frac{\partial h_o}{\partial x_j} + \rho_{ro}\mathbf{u}_j\right), \tag{1b}$$

where q_{wi} and q_{oi} are velocity components in the i direction (i, $j = 1, 2, 3$) for water and oil phases $[\mathrm{L^3\,L^{-2}\,T^{-1}}]$, x_j are Cartesian spatial coordinates, h_w and h_o are water height-equivalent pressure heads in water and oil [L] of the form $h_p = P_p/\rho_w g$ ($p = o, w$) where P_p is the p-phase pressure $[\mathrm{F\,L^{-2}}]$, ρ_w is the density of water $[\mathrm{M\,L^{-3}}]$ and g is gravitational acceleration $[\mathrm{L^2T^{-1}}]$, $\mathbf{K}_{pij}$ are p-phase conductivity tensors $[\mathrm{L\,T^{-1}}]$, ρ_{ro} is the ratio of oil to water density $[\mathrm{L^0}]$, and $u_j = \partial z/\partial x_j$

is a unit gravitational vector [L^0] where z is elevation. Phase conductivities are conventionally assumed to be of the form

$$\mathbf{K}_{w_{ij}} = k_{rw}\mathbf{K}_{sw_{ij}}\,, \tag{2a}$$

$$\mathbf{K}_{o_{ij}} = k_{ro}\mathbf{K}_{sw_{ij}}/\eta_{ro}\,, \tag{2b}$$

where k_{rw} and k_{ro} are relative permeabilities of water and oil [L^0], respectively, η_{ro} is the ratio of oil to water absolute viscosity [L^0], and $\mathbf{K}_{sw_{ij}}$ is the saturated conductivity tensor for water. (Note: ρ_{ro} is absent from the numerator of Equation (2b) due to use of water-height equivalent head h_0 in Equation (1b).) An equation of the same form as (1b) may be written for gas-phase convection. However, we shall restrict our attention here to cases in which it is reasonable to invoke Richard's assumption – that gas pressure gradients are negligibly small due to atmospheric boundary control and low gas impedance – thus avoiding explicit consideration of gas flow.

Assuming negligible compressibility of the water and oil phases and of the soil matrix, liquid-phase continuity equations may be written as

$$\Phi\frac{\partial S_w}{\partial t} = -\frac{\partial q_{wi}}{\partial x_j} + J_w\,, \tag{3a}$$

$$\Phi\frac{\partial S_o}{\partial t} = -\frac{\partial q_{oi}}{\partial x_j} + J_o\,, \tag{3b}$$

where Φ is porosity [$L^3\,L^{-3}$], S_p is p-phase saturation [L^3L^{-3}], t is time [T], x_j are Cartesian coordinates ($i, j = 1, 2, 3$), and J_p are p-phase volumetric source-sink terms [$L^3\,L^{-3}T^{-1}$].

2.2. VERTICAL EQUILIBRIUM HEAD DISTRIBUTIONS

To proceed further, it is useful to introduce the concept of piezometric head for water and oil phases and define

$$\Psi_w = h_w + z, \tag{4a}$$

$$\Psi_o = h_o + \rho_{ro}z, \tag{4b}$$

where Ψ_w and Ψ_o and water and oil piezometric heads and z is elevation above an arbitrary datum. We wish to consider the situation in which liquid velocities in the vertical direction may be regarded as small relative to those in the horizontal. More specifically, we assume that vertical fluid redistribution occurs on a sufficiently short time-scale such that vertical pressure distributions constantly approximate hydrostatic conditions, i.e. $\partial\Psi_w/\partial z$ and $\partial\Psi_o/\partial z \to 0$.

In such circumstances, it is possible to characterize the vertical pressure distributions in all phases in terms of various fluid 'table' elevations. Consider a (locally) static system containing air, water and lighter-than-water oil in which we install a hypothetical screened well (Figure 1). An oil lens is observed which may be characterized by an air-oil table elevation, z_{ao}, at which location the gauge oil pressure is zero, and an oil-water table elevation, z_{ow}, at which water and oil pressures are equal. We may also theoretically define an air-water table elevation, z_{aw}, at which the gauge water pressure is zero. Hydrostatic conditions require that $\partial \Psi_w/\partial z = 0$ and $\partial \Psi_o/\partial z = 0$, hence

$$\Psi_w = z_{aw}, \tag{5a}$$

$$\Psi_o = \rho_{ro} z_{ao} \tag{5b}$$

and

$$h_w = z_{aw} - z, \tag{6a}$$

$$h_o = \rho_{ro}(z_{ao} - z). \tag{6b}$$

From (6) and the definitions of z_{aw}, z_{ao}, and z_{ow}, we observe that

$$z_{ow} = z_{aw} - \rho_{ro} H_o, \tag{7a}$$

where $H_o = z_{ao} - z_{ow}$ is the 'piezometric oil height' (see Figure 1). The various

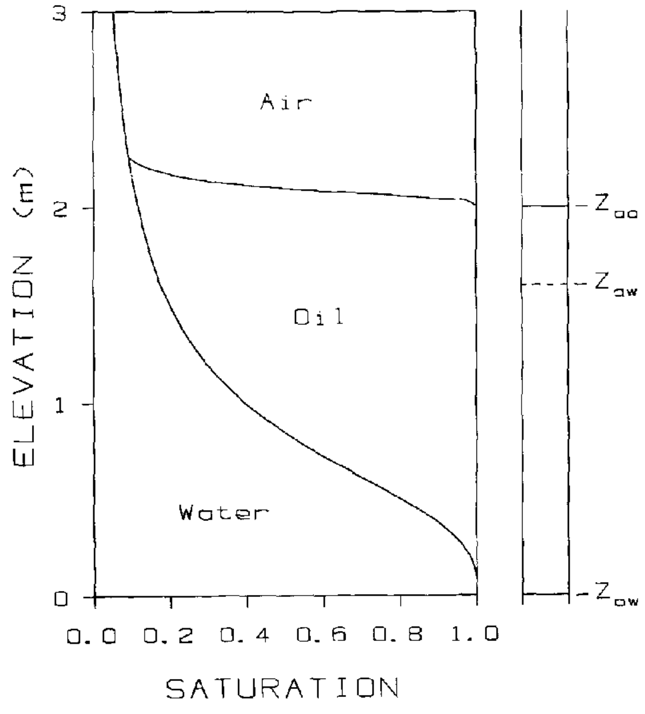

Fig. 1. Water and total liquid distributions in equilibrium with well (for VG model properties given in Table 1 with $H_o = 2$ m).

table elevations are thus related by

$$z_{ow} = \frac{z_{aw} - \rho_{ro} z_{ao}}{1 - \rho_{ro}} \tag{7b}$$

such that stipulation of any two of the three table elevations completely defines the three-phase static vertical head distributions.

