Chapter 2

Flow and Transport Equations

2.1 Introduction

Mathematical models of petroleum reservoirs have been utilized since the late 1800s. A mathematical model consists of a set of equations that describe the flow of fluids in a petroleum reservoir, together with an appropriate set of boundary and/or initial conditions. This chapter is devoted to the development of such a model.

Fluid motion in a petroleum reservoir is governed by the conservation of mass, momentum, and energy. In the simulation of flow in the reservoir, the momentum equation is given in the form of Darcy’s law (Darcy, 1856). Derived empirically, this law indicates a linear relationship between the fluid velocity relative to the solid and the pressure head gradient. Its theoretical basis was provided by, e.g., Whitaker (1966); also see the books by Bear (1972) and Scheidegger (1974). The present chapter reviews some models that are known to be of practical importance.

There are several books available on fluid flow in porous media. The books by Muskat (1937; 1949) deal with the mechanics of fluid flow, the one by Collins (1961) is concerned with the practical and theoretical bases of petroleum reservoir engineering, and the one by Bear (1972) treats the dynamics and statics of fluids. The books by Peaceman (1977) and Aziz and Settari (1979) (also see Mattax and Dalton, 1990) present the application of finite difference methods to fluid flow in porous media. While the book by Chavent and Jaffré (1986) discusses finite element methods, the discussion is very brief, and most of their book is devoted to the mathematical formulation of models. The proceedings edited by Ewing (1983), Wheeler (1995), and Chen et al. (2000A) contain papers on finite elements for flow and transport problems. There are also books available on ground water hydrology; see Polubarinova-Kochina (1962), Wang and Anderson (1982), and Helmig (1997), for example.

The material presented in this chapter is very condensed. We do not attempt to derive differential equations that govern the flow and transport of fluids in porous media, but rather we review these equations to introduce the terminology and notation used throughout this book. The chapter is organized as follows. We consider the single phase flow of a fluid in a porous medium in Section 2.2. While this book concentrates on an ordinary porous...
medium, deformable and fractured porous media for single phase flow are also studied as an example. Furthermore, flow equations that include non-Darcy effects are described, and boundary and initial conditions are also presented. We develop the governing equations for two-phase immiscible flow in a porous medium in Section 2.3; attention is paid to the development of alternative differential equations for such a flow. Boundary and initial conditions associated with these alternative equations are established. We consider flow and transport of a component in a fluid phase and the problem of miscible displacement of one fluid by another in Section 2.4; diffusion and dispersion effects are discussed. We deal with transport of multicomponents in a fluid phase in Section 2.5; reactive flow problems are presented. We present the black oil model for three-phase flow in Section 2.6. A volatile oil model is defined in Section 2.7; this model includes the oil volatility effect. We construct differential equations for multicomponent, multiphase compositional flow, which involves mass transfer between phases in a general fashion, in Section 2.8. Although most mathematical models presented deal with isothermal flow, we also present a section on nonisothermal flow in Section 2.9. In Section 2.10, we consider chemical compositional flooding, where ASP+foam (alkaline, surfactant, and polymer) flooding is described. In Section 2.11, flows in fractured porous media are studied in more detail. Section 2.12 is devoted to discussing the relationship among all the flow models presented in this chapter. Finally, bibliographical information is given in Section 2.13. The mathematical models are briefly described in this chapter; more details on the governing differential equations and constitutive relations will be given in each of the subsequent chapters where a specific model is treated.

The term *phase* stands for matter that has a homogeneous chemical composition and physical state. Solid, liquid, and gaseous phases can be distinguished. Although there may be several liquid phases present in a porous medium, only a gaseous phase can exist. The phases are separate from each other. The term *component* is associated with a unique chemical species, and components constitute the phases.

### 2.2 Single Phase Flow

In this section, we consider the transport of a *Newtonian fluid* that occupies the entire void space in a porous medium under the isothermal condition.

#### 2.2.1 Single phase flow in a porous medium

The governing equations for the *single phase flow* of a fluid (a single component or a homogeneous mixture) in a porous medium are given by the *conservation of mass*, *Darcy’s law*, and an *equation of state*. We make the assumptions that the mass fluxes due to dispersion and diffusion are so small (relative to the advective mass flux) that they are negligible and that the fluid-solid interface is a material surface with respect to the fluid mass so that no mass of this fluid can cross it.

The spatial and temporal variables will be represented by \( \mathbf{x} = (x_1, x_2, x_3) \) and \( t \), respectively. Denote by \( \phi \) the *porosity* of the porous medium (the fraction of a representative elementary volume available for the fluid), by \( \rho \) the density of the fluid per unit volume, by \( \mathbf{u} = (u_1, u_2, u_3) \) the superficial *Darcy velocity*, and by \( q \) the external sources and sinks. Con-
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Consider a rectangular cube such that its faces are parallel to the coordinate axes (cf. Figure 2.1). The centroid of this cube is denoted \((x_1, x_2, x_3)\), and its length in the \(x_i\)-coordinate direction is \(\Delta x_i\), \(i = 1, 2, 3\). The \(x_i\)-component of the mass flux (mass flow per unit area per unit time) of the fluid is \(\rho u_i\). Referring to Figure 2.1, the mass inflow across the surface at \(x_1 - \frac{\Delta x_1}{2}\) per unit time is

\[
\left(\rho u_1\right)_{x_1 - \frac{\Delta x_1}{2}, x_2, x_3} \Delta x_1 \Delta x_2 \Delta x_3,
\]

and the mass outflow at \(x_1 + \frac{\Delta x_1}{2}\) is

\[
\left(\rho u_1\right)_{x_1 + \frac{\Delta x_1}{2}, x_2, x_3} \Delta x_1 \Delta x_2 \Delta x_3.
\]

Similarly, in the \(x_2\)- and \(x_3\)-coordinate directions, the mass inflows and outflows across the surfaces are, respectively,

\[
\left(\rho u_2\right)_{x_1, x_2 - \frac{\Delta x_2}{2}, x_3} \Delta x_1 \Delta x_2 \Delta x_3, \quad \left(\rho u_2\right)_{x_1, x_2 + \frac{\Delta x_2}{2}, x_3} \Delta x_1 \Delta x_2 \Delta x_3
\]

and

\[
\left(\rho u_3\right)_{x_1, x_2, x_3 - \frac{\Delta x_3}{2}} \Delta x_1 \Delta x_2 \Delta x_3, \quad \left(\rho u_3\right)_{x_1, x_2, x_3 + \frac{\Delta x_3}{2}} \Delta x_1 \Delta x_2 \Delta x_3.
\]

With \(\partial / \partial t\) being the time differentiation, mass accumulation due to compressibility per unit time is

\[
\frac{\partial (\phi \rho)}{\partial t} \Delta x_1 \Delta x_2 \Delta x_3,
\]

and the removal of mass from the cube, i.e., the mass decrement (accumulation) due to a sink of strength \(q\) (mass per unit volume per unit time) is

\[-q \Delta x_1 \Delta x_2 \Delta x_3.\]

The difference between the mass inflow and outflow equals the sum of mass accumulation.
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within this cube:

\[
\left[ (\rho u_1)_{x_1, x_2, x_3} - (\rho u_1)_{x_1 + \Delta x_1, x_2, x_3} \right] \Delta x_2 \Delta x_3
\]

\[
+ \left[ (\rho u_2)_{x_1, x_2, x_3} - (\rho u_2)_{x_1, x_2 + \Delta x_2, x_3} \right] \Delta x_1 \Delta x_3
\]

\[
+ \left[ (\rho u_3)_{x_1, x_2, x_3 + \Delta x_3} - (\rho u_3)_{x_1, x_2, x_3} \right] \Delta x_1 \Delta x_2
\]

\[
= \left( \frac{\partial (\phi \rho)}{\partial t} - q \right) \Delta x_1 \Delta x_2 \Delta x_3.
\]

