

NOTES ON FLOW AND TRANSPORT IN POROUS MEDIA

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1. SINGLE PHASE FLOW

1.1. **Model Equations.** If only one fluid phase occupies the porous medium then the model is

$$\frac{\partial(\omega\rho)}{\partial t} + \nabla \cdot (\rho\mathbf{v}) + c = d \quad (1)$$

$$\mathbf{v} = -\frac{\bar{\mathbf{k}}_i}{\mu}(\nabla p - \rho\mathbf{g}) \quad (2)$$

$$\bar{\mathbf{k}}_i = \bar{\mathbf{k}}(\mathbf{x}) \quad (3)$$

$$\omega = \omega(\mathbf{x}, p) \quad (4)$$

$$\rho = \rho(p) \quad (5)$$

$$\mu = \mu(p) \quad (6)$$

Equation 1 is the mass balance. Equation 2, Darcy's law, can be derived from a momentum balance if inertia of the fluid is neglected. The proportionality constant depends on the fluid through the viscosity, μ_w , and through the medium permeability, $\bar{\mathbf{k}}_i$. The porosity, ω , is the volumetric fraction of the porous medium that can transmit fluid. It is usually assumed to be a (spatially variable) constant or a weakly nonlinear function of pressure. The density, ρ , is the mass of water per unit volume of water, also usually assumed to be constant or a weakly nonlinear function of the pressure. The Darcy velocity, \mathbf{v} , is the velocity such that the volumetric flux (flow) through a surface with area dA with unit normal $\boldsymbol{\nu}$ is $\mathbf{v} \cdot \boldsymbol{\nu} dA$ [Chavent and Jaffré, 1986]. The sources and sinks are represented by c and d respectively. Since the domain is not entirely open to flow due to the presence of the solid matrix, the Darcy velocity is sometimes called the filtration velocity, the macroscopic apparent velocity, or a fictitious velocity (c.f. [de Marsily, 1986, Chavent and Jaffré, 1986]). Another relevant velocity is \mathbf{v}/ω , which is the average fluid velocity in the pores, sometimes called the microscopic velocity or fictitious mean pore velocity. The intrinsic permeability of the medium, $\bar{\mathbf{k}}_i$, is the part of the proportionality constant in Darcy's law that reflects the flow properties of the medium (the porosity and the connectivity of the pore space). The pressure is p and the gravitational acceleration vector is \mathbf{g} . The fluid viscosity, μ , is the dynamic viscosity of the fluid. Technically all of these quantities are porous medium-scale quantities, which means that they are different from their counterparts in classical fluid dynamics in that they are obtained from some upscaling procedure such as volume averaging. Furthermore, all of the media properties are usually functions of space, and $\bar{\mathbf{k}}_i$ is usually anisotropic.

1.1.1. *Closure Relations.* Density and porosity equations are often based on their coefficients of compressibility at a reference pressure p_0 :

$$\beta_f = \left(\frac{1}{\rho} \frac{\partial \rho}{\partial p} \right)_{p_0} = \left(\frac{\partial \log(\rho)}{\partial p} \right)_{p_0} \quad (7)$$

$$\beta_m = \left(\frac{1}{\omega} \frac{\partial \omega}{\partial p} \right)_{p_0} = \left(\frac{\partial \log(\omega)}{\partial p} \right)_{p_0} \quad (8)$$

Exponential constitutive laws can be written as

$$\rho(p) = \rho_0 e^{\beta_f(p-p_0)} \quad (9)$$

$$\omega(\mathbf{x}, p) = \omega_0(\mathbf{x}) e^{\beta_m(p-p_0)} \quad (10)$$

Typically $\beta_f, \beta_m \ll 1$ so that first order Taylor series approximations about p_0 are accurate:

$$\rho(p) = \rho_0 (1 + \beta_f p) \quad (11)$$

$$\omega(\mathbf{x}, p) = \omega_0(\mathbf{x}) (1 + \beta_m p) \quad (12)$$

We note that $\omega(p)$ is more complex than $\rho(p)$ in that it incorporates compressibility of the solid as well as other effects such as rearrangement of the pore structure. To be consistent these effects would also need to be represented with a nonlinear permeability \bar{k}_i , but in practice the simple linear expression above is used.

For gases, density relations based on ideal or real gases can be used such as [Helmig, 1997]

$$\rho = \frac{p - p_0}{ZRT} \quad (13)$$

where Z is the real gas factor, R is the gas constant, and T is the temperature.

1.2. Working Formulations.

1.2.1. *Dimensionless Variables .* The dimensions of the variables are

$$\omega[-] \quad \rho[ML^{-3}] \quad \mathbf{v}[LT^{-1}] \quad \bar{k}_i[L^2] \quad \mu_w[ML^{-1}T^{-1}] \quad p[ML^{-1}T^{-2}] \quad \mathbf{g}[LT^{-2}]$$

Let p_0 be some reference pressure, say atmospheric pressure, and \mathbf{x}_0 be a reference coordinate, say the lowest point in the domain in some coordinate system. The rank of the dimensional matrix is 3, which means we can put the equation in dimensionless form with the choice of three reference scales. We will use a reference length l , the magnitude of gravitational acceleration, $g = \|g\|$, and a reference density $\rho_0 = \rho(p_0)$. This

yields the following dimensionless variables:

$$\tilde{t} = t\sqrt{\frac{g}{l}} \quad (14)$$

$$\tilde{\mathbf{x}} = \mathbf{x}\frac{1}{l} \quad (15)$$

$$\tilde{\psi} = \frac{p - p_0}{\rho_0 g l} \quad (16)$$

$$\tilde{\rho} = \frac{\rho}{\rho_0} \quad (17)$$

$$\tilde{\bar{\mathbf{K}}} = \frac{\rho_0 g \bar{\mathbf{k}}}{\mu \sqrt{g l}} \quad (18)$$

$$\tilde{\mathbf{v}} = \mathbf{v} \frac{1}{\sqrt{g l}} \quad (19)$$

$$\tilde{\mathbf{g}} = \frac{\mathbf{g}}{g} \quad (20)$$

$$\tilde{z} = -\tilde{\mathbf{g}} \cdot (\tilde{\mathbf{x}} - \tilde{\mathbf{x}}_0) \quad (21)$$

$$\tilde{c} = \frac{c}{\rho_0} \sqrt{\frac{l}{g}} \quad (22)$$

$$\tilde{d} = \frac{d}{\rho_0} \sqrt{\frac{l}{g}} \quad (23)$$

$$(24)$$

We will assume that for the remainder of this chapter the variables are dimensionless unless otherwise stated (we will drop the tilde's). After substituting the dimensionless variables into equations 1 and 2, we obtain the general dimensionless form of the single phase flow equation

$$\frac{\partial \omega \rho}{\partial t} - \nabla \cdot \rho \bar{\mathbf{K}} (\nabla \psi + \rho \nabla z) + c = d \quad (25)$$