2.3. VERTICALLY INTEGRATED FLOW EQUATIONS

Let us assume that the flow domain of interest is bounded at the top by the soil-atmosphere boundary and at the bottom by an effective lower bound of the unconfined aquifer. (In principal, this would be an impermeable layer, but if partially penetrating wells are modeled, the effective lower boundary of the well-coning zone would be relevant in practice.) We designate the elevations of these physical boundaries as z_u and z_l, respectively. Integration of Darcy's equation (1) in the vertical direction subject to the assumption of local vertical equilibrium represented by (4) and (5) yields

$$Q_{w_i} = -\mathbf{T}_{w_{ij}} \frac{\partial z_{aw}}{\partial x_j}, \tag{8a}$$

$$Q_{o_i} = -\mathbf{T}_{o_{ij}} \frac{\partial z_{ao}}{\partial x_j}, \tag{8b}$$

where Q_{wi} and Q_{oi} are vertically integrated fluxes of water and oil [$\mathrm{L}^3\ \mathrm{L}^{-1}\ \mathrm{T}^{-1}$] in the i direction ($i, j = 1, 2$) of the form

$$Q_{p_i} = \int_{z_l}^{z_u} q_{p_i}\,\mathrm{d}z \tag{9}$$

for the p-phase ($p = o, w$), and $\mathbf{T}_{w_{ij}}$ and $\mathbf{T}_{o_{ij}}$ are water and oil transmissivity tensors defined by

$$\mathbf{T}_{w_{ij}} = \int_{z_l}^{z_u} K_{w_{ij}}\,\mathrm{d}z, \tag{10a}$$

$$\mathbf{T}_{o_{ij}} = \rho_{ro} \int_{z_l}^{z_u} K_{o_{ij}}\,\mathrm{d}z. \tag{10b}$$

Likewise, integrating the continuity equations (3) over the vertical domain yields

$$\frac{\partial V_w}{\partial t} = -\frac{\partial Q_{wi}}{\partial x_j} + \bar{J}_w, \tag{11a}$$

$$\frac{\partial V_o}{\partial t} = -\frac{\partial Q_{oi}}{\partial x_j} + \bar{J}_o, \tag{11b}$$

where V_w and V_o are total water and oil volumes per horizontal area $[\mathrm{L}^3\ \mathrm{L}^{-2}]$ at a point in the areal plane defined by

$$V_w = \int_{z_l}^{z_u} \Phi S_w \, \mathrm{d}z, \tag{12a}$$

$$V_o = \int_{z_l}^{z_u} \Phi S_o \, \mathrm{d}z, \tag{12b}$$

and $\bar{J}_w$ and $\bar{J}_o$ are vertically integrated source-sink terms $[\mathrm{L}^3\ \mathrm{L}^{-2}\ \mathrm{T}^{-1}]$.

Combining (8) and (11) yields the governing equations for areal flow of water and oil as

$$\frac{\partial V_w}{\partial t} = \frac{\partial}{\partial x_i}\left[\mathbf{T}_{w_{ij}} \frac{\partial z_{aw}}{\partial x_j}\right] + \bar{J}_w, \tag{13a}$$

$$\frac{\partial V_o}{\partial t} = \frac{\partial}{\partial x_i}\left[\mathbf{T}_{o_{ij}} \frac{\partial z_{ao}}{\partial x_j}\right] + \bar{J}_0. \tag{13b}$$

Since V_w and V_o will, in general, be functions of both z_{aw} and z_{ao}, implicit solution of the coupled PDEs (13a) and (13b) for fluid-table elevations requires expansion of the left-hand sides as

$$\gamma_{ww} \frac{\partial z_{aw}}{\partial t} + \gamma_{wo} \frac{\partial z_{ao}}{\partial t} = \frac{\partial}{\partial x_i}\left[T_{w_{ij}} \frac{\partial z_{aw}}{\partial x_j}\right] + \bar{J}_w, \tag{14a}$$

$$\gamma_{ow} \frac{\partial z_{aw}}{\partial t} + \gamma_{oo} \frac{\partial z_{ao}}{\partial t} = \frac{\partial}{\partial x_i}\left[T_{o_{ij}} \frac{\partial z_{ao}}{\partial x_j}\right] + \bar{J}_0, \tag{14b}$$

where γ_{pq} $[\mathrm{L}\ \mathrm{L}^{-1}]$ are pq-phase storage coefficients defined by

$$\gamma_{pq} = \partial V_p / \partial z_{aq} \tag{15}$$

in which p, $q = o$, w are phase indices. It may be noted that γ_{ww} corresponds to the storage coefficient of conventional single-phase groundwater-flow analyses.

3. Vertically Integrated Saturation-Pressure Relations

3.1. DERIVATION OF FUNCTIONAL RELATIONS

To solve the vertically integrated flow equations, (14a) and (14b), expressions are required for the integrated saturation-pressure functions, $V_w(z_{aw}, z_{ao})$ and $V_o(z_{aw}, z_{ao})$. We proceed to obtain these by assuming local three-phase saturation-pressure relations may be described by scaled relations of the form proposed by Parker *et al.* (1987), namely

$$\bar{S}_w(\beta_{ow} h_{ow}) = S^*(h^*), \tag{16a}$$

$$\bar{S}_t(\beta_{ao} h_{ao}) = S^*(h^*), \tag{16b}$$

where h_{ow} and h_{ao} are oil-water and air-oil capillary heads, β_{ow} and β_{ao} are fluid pair-dependent scaling coefficients, and $S^*(h^*)$ is a scaled saturation-capillary head function defined by

$$S^*(h^*) \equiv \bar{S}_w^{\text{prist}}(h_{aw}), \tag{16c}$$

where $\bar{S}_w^{\text{prist}}$ denotes the effective saturation of water in the pristine air-water system and h_{aw} is the air-water capillary head. Effective water and total liquid saturations are defined, respectively, by

$$\bar{S}_w = \frac{S_w - S_m}{1 - S_m}, \tag{17a}$$

$$\bar{S}_t = \frac{S_w + S_o - S_m}{1 - S_m}, \tag{17b}$$

where S_w and S_o are actual water and oil saturations and S_m is the 'irreducible' water saturation. The pertinent capillary heads are defined by

$$h_{ao} = h_a - h_o, \tag{18a}$$

$$h_{ow} = h_o - h_w, \tag{18b}$$

$$h_{aw} = h_a - h_w, \tag{18c}$$

where h_w and h_o are as previously introduced and h_a is the gas-phase head which is assumed here to be zero (i.e., atmospheric pressure).