Divide this equation by \( \Delta x_1 \Delta x_2 \Delta x_3 \) to see that

\[
- (\rho u_1)_{x_1 + \Delta x_1, x_2, x_3} + (\rho u_1)_{x_1, x_2, x_3}
\]

\[
= \left( \frac{\partial (\phi \rho)}{\partial t} - q \right) \Delta x_1 \Delta x_2 \Delta x_3.
\]

Letting \( \Delta x_i \to 0, i = 1, 2, 3 \), we obtain the mass conservation equation

\[
\frac{\partial (\phi \rho)}{\partial t} = - \nabla \cdot (\rho u) + q,
\]

where \( \nabla \cdot \) is the divergence operator:

\[
\nabla \cdot u = \frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3}.
\]

Note that \( q \) is negative for sinks and positive for sources.

Equation (2.1) is established for three space dimensions. It also applies to the one-dimensional (in the \( x_1 \)-direction) or two-dimensional (in the \( x_1, x_2 \)-plane) flow if we introduce the factor

\[
\tilde{\alpha}(x) = \Delta x_2(x) \Delta x_3(x) \quad \text{in one dimension},
\]

\[
\tilde{\alpha}(x) = \Delta x_3(x) \quad \text{in two dimensions},
\]

\[
\tilde{\alpha}(x) = 1 \quad \text{in three dimensions}.
\]

For these three cases, (2.1) becomes

\[
\tilde{\alpha} \frac{\partial (\phi \rho)}{\partial t} = - \nabla \cdot (\tilde{\alpha} \rho u) + \tilde{\alpha} q.
\]

The formation volume factor, \( B \), is defined as the ratio of the volume of the fluid measured at reservoir conditions to the volume of the same fluid measured at standard conditions:

\[
B(p, T) = \frac{V(p, T)}{V_s},
\]

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where \( s \) denotes the standard conditions and \( p \) and \( T \) are the fluid pressure and temperature (at reservoir conditions), respectively. Let \( W \) be the weight of the fluid. Because \( V = W/\rho \) and \( V_s = W/\rho_s \), where \( \rho_s \) is the density at standard conditions, we see that

\[
\rho = \frac{\rho_s}{B}.
\]

Substituting \( \rho \) into (2.2), we have

\[
\tilde{\alpha} \frac{\partial}{\partial t} \left( \frac{\phi}{B} \right) = -\nabla \cdot \left( \frac{\tilde{\alpha}}{B} \mathbf{u} \right) + \tilde{\alpha} q \rho_s. \tag{2.3}
\]

While (2.1) and (2.3) are equivalent, the former will be utilized in this book except for the black oil and volatile oil models.

In addition to (2.1), we state the momentum conservation in the form of Darcy’s law (Darcy, 1856). This law indicates a linear relationship between the fluid velocity and the pressure head gradient:

\[
\mathbf{u} = -\frac{1}{\mu} \mathbf{k} (\nabla p - \rho \varphi \nabla z), \tag{2.4}
\]

where \( \mathbf{k} \) is the absolute permeability tensor of the porous medium, \( \mu \) is the fluid viscosity, \( \varphi \) is the magnitude of the gravitational acceleration, \( z \) is the depth, and \( \nabla \) is the gradient operator:

\[
\nabla p = \left( \frac{\partial p}{\partial x_1}, \frac{\partial p}{\partial x_2}, \frac{\partial p}{\partial x_3} \right).
\]

The \( x_3 \)-coordinate in (2.4) is in the vertical downward direction. The permeability is an average medium property that measures the ability of the porous medium to transmit fluid. In some cases, it is possible to assume that \( \mathbf{k} \) is a diagonal tensor

\[
\mathbf{k} = \begin{pmatrix}
  k_{11} & 0 & 0 \\
  0 & k_{22} & 0 \\
  0 & 0 & k_{33}
\end{pmatrix} = \text{diag}(k_{11}, k_{22}, k_{33}).
\]

If \( k_{11} = k_{22} = k_{33} \), the porous medium is called isotropic; otherwise, it is anisotropic.

### 2.2.2 General equations for single phase flow

Substituting (2.4) into (2.1) yields

\[
\frac{\partial (\phi \rho)}{\partial t} = \nabla \cdot \left( \frac{\rho}{\mu} \mathbf{k} (\nabla p - \rho \varphi \nabla z) \right) + \tilde{q}. \tag{2.5}
\]

An equation of state is expressed in terms of the fluid compressibility \( c_f \):

\[
c_f = -\frac{1}{V} \frac{\partial V}{\partial p} \bigg|_T = \frac{1}{\rho} \frac{\partial \rho}{\partial p} \bigg|_T, \tag{2.6}
\]

at a fixed temperature \( T \), where \( V \) stands for the volume occupied by the fluid at reservoir conditions. Combining (2.5) and (2.6) gives a closed system for the main unknown \( p \).
or \( \rho \). Simplified expressions such as a linear relationship between \( p \) and \( \rho \) for a slightly compressible fluid can be used; see the next subsection.

It is sometimes convenient in mathematical analysis to write (2.5) in a form without the explicit appearance of gravity, by the introduction of a pseudopotential (Hubbert, 1956):

\[
\Phi' = \int_{p^o}^{p} \frac{1}{\rho(\xi) \Phi} \, d\xi - z,
\]

(2.7)

where \( p^o \) is a reference pressure. Using (2.7), equation (2.5) reduces to

\[
\frac{\partial (\Phi \rho)}{\partial t} = \nabla \cdot \left( \frac{\rho^2 \Phi}{\mu} \nabla \Phi' \right) + q.
\]

(2.8)

In numerical computations, more often we use the usual potential (piezometric head)

\[
\Phi = p - \rho \varphi z,
\]

which is related to \( \Phi' \) (with, e.g., \( p^o = 0 \) and constant \( \rho \)) by

\[
\Phi = \rho \varphi \Phi'.
\]

If we neglect the term \( \varphi z \nabla \rho \), in terms of \( \Phi \), (2.5) becomes

\[
\frac{\partial (\Phi \rho)}{\partial t} = \nabla \cdot \left( \frac{\rho^2 \Phi}{\mu} \nabla \Phi \right) + q.
\]

(2.9)

In general, there is not a distributed mass source or sink in single phase flow in a three-dimensional medium. However, as an approximation, we may consider the case where sources and sinks of a fluid are located at isolated points \( x^{(i)} \). Then these point sources and sinks can be surrounded by small spheres that are excluded from the medium. The surfaces of these spheres can be treated as part of the boundary of the medium, and the mass flow rate per unit volume of each source or sink specifies the total flux through its surface.