1.2.2. *Potentials.* A trick for rewriting nonlinear diffusion terms [Kirchoff, 1894, Carslaw and Jaeger, 1959] is to use the fact that $a(u)\nabla u = \nabla \phi$ where

$$\phi = \int_{u_0}^u a(w) dw \quad (26)$$

We can define a potential

$$\phi = \int_0^\psi \frac{1}{\rho(w)} dw + z \quad (27)$$

so that

$$\rho \nabla \phi = \rho \left(\frac{1}{\rho} \nabla \psi + \nabla z \right) = \nabla \psi + \rho \nabla z \quad (28)$$

which in the case of an incompressible fluid is just $\phi = \psi + z$. Since $\frac{d\phi}{d\psi} > 0$, we can assume the existence of $\psi(\phi, z)$. This potential is sometimes known as the Hubbert potential, and, in the incompressible case, it is known as the total hydraulic head. The single phase model can then be reduced to a nonlinear heat equation for ϕ , which we write as

$$\frac{\partial(\omega \rho)}{\partial t} - \nabla \cdot \rho^2 \bar{\mathbf{K}} \nabla \phi + c = d \quad (29)$$

Another useful potential is

$$\phi = \int_0^\psi \rho(u) du \quad (30)$$

which yields

$$\frac{\partial(\omega \rho)}{\partial t} - \nabla \cdot (\bar{\mathbf{K}} \nabla \phi + \rho^2 \bar{\mathbf{K}} \nabla z) + c = d \quad (31)$$

1.2.3. *Incompressible Fluid and Medium.* In this case ω is a constant and $\rho = 1$ (it's dimensionless), which yields

$$\nabla \cdot \bar{\mathbf{K}} \nabla \phi + c = d \quad (32)$$

with $\phi = \psi + z$.

1.2.4. *Slightly Compressible Fluid.* In dimensionless form equations 11 and 12 are

$$\rho = 1 + \beta_f \rho_0 g l = 1 + \epsilon_f \psi \quad (33)$$

$$\omega = \omega_0 (1 + \beta_m \rho_0 g l) = \omega_0 (1 + \epsilon_m \psi) \quad (34)$$

If we neglect higher order terms in ϵ_f and ϵ_m and spatial gradients of ρ [Chavent and Jaffré, 1986] we obtain

$$\omega_0 (\epsilon_f + \epsilon_m) \frac{\partial \psi}{\partial t} - \nabla \cdot \bar{\mathbf{K}} (\nabla \psi + \nabla z) + c = d \quad (35)$$

Often a specific storage coefficient is defined as

$$S_s = \omega_0 (\hat{\beta}_r + \hat{\beta}_f) \quad (36)$$

1.2.5. *The Classical Porous Medium Equation.* In the case of gas $\rho = C\psi^\gamma$ ($\gamma = 1$ for ideal gases and the real gas law given above) so the fully compressible model above is

$$\frac{\partial(\omega C \psi^\gamma)}{\partial t} + \nabla \cdot (C^2 \psi^{2\gamma} \bar{\mathbf{K}} \mathbf{g} - \bar{\mathbf{K}} C \nabla \psi^{\gamma+1}) = 0 \quad (37)$$

which is a form of the classical porous medium equation.

1.3. Boundary and Initial Conditions. In field applications usually either the pressure (or pressure head or total head) is specified or the normal flux is specified at each point of the boundary. In some applications a mixed (Robin) boundary condition is specified to simulate various other physical situations (e.g. river and lake boundaries).

$$\phi = \phi_d(t, \mathbf{x}) \quad \mathbf{x} \in \Gamma^D \quad (38)$$

$$\mathbf{v} \cdot \boldsymbol{\nu} = q_n(t, \mathbf{x}) \quad \mathbf{x} \in \Gamma^N \quad (39)$$

$$\alpha_r [\phi - \phi_d(t, \mathbf{x})] + \beta_r [\mathbf{v} \cdot \boldsymbol{\nu} - q_n(t, \mathbf{x})] = 0 \quad \mathbf{x} \in \Gamma^R \quad (40)$$

where $\boldsymbol{\nu}$ is the outward unit normal on Γ . Initial conditions are often taken as a static equilibrium condition, which yields $\phi(\mathbf{x}) = c$. Steady flow initial conditions can also be specified easily in a homogeneous medium with simple boundary conditions. In the heterogeneous case or for complex boundary conditions/geometries we may have to solve the steady state problem for the initial conditions to the transient problem.

1.4. Sources and Sinks. Wells can be specified as “holes” in the domain and therefore represented as boundary conditions or as point sources if the domain is large enough with respect to the well diameter. Recharge to the aquifer can be represented through boundary conditions but is often represented as a spatially distributed source as well.

1.5. **Summary.** Single Phase Flow Equation

$$m_t + \nabla \cdot (\mathbf{f} - \bar{\mathbf{a}} \nabla \phi) + c = d \quad (41)$$

Primitive Form Coefficients

$$m = \omega \rho \quad (42)$$

$$f = -\rho^2 \bar{\mathbf{K}} \nabla z \quad (43)$$

$$\bar{\mathbf{a}} = \rho \bar{\mathbf{K}} \quad (44)$$

$$\phi = \psi \quad (45)$$

$$c, d = \text{problem dependent wells and sources} \quad (46)$$

$$u = \phi = \psi \quad (47)$$

Potential Form Coefficients

$$m = \omega \rho \quad (48)$$

$$f = 0 \quad (49)$$

$$a = \rho \bar{\mathbf{K}} \quad (50)$$

$$\phi = \int_0^\psi \frac{1}{\rho(s)} ds + z, \text{ or if incompressible } = \psi + z \quad (51)$$

$$u = \psi \text{ or } u = \phi \quad (52)$$

Density Closure Relations (Dimensionless)

$$\rho = 1 \quad (\text{constant}) \quad (53)$$

$$\rho = e^{\beta_f \psi} \quad (\text{exponential}) \quad (54)$$

$$\rho = 1 + \beta_f \psi \quad (\text{linear}) \quad (55)$$

$$\rho = p/Z(p, T)RT \quad (\text{real gas, } Z=1 \text{ for ideal}) \quad (56)$$

$$\rho = (\psi/\psi_0)^m e^{\beta_f \psi} \quad (\text{general}) \quad (57)$$

Porosity Closure Relations (Dimensionless)

$$\rho = \omega_0 \quad (\text{constant}) \quad (58)$$

$$\rho = 1 + \beta_m \psi \quad (\text{linear}) \quad (59)$$

Dimesional Quantities (Examples–Source <http://www.hbcpnetbase.com>)

$$\rho_0 = 997.0 \quad [kg/m^3] \text{ for water at } 25^\circ \text{ C and } 101325\text{Pa} \quad (60)$$

$$\rho_0 = 1.205 \quad [kg/m^3] \text{ for air at } 20^\circ \text{ C and } 101325\text{Pa} \quad (61)$$

$$\beta_f = \rho_0 g l \cdot 4.524 \times 10^{-10} \quad [(kg \cdot m/s^2)^{-1} = Pa^{-1}] \text{ for water at } 25^\circ \text{ C} \quad (62)$$

$$\beta_f = \rho_0 g l \cdot 9.87 \times 10^{-6} \quad [(kg \cdot m/s^2)^{-1} = Pa^{-1}] \text{ for air at } 25^\circ \text{ C} \quad (63)$$

$$\beta_m = \rho_0 g l \cdot 10^{-6} \text{—} 10^{-11} \quad [(kg \cdot m/s^2)^{-1} = Pa^{-1}] \text{ for various media} \quad (64)$$

$$\mu = 8.9 \times 10^{-4} \quad [kg/m \cdot s = Pa \cdot s] \text{ for water at } 25^\circ \quad (65)$$

$$\mu = 7.1 \times 10^{-6} \quad [kg/m \cdot s = Pa \cdot s] \text{ for air at } 25^\circ \quad (66)$$

$$g = 9.8 \quad [m/s^2] \text{ for Mississippi} \quad (67)$$

$$\bar{\mathbf{k}} = 10^{-7} \text{—} 10^{-16} \quad [m^2] \text{ for various media} \quad (68)$$

$$\omega = 0.01 \text{—} 0.9 \quad [-] \text{ for various media} \quad (69)$$

$$R = 8.314 \quad [kg \cdot m^2 / K \text{mols}^2] \quad (70)$$

2. TWO-PHASE FLOW

When two mobile fluid phases occupy the pore space there are two ways of modeling the problem, and we will consider both of them. The first conceptualizes the system as consisting of two distinct, time-dependent single phase domains. The second conceptualizes the system as a single domain with a variable composition. We refer to one phase as the wetting phase and the other the non-wetting phase according to which fluid has a stronger attraction to the solid phase.