It may be shown theoretically that the scaling factors β_{ao} and β_{ow} are approximated by

$$\beta_{ao} = \sigma_{aw}/\sigma_{ao}, \tag{19a}$$

$$\beta_{ow} = \sigma_{aw}/\sigma_{ow}, \tag{19b}$$

where σ_{aw} is the surface tension of uncontaminated water, σ_{ao} is the surface tension of the organic liquid, and σ_{ow} is the interfacial tension between oil and water (Lenhard and Parker, 1987; 1988). Contamination of the air-water system by an infinitesimal volume of oil such that (16a) and (16b) hold and $S_t \rightarrow 0$ indicates that the form of the contaminated air-water saturation-pressure relation is

$$\bar{S}_w^{\text{contam}}(\beta'_{aw}h_{aw}) = \bar{S}_w^{\text{prist}}(h_{aw}), \tag{20a}$$

where

$$\beta'_{aw} = \sigma_{aw}/\sigma'_{aw} \tag{20b}$$

in which σ'_{aw} is the surface tension of organic contaminated water.

In previous studies, we have taken the form of $S^*(h^*)$ to be given by Van Genuchten's (1980) model

$$S^*(h^*) = [1 + (\alpha h^*)^n]^{-m}, \quad h^* > 0, \tag{21a}$$

$$S^*(h^*) = 1, \quad h^* \leq 0, \tag{21b}$$

where α $[L^{-1}]$ and n $[L^0]$ are Van Genuchten parameters and $m = 1 - 1/n$. From (21) and (16), the three-phase saturation-pressure relations are given by

$$S_w = (1 - S_m)\{1 + (\alpha\beta_{ow}h_{ow})^n\}^{-m} + S_m, \quad h_{ow} > 0, \tag{22a}$$

$$S_w = 1, \quad h_{ow} \leq 0, \tag{22b}$$

$$S_t = (1 - S_m)\{1 + (\alpha\beta_{ao}h_{ao})^n\}^{-m} + S_m, \quad h_{ao} > 0, \tag{22c}$$

$$S_t = 1, \quad h_{ao} \leq 0. \tag{22d}$$

Substitution of (22) into (12) yields integral expressions for water and oil volumes, V_w and V_o. Unfortunately, while (22) has been shown to provide an accurate representation of two- or three-phase saturation-pressure relations (Parker *et al.*, 1987; Lenhard and Parker, 1987; Lenhard and Parker, 1988; Lenhard *et al.*, 1988), it suffers a distinct disadvantage for our present purpose because it cannot be integrated exactly in (12) to obtain closed-form expressions for V_w and V_o.

A more suitable choice for $S^*(h^*)$ which avoids this difficulty is the model of Brooks and Corey (1966) which has the form

$$S^*(h^*) = [h_d/h^*]^\lambda, \quad h^* > h_d, \tag{23a}$$

$$S^*(h^*) = 1, \quad h^* \leq h_d, \tag{23b}$$

where h_d [L] is the air-entry head of the pristine air-water system and λ $[L^0]$ is a parameter governed by the pore-size distribution. From (23) and (16), water and total liquid saturations for the Brooks–Corey model are described by

$$S_w = (1 - S_m)\{h_d/\beta_{ow}h_{ow}\}^\lambda + S_m, \quad h_{ow} > h_d/\beta_{ow}, \tag{24a}$$

$$S_w = 1, \quad h_{ow} \leq h_d/\beta_{ow}, \tag{24b}$$

$$S_t = (1 - S_m)\{h_d/\beta_{ao}h_{ao}\}^\lambda + S_m, \quad h_{ao} > h_d/\beta_{ao}, \tag{24c}$$

$$S_t = 1, \quad h_{ao} \leq h_d/\beta_{ao}, \tag{24d}$$

and oil saturation is $S_o = S_t - S_w$. The expression for vertically integrated water volume (Equation (12a)) can now be expressed as

$$V_w = \Phi(\Omega - z_l) + \int_{\Omega}^{z_u} \Phi\, S_w(z)\, dz, \tag{25}$$

with

$$\Omega = \mathrm{Min}(z_u, z_{fow})$$

$$z_{fow} = z_{ow} + h_d/\beta_{ow}(1 - \rho_{ro}),$$

where z_{fow} represents the elevation below which complete water saturation occurs (upper boundary of saturated oil-water capillary fringe). Substituting (24) for $S_w(h_{ow})$, making a change of variables from z to h_{ow} via (6) and integrating assuming uniform soil properties with depth yields for $z_{fow} < z_u$

$$V_w = \Phi\left(z_{ow} + \frac{h_d}{\beta_{ow}(1-\rho_{ro})} - z_l\right) + \\ + \frac{\Phi(1-S_m)}{(1-\lambda)(1-\rho_{ro})}\mathscr{B}^{\lambda}(\mathscr{A}^{1-\lambda} - \mathscr{B}^{1-\lambda}\Big) + \frac{\Phi S_m}{1-\rho_{ro}}(\mathscr{A} - \mathscr{B}), \tag{26a}$$

where

$$\mathscr{A} = (1-\rho_{ro})(z_u - z_{ow}), \qquad \mathscr{B} = h_d/\beta_{ow}$$

For $z_{fow} \geqslant z_u$ we have simply

$$V_w = \Phi(z_u - z_l). \tag{26b}$$

Note that in both (26a) and (26b), V_w is a function of z_{ow} only.

The expression for vertically integrated oil volume (Equation (12b)) can likewise be expressed in integral form as

$$V_o = \Phi\int_{\Omega}^{\Gamma}[1 - S_w(z)]\,\mathrm{d}z + \Phi\int_{\Gamma}^{z_u} S_t(z)\,\mathrm{d}z - \Phi\int_{\Gamma}^{z_u} S_w(z)\,\mathrm{d}z, \tag{27}$$

in which

$$\Gamma = \mathrm{Min}(z_u, z_{fao}), \qquad z_{fao} = z_{ao} + h_d/\beta_{ao}\rho_{ro},$$

where z_{fao} represents the elevation below which complete liquid saturation occurs (upper boundary of saturated air-oil capillary fringe). Substituting $S_w(h_{ow})$ and $S_t(h_{ao})$ from (24), changing variables via (6), and integrating yields for $z_{fao} \geqslant z_u$

$$V_0 = \frac{(1-S_m)\Phi}{1-\rho_{ro}}[\mathscr{A} - \mathscr{B}] - \frac{(1-S_m)\Phi}{(1-\rho_{ro})(1-\lambda)}\mathscr{B}^{\lambda}(\mathscr{A}^{1-\lambda} - \mathscr{B}^{1-\lambda}), \tag{28a}$$