Another approach to handling point sources and sinks is to insert them in the mass conservation equation. That is, for point sinks, we define \( q \) in (2.5) by

\[
q = - \sum_i \rho q^{(i)} \delta(x - x^{(i)}),
\]

(2.10)

where \( q^{(i)} \) indicates the volume of the fluid produced per unit time at \( x^{(i)} \) and \( \delta \) is the Dirac delta function. For point sources, \( q \) is given by

\[
q = \sum_i \rho^{(i)} q^{(i)} \delta(x - x^{(i)}),
\]

(2.11)

where \( q^{(i)} \) and \( \rho^{(i)} \) denote the volume of the fluid injected per unit time and its density (which is known) at \( x^{(i)} \), respectively. The treatment of sources and sinks will be discussed in more detail in later chapters (cf. Chapter 13).
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2.2.3 Equations for slightly compressible flow and rock

It is sometimes possible to assume that the fluid compressibility $c_f$ is constant over a certain range of pressures. Then, after integration (cf. Exercise 2.1), we write (2.6) as

$$\rho = \rho^o e^{c_f(p - p^o)},$$  \hfill (2.12)

where $\rho^o$ is the density at the reference pressure $p^o$. Using a Taylor series expansion, we see that

$$\rho = \rho^o \left\{1 + c_f(p - p^o) + \frac{1}{2!} c_f^2 (p - p^o)^2 + \cdots\right\},$$

so an approximation results:

$$\rho \approx \rho^o \left(1 + c_f(p - p^o)\right).$$  \hfill (2.13)

The rock compressibility is defined by

$$c_R = \frac{1}{\phi} \frac{d\phi}{dp}.$$  \hfill (2.14)

After integration, it is given by

$$\phi = \phi^o e^{c_R(p - p^o)},$$  \hfill (2.15)

where $\phi^o$ is the porosity at $p^o$. Similarly, it is approximated by

$$\phi \approx \phi^o \left(1 + c_R(p - p^o)\right).$$  \hfill (2.16)

Then it follows that

$$\frac{d\phi}{dp} \approx \phi^o c_R.$$  \hfill (2.17)

After carrying out the time differentiation in the left-hand side of (2.5), the equation becomes

$$\left(\phi \frac{\partial \rho}{\partial p} + \rho \frac{d\phi}{dp} \right) \frac{\partial p}{\partial t} = \nabla \cdot \left(\frac{\rho}{\mu} k \left(\nabla p - \rho \phi \nabla z\right)\right) + q.$$  \hfill (2.18)

Substituting (2.6) and (2.17) into (2.18) gives

$$\rho \left(\phi c_f + \phi^o c_R\right) \frac{\partial p}{\partial t} = \nabla \cdot \left(\frac{\rho}{\mu} k \left(\nabla p - \rho \phi \nabla z\right)\right) + q.$$  

Defining the total compressibility

$$c_t = c_f + \phi^o c_R,$$  \hfill (2.19)

we see that

$$\phi \rho c_t \frac{\partial p}{\partial t} = \nabla \cdot \left(\frac{\rho}{\mu} k \left(\nabla p - \rho \phi \nabla z\right)\right) + q,$$  \hfill (2.20)

which is a parabolic equation in $p$ (cf. Section 2.3.2), with $\rho$ given by (2.12).
2.2.4 Equations for gas flow

For gas flow, the compressibility $c_g$ of gas is usually not assumed to be constant. In such a case, the general equation (2.18) applies; i.e.,

$$c(p) \frac{\partial p}{\partial t} = \nabla \cdot \left( \frac{\rho}{\mu} k (\nabla p - \rho \phi \nabla z) \right) + q, \quad (2.21)$$

where

$$c(p) = \phi \frac{\partial \rho}{\partial p} + \rho \frac{d\phi}{dp}.$$

A different form of (2.21) can be derived if we use the gas law (the pressure-volume-temperature (PVT) relation)

$$\rho = \frac{pW}{ZRT}, \quad (2.22)$$

where $W$ is the molecular weight, $Z$ is the gas compressibility factor, and $R$ is the universal gas constant. If pressure, temperature, and density are in atm, K, and g/cm$^3$, respectively, the value of $R$ is 82.057. For a pure gas reservoir, the gravitational constant is usually small and neglected. We assume that the porous medium is isotropic; i.e., $k = k\mathbf{I}$, where $\mathbf{I}$ is the identity tensor. Furthermore, we assume that $\phi$ and $\mu$ are constants. Then, substituting (2.22) into (2.5), we see that

$$\phi \frac{\partial}{\partial t} \left( \frac{p}{Z} \right) = \nabla \cdot \left( \frac{p}{\mu Z} \nabla p \right) + \frac{RT}{WK} q. \quad (2.23)$$

Note that $2p \nabla p = \nabla p^2$, so (2.23) becomes

$$\frac{2\phi \mu Z}{k} \frac{\partial}{\partial t} \left( \frac{p}{Z} \right) = \Delta p^2 + 2pZ \frac{d}{dp} \left( \frac{1}{Z} \right) |\nabla p|^2 + \frac{2\mu Z RT}{WK} q, \quad (2.24)$$

where $\Delta$ is the Laplacian operator:

$$\Delta p = \frac{\partial^2 p}{\partial x_1^2} + \frac{\partial^2 p}{\partial x_2^2} + \frac{\partial^2 p}{\partial x_3^2}.$$

Because

$$c_g = \frac{1}{\rho} \left| \frac{\partial \rho}{\partial p} \right|_T = \frac{1}{p} - \frac{1}{Z} \frac{dZ}{dp},$$

we have

$$\frac{\partial}{\partial t} \left( \frac{p}{Z} \right) = \frac{pc_g \partial p}{Z}.$$

Inserting this equation into (2.24) and neglecting the term involving $|\nabla p|^2$ (often smaller than other terms in (2.24)), we obtain

$$\frac{\phi \mu c_g}{k} \frac{\partial p^2}{\partial t} = \Delta p^2 + \frac{2ZRT\mu}{WK} q, \quad (2.25)$$

which is a parabolic equation in $p^2$. 

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There is another way to derive an equation similar to (2.25). Define a pseudopressure by

\[ \psi = 2 \int_{p_0}^{p} \frac{p}{Z\mu} dp. \]

Note that

\[ \nabla \psi = \frac{2p}{Z\mu} \nabla p, \quad \frac{\partial \psi}{\partial t} = \frac{2p}{Z\mu} \frac{\partial p}{\partial t}. \]

Equation (2.23) becomes

\[ \frac{\phi_{\kappa}}{c_{\kappa}} \frac{\partial \psi}{\partial t} = \frac{\Delta \psi}{\Delta_1} + \frac{2RT}{W_k} q. \]  
(2.26)

The derivation of (2.26) does not require us to neglect the second term in the right-hand side of (2.24).

2.2.5 Single phase flow in a deformable medium

Consider a deformable porous medium whose solid skeleton has compressibility and shearing rigidity. The medium is assumed to be composed of a linear elastic material, and its deformation to be small.

Let \( w_s \) and \( w \) be the displacements of the solid and fluid, respectively. For a deformable medium, Darcy’s law in (2.4) is generalized as follows (Biot, 1955; Chen et al., 2004B):

\[ \dot{w} - \dot{w}_s = -\frac{1}{k} (\nabla p - \rho \nabla z), \]  
(2.27)

where \( \dot{w} = \partial w / \partial t \). Note that \( u = \dot{w} \), so (2.27) just introduces a new dependent variable \( w_s \). Additional equations are needed for a closed system.