2.1. Abrupt Interface Approximation. The wetting and non-wetting phases are described by single phase flow equations in the domains $\Omega_w(t)$ and $\Omega_n(t)$ respectively, and suitable boundary conditions on the fixed (external) boundaries of $\Omega = \Omega_w(t) \cup \Omega_n(t)$ are given. We describe the surface separating the two fluids (the abrupt interface or internal boundary) as $\mathbf{x}_s(s_1, s_2, t)$, which is unknown. To complete the description of the problem we need boundary conditions for the fluids on \mathbf{x}_s and an equation and boundary conditions for \mathbf{x}_s . The assumption that the surface is a fluid interface means that the normal velocity (physical/microscopic velocity not the Darcy velocity) of the fluids is equal to the normal velocity of the surface, which provides along $x_s(s_1, s_2, t)$

$$\frac{\mathbf{v}_w}{\omega} \cdot \nu_s = \frac{\mathbf{v}_n}{\omega} \cdot \nu_s = \frac{d\mathbf{x}_s}{dt} \cdot \nu_s \quad (71)$$

where $\nu_s = \frac{\partial \mathbf{x}}{\partial s_1} \times \frac{\partial \mathbf{x}}{\partial s_2} / \|\frac{\partial \mathbf{x}}{\partial s_1} \times \frac{\partial \mathbf{x}}{\partial s_2}\|$. An additional condition at the interface is obtained by assuming that the pressure is continuous (or discontinuous with a suitably defined jump):

$$p_w[\mathbf{x}_s(s_1, s_2, t)] = p_n[\mathbf{x}_s(s_1, s_2, t)] \quad (72)$$

As an example consider a surface that can be parameterized as $[x, y, h(x, y, t)]$ with Dirichlet conditions on h along the external boundary. Then

$$\nu_s = \frac{(-h_x, -h_y, 1)}{\sqrt{h_x^2 + h_y^2 + 1}} \quad (73)$$

and the equation for h is then

$$\frac{\partial h}{\partial t} + \frac{1}{\omega} \mathbf{v}_w \cdot (-h_x, -h_y, 1)^t = 0 \quad (74)$$

which together with equations 71 and 72 closes the system for h, p_w, p_n .

2.1.1. The Dupuit Hypothesis for Unconfined Aquifers. If we consider the model given in the previous section with the non-wetting phase occupying the region above $h(x, y, t)$, then we can try to use physical reasoning to simplify the model further. First we assume that $p_n \approx 0$. That is, we neglect the model of the non-wetting phase (air) and consider only the model over $\Omega_w(t)$ with boundary condition

$$p_w(x, y, h(x, y, t)) = 0 \quad (75)$$

and with h still governed by equation 74. We next eliminate the free boundary from the problem by integrating in the z direction. To integrate in the z direction we use Dupuit's hypothesis, which is that flow in the z direction is negligible. No flow in the z direction implies that the total head, ϕ , is a constant in the z direction. Furthermore, since unconfined aquifers are generally shallow, compressibility of the fluid and medium are neglected. We have then that

$$\phi(x, y, t) = \phi(x, y, h(x, y, t), t) = p_w(x, y, h(x, y, t), t) + \rho_w g z = h(x, y, t) \quad (76)$$

Defining $z_0(x, y)$ as the bottom of the aquifer we can integrate the incompressible single phase flow equation to yield a two-dimensional (quasi-three dimensional) model for an unconfined aquifer (see [de Marsily, 1986]).

$$\omega_d \frac{\partial h}{\partial t} + \nabla \cdot \mathbf{v} = 0 \quad (77)$$

$$\mathbf{v} = \bar{\mathbf{T}} \nabla h \quad (78)$$

$$T_* = \int_{z_0(x, y)}^{h(x, y, t)} K_{*,*} dz \quad (79)$$

where ω_d is the so-called drainable porosity or specific yield. If $\bar{\mathbf{K}}$ is constant in the z -direction the model simplifies further to

$$\omega_d \frac{\partial \hat{h}}{\partial t} + \nabla \cdot \hat{h} \bar{\mathbf{K}} \nabla \hat{h} = 0 \quad (80)$$

where $\hat{h} = h - z_0$.

2.2. Continuum Model Equations. Now we consider the second approach to modeling two-phase flow. For a mixture of two mobile, immiscible fluid phases (labeled wetting, w , and a non-wetting, n) the standard model is

$$\frac{\partial(\omega s_w \rho_w)}{\partial t} + \nabla \cdot (\rho_w \mathbf{v}_w) + c_w = d_w \quad (81)$$

$$\frac{\partial(\omega s_n \rho_n)}{\partial t} + \nabla \cdot (\rho_n \mathbf{v}_n) + c_n = d_n \quad (82)$$

$$\mathbf{v}_w = -\frac{\bar{\mathbf{k}}_i \bar{\mathbf{k}}_{rw}}{\mu_w} (\nabla p_w - \rho_w \mathbf{g}) \quad (83)$$

$$\mathbf{v}_n = -\frac{\bar{\mathbf{k}}_i \bar{\mathbf{k}}_{rn}}{\mu_n} (\nabla p_n - \rho_n \mathbf{g}) \quad (84)$$

$$s_n = 1 - s_w \quad (85)$$

$$p_n - p_w = p_c(\mathbf{x}, s_w) \quad (86)$$

$$\bar{\mathbf{k}}_{r\alpha} = \bar{\mathbf{k}}_{r\alpha}(\mathbf{x}, s_w) \quad (87)$$

$$\bar{\mathbf{k}}_i = \bar{\mathbf{k}}_i(\mathbf{x}) \quad (88)$$

$$\rho_\alpha = \rho_\alpha(p_\alpha) \quad (89)$$

$$\omega = \omega(\mathbf{x}, p_n, p_w) \quad (90)$$

$$\mu_\alpha = \mu_\alpha(p_\alpha) \quad (91)$$

The multiphase extensions of Darcy's law, equations 83 and 84, are apparently due to Muskat (c.f. [Chavent and Jaffré, 1986]). The phase pressures, p_w and p_n , are porous medium scale pressures derived for each phase separately. The saturations, s_w and s_n , are the fractions of the pore space occupied by the fluid phases. The relative permeabilities, $\bar{\mathbf{k}}_{rw}$ and $\bar{\mathbf{k}}_{rn}$, are the fractions of the intrinsic permeability “available” to the fluids. The equations couple through equations 85–87. The remainder of the quantities are defined analogously to the single phase case.