and for $z_{fao} < z_u$

$$V_0 = \frac{(1-S_m)\Phi}{1-\rho_{ro}}(\mathscr{C} - \mathscr{B}) - \frac{(1-S_m)\Phi}{(1-\rho_{ro})(1-\lambda)}\mathscr{B}^{\lambda}(\mathscr{C}^{1-\lambda} - \mathscr{B}^{1-\lambda}) + \\ + \frac{S_m\Phi}{\rho_{ro}}(\mathscr{D} - \mathscr{E}) + \frac{(1-S_m)\Phi}{\rho_{ro}(1-\lambda)}\mathscr{E}^{\lambda}(\mathscr{D}^{1\;\;\lambda} - \mathscr{E}^{1\;\;\lambda}) - \\ - \frac{S_m\Phi}{1-\rho_{ro}}(\mathscr{A} - \mathscr{C}) - \frac{(1-S_m)\Phi}{(1-\lambda)(1-\rho_{ro})}\mathscr{B}^{\lambda}(\mathscr{A}^{1-\lambda} - \mathscr{C}^{1-\lambda}), \tag{28b}$$

where

$$\mathscr{C} = z_{ao} + \frac{h_d(1-\rho_{ro})}{\beta_{ao}\rho_{ro}} - z_{aw}, \qquad \mathscr{D} = \rho_{ro}(z_u - z_{ao}), \qquad \mathscr{E} = h_d/\beta_{ao}.$$

Partial derivatives of vertically integrated water and oil volumes with respect to

z_{aw} and z_{ao} may be readily obtained by differentiating (26) and (28) to obtain storage coefficients. The results are

$$\gamma_{ww} = \frac{\Phi}{1-\rho_{ro}}(1-(1-S_m)\mathscr{B}^{\lambda}\mathscr{A}^{-\lambda}-S_m), \tag{29a}$$

$$\gamma_{wo} = \frac{-\rho_{ro}\Phi}{1-\rho_{ro}}(1-(1-S_m)\,\mathscr{B}^{\lambda}\mathscr{A}^{-\lambda}-S_m), \tag{29b}$$

$$\gamma_{oo} = \Phi(1-S_m)\left(\frac{1}{1-\rho_{ro}} - \mathscr{E}^{\lambda}\mathscr{D}^{-\lambda} - \frac{\rho_{ro}}{1-\rho_{ro}}\mathscr{B}^{\lambda}\mathscr{A}^{-\lambda}\right), \tag{29c}$$

$$\gamma_{ow} = \frac{\Phi(1-S_m)}{1-\rho_{ro}}(\mathscr{B}^{\lambda}\mathscr{A}^{-\lambda}-1), \tag{29d}$$

where the constants $\mathscr{A}$, $\mathscr{B}$, etc. are as previously defined.

3.2. EVALUATION OF MODEL PREDICTIONS

Experimental validation of multiphase saturation-pressure relations based on the Van Genuchten model has been presented by Parker *et al.* (1987) and Lenhard and Parker (1987, 1988) for conditions involving monotonic water and total liquid drainage. Therefore, we choose here to evaluate the vertically integrated Brooks–Corey model by comparison with its Van Genuchten analog. Since the Van Genuchten model does not yield closed form expressions for integrated water and oil volumes, these quantities were evaluated numerically from the integral expressions using Gauss quadrature in conjunction with bisection procedures to refine integration limits.

In order to compare the two models, a procedure must be first determined for converting Van Genuchten (VG) model parameters to 'equivalent' Brooks–Corey (BC) parameters or vice-versa. A simple method for accomplishing this is to equate $\mathrm{d}S^*/\mathrm{d}h^*$ for the two models at $S^* = 0.5$ and to force the models through a specified match-point saturation (Lenhard *et al.*, 1988). The resulting expressions for BC model parameters in terms of VG parameters are

$$\lambda = \frac{m}{1-m}(1-0.5^{1/m}), \tag{30a}$$

$$h_d = \alpha^{-1}\bar{S}_x^{1/\lambda}(\bar{S}_x^{-1/m}-1)^{1/n}, \tag{30b}$$

where λ and h_d are BC parameters, α, n and $m = 1 - 1/n$ are VG parameters, and $\bar{S}_x$ is the match-point effective saturation which will typically lie between 0.5 and 0.9 depending on the criterion used to define 'equivalence' — i.e., where on the curves differences are minimized.

Consider a porous medium with $S^*(h^*)$ as shown in Figure 2 for Van Genuchten parameters listed in Table I. The material corresponds to a rather uniformly

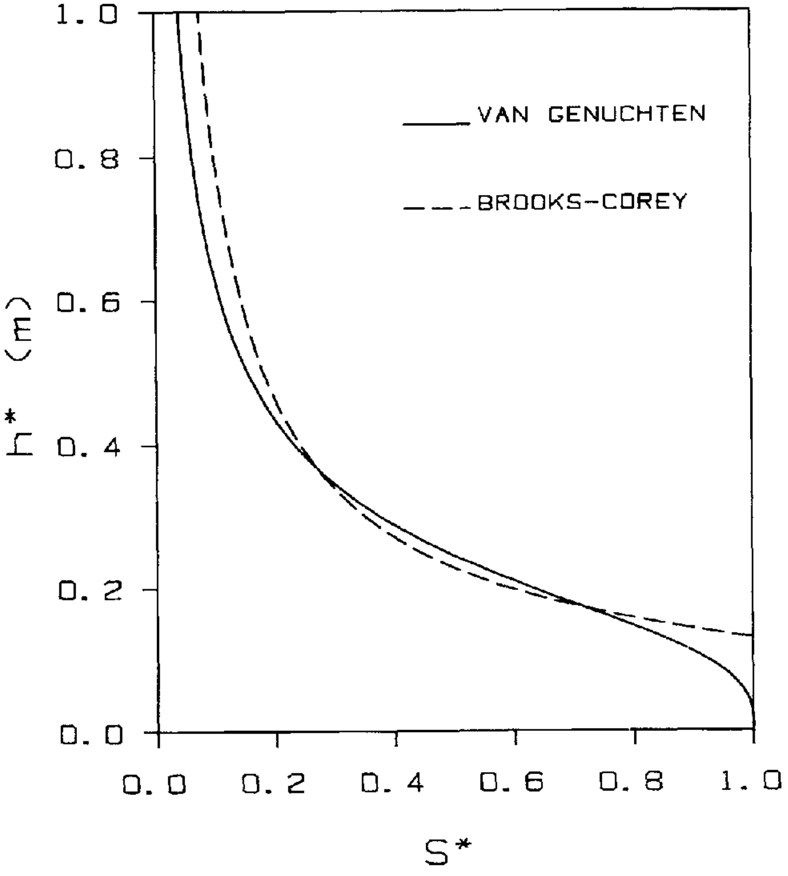

Fig. 2. Comparison of VG and BC scaled saturation-capillary head functions for parameters in Table I.