Let \( I \) be the identity matrix. The total stress tensor of the bulk material is

\[ \sigma + \sigma_1 \equiv \left( \begin{array}{ccc} \sigma_{11} + \sigma & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} + \sigma & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} + \sigma \end{array} \right) \]

with the symmetry property \( \sigma_{ij} = \sigma_{ji} \). To understand the meaning of this tensor, consider a cube of the bulk material with unit size. Then \( \sigma \) represents the total normal tension force applied to the fluid part of the faces of the cube, while the remaining components \( \sigma_{ij} \) are the forces applied to the portion of the cube faces occupied by the solid. The stress tensor satisfies the equilibrium relation

\[ \nabla \cdot (\sigma + \sigma_1) + \rho_t \nabla z = 0, \]  
(2.28)

where \( \rho_t = \rho (1 - \phi) \rho_s + (1 - \phi) \rho_s \) is the mass density of the bulk material and \( \rho_s \) is the solid density. To relate \( \sigma \) to \( w_s \), we need a constitutive relationship between the stress and strain tensors.

Denote the strain tensors of the solid and fluid by \( \epsilon_s \) and \( \epsilon_f \), respectively, defined by

\[ \epsilon_{s,ij} = \frac{1}{2} \left( \frac{\partial w_{s,j}}{\partial x_i} + \frac{\partial w_{s,i}}{\partial x_j} \right), \quad \epsilon_{ij} = \frac{1}{2} \left( \frac{\partial w_{i,j}}{\partial x_j} + \frac{\partial w_{j,i}}{\partial x_i} \right), \quad i, j = 1, 2, 3. \]
Also, define \( \epsilon = \epsilon_{11} + \epsilon_{22} + \epsilon_{33} \). The stress-strain relationship is

\[
\begin{pmatrix}
\sigma_{11} \\
\sigma_{22} \\
\sigma_{33} \\
\sigma_{23} \\
\sigma_{31} \\
\sigma_{12}
\end{pmatrix} = \begin{pmatrix}
\epsilon_{11} & c_{12} & c_{13} & c_{14} & c_{15} & c_{16} & c_{17} \\
0 & c_{22} & c_{23} & c_{24} & c_{25} & c_{26} & c_{27} \\
0 & 0 & c_{33} & c_{34} & c_{35} & c_{36} & c_{37} \\
0 & 0 & 0 & c_{44} & c_{45} & c_{46} & c_{47} \\
0 & 0 & 0 & 0 & c_{55} & c_{56} & c_{57} \\
0 & 0 & 0 & 0 & 0 & c_{66} & c_{67}
\end{pmatrix} \begin{pmatrix}
\epsilon_{r,11} \\
\epsilon_{r,22} \\
\epsilon_{r,33} \\
\epsilon_{r,23} \\
\epsilon_{r,31} \\
\epsilon_{r,12}
\end{pmatrix},
\]

where \( c_{ij} = c_{ji} \) (i.e., the coefficient matrix is symmetric). Now, substitute this relationship into (2.28) to give three equations for the three unknowns \( w_s,1, \) \( w_s,2, \) and \( w_s,3. \)

As an example of the stress-strain relationship, we consider the case where the solid matrix is isotropic. In this case, with \( \epsilon_s = \epsilon_{s,11} + \epsilon_{s,22} + \epsilon_{s,33} \), the relationship is given by

\[
\sigma_{ii} = 2G \left( \epsilon_{s,ii} + \frac{\nu \epsilon_s}{1 - 2\nu} \right) - H p, \quad i = 1, 2, 3,
\]

\[
\sigma_{ij} = 2G \epsilon_{s,ij}, \quad i, j = 1, 2, 3; \ i \neq j,
\]

where \( G \) and \( \nu \) are the Young modulus and the Poisson ratio for the solid skeleton, and \( H \) is a physical constant whose value must be determined by experiments or by numerical methods (Biot, 1955; Chen et al., 2004B).

### 2.2.6 Single phase flow in a fractured medium

A fractured porous medium is a medium that is intersected by a network of interconnected fractures, or solution channels (cf. Figure 2.2). Such a medium could be modeled by allowing the porosity and permeability to vary rapidly and discontinuously over the whole domain. Both these quantities are much larger in the fractures than in the blocks of porous rock (called matrix blocks). However, the data requirement and computational cost for simulating such a single porosity model would be too great to approximate the flow in the entire medium. Instead, it is more convenient to regard the fluid in the void space as made

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up of two parts, one part in the fractures and the other in the matrix, and to treat each part as a continuum that occupies the entire domain. These two overlapping continua are allowed to coexist and interact with each other. There are two distinct dual concepts: dual porosity (and single permeability) and dual porosity/permeability. The former is considered in this section, while the latter will be studied in Section 2.11.

Since fluid flows more rapidly in the fractures than in the matrix, we assume that it does not flow directly from one block to another. Rather, it first flows into the fractures, and then it flows into another block or remains in the fractures (Douglas and Arbogast, 1990). Also, the equations that describe the flow in the fracture continuum contain a source term that represents the flow of fluid from the matrix to the fractures; this term is assumed to be distributed over the entire medium. Finally, we assume that the external sources and sinks interact only with the fracture system, which is reasonable since flow is much faster in this system than in the matrix blocks. Based on these assumptions, flow through each block in a fractured porous medium is given by

\[
\frac{\partial (\phi \rho)}{\partial t} = - \nabla \cdot (\rho \mathbf{u}), \tag{2.29}
\]

The flow in the fractures is described by

\[
\frac{\partial (\phi_f \rho_f)}{\partial t} = - \nabla \cdot (\rho_f \mathbf{u}_f) + q_{mf} + q_{ext}, \tag{2.30}
\]

where the subscript \(f\) represents the fracture quantities, \(q_{mf}\) denotes the flow from the matrix to the fractures, and \(q_{ext}\) indicates the external sources and sinks. The velocities \(\mathbf{u}\) and \(\mathbf{u}_f\) are determined by Darcy’s law as in (2.4).

The matrix-fracture transfer term \(q_{mf}\) can be defined by two different approaches: one approach using matrix shape factors (Warren and Root, 1963; Kazemi, 1969) and the other based on boundary conditions imposed explicitly on matrix blocks (Pirson, 1953; Barenblatt et al., 1960). The latter approach is presented here; the former will be described in Section 2.11 and Chapter 12. The total mass of fluid leaving the \(i\)th matrix block \(\Omega_i\) per unit time is

\[
\int_{\partial \Omega_i} \rho \mathbf{u} \cdot \mathbf{n} d\ell,
\]

where \(\mathbf{n}\) is the outward unit normal to the surface \(\partial \Omega_i\) of \(\Omega_i\) and the dot product \(\mathbf{u} \cdot \mathbf{n}\) is defined by

\[
\mathbf{u} \cdot \mathbf{n} = u_1 v_1 + u_2 v_2 + u_3 v_3.
\]

The divergence theorem and (2.29) imply

\[
\int_{\partial \Omega_i} \rho \mathbf{u} \cdot \mathbf{n} d\ell = \int_{\Omega_i} \nabla \cdot (\rho \mathbf{u}) d\mathbf{x} = - \int_{\Omega_i} \frac{\partial (\phi \rho)}{\partial t} d\mathbf{x}.
\]