2.2.1. Closure Relations. We will use the following scaled saturation and capillary pressure for expressing constitutive relations

$$s_e = \frac{s_w - s_m(\mathbf{x})}{s_M(\mathbf{x}) - s_m(\mathbf{x})} \quad (92)$$

$$p_{ce} = \frac{p_c}{p_{cM}(\mathbf{x})} \quad (93)$$

The effective saturation, s_e , is defined for two reasons. First, for most constitutive laws, the saturation cannot usually vary between 0 and 1 (i.e. from full saturation of one phase to full saturation of the other). Usually the wetting phase cannot be fully removed from the grains of the solid phase by flow alone, so the minimum saturation $s_m(\mathbf{x}) > 0$. Sometimes s_m is called the irreducible saturation or residual saturation but these terms are not always synonymous [Parker et al., 1987]. When we introduce other processes besides flow, the definitions of s_e will have to be extended for $S > s_M$ and $S < s_m$. The second reason for the scaling is that it is often useful if the \mathbf{x} dependence can be factored out of the nonlinearities, and in many kinds of media a good approximation for the soil properties is that the $s_e - p_{ce}$ nonlinearity is independent of \mathbf{x} (i.e. $p_c(\mathbf{x}, S) = p_{cM}(\mathbf{x}) p_{ce}(s_e)$). We have labeled p_{cM} after [Chavent and Jaffré, 1986] as the maximum capillary pressure, although in general we will use a scaling factor motivated by the particular constitutive relations (e.g. the so-called displacement pressure).

We dealt with some models of density in the single phase case, where we essentially used microscopic equations of state. In the two-phase case it seems like the porous medium scale density concept begins to get complicated much like the porous medium compressibility in the single phase case. In addition to compression of the phase under pressure forces, for small and intermediate saturations it would seem that the fluid density relations might also be affected by attraction to the solid grains and the other phase. While we have assumed the fluids are immiscible, there are probably also changes due to dissolution or evaporation [Helmig, 1997]. In any case the density and porosity closure relations are generally only weakly nonlinear so we will focus primarily on the relations for p_{ce} , s_e and $k_{r\alpha}$, which we refer to as the $p - s - k$ relations.

FIGURE 1. p_{ce} vs. s_e

The commonly used relations between the effective saturation and effective capillary pressure generally have the same shape, which we discuss briefly before presenting the details of the actual $p - s - k$ models.

Common $p_{ce} - s_e$ relations have the shapes in figure 1. Common features are unboundedness as $s_e \rightarrow 0$ and discontinuities or unbounded slope at $s_e = 1$. The inverse of the relationship (i.e. $s_e(p_{ce})$) can be useful since the slope of the inverse is usually bounded—although there is a set of relations that have unbounded second derivative for the inverse at $s_e = 1$. The slope of the inverse is often discontinuous at $s_e = 1$ so dealing with the nonlinearities at $s_e = 1$ is important to consider. If we think of the $p_{ce} - s_e$ relation as algebraic constraints we can describe the difficulties as follows. For the “forward” constraint

$$p_{ce}(s_e) - s_e = 0 \quad (94)$$

we have a nice constraint for either variable except as $s_e \rightarrow 0, 1$ in which case the derivative with respect to s_e blows up. On the other hand if we use the “inverse” constraint

$$s_e(p_{ce}) - s_e = 0 \quad (95)$$

we always have a nice constraint for s_e , but $\frac{ds_e}{dp_{ce}}(0) = 0$. This means that in order to have a closed system of equations for p_{ce} and s_e we need some other constraint on p_{ce} . Unfortunately the coefficients of p_{ce} in the mass balance equations are often zero at $s_e = 1$ so finding such a constraint can be a problem.

Common $k_{r\alpha} - s_e$ relations have the shapes in figure 2. The slopes can be unbounded at $s_e = 1$. It turns out that if you compose the $k_{r\alpha} - s_e$ relation with the inverse of the $s_e(p_{ce})$ relation then the slopes of the resulting $k_{r\alpha} - p_{ce}$ relations are bounded for all but a small range of cases (figure 3). As with the $p_{ce} - s_e$ relation, the $s_e = 1$ case can be troublesome. Note that the following simplified $k_{r\alpha} - s_e$ relations are sometimes used for analysis and computations, but they do not exhibit all of the behavior discussed above $s_e = 1$.

$$k_{rw} = s_e^2 \quad (96)$$

$$k_{rn} = \frac{1}{2}(1 - s_e)^2 \quad (97)$$

The following sections work out the details of common $p - s - k$ relations for the sake of completeness. First we present $p - s$ relations. The $s - k$ relations will then be formulated independently of the $p - s$ model. Skip to section equation 2.3.2 if you don’t need these details, the equations and closure relations will be summarized at the end of the chapter.

Van Genuchten. The Van Genuchten relation is [van Genuchten, 1980]

FIGURE 2. $k_{r\alpha}$ vs. s_e FIGURE 3. $k_{r\alpha}$ vs. p_{ce}

$$p_c = p_{ce}/\alpha \quad (98)$$

$$p_{ce} = \left(s_e^{-1/m} - 1\right)^{1/n} \quad (99)$$

where $n > 1$, $0 < m < 1$, and $\alpha > 0$ ($p_{cM} = 1/\alpha$). Hence $p_{ce} : [0, 1] \rightarrow [0, \infty)$ is unbounded as $s_e \rightarrow 0$. Furthermore

$$\frac{dp_{ce}}{ds_e} = \frac{-1}{nm} \left(s_e^{-1/m} - 1\right)^{1/n-1} s_e^{-1/m-1} \quad (100)$$

is unbounded as $s_e \rightarrow 1$ and $s_e \rightarrow 0$ because $n > 1$.

If we deal with the inverse instead we have

$$s_e = (1 + p_{ce}^n)^{-m} \quad (101)$$

$$\frac{ds_e}{dp_{ce}} = -mn(1 + p_{ce}^n)^{-m-1} p_{ce}^{n-1} \quad (102)$$

which is C^1 on $[0, \infty)$, but not C^2 at $p_{ce} = 0$ if $1 < n < 2$.

Brooks-Corey. The Brooks-Corey $p - s$ relation is Brooks and Corey [1966]

$$p_c = p_d p_{ce} \quad (103)$$

$$p_{ce} = \begin{cases} s_e^{-1/\lambda} & s_e < 1 \\ 0 & s_e = 1 \end{cases} \quad (104)$$

where $\lambda > 0$ and $p_d > 0$ ($p_{cM} = p_d$ is known as the displacement or entry pressure). Thus p_{ce} and $\frac{dp_{ce}}{ds_e}$ are discontinuous at $s_e = 1$ and unbounded as $s_e \rightarrow 0$. On $(0, 1)$, however, $\frac{dp_{ce}}{ds_e}$ is bounded, as opposed to the unbounded behavior of the van Genuchten relation.

The inverse is

$$s_e = \begin{cases} p_{ce}^{-\lambda} & p_{ce} \geq 1 \\ 1 & p_{ce} < 1 \end{cases} \quad (105)$$

This function is C^∞ except at $p_{ce} = 1$, where it is Lipschitz continuous.

Summary. As $s_e \rightarrow 0$, both the $p - S$ models have $p_{ce} \rightarrow \infty$. In fact, for small s_e the curves are nearly identical if $\lambda = nm$.