graded medium sand. If, following Lenhard *et al.* (1988), we select $\bar{S}_x = 0.72$ as the optimum match point then corresponding h_d and λ are as given in Table I. The resulting $S^*(h^*)$ function for the BC model exhibits good correspondence with the VG model except at low capillary pressures where the former overpredicts fluid saturation due to the assumption of a distinct air entry pressure at which C^1 discontinuity occurs (Figure 2). The VG model will asymptotically approach the behavior of the BC model as $n \rightarrow \infty$ and $\lambda \rightarrow \infty$, in which case $S^*(h^*)$ for both models approaches a step function with discontinuity at $h^* = h_d = 1/\alpha$.

To investigate the behavior of integrated saturation-pressure relations, we consider fluid properties typical of a light hydrocarbon spill (e.g., gasoline) in an unconfined aquifer bounded by an impermeable layer at $z_l = 0$ and with the soil surface at $z_u = 10$ m (Table I). Vertically integrated water volume, V_w, as a function of oil-water table elevation, z_{ow}, given by (26) is illustrated for the hypothet-

Table I. Soil and fluid properties employed in example calculations

Scaled retention function			
VG model:	$\alpha = 5.0\ \mathrm{m}^{-1}$	BC model:	$h_d = 0.133$ m
	$n = 3.0$		$\lambda = 1.29$
Other soil properties			
	$S_m = 0.0$		$z_u = 10.0$ m
	$\Phi = 0.4$		$z_l = 0.0$ m
	$K_{sw} = 10.0\ \mathrm{m\ d}^{-1}$		
Fluid properties			
	$\rho_{ro} = 0.8$		$\beta_{ao} = 3.2$
	$\eta_{ro} = 0.8$		$\beta_{ow} = 1.45$

ical soil in Figure 3. Linearity of $V_w(z_{ow})$ is observed for $z_u - z_{ow} > 3$ m corresponding to the thickness of the capillary water zone in which S_w substantially exceeds S_m that for larger z_{ow} begins to intersect the soil surface. Storage coefficients for water, γ_{ww} and γ_{wo}, are accordingly nearly constant over a similar

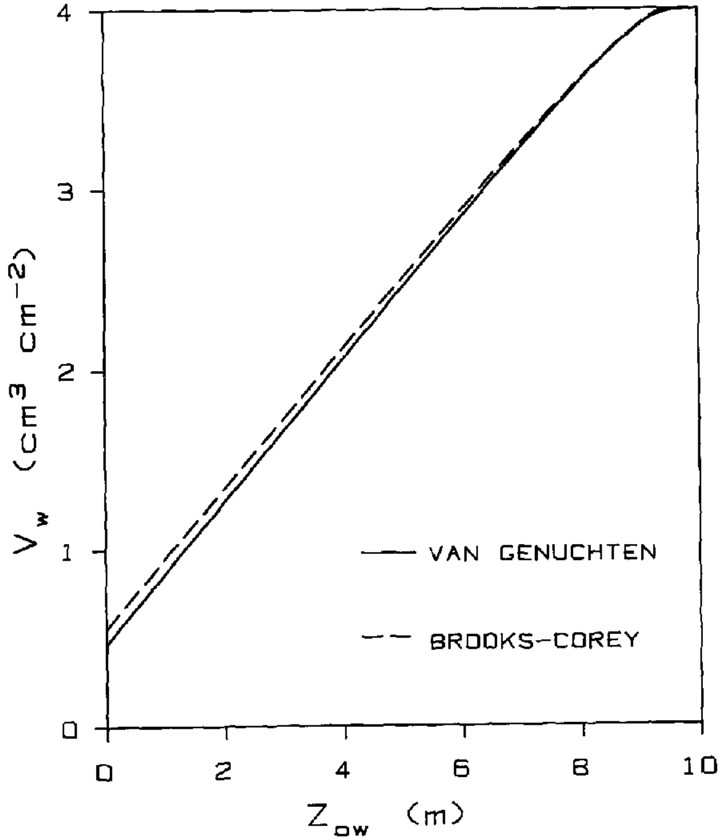

Fig. 3. Comparison of vertically integrated water volume as a function of oil-water table elevation for VG and BC models.

range in z_{ow} (Figure 4) and for large $z_u - z_{ow}$ approach values given by

$$\gamma_{ww}^{\infty} = \Phi(1 - S_m)/(1 - \rho_{ro}), \tag{31a}$$

$$\gamma_{wo}^{\infty} = -\Phi\rho_{ro}(1 - S_m)/(1 - \rho_{ro}). \tag{31b}$$

Although V_w, γ_{ww} and γ_{wo} are shown as functions of z_{ow}, the water flow equation (14a) is in terms of z_{aw} and z_{ao}. However, from (7) it is evident that z_{ow} is linearly related to z_{aw} and z_{ao} so that the water equation is effectively linear in the storage terms excluding effects of coupling with the oil flow equation.

Unlike problems in petroleum reservoir modeling which commonly involve piezometric oil heights, $H_o = z_{ao} - z_{ow}$, of many meters, hydrocarbon spill problems rarely yield H_0 greater than $1 - 2$ m (e.g., Parker *et al.*, 1988). We confine our attention here to the latter narrow range. Furthermore, in normal circumstances, the maximum elevation of the zone exhibiting nonzero oil saturation is considerably less than z_u in which case V_0 becomes a unique function of H_o. For