Now, define \(q_{mf}\) by

\[
q_{mf} = - \sum_i \chi_i(\mathbf{x}) \frac{1}{|\Omega_i|} \int_{\Omega_i} \frac{\partial (\phi \rho)}{\partial t} d\mathbf{x}, \tag{2.31}
\]

where \(|\Omega_i|\) denotes the volume of \(\Omega_i\) and \(\chi_i(\mathbf{x})\) is its characteristic function, i.e.,

\[
\chi_i(\mathbf{x}) = \begin{cases} 
1 & \text{if } \mathbf{x} \in \Omega_i, \\
0 & \text{otherwise}.
\end{cases}
\]
With the definition of $q_{mf}$, we now establish a boundary condition on the surface of each matrix block in a general fashion. Gravitational forces have a special effect on this condition. Moreover, pressure gradient effects must be treated on the same footing as the gravitational effects. To that end, following Arbogast (1993), we employ the pseudopotential $\Phi'$ defined in (2.7) to impose a condition on the surface of each matrix block by

$$\Phi' = \Phi'_f - \Phi^o \text{ on } \partial \Omega_i,$$  \hspace{1cm} (2.32)

where, for a given $\Phi'_f$, $\Phi^o$ is a pseudopotential reference value on each block $\Omega_i$ determined by

$$\frac{1}{|\Omega_i|} \int_{\Omega_i} (\phi \rho) \left( \psi(\Phi'_f - \Phi^o + x_i) \right) \, dx = (\phi \rho)(p_f),$$  \hspace{1cm} (2.33)

with the function $\psi'$ equal to the inverse of the integral in (2.7) as a function of $p$. Monotonicity of $\phi \rho$ insures a unique solution to (2.33) unless the rock and fluid are incompressible. In that case, set $\Phi^o = 0$.

For the model described, the highly permeable fracture system rapidly comes into equilibrium on the fracture spacing scale locally. This equilibrium is defined in terms of the pseudopotential, and is reflected in the matrix equations through the boundary condition (2.32).

### 2.2.7 Non-Darcy's law

Strictly speaking, Darcy’s law holds only for a Newtonian fluid over a certain range of flow rates. As the flow rate increases, a deviation from this law has been noticed (Dupuit, 1863; Forchheimer, 1901). It has been experimentally and mathematically observed that this deviation is due to inertia, turbulence, and other high-velocity effects (Fancher and Lewis, 1933; Hubbert, 1956; Mei and Auriault, 1991; Chen et al., 2000B). Hubbert (1956) observed a deviation from the usual Darcy law at a Reynolds’ number of flow of about one (based on the grain diameter of an unconsolidated medium), whereas turbulence was not noticed until the Reynolds’ number approached 600 (Aziz and Settari, 1979).

A correction to Darcy’s law for high flow rates can be described by a quadratic term (Forchheimer, 1901; Ward, 1964; Chen et al., 2000B):

$$(\mu I + \beta \rho |u|k)u = -k (\nabla p - \rho \phi \nabla z),$$

where $\beta$ indicates the inertial or turbulence factor and

$$|u| = \sqrt{u_1^2 + u_2^2 + u_3^2}.$$ 

This equation is generally called Forchheimer’s law and incorporates laminar, inertial, and turbulence effects. It has been the subject of many experimental and theoretical investigations. These investigations have centered on the issue of providing a physical or theoretical basis for the derivation of Forchheimer’s law. Many approaches have been developed and analyzed for this purpose such as empiricism fortified with dimensional analysis (Ward, 1964), experimental study (MacDonald et al., 1979), averaging methods (Chen et al., 2000B), and variational principles (Knupp and Lage, 1995).
2.2. Single Phase Flow

![Darcy's Law Diagram](image)

Figure 2.3. Threshold phenomenon.

2.2.8 Other effects

There exist several effects that introduce additional complexity in the basic flow equations. Some fluids (e.g., polymer solutions; cf. Section 2.10 and Chapter 11) exhibit non-Newtonian phenomena, characterized by nonlinear dependence of shear stress on shear rate. The study of non-Newtonian fluids is beyond the scope of this book, but can be found in the literature on rheology. In practice, the resistance to flow in a porous medium can be represented by Darcy’s law with viscosity \( \mu \) depending on flow velocity; i.e.,

\[
 u = -\frac{1}{\mu(\mathbf{u})} \mathbf{k} (\nabla p - \rho \phi \nabla z) .
\]

Over a certain range of the velocity (the pseudoplastic region of flow), the viscosity can be approximated by a power law (Bird et al., 1960):

\[
 \mu(\mathbf{u}) = \mu_o |\mathbf{u}|^{m-1},
\]

where the constants \( \mu_o \) and \( m \) are empirically determined.

Other effects are related to threshold and slip phenomena. It has been experimentally observed that a certain nonzero pressure gradient is required to initiate flow. The threshold phenomenon can be seen in the relationship between \( q \) and \( \partial p/\partial x \) for low rates, as shown in Figure 2.3. The slip (or Klinkenberg) phenomenon occurs in gas flow at low pressures and results in an increase of effective permeability compared to that measured for liquids. These two phenomena are relatively unimportant, and can be incorporated with a modification of Darcy’s law (Bear, 1972).

2.2.9 Boundary conditions

The mathematical model described so far for single phase flow is not complete unless necessary boundary and initial conditions are specified. Below we present boundary conditions of three kinds that are relevant to (2.5). A similar discussion can be given for (2.28), which defines the displacement of the solid. Also, similar boundary conditions can be described for the dual porosity model. We denote by \( \Gamma \) the external boundary or a boundary segment of the porous medium domain \( \Omega \) under consideration.

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Chapter 2. Flow and Transport Equations

Prescribed pressure

When the pressure is specified as a known function of position and time on \( \Gamma \), the boundary condition is

\[
p = g_1 \quad \text{on } \Gamma.
\]

In the theory of partial differential equations, such a condition is termed a boundary condition of the first kind, or a Dirichlet boundary condition.

Prescribed mass flux

When the total mass flux is known on \( \Gamma \), the boundary condition is

\[
\rho \mathbf{u} \cdot \mathbf{n} = g_2 \quad \text{on } \Gamma,
\]

where \( \mathbf{n} \) indicates the outward unit normal to \( \Gamma \). This condition is called a boundary condition of the second kind, or a Neumann boundary condition. For an impervious boundary, \( g_2 = 0 \).

Mixed boundary condition

A boundary condition of mixed kind (or third kind) takes the form

\[
g_p p + g_u \rho \mathbf{u} \cdot \mathbf{n} = g_3 \quad \text{on } \Gamma,
\]

where \( g_p, g_u \), and \( g_3 \) are given functions. This condition is referred to as a Robin or Darcy-Werts boundary condition. Such a condition occurs when \( \Gamma \) is a semipervious boundary. Finally, the initial condition can be defined in terms of \( p \):

\[
p(\mathbf{x}, 0) = p_0(\mathbf{x}), \quad \mathbf{x} \in \Omega.
\]

2.3 Two-Phase Immiscible Flow

In reservoir simulation, we are often interested in the simultaneous flow of two or more fluid phases within a porous medium. We now develop basic equations for multiphase flow in a porous medium. In this section, we consider two-phase flow where the fluids are immiscible and there is no mass transfer between the phases. One phase (e.g., water) wets the porous medium more than the other (e.g., oil), and is called the wetting phase and indicated by a subscript \( w \). The other phase is termed the nonwetting phase and indicated by \( o \). In general, water is the wetting fluid relative to oil and gas, while oil is the wetting fluid relative to gas.

2.3.1 Basic equations

Several new quantities peculiar to multiphase flow, such as saturation, capillary pressure, and relative permeability, must be introduced. The saturation of a fluid phase is defined as the fraction of the void volume of a porous medium filled by this phase. The fact that the two fluids jointly fill the voids implies the relation

\[
S_w + S_o = 1,
\]
2.3. Two-Phase Immiscible Flow

where $S_w$ and $S_o$ are the saturations of the wetting and nonwetting phases, respectively. Also, due to the curvature and surface tension of the interface between the two phases, the pressure in the wetting fluid is less than that in the nonwetting fluid. The pressure difference is given by the capillary pressure

$$p_c = p_o - p_w.$$  \hspace{1cm} (2.35)

Empirically, the capillary pressure is a function of saturation $S_w$.