At $s_e = 1$ the two models differ significantly. The Brooks-Corey model has a jump discontinuity in capillary pressure equal to the displacement pressure (or a jump of 1 in p_{ce}) whereas Van Genuchten varies continuously, but very quickly, to $p_{ce} = 0$. The non-smoothness at $s_e = 1$ is significant because $s_e = 1$ can be reached with only flow processes and is often the initial condition for a portion of the domain. We may deal with the inverses, $s_e(p_{ce})$, in which case both curves are Lipschitz continuous on $[0, \infty)$. The Van Genuchten curve is C^1 at $p_{ce} = 0$ while Brooks-Corey is Lipschitz continuous at $p_{ce} = 1$. The difference in the two curves near $S = 1$ is physically significant. The Brooks-Corey model includes the concept of finite entry pressure, which implies that the non-wetting phase cannot jointly occupy the pore space with the wetting phase until the non-wetting phase pressure exceeds p_d . Recent work suggests that the Van Genuchten curves should be augmented with a finite entry pressure [Gerhard and Kueper, 2003a,b].

Permeability Models. The permeability models are based on empirical and theoretical considerations that relate the saturation and the capillary pressure to the permeability. For that reason they depend on the $p - S$ relations above. We first present the general permeability models and then derive closed form expressions for the permeability functions using the Brooks-Corey and Van Genuchten $p - s$ relations.

Mualem. Mualem's general permeability model is [Mualem, 1976]

$$k_{rw} = s_e^{1/2} \left\{ \frac{\int_0^{s_e} \frac{1}{p_c} ds}{\int_0^1 \frac{1}{p_c} ds} \right\}^2 \quad (106)$$

$$k_{rn} = (1 - s_e)^{1/2} \left\{ \frac{\int_{s_e}^1 \frac{1}{p_c} ds}{\int_0^1 \frac{1}{p_c} ds} \right\}^2 \quad (107)$$

Burdine. Burdine's general permeability model is [Burdine, 1953]

$$k_{rw} = s_e^2 \left\{ \frac{\int_0^{s_e} \frac{1}{p_c^2} ds}{\int_0^1 \frac{1}{p_c^2} ds} \right\} \quad (108)$$

$$k_{rn} = (1 - s_e)^2 \left\{ \frac{\int_{s_e}^1 \frac{1}{p_c^2} ds}{\int_0^1 \frac{1}{p_c^2} ds} \right\} \quad (109)$$

Van Genuchten-Mualem. Note that both models above are independent of scalings of p_c , so that we simply use p_{ce} for the calculations. If we substitute the Van Genuchten $p - s$ model into the Mualem

permeability model we need to calculate the integral

$$\int_0^{s_e} \left(s_e^{-1/m} - 1 \right)^{-1/n} ds \quad (110)$$

Making the substitution $y^m = s_e$ and requiring that $m = 1 - 1/n$ we obtain [van Genuchten, 1980]

$$m \int_0^{y^m} (y^{-1} - 1)^{-1/n} y^{m-1} dy = m \int_0^{y^m} \left(\frac{1-y}{y} \right)^{-1/n} y^{m-1} dy \quad (111)$$

$$= m \int_0^{y^m} (1-y)^{-1/n} y^{m-1+1/n} dy \quad (112)$$

$$= m \int_0^{y^m} (1-y)^{-1/n} dy \quad (113)$$

$$= -\frac{m}{1-1/n} (1-y)^{1-1/n} \Big|_0^{y^m} \quad (114)$$

$$= 1 - (1 - s_e^{1/m})^m \quad (115)$$

Hence

$$k_{rw} = s_e^{1/2} \left[1 - (1 - s_e^{1/m})^m \right]^2 \quad (116)$$

$$k_{rn} = (1 - s_e)^{1/2} (1 - s_e^{1/m})^{2m} \quad (117)$$

and

$$\frac{dk_{rw}}{ds_e} = \frac{1}{2} s_e^{-1/2} \left[1 - (1 - s_e^{1/m})^m \right]^2 \quad (118)$$

$$+ 2 \left[1 - (1 - s_e^{1/m})^m \right] (1 - s_e^{1/m})^{m-1} s_e^{1/m-1/2} \quad (119)$$

$$\frac{dk_{rn}}{ds_e} = -\frac{1}{2} (1 - s_e)^{-1/2} (1 - s_e^{1/m})^{2m} \quad (120)$$

$$- 2(1 - s_e)^{1/2} (1 - s_e^{1/m})^{2m-1} s_e^{1/m-1} \quad (121)$$

Since $0 < m < 1$, $\frac{dk_{rw}}{ds_e}$ and $\frac{dk_{rn}}{ds_e}$ may be unbounded as $s_e \rightarrow 1$.

Substituting the Van Genuchten $s - p$ relationship we obtain

$$k_{rw} = \frac{\left[1 - p_{ce}^{n-1} (1 + p_{ce}^n)^{-m} \right]^2}{(1 + p_{ce}^n)^{m/2}} \quad (122)$$

$$k_{rn} = \left[1 - (1 + p_{ce}^n)^{-m} \right]^{1/2} \left[p_{ce}^{n-1} (1 + p_{ce}^n)^{-m} \right]^2 \quad (123)$$

and

$$k_{rw} = \frac{-nm}{2} (1 + p_{ce}^n)^{-m/2-1} p_{ce}^{n-1} \left[1 - p_{ce}^{n-1} (1 + p_{ce}^n)^{-m} \right]^2 + \quad (124)$$

$$- 2(1 + p_{ce}^n)^{-m/2} \left[1 - p_{ce}^{n-1} (1 + p_{ce}^n)^{-m} \right]. \quad (125)$$

$$\left[(n-1) p_{ce}^{n-2} (1 + p_{ce}^n)^{-m} - m n p_{ce}^{n-1} (1 + p_{ce}^n)^{-m-1} p_{ce}^{n-1} \right] \quad (126)$$

$$k_{rn} = \frac{-nm}{2} \left[1 - (1 + p_{ce}^n)^{-m} \right]^{-1/2} (1 + p_{ce}^n)^{-m-1} p_{ce}^{n-1} \left[p_{ce}^{n-1} (1 + p_{ce}^n)^{-m} \right]^2 \quad (127)$$

$$2 \left[1 - (1 + p_{ce}^n)^{-m} \right]^{1/2} \left[p_{ce}^{n-1} (1 + p_{ce}^n)^{-m} \right]. \quad (128)$$

$$\left[(n-1) p_{ce}^{n-2} (1 + p_{ce}^n)^{-m} - m n p_{ce}^{n-1} (1 + p_{ce}^n)^{-m-1} p_{ce}^{n-1} \right] \quad (129)$$

Using this form of the relations we only get unbounded derivatives in k_{rw} at $p_c = 0$ in the case $1 < n < 2$, which is the same range where the second derivative of the Van Genuchten $p - S$ relation is unbounded at $p_c = 0$.