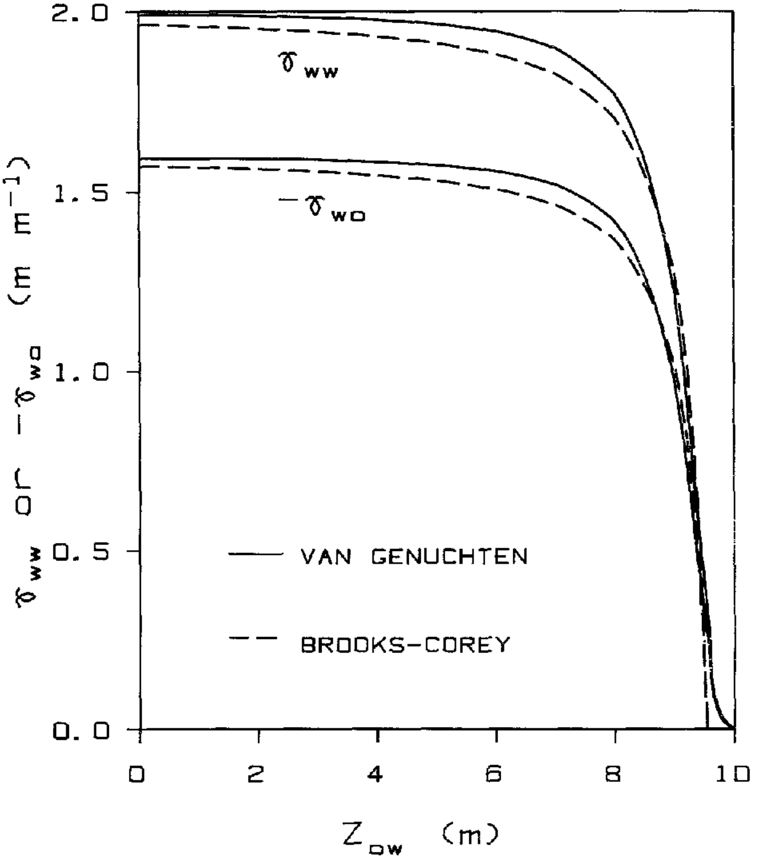

Fig. 4. Comparison of water–water and water–oil storage coefficients as a function of oil–water table elevation for VG and BC models.

the example problem with $H_o \leqslant 2$ m, this condition is met if $z_u - z_{ao} \geqslant 25$ cm. A comparison of BC and VG model $V_o(H_o)$ relations subject to this restriction is shown in Figure 5. For $H_0 > 1$ m, the two models correspond closely and are only mildly nonlinear. At smaller H_o, the functions become markedly nonlinear and the BC model increasingly underpredicts V_o. While the VG model predicts $V_o \rightarrow 0$ as $H_o \rightarrow 0$, the BC model indicates $V_o \rightarrow 0$ as $H_o \rightarrow H_o^{\min}$, where

$$H_o^{\min} = H_o\big|_{zfao=zfow} = h_d\left(\frac{1}{\beta_{ow}(1-\rho_{ro})} - \frac{1}{\beta_{ao}\rho_{ro}}\right). \tag{32}$$

It may be noted that selection of the match point for relating BC and VG parameters which controls h_d will directly influence the degree of deviation between BC and VG models at low oil volumes. Since h_d is, after all, simply an empirical model parameter, it may be adjusted in practice so that the integrated BC model

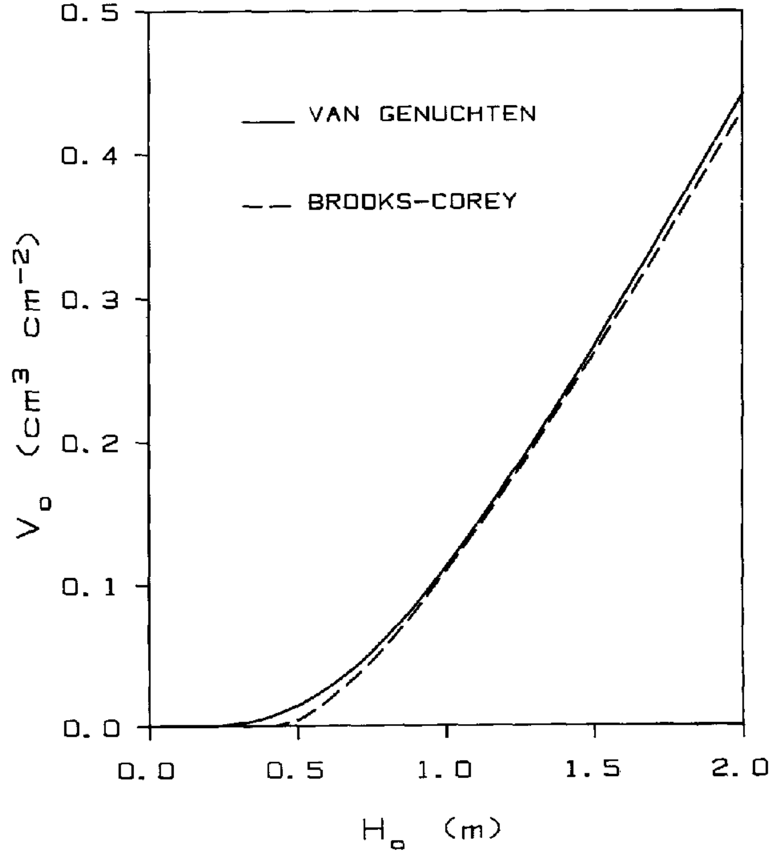

Fig. 5. Comparison of vertically integrated oil volume as a function of piezometric oil height for VG and BC models.

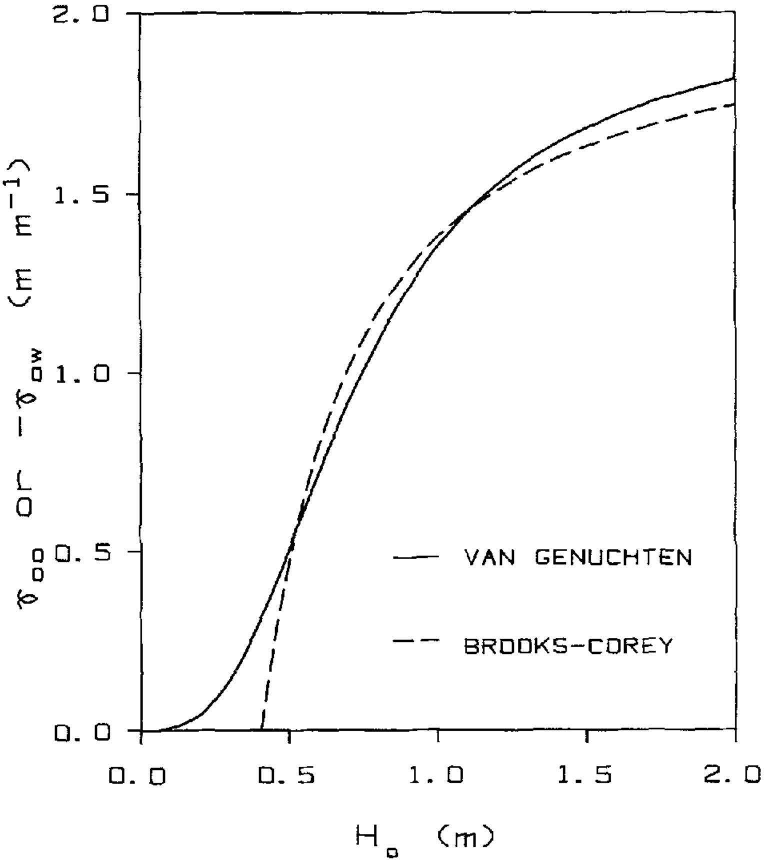

Fig. 6. Comparison of oil–water and oil–oil storage coefficients as a function of piezometric oil height for VG and BC models.

provides a suitable statistical fit to the true $V_o(H_o)$ function over the range of interest.