Except for the accumulation term, the same derivation that led to (2.1) also applies to the mass conservation equation for each fluid phase (cf. Exercise 2.2). Mass accumulation in a differential volume per unit time is

$$\frac{\partial (\phi \rho \alpha S_\alpha)}{\partial t} \Delta x_1 \Delta x_2 \Delta x_3.$$  

Taking into account this and the assumption that there is no mass transfer between phases in the immiscible flow, mass is conserved within each phase:

$$\frac{\partial (\phi \rho \alpha S_\alpha)}{\partial t} = -\nabla \cdot (\rho \alpha u_\alpha) + q_\alpha, \hspace{0.5cm} \alpha = w, o,$$  \hspace{1cm} (2.36)

where each phase has its own density $\rho_\alpha$, Darcy velocity $u_\alpha$, and mass flow rate $q_\alpha$. Darcy’s law for single phase flow can be directly extended to multiphase flow:

$$u_\alpha = -\frac{1}{\mu_\alpha} k_\alpha (\nabla p_\alpha - \rho_\alpha \phi \nabla z), \hspace{0.5cm} \alpha = w, o,$$  \hspace{1cm} (2.37)

where $k_\alpha$, $p_\alpha$, and $\mu_\alpha$ are the effective permeability, pressure, and viscosity for phase $\alpha$.

Since the simultaneous flow of two fluids causes each to interfere with the other, the effective permeabilities are not greater than the absolute permeability $k$ of the porous medium. The relative permeabilities $k_{\alpha\alpha}$ are widely used in reservoir simulation:

$$k_\alpha = k_{\alpha\alpha} k, \hspace{0.5cm} \alpha = w, o.$$  \hspace{1cm} (2.38)

The function $k_{\alpha\alpha}$ indicates the tendency of phase $\alpha$ to wet the porous medium.

Typical functions of $p_c$ and $k_{\alpha\alpha}$ will be described in the next chapter. When $q_w$ and $q_o$ represent a finite number of point sources or sinks, they can be defined as in (2.10) or (2.11). Also, the densities $\rho_w$ and $\rho_o$ are functions of their respective pressures. Thus, after substituting (2.37) into (2.36) and using (2.34) and (2.35), we have a complete system of two equations for two of the four main unknowns $p_\alpha$ and $S_\alpha, \alpha = w, o$. Other mathematical formulations will be discussed in this section. The development of single phase flow in deformable and fractured porous media is applicable to two-phase flow. We do not pursue this similar development.

2.3.2 Alternative differential equations

In this section, we derive several alternative formulations of the differential equations in (2.34)–(2.37).
Chapter 2. Flow and Transport Equations

Formulation in phase pressures

Assume that the capillary pressure $p_c$ has a unique inverse function:

$$S_w = p_c^{-1}(p_o - p_w).$$

We use $p_w$ and $p_o$ as the main unknowns. Then it follows from (2.34)–(2.37) that

$$\nabla \cdot \left( \frac{\rho_w}{\mu_w} k_w \left( \nabla p_w - \rho_w \phi \nabla z \right) \right) = \frac{\partial (\phi \rho_w p_c^{-1})}{\partial t} - q_w,$$

$$\nabla \cdot \left( \frac{\rho_o}{\mu_o} k_o \left( \nabla p_o - \rho_o \phi \nabla z \right) \right) = \frac{\partial (\phi \rho_o (1 - p_c^{-1}))}{\partial t} - q_o. \quad (2.39)$$

This system was employed in the simultaneous solution (SS) scheme in petroleum reservoirs (Douglas et al., 1959). The equations in this system are strongly nonlinear and coupled. More details will be given in Chapter 7.

Formulation in phase pressure and saturation

We use $p_o$ and $S_w$ as the main variables. Applying (2.34), (2.35), and (2.37), equation (2.36) can be rewritten as

$$\nabla \cdot \left( \frac{\rho_w}{\mu_w} k_w \left( \nabla p_o - \frac{dp_c}{dS_w} \nabla S_w - \rho_w \phi \nabla z \right) \right) = \frac{\partial (\phi \rho_w S_w)}{\partial t} - q_w,$$

$$\nabla \cdot \left( \frac{\rho_o}{\mu_o} k_o \left( \nabla p_o - \rho_o \phi \nabla z \right) \right) = \frac{\partial (\phi \rho_o (1 - S_w))}{\partial t} - q_o. \quad (2.40)$$

Carrying out the time differentiation in (2.40), dividing the first and second equations by $\rho_w$ and $\rho_o$, respectively, and adding the resulting equations, we obtain

$$\frac{1}{\rho_w} \nabla \cdot \left( \frac{\rho_w}{\mu_w} k_w \left( \nabla p_o - \frac{dp_c}{dS_w} \nabla S_w - \rho_w \phi \nabla z \right) \right) + \frac{1}{\rho_o} \nabla \cdot \left( \frac{\rho_o}{\mu_o} k_o \left( \nabla p_o - \rho_o \phi \nabla z \right) \right)
= \frac{S_w}{\rho_w} \frac{\partial (\phi \rho_o)}{\partial t} + \frac{1 - S_w}{\rho_o} \frac{\partial (\phi \rho_o)}{\partial t} - \frac{q_w}{\rho_w} - \frac{q_o}{\rho_o}. \quad (2.41)$$

Note that if the saturation $S_w$ in (2.41) is explicitly evaluated, we can use this equation to solve for $p_o$. After computing this pressure, the second equation in (2.40) can be used to calculate $S_w$. This is the implicit pressure-explicit saturation (IMPES) scheme and has been widely exploited for two-phase flow in petroleum reservoirs (cf. Chapter 7).

Formulation in a global pressure

The equations in (2.39) and (2.40) are strongly coupled, as noted. To reduce the coupling, we now write them in a different formulation, where a global pressure is used. For simplicity,
2.3. Two-Phase Immiscible Flow

we assume that the densities are constant; the formulation does extend to variable densities (Chen et al., 1995; Chen et al., 1997A). Introduce the phase mobilities

\[ \lambda_\alpha = \frac{k_{r\alpha}}{\mu_\alpha}, \quad \alpha = w, o, \]

and the total mobility

\[ \lambda = \lambda_w + \lambda_o. \]

Also, define the fractional flow functions

\[ f_\alpha = \frac{\lambda_\alpha}{\lambda}, \quad \alpha = w, o. \]

With \( S = S_w \), define the global pressure (Antoncev, 1972; Chavent and Jaffré, 1986)

\[ p = p_o - \int_{p_c}^{p_c(S)} f_w(p_c^{-1}(\xi))d\xi, \quad (2.42) \]

and the total velocity

\[ \mathbf{u} = \mathbf{u}_w + \mathbf{u}_o. \quad (2.43) \]

It follows from (2.35), (2.37), and (2.42) that the total velocity is

\[ \mathbf{u} = -k\lambda (\nabla p - (\rho_w f_w + \rho_o f_o)\phi \nabla z). \quad (2.44) \]