Van Genuchten-Burdine. Similar manipulations to the Mualem model requiring that $m = 1 - 2/n$ lead to

$$k_{rw} = s_e^2 \left[1 - \left(1 - s_e^{1/m} \right)^m \right] \quad (130)$$

$$k_{rn} = (1 - s_e)^2 \left(1 - S^{1/m} \right)^m \quad (131)$$

or

$$k_{rw} = \frac{1 - p_{ce}^{n-1} (1 + p_{ce}^n)^{-m}}{(1 + p_{ce}^n)^{2m}} \quad (132)$$

$$k_{rn} = \left[1 - (1 + p_{ce}^n)^{-m} \right]^2 \left[p_{ce}^{n-1} (1 + p_{ce}^n)^{-m} \right] \quad (133)$$

Brooks-Corey-Mualem. Again substituting the $p_c - S$ relation into the Mualem expression we obtain

$$k_{rw} = s_e^{(4+5\lambda)/2\lambda} \quad (134)$$

$$k_{rn} = (1 - s_e)^{1/2} (1 - s_e^{1/\lambda+1})^2 \quad (135)$$

or

$$k_{rw} = p_{ce}^{-(4+5\lambda)} \quad (136)$$

$$k_{rn} = (1 - p_{ce}^{-\lambda})^{1/2} (1 - p_{ce}^{-(\lambda+1)})^2 \quad (137)$$

Brooks-Corey-Burdine. Using the Burdine model (which is typically used in conjunction with Brooks-Corey) gives

$$k_{rw} = s_e^{(2+3\lambda)/\lambda} \quad (138)$$

$$k_{rn} = (1 - s_e)^2 (1 - s_e^{(2+\lambda)/\lambda}) \quad (139)$$

or

$$k_{rw} = p_{ce}^{-(2+3\lambda)} \quad (140)$$

$$k_{rn} = (1 - p_{ce}^{-\lambda})^2 (1 - p_{ce}^{-(2+\lambda)}) \quad (141)$$

2.3. Working Formulations.

2.3.1. *Dimensionless Variables.*

$$\tilde{t} = t \sqrt{\frac{g}{l}} \quad (142)$$

$$\tilde{\mathbf{x}} = \mathbf{x} \frac{1}{l} \quad (143)$$

$$\tilde{\psi}_\alpha = \frac{p_\alpha - p_{w,0}}{\rho_{w,0} g l} \quad (144)$$

$$\tilde{\psi}_c = \tilde{\psi}_n - \tilde{\psi}_w \quad (145)$$

$$\tilde{\rho}_\alpha = \frac{\rho_\alpha}{\rho_{\alpha,0}} \quad (146)$$

$$\tilde{\bar{K}} = \frac{\rho_{w,0} g \bar{\mathbf{k}}}{\mu_w \sqrt{g l}} \quad (147)$$

$$\tilde{\mathbf{v}}_\alpha = \mathbf{v}_\alpha \frac{1}{\sqrt{g l}} \quad (148)$$

$$\tilde{\mathbf{g}} = \frac{\mathbf{g}}{g} \quad (149)$$

$$\tilde{z} = -\tilde{\mathbf{g}} \cdot (\tilde{\mathbf{x}} - \tilde{\mathbf{x}}_0) \quad (150)$$

$$\tilde{\mu}_\alpha = \frac{\mu_\alpha}{\mu_w} \quad (151)$$

$$\tilde{\lambda}_w = \frac{\tilde{\rho}_w k_{rw}}{\tilde{\mu}_w} \quad (152)$$

$$\tilde{\lambda}_n = \frac{\tilde{\rho}_n k_{rn}}{\tilde{\mu}_n} \quad (153)$$

$$\tilde{c}_\alpha = \frac{c_\alpha}{\rho_{\alpha,0}} \sqrt{\frac{l}{g}} \quad (154)$$

$$\tilde{d}_\alpha = \frac{d_\alpha}{\rho_{\alpha,0}} \sqrt{\frac{l}{g}} \quad (155)$$

$$b = \frac{\rho_{n,0}}{\rho_{w,0}} \quad (156)$$

2.3.2. *Pressure-Saturation Equations* . Substituting equations 83–91 into equations 81 and 82 and writing the result in terms of the dimensionless variables above (dropping the tilde's) yields:

$$\frac{\partial \omega s_w \rho_w}{\partial t} + \nabla \cdot (\rho_w \mathbf{v}_w) + c_w = d_w \quad (157)$$

$$\rho_w \mathbf{v}_w = -\bar{\mathbf{K}} \lambda_w (\nabla \psi_w + \rho_w \nabla z) \quad (158)$$

$$\frac{\partial \omega (1 - s_w) \rho_n}{\partial t} + \nabla \cdot (\rho_n \mathbf{v}_n) + c_n = d_n \quad (159)$$

$$\rho_n \mathbf{v}_n = -\bar{\mathbf{K}} \lambda_n (\nabla \psi_w + \nabla \psi_c + b \rho_n \nabla z) \quad (160)$$

The choice of the two unknowns depends on how general we wish the model to be. Since incompressible fluids and media are often used in practice ω and ρ_α are ruled out. On the other hand the phase pressures cannot be determined as functions of S_n , S_w , and p_c , so at least one phase pressure is usually included as a dependent variable. Lastly, in the case of the disappearance of one of the phases under incompressibility assumptions, the Darcy's law for that phase has zero coefficients in the spatial terms so only the temporal accumulation term remains, leaving only the temporal term for the saturation. If $\frac{dS}{dp_c} = 0$ under these conditions (i.e. the Van Genuchten $p - S$ relation), applying the chain rule will still not produce an equation for p_c . For these reasons the most versatile choice appears to be a phase pressure and a saturation, say (S_w, p_w) . This formulation is called the pressure-saturation formulation (c.f. [Aziz and Settari, 1979, Chavent and Jaffré, 1986, Helmig, 1997]). Further discussion of the choice of variables can be found in [Kueper and Frind, 1991, Kees and Miller, 2002]. Since the constitutive theory is based on wetting phase fluid being present at every point in the medium, S_w and p_w always have physical meaning.

2.3.3. *Fractional Flow Formulations.* The petroleum industry generally uses formulations based on the total fluid velocity, that is, the sum of both phase velocities. The wetting phase mass balance is then rewritten in terms of this total velocity by formulating the so-called “fractional flow” function. We explore several formulations based on this approach (c.f. [Chavent and Jaffré, 1986]).

Summing equations 157–160 we obtain

$$\frac{\partial \omega [\rho_w s_w + \rho_n (1 - s_w)]}{\partial t} + \nabla \cdot (\rho_w \mathbf{v}_w + \rho_n \mathbf{v}_n) = 0 \quad (161)$$

$$\rho_w \mathbf{v}_w + \rho_n \mathbf{v}_n = -\bar{\mathbf{K}} [(\lambda_w + \lambda_n) \nabla \psi_w + \lambda_n \nabla \psi_c] \quad (162)$$

$$+ (\lambda_w \rho_w + \lambda_n b \rho_n) \nabla z \quad (163)$$

To simplify further we define

$$\mathbf{q}_t = \rho_w \mathbf{v}_w + \rho_n \mathbf{v}_n \quad (164)$$

$$\lambda_t = \lambda_w + \lambda_n \quad (165)$$

$$f_n = \frac{\lambda_n}{\lambda_t} \quad (166)$$

$$f_w = \frac{\lambda_w}{\lambda_t} \quad (167)$$

$$\rho_t = f_w \rho_w + f_n b \rho_n = \rho_w + f_n (b \rho_n - \rho_w) \quad (168)$$

Note that $f_n + f_w = 1$. Substituting these definitions yields

$$\frac{\partial \omega [s_w (\rho_w - \rho_n) + \rho_n]}{\partial t} + \nabla \cdot \mathbf{q}_t = 0 \quad (169)$$

$$\mathbf{q}_t = -\bar{\mathbf{K}} \lambda_t (\nabla \psi_w + f_n \nabla \psi_c + \rho_t \nabla z) \quad (170)$$

Now we express $\rho_w \mathbf{v}_w$ in terms of \mathbf{q}_t . Note first that

$$f_w \mathbf{q}_t = -\bar{\mathbf{K}} \{ \lambda_w \nabla \psi_w + \lambda_w f_n \nabla \psi_c + \lambda_w [\rho_w + f_n (b \rho_n - \rho_w)] \nabla z \} \quad (171)$$