Relations between the oil storage coefficients, γ_{oo} and γ_{ow}, and H_o over the same range of $0 < H_o \leq 2$ m also clearly illustrate the nonlinearity in the oil-storage terms for low oil volumes (Figure 6). Although, in general, $\gamma_{oo} \neq -\gamma_{ow}$, for the specific circumstances employed here these quantities are indistinguishable within the precision of plotting in Figure 6 and are shown as single curves. For sufficiently large oil volumes ($H_o \gg 2$ m, $\gamma_{oo} \to \gamma_{ww}^{\infty}$ and $\gamma_{ow} \to -\gamma_{ww}^{\infty}$ as given by (31a).

4. Water and Oil Transmissivity Relations

4.1. DERIVATION OF TRANSMISSIVITY RELATIONS

Water transmissivity will be largely due to flow in the water saturated zone owing to the rapid reduction in permeability with decreasing water saturation. Ignoring any contribution of water flow above z_{ow} yields via (10a) the classical definition of transmissivity

$$\mathbf{T}_{w_{ij}} = \mathbf{K}_{sw_{ij}}(z_{ow} - z_l). \tag{33}$$

In the case of the Brooks–Corey model, a well-defined water saturated capillary fringe is described which has an upper elevation z_{fow}. Including the contribution of this water saturated fringe to water transmissivity yields a modified expression for $\mathbf{T}_{w_{ij}}$

$$\mathbf{T}_{w_{ij}} = \mathbf{K}_{sw_{ij}}(z_{fow} - z_l) \tag{34}$$

which may be utilized when the Brooks–Corey model is employed. Except for very thin aquifers or very fine grained sediments, the distinction between (33) and (34) will generally be small.

To evaluate oil transmissivity, explicit consideration must be given to variations in oil relative permeability with water and oil saturations which in turn depend on elevation. Parker *et al.* (1987) have derived an expression for oil relative permeability for the Van Genuchten model as

$$k_{ro} = (\bar{S}_t - \bar{S}_w)^{1/2}\{[1 - \bar{S}_w^{1/m}]^m - [1 - \bar{S}_t^{1/m}]^m\}^2. \tag{35}$$

Substituting (35) into (10b) and employing (6), (17) and (22) to define $\bar{S}_w(z)$ and $\bar{S}_t(z)$ yields an integral expression for oil transmissivity which is analytically intractable but which may be, nevertheless, evaluated numerically.

In the case of the Brooks–Corey model, relative permeability-saturation relations may be derived by application of Burdine's (1953) method which defines oil relative permeability as

$$k_{ro} = (\bar{S}_t - \bar{S}_w)^2 \frac{\displaystyle\int_{\bar{S}_w}^{\bar{S}_t} \frac{\mathrm{d}S^*}{h^{*2}}}{\displaystyle\int_0^1 \frac{\mathrm{d}S^*}{h^{*2}}}. \tag{36}$$

Substitution of the Brooks–Corey function for $S^*(h^*)$ yields

$$k_{ro} = (\bar{S}_t - \bar{S}_w)^2\,(\bar{S}_t^{(2-\lambda)/\lambda} - \bar{S}_w^{(2-\lambda)/\lambda})\,. \tag{37}$$

To evaluate oil transmissivity for the Brooks–Corey model, it is convenient to first separate the integral expression for $\mathbf{T}_o$ (Equation (10b)) into two terms corresponding to regions which are liquid saturated (no air present) and unsaturated (air present) as

$$\mathbf{T}_{o_{ij}} = \mathbf{T}'_{o_{ij}} + \mathbf{T}''_{o_{ij}} \tag{38a}$$

in which

$$\mathbf{T}'_{o_{ij}} = \frac{\mathbf{K}_{sw_{ij}}\rho_{ro}}{\eta_{ro}} \int_{\Omega}^{\Gamma} k_{ro}(z)\,\mathrm{d}z \tag{38b}$$

and

$$\mathbf{T}''_{o_{ij}} = \frac{\mathbf{K}_{sw_{ij}}\rho_{ro}}{\eta_{ro}} \int_{\Gamma}^{z_u} k_{ro}(z)\,\mathrm{d}z \tag{38c}$$

where $\mathbf{T}'_{o_{ij}}$ and $\mathbf{T}''_{o_{ij}}$ are contributions of the liquid saturated and unsaturated regions, respectively, to total transmissivity, Ω is the lowest elevation at which air occurs (see Equation (25)), and Γ is the lowest elevation at which air occurs (see Equation (27)).

For the liquid saturated region, employing (38b) and making a change of variables from z to h_{ow} via (6) yields

$$\mathbf{T}'_{o_{ij}} = \frac{\mathbf{K}_{sw}\rho_{ro}}{\eta_{ro}(1-\rho_{ro})} \int_{h_d/\beta_{ow}}^{(1-\rho_{ro})(\Gamma+z_{ow})} k_{ro}\,\mathrm{d}h_{ow}\,. \tag{39}$$

For the case of total liquid saturation (i.e., $\bar{S}_t = 1$), (37) can be expressed in polynomial form as a function of h_{ow} via (24) as

$$k_{ro} = 1 - 2\Pi^{\lambda} + \Pi^{2\lambda} - \Pi^{2+\lambda} + 2\Pi^{2+2\lambda} - \Pi^{2-3\lambda}, \tag{40}$$