Also, carrying out the differentiation in (2.36), dividing by \( \rho_\alpha \), adding the resulting equations with \( \alpha = w \) and \( o \), and applying (2.42), we obtain

\[ \nabla \cdot \mathbf{u} = -\frac{\partial \phi}{\partial t} + \frac{q_w}{\rho_w} + \frac{q_o}{\rho_o}. \quad (2.45) \]

Substituting (2.44) into (2.45) gives a pressure equation for \( p \):

\[ -\nabla \cdot (k\lambda (\nabla p - (\rho_w f_w + \rho_o f_o)\phi \nabla z)) = -\frac{\partial \phi}{\partial t} + \frac{q_w}{\rho_w} + \frac{q_o}{\rho_o}. \quad (2.46) \]

The phase velocities are related to the total velocity by (cf. Exercise 2.3)

\[ \mathbf{u}_w = f_w \mathbf{u} + k\lambda_w f_w \nabla p_c + k\lambda_o f_w (\rho_w - \rho_o)\phi \nabla z, \]
\[ \mathbf{u}_o = f_o \mathbf{u} - k\lambda_w f_o \nabla p_c + k\lambda_o f_o (\rho_o - \rho_w)\phi \nabla z. \quad (2.47) \]

From the first equation of (2.47) and (2.36) with \( \alpha = w \), we have a saturation equation for \( S = S_w \):

\[ \frac{\phi}{\partial t} \frac{\partial S}{\partial \phi} + \nabla \cdot \left( k\lambda_w f_w \left( \frac{\partial p}{\partial S} \nabla S - (\rho_o - \rho_w)\phi \nabla z \right) + f_w \mathbf{u} \right) \]
\[ = -\frac{S}{\rho_w} \frac{\partial \phi}{\partial t} + \frac{q_w}{\rho_w}. \quad (2.48) \]

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Chapter 2. Flow and Transport Equations

Classification of differential equations

There are basically three types of second-order partial differential equations: elliptic, parabolic, and hyperbolic. We must be able to distinguish among these types when numerical methods for their solution are devised.

If two independent variables (either \((x_1, x_2)\) or \((x_1, t)\)) are considered, then second-order partial differential equations have the form, with \(x = x_1\),

\[
a \frac{\partial^2 p}{\partial x^2} + b \frac{\partial^2 p}{\partial t^2} = f \left( \frac{\partial p}{\partial x}, \frac{\partial p}{\partial t}, p \right).
\]

This equation is (1) elliptic if \(ab > 0\), (2) parabolic if \(ab = 0\), or (3) hyperbolic if \(ab < 0\).

The simplest elliptic equation is the Poisson equation

\[
\frac{\partial^2 p}{\partial x_1^2} + \frac{\partial^2 p}{\partial x_2^2} = f(x_1, x_2).
\]

A typical parabolic equation is the heat conduction equation

\[
\phi \frac{\partial p}{\partial t} = \frac{\partial^2 p}{\partial x_1^2} + \frac{\partial^2 p}{\partial x_2^2}.
\]

Finally, the prototype hyperbolic equation is the wave equation

\[
\frac{1}{v^2} \frac{\partial^2 p}{\partial t^2} = \frac{\partial^2 p}{\partial x_1^2} + \frac{\partial^2 p}{\partial x_2^2}.
\]

In the one-dimensional case, this equation can be “factorized” into two first-order parts:

\[
\left( \frac{1}{v} \frac{\partial}{\partial t} - \frac{\partial}{\partial x} \right) \left( \frac{1}{v} \frac{\partial}{\partial t} + \frac{\partial}{\partial x} \right) p = 0.
\]

The second part gives the first-order hyperbolic equation

\[
\frac{\partial p}{\partial t} + v \frac{\partial p}{\partial x} = 0.
\]

We now turn to the two-phase flow equations. While the phase mobilities \(\lambda_\alpha\) can be zero (cf. Chapter 3), the total mobility \(\lambda\) is always positive, so the pressure equation (2.46) is elliptic. If one of the densities varies, this equation becomes parabolic. In general, \(-k\lambda_\alpha f_\alpha dp_{\alpha}/dS\) is semipositive definite, so the saturation equation (2.48) is a parabolic equation, which is degenerate in the sense that the diffusion can be zero. This equation becomes hyperbolic if the capillary pressure is ignored. The total velocity is used in the global pressure formulation. This velocity is smoother than the phase velocities. It can also be used in the phase formulations (2.39) and (2.40) (Chen and Ewing, 1997B). We remark that the coupling between (2.46) and (2.48) is much less strong than between the equations in (2.39) and (2.40). Finally, with \(p_c = 0\), (2.48) becomes the known Buckley–Leverett equation whose flux function \(f_\alpha\) is generally nonconvex over the range of saturation values where this function is nonzero, as illustrated in Figure 2.4; see the next subsection for the formulation in hyperbolic form.
2.3. Two-Phase Immiscible Flow

![Figure 2.4. A flux function $f_w$.](image)

**Formulation in hyperbolic form**

Assume that $p_c = 0$ and that rock compressibility is neglected. Then (2.48) becomes

$$
\phi \frac{\partial S}{\partial t} + \nabla \cdot (f_w \mathbf{u} - \lambda_o f_w (\rho_o - \rho_w) \phi k \nabla z) = \frac{q_w}{\rho_w}.
$$

(2.49)

Using (2.45) and the fact that $f_w + f_o = 1$, this equation can be manipulated into

$$
\phi \frac{\partial S}{\partial t} + \left( \frac{df_w}{dS} \mathbf{u} - \frac{d(\lambda_o f_w)}{dS} (\rho_o - \rho_w) \phi k \nabla z \right) \cdot \nabla S = \frac{f_o q_w}{\rho_w} - \frac{f_w q_o}{\rho_o},
$$

(2.50)

which is a hyperbolic equation in $S$. Finally, if we neglect the gravitational term, we obtain

$$
\phi \frac{\partial S}{\partial t} + \frac{df_w}{dS} \mathbf{u} \cdot \nabla S = \frac{f_o q_w}{\rho_w} - \frac{f_w q_o}{\rho_o},
$$

(2.51)

which is the familiar form of waterflooding equation, i.e., the Buckley–Leverett equation. The source term in (2.51) is zero for production since

$$
\frac{q_w}{\rho_w} = f_w \left( \frac{q_w}{\rho_w} + \frac{q_o}{\rho_o} \right),
$$

by Darcy’s law. For injection, this term may not be zero since it equals $(1 - f_w)q_w/\rho_w \neq 0$ in this case.

**2.3.3 Boundary conditions**

As for single phase flow, the mathematical model described so far for two-phase flow is not complete unless necessary boundary and initial conditions are specified. Below we present boundary conditions of three kinds that are relevant to systems (2.39), (2.40), (2.46), and (2.48). We denote by $\Gamma$ the external boundary or a boundary segment of the porous medium domain $\Omega$ under consideration.
Boundary conditions for system (2.39)

The symbol \( \alpha \), as a subscript, with \( \alpha = w, o \), is used to indicate a considered phase. When a phase pressure is specified as a known function of position and time on \( \Gamma \), the boundary condition reads

\[
p_{\alpha} = g_{\alpha,1} \quad \text{on } \Gamma.
\]  

(2.52)

When the mass flux of phase \( \alpha \) is known on \( \Gamma \), the boundary condition is

\[
\rho_{\alpha} u_{\alpha} \cdot v = g_{\alpha,2} \quad \text{on } \Gamma,
\]  

(2.53)

where \( v \) indicates the outward unit normal to \( \Gamma \) and \( g_{\alpha,2} \) is given. For an impervious boundary for the \( \alpha \)-phase, \( g_{\alpha,2} = 0 \).