Hence, we obtain for $\rho_w \mathbf{v}_w$

$$\rho_w \mathbf{v}_w = f_w \mathbf{q}_t + \bar{\mathbf{K}} \lambda_w f_n \nabla \psi_c + \bar{\mathbf{K}} \lambda_w f_n (b \rho_n - \rho_w) \nabla z \quad (172)$$

Combining the results yields

$$\frac{\partial \omega \rho_w s_w}{\partial t} + \nabla \cdot \mathbf{q}_w = 0 \quad (173)$$

$$\mathbf{q}_w = f_w \mathbf{q}_t + \bar{\mathbf{K}} \lambda_w f_n \nabla \psi_c + \bar{\mathbf{K}} \lambda_w f_n (b \rho_n - \rho_w) \nabla z \quad (174)$$

$$\frac{\partial \omega [s_w (\rho_w - \rho_n) + \rho_n]}{\partial t} + \nabla \cdot \mathbf{q}_t = 0 \quad (175)$$

$$\mathbf{q}_t = -\bar{\mathbf{K}} \lambda_t (\nabla \psi_w + f_n \nabla \psi_c + \rho_t \nabla z) \quad (176)$$

If we choose s_w, ψ_w as the dependent variables and assume $\psi_c = \psi_{cM}(\mathbf{x}) \bar{\psi}_c(S_w)$ then using the chain rule on $\nabla \psi_c$ yields

$$\frac{\partial \omega \rho_w S_w}{\partial t} + \nabla \cdot (\mathbf{q}_w) = 0 \quad (177)$$

$$\mathbf{q}_w = f_w \mathbf{q}_t + \bar{\mathbf{K}} \lambda_w f_n \left(\psi_{cM} \frac{d\bar{\psi}_c}{dS_w} \nabla S_w + \bar{\psi}_c \nabla \psi_{cM} \right) \quad (178)$$

$$+ \bar{\mathbf{K}} \lambda_w f_n (b \rho_n - \rho_w) \nabla z \quad (179)$$

$$\frac{\partial \omega [S_w (\rho_w - \rho_n) + \rho_n]}{\partial t} + \nabla \cdot \mathbf{q}_t = 0 \quad (180)$$

$$\mathbf{q}_t = -\bar{\mathbf{K}} \lambda_t \left(\nabla \psi_w + f_n \frac{d\psi_c}{dS_w} \nabla S_w + \rho_t \nabla z \right) \quad (181)$$

2.3.4. *Potentials.* Defining potentials to remove nonlinear diffusion terms can be more complicated in the two-phase case because nonlinearities may have more complicated dependencies. In general we may have a term like $a(u, v, \mathbf{x})\nabla u$ that we would like to write as $\nabla\phi$ for some ϕ . Using the Kirchoff transform we get for $i = 1, 2, 3$

$$\frac{\partial \int_{u_0}^u a(w, v, \mathbf{x}) dw}{\partial x_i} = a(u, v, w)u_{x_i} + \int_{u_0}^u \frac{\partial a}{\partial v}(w, v, \mathbf{x}) dw \frac{\partial v}{\partial x_i} + \int_{u_0}^u \frac{\partial a}{\partial x_i}(w, v, \mathbf{x}) dw \quad (182)$$

so in general to employ a potential we have to incorporate “correction” terms (the last two terms on the rhs)

$$a(u, v, \mathbf{x})\nabla u = \nabla\phi - \chi\nabla v - \nabla A \quad (183)$$

where

$$\phi = \int_{u_0}^u a(w, v, \mathbf{x}) dw \quad (184)$$

$$\chi = \int_{u_0}^u \frac{\partial a}{\partial v}(w, v, \mathbf{x}) dw \quad (185)$$

$$(\nabla A)_i = \int_{u_0}^u \frac{\partial a}{\partial x_i}(w, v, \mathbf{x}) dw \quad i = 1, 2, 3 \quad (186)$$

2.3.5. *Global Pressure Formulation.* In the total flow equation if we use the approach in the previous section to define a potential

$$\phi = \int_{-\infty}^{\psi_c} f_n(w) dw \quad (187)$$

then

$$\mathbf{q}_t = -\bar{K}\lambda_t (\nabla\psi_w + \nabla\phi - \chi\nabla\psi_w - \nabla A + \rho_t\nabla z) \quad (188)$$

This form motivates the definition of a global pressure head

$$\psi_t = \psi_w + \phi = \psi_w + \int_{-\infty}^{\psi_c} f_n(w) dw \quad (189)$$

The global pressure can also be rewritten in a more intuitive form using the facts that $f_n = 1 - f_w$ and $\psi_c = \psi_n - \psi_w$:

$$\psi_t = \frac{\psi_w + \psi_n}{2} + \phi^* = \frac{\psi_w + \psi_n}{2} + \int_{-\infty}^{\psi_c} \left[\frac{1}{2} - f_w(w) \right] dw \quad (190)$$

If we assume that the densities involved in ϕ (through f_n) are evaluated at ψ_t rather than ψ_w , we can make equation 189 or equation 190 an implicit definition of ψ_t , and we obtain for the global flow

$$\mathbf{q}_t = -\bar{K}\lambda_t ((1 - \chi)\nabla\psi_t - \nabla A + \rho_t\nabla z) \quad (191)$$

The global pressure gathers all the pressure effects into a single potential, which from equation 190 we see is an extension of the arithmetic average of the phase pressures, which incorporates capillary effects.

2.3.6. *Homogeneous Relative Permeabilities.* If we can write the relative permeabilities as

$$k_{r\alpha} = k_r(\mathbf{x})k_{r\alpha}(s_e) \quad (192)$$

then the spatial dependence is essentially part of the hydraulic conductivity anyway, so we can assume it is incorporated into \bar{K} and the term ∇A is then zero.

2.3.7. *Incompressible Fluids.* If, additionally, the fluids are incompressible then $\rho_n = \rho_w = 1$ (recall that we’re using dimensionless variables) and the cross term χ above is zero, which yields

$$\nabla \cdot \mathbf{q}_t = 0 \quad (193)$$

$$\mathbf{q}_t = -\bar{K}\lambda_t (\nabla\psi_t + \rho_t\nabla z) \quad (194)$$

In one dimension this reduces to $\mathbf{q}(\mathbf{x}, t) = \mathbf{q}(t)$ and the system effectively reduced to a single nonlinear equation for the s_w .

2.3.8. *Light, Inviscid Non-Wetting Phase.* If we assume $\mu_n/\mu_w = 0$ then $f_n = 1$ and $f_w = 0$ except possibly in the limits as $s_w \rightarrow 0, 1$ so that the saturation equation reduces to

$$\frac{\partial \omega \rho_w s_w}{\partial t} + \nabla \cdot \mathbf{q}_w = 0 \quad (195)$$

$$\mathbf{q}_w = \bar{\mathbf{K}} \lambda_w \nabla \psi_c + \bar{\mathbf{K}} \lambda_w (b \rho_n - \rho_w) \nabla z \quad (196)$$

Furthermore if we assume $b = \rho_{n,0}/\rho_{w,0} = 0$ then no terms depend on the properties of the non-wetting fluid.