where

$$\Pi = h_d/\beta_{ow}h_{ow}\,.$$

Substitution of (40) into (39) yields

$$\begin{aligned}\mathbf{T}'_{o_{ij}} = \frac{\mathbf{K}_{sw_{ij}}\rho_{ro}}{\eta_{ro}(1-\rho_{ro})}\Bigg\{ &\mathscr{F} - \mathscr{B} - \frac{2}{1-\lambda}\mathscr{B}^{\lambda}\left(\mathscr{F}^{1-\lambda} - \mathscr{B}^{1-\lambda}\right)\\ &+ \frac{1}{1-2\lambda}\mathscr{B}^{2\lambda}\left(\mathscr{F}^{1-2\lambda} - \mathscr{B}^{1-2\lambda}\right) + \frac{1}{1+\lambda}\mathscr{B}^{2+\lambda}\left(\mathscr{F}^{-1-\lambda} - \mathscr{B}^{-1-\lambda}\right)\\ &+ \frac{2}{2\lambda-1}\mathscr{B}^{2+2\lambda}\left(\mathscr{F}^{-1-2\lambda} - \mathscr{B}^{-1-2\lambda}\right) + \frac{1}{1+3\lambda}\mathscr{B}^{2-3\lambda}\left(\mathscr{F}^{-1-3\lambda} - \mathscr{B}^{-1-3\lambda}\right)\Bigg\}\end{aligned} \tag{41}$$

where

$$\mathscr{F} = \mathscr{A}, \qquad \text{for } z_{fao} \geqslant z_u\,,$$

$$\mathscr{F} = z_{ao} - z_{aw} + \frac{h_d(1-\rho_{ro})}{\beta_{ao}\rho_{ro}}, \quad \text{for } z_{fao} < z_u\,,$$

and other terms are as previously defined.

Evaluation of the second oil transmissivity term, $\mathbf{T}''_o$, corresponding to the liquid unsaturated zone cannot be carried out in closed form. Since oil relative permeability decreases exponentially as both total liquid saturation and water saturation decrease above z_{fao}, it may be anticipated that the contribution of $\mathbf{T}''_o$ to oil transmissivity will be small compared to that of $\mathbf{T}_o'$. Using numerical quadrature to evaluate $\mathbf{T}_o''$, we find this to indeed be the case. In general, $\mathbf{T}_o''$ is found to be rarely greater than 2% of $\mathbf{T}_o$ except for very low oil volumes when the absolute magnitude of $\mathbf{T}_o$ becomes in any case very low. Therefore, for the Brooks–Corey model we subsequently disregard $\mathbf{T}_o''$ and take $\mathbf{T}_o = \mathbf{T}_o'$ given by (41) as the oil transmissivity function.

4.2. EVALUATION OF MODEL PREDICTIONS

If effects of the unsaturated zone on water flow are ignored, water transmissivity is a simple linear function of z_{ow} as given by (33) or (34). However, unless piezometric oil height, H_o, is constant, nonlinearity nevertheless arises due to coupling with the oil flow equation, which is itself inherently more nonlinear as demonstrated by the behavior of oil storage coefficient terms.

Under the same conditions that V_o is uniquely defined by H_o as discussed

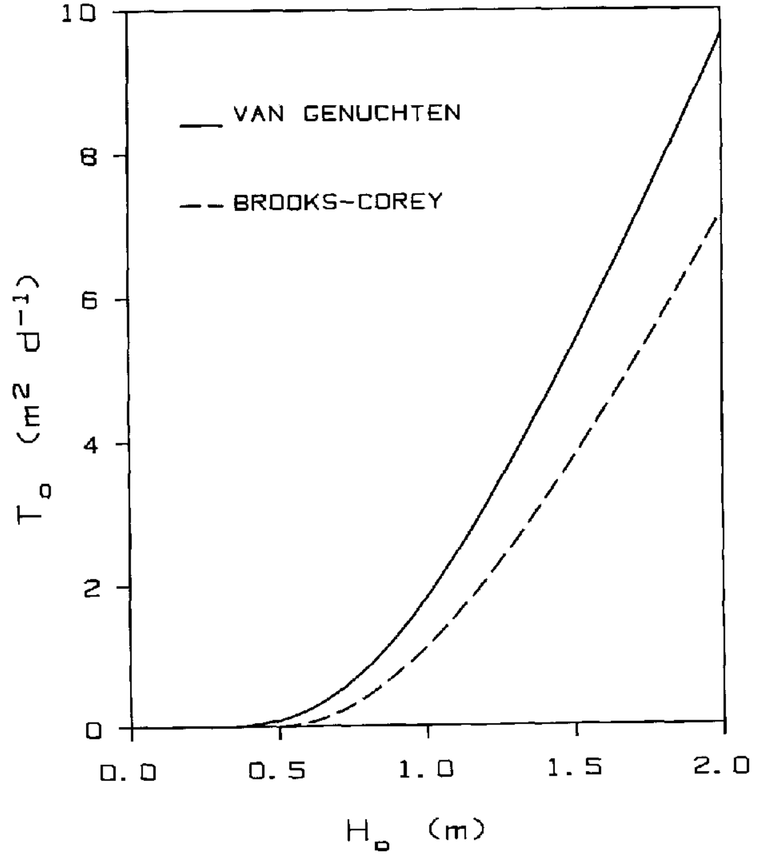

Fig. 7. Comparison of oil transmissivity as a function of piezometric oil height for VG and BC models.

previously, oil transmissivity, $\mathbf{T}_o$, will also be a function only of H_o. The relationship between $\mathbf{T}_o$ and H_o for the example fluid-porous media system over the range $0 < H_o \leq 2$ m is shown in Figure 7. Substantial nonlinearity of $\mathbf{T}_o$ is exhibited over the same range for which $V_o(H_o)$ was observed to be significantly nonlinear, i.e., for $H_o < 1$ m. The Brooks–Corey model consistently predicts lower oil transmissivities than those from the Van Genuchten model.

5. Summary and Conclusions

A mathematical model was derived to describe flow of water and oil in the presence of air at atmospheric pressure in an areal domain subject to the assumption of local vertical equilibrium. Independent variables in the model are air-oil table elevation where gauge oil pressure is zero and air-water table where gauge water pressure is zero. These elevations may, in turn, be related to the oil-water table elevation where oil-water capillary pressure is zero corresponding to the oil-water separation level which would theoretically be observed in an observation well in equilibrium with the soil. Constitutive relations in the model consist of vertically integrated water and oil volumes and their derivatives with respect to fluid table elevations and water and oil transmissivities. Closed-form expressions for the constitutive relations are derived based on a three-phase extension of the Brooks–Corey saturation-capillary pressure function.

Vertical integration of the governing equations leads to reduced dimensionality and nonlinearity and, thus, provides a computationally efficient formulation for the analysis of hydrocarbon spreading from leaking storage tanks or removal from well or trench systems. Nonlinearity in the constitutive equations is virtually absent for large oil lens thicknesses but increases as oil volume diminishes. Agreement between the Brooks–Corey model, which yields analytic vertically integrated functions, and the Van Genuchten model, which is not amenable to closed form solution, is close except at very low oil lens thicknesses due the assumption of a distinct air-entry pressure for the Brooks–Corey model.

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