2.3.9. *Richards' Equation.* If we fix $\psi_n = 0$ then $\psi_c = -\psi_w$ and we obtain Richards' equation

$$\frac{\partial \omega \rho_w s_w}{\partial t} + \nabla \cdot \mathbf{q}_w = 0 \quad (197)$$

$$\mathbf{q}_w = -\bar{\mathbf{K}} \lambda_w (\nabla \psi_w + \rho_w \nabla z) \quad (198)$$

2.4. Boundary and Initial Conditions. Boundary conditions can get very complicated in two-phase flow because of the wide range of variable choices. As mentioned above the most versatile model of two-phase flow outside of the fractional flow model uses s_w and ψ_w . This choice can also be used in the fractional flow model. On the other hand if ψ_t is used instead, then of course simple linear Dirichlet conditions on ψ_w, s_w become nonlinear Dirichlet conditions on ψ_t, s_w .

2.5. Summary. Two-Phase Flow Equations

$$m_{1,t} + \nabla \cdot \left(\mathbf{f}_1 - \sum_{j=1}^2 \bar{\mathbf{a}}_{1,j} \nabla \phi_j \right) + c_1 = d_1 \quad (199)$$

$$m_{2,t} + \nabla \cdot \left(\mathbf{f}_2 - \sum_{j=1}^2 \bar{\mathbf{a}}_{2,j} \nabla \phi_j \right) + c_2 = d_2 \quad (200)$$

$$c_\alpha, d_\alpha = \text{problem dependent wells and sources} \quad (201)$$

Auxiliary Variables (Dimensionless)

$$\lambda_w = \frac{\rho_w k_{rw}}{\mu_w} \quad (202)$$

$$\lambda_n = \frac{\rho_n k_{rn}}{\mu_n} \quad (203)$$

$$\lambda_t = \lambda_w + \lambda_n \quad (204)$$

$$f_n = \frac{\lambda_n}{\lambda_t} \quad (205)$$

$$f_w = \frac{\lambda_w}{\lambda_t} \quad (206)$$

$$\rho_t = f_w \rho_w + f_n b \rho_n = \rho_w + f_n (b \rho_n - \rho_w) \quad (207)$$

$$(208)$$

Primitive Form Coefficients

$$m_1 = \omega \rho_w s_w \quad (209)$$

$$m_2 = \omega \rho_n (1 - s_w) \quad (210)$$

$$f_1 = -\rho_w^2 \bar{K} \lambda_w \nabla z \quad (211)$$

$$f_2 = -\rho_n^2 \bar{K} \lambda_n b \nabla z \quad (212)$$

$$\bar{a}_{1,1} = \rho_w \bar{K} \lambda_w \quad (213)$$

$$\bar{a}_{2,2} = \rho_n \bar{K} \lambda_n \quad (214)$$

$$\phi_1 = \psi_w \quad (215)$$

$$\phi_2 = \psi_c(s_w) + \psi_w \quad (216)$$

$$u_1 = s_w \quad (217)$$

$$u_2 = \psi_w \quad (218)$$

Fractional Flow (“Phase Form”) Coefficients

$$m_1 = \omega \rho_w s_w \quad (219)$$

$$m_2 = \omega [s_w (\rho_w - \rho_n) + \rho_n] \quad (220)$$

$$f_1 = f_w q_t + \bar{K} \lambda_w f_n (b \rho_n - \rho_w) \nabla z \quad (221)$$

$$f_2 = \bar{K} \lambda_t \rho_t \nabla z \quad (222)$$

$$a_{1,1} = -\bar{K} \lambda_w f_n \quad (223)$$

$$a_{2,1} = \bar{K} \lambda_n \quad (224)$$

$$a_{2,2} = \bar{K} \lambda_t \quad (225)$$

$$\phi_1 = \psi_c(s_w) \quad (226)$$

$$\phi_2 = \psi_w \quad (227)$$

$$u_1 = s_w \quad (228)$$

$$u_2 = \psi_w \quad (229)$$

Fractional Flow (“Global Pressure”)

$$m_1 = \omega \rho_w s_w \quad (230)$$

$$m_2 = \omega [s_w (\rho_w - \rho_n) + \rho_n] \quad (231)$$

$$f_1 = f_w q_t + \bar{K} \lambda_w f_n (b \rho_n - \rho_w) \nabla z \quad (232)$$

$$f_2 = \bar{K} \lambda_t \rho_t \nabla z \quad (233)$$

$$a_{1,1} = -\bar{K} \lambda_w f_n \quad (234)$$

$$a_{2,2} = \bar{K} \lambda_t (1 - \chi) \quad (235)$$

$$\phi_1 = \psi_c(s_w) \quad (236)$$

$$\phi_2 = \psi_t = \psi_w + \int_{-\infty}^{\psi_c} f_n(w) dw = \frac{\psi_w + \psi_n}{2} + \int_0^{s_e} \left(\frac{1}{2} - f_w \right) \frac{d\psi_c}{ds_e} dw \quad (237)$$

$$u_1 = s_w \quad (238)$$

$$u_2 = \psi_t \quad (239)$$

Richards’ Equation

$$m_1 = \omega \rho_w s_w \quad (240)$$

$$f_1 = -\bar{K} \lambda_w \rho_w \nabla z \quad (241)$$

$$a_1 = \bar{K} \lambda_w \quad (242)$$

$$\phi_1 = \psi_w \quad (243)$$

$$u_1 = \psi_w \quad (244)$$

p-s-k Closure Relations

$$s_e = \frac{s_w - s_m(\mathbf{x})}{s_M(\mathbf{x}) - s_m(\mathbf{x})} \quad (\text{effective saturation}) \quad (245)$$

$$p_{ce} = \frac{p_c}{p_{cM}(\mathbf{x})} \quad (\text{effective capillary pressure}) \quad (246)$$

Simple Model

$$p_{ce} = s_e \quad (247)$$

$$k_{rw} = s_e^2 \quad (248)$$

$$k_{rn} = \frac{1}{2}(1 - s_e)^2 \quad (249)$$

Van Genuchten-Mualem

$$p_{cM} = \frac{1}{\alpha(\mathbf{x})} \quad \alpha > 0 \quad (250)$$

$$p_{ce} = \left(s_e^{-1/m} - 1 \right)^{1-m} \quad 0 < m < 1 \quad (251)$$

$$k_{rw} = s_e^{1/2} \left[1 - (1 - s_e^{1/m})^m \right]^2 \quad (252)$$

$$k_{rn} = (1 - s_e)^{1/2} (1 - s_e^{1/m})^{2m} \quad (253)$$

Brooks-Corey-Burdine

$$p_{cM} = p_d(\mathbf{x}) \quad p_d > 0 \quad (254)$$

$$p_{ce} = \begin{cases} s_e^{-1/\lambda} & s_e < 1 \\ 0 & s_e = 1 \end{cases} \quad \lambda > 0 \quad (255)$$

$$k_{rw} = s_e^{(2+3\lambda)/\lambda} \quad (256)$$

$$k_{rn} = (1 - s_e)^2 (1 - s_e^{(2+\lambda)/\lambda}) \quad (257)$$

Notes: i) In any of the above formulations a nonlinear potential, such as $\psi_c(s_w)$ can be chained out to get a diffusion term with respect to the unknown (s_w). It's probably better to avoid doing that because 1) it makes the Jacobian of the fully discrete model more complicated 2) it relies on more smoothness in $\psi_c(s_w)$, and 3) I have a vague idea that you want to avoid putting nonlinearity in the diffusion coefficients (the a's).
ii) The density and porosity closure relations are the same as for the saturated case.

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