When \( \Gamma \) is a semipervious boundary for the \( \alpha \)-phase, a boundary condition of mixed kind occurs:

\[
g_{\alpha,p} p_{\alpha} + g_{\alpha,u} \rho_{\alpha} u_{\alpha} \cdot v = g_{\alpha,3} \quad \text{on } \Gamma,
\]  

(2.54)

where \( g_{\alpha,p}, g_{\alpha,u}, \) and \( g_{\alpha,3} \) are given functions.

Initial conditions specify the values of the main unknowns \( p_w \) and \( p_o \) over the entire domain at some initial time, usually taken at \( t = 0 \):

\[
p_{\alpha}(x, 0) = p_{\alpha,0}(x), \quad \alpha = w, o,
\]

where \( p_{\alpha,0}(x) \) are known functions.

Boundary conditions for system (2.40)

Boundary conditions for system (2.40) can be imposed as for system (2.39); i.e., (2.52)–(2.54) are applicable to system (2.40). The only difference between the boundary conditions for these two systems is that a prescribed saturation is sometimes given on \( \Gamma \) for system (2.40):

\[
S_w = g_4 \quad \text{on } \Gamma.
\]

In practice, this prescribed saturation boundary condition seldom occurs. However, a condition \( g_4 = 1 \) does occur when a medium is in contact with a body of this wetting phase. The condition \( S_w = 1 \) can be exploited on the bottom of a water pond on the ground surface, for example. An initial saturation is also specified:

\[
S_{w}(x, 0) = S_{w,0}(x),
\]

where \( S_{w,0}(x) \) is given.

Boundary conditions for (2.46) and (2.48)

Boundary conditions are usually specified in terms of phase quantities like those in (2.52)–(2.54). These conditions can be transformed into those in terms of the global quantities introduced in (2.42) and (2.43). For the prescribed pressure boundary condition in (2.52), for example, the corresponding boundary condition is given by

\[
p = g_1 \quad \text{on } \Gamma,
\]  

(2.55)
2.4 Transport of a Component in a Fluid Phase

where \( p \) is defined by (2.42) and \( g_1 \) is determined by

\[
g_1 = g_{o.1} - \int_{\xi=1}^{\xi=0} f_w \left( p_c^{-1}(\xi) \right) d\xi.
\]

Also, when the total mass flux is known on \( \Gamma \), it follows from (2.53) that

\[
u \cdot n = g_2 \quad \text{on} \quad \Gamma,
\]

where

\[
g_2 = \frac{g_{o.2}}{\rho_o} + \frac{g_{w.2}}{\rho_w}.
\]

For an impervious boundary for the total flow, \( g_2 = 0 \).

### 2.4 Transport of a Component in a Fluid Phase

Now, we consider the transport of a component (e.g., a solute) in a fluid phase that occupies the entire void space in a porous medium. We do not consider the effects of chemical reactions between the components in the fluid phase, radioactive decay, biodegradation, or growth due to bacterial activities that cause the quantity of this component to increase or decrease. Conservation of mass of the component in the fluid phase is given by

\[
\frac{\partial (\phi c \rho)}{\partial t} = - \nabla \cdot \left( c \rho \mathbf{u} - \rho \mathbf{D} \nabla c \right) - \sum_i q_1^{(i)}(\mathbf{x}^{(i)}, t) \delta(\mathbf{x} - \mathbf{x}^{(i)}) (\rho c)(\mathbf{x}, t) + \sum_j q_2^{(j)}(\mathbf{x}^{(j)}, t) \delta(\mathbf{x} - \mathbf{x}^{(j)}) (\rho^{(j)} c^{(j)})(\mathbf{x}, t),
\]

where \( c \) is the concentration (volumetric fraction in the fluid phase) of the component, \( \mathbf{D} \) is the diffusion-dispersion tensor, \( q_1^{(i)} \) and \( q_2^{(j)} \) are the rates of production and injection (in terms of volume per unit time) at points \( x^{(i)} \) and \( x^{(j)} \), respectively, and \( c^{(j)} \) is the specified concentration at source points.

Darcy’s law for the fluid is expressed as in (2.4); namely,

\[
\mathbf{u} = -\frac{1}{\mu} k (\nabla p - \rho \phi \nabla z).
\]

The mass balance of the fluid is written as

\[
\frac{\partial (\phi \rho)}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = - \sum_i \rho q_1^{(i)}(\mathbf{x}^{(i)}, t) \delta(\mathbf{x} - \mathbf{x}^{(i)}) + \sum_j \rho^{(j)} q_2^{(j)}(\mathbf{x}^{(j)}, t) \delta(\mathbf{x} - \mathbf{x}^{(j)}).
\]

The diffusion-dispersion tensor \( \mathbf{D} \) in (2.55) in three space dimensions is defined by

\[
\mathbf{D}(\mathbf{u}) = \phi \left\{ d_\infty \mathbf{l} + |\mathbf{u}| \left( d\mathbf{E}(\mathbf{u}) + d\mathbf{E}^t(\mathbf{u}) \right) \right\},
\]
where $d_m$ is the molecular diffusion coefficient; $d_l$ and $d_t$ are, respectively, the longitudinal and transverse dispersion coefficients; $|\mathbf{u}|$ is the Euclidean norm of $\mathbf{u} = (u_1, u_2, u_3)$, $|\mathbf{u}| = \sqrt{u_1^2 + u_2^2 + u_3^2}$; $\mathbf{E}(\mathbf{u})$ is the orthogonal projection along the velocity,

$$
\mathbf{E}(\mathbf{u}) = \frac{1}{|\mathbf{u}|^2} \begin{pmatrix}
    u_1^2 & u_1u_2 & u_1u_3 \\
    u_2u_1 & u_2^2 & u_2u_3 \\
    u_3u_1 & u_3u_2 & u_3^2
\end{pmatrix},
$$

and $\mathbf{E}^\bot(\mathbf{u}) = \mathbf{I} - \mathbf{E}(\mathbf{u})$.

Physically, the tensor dispersion is more significant than the molecular diffusion; also, $d_l$ is usually considerably larger than $d_t$. The density and viscosity are known functions of $p$ and $c$:

$$
\rho = \rho(p, c), \quad \mu = \mu(p, c).
$$

After the substitution of (2.56) into (2.55) and (2.57), we have a coupled system of two equations in $c$ and $p$. Boundary and initial conditions for this system can be developed as in the earlier sections. Note that the equations described here apply to the problem of miscible displacement of one fluid by another in a porous medium. Various simplifications discussed in Section 2.2 apply to (2.56) and (2.57).

### 2.5 Transport of Multicomponents in a Fluid Phase

The equation used to model the transport of multicomponents in a fluid phase in a porous medium is similar to (2.55); i.e.,

$$
\frac{\partial (\phi c_i \rho)}{\partial t} = - \nabla \cdot (c_i \rho \mathbf{u} - \rho \mathbf{D}_i \nabla c_i) + q_i, \quad i = 1, 2, \ldots, N_c, \tag{2.59}
$$

where $c_i$, $q_i$, and $\mathbf{D}_i$ are the (volumetric) concentration, the source/sink term, and the diffusion-dispersion tensor of the $i$th component, respectively, and $N_c$ is the number of the components in the fluid. The constraint for the concentrations is

$$
\sum_{i=1}^{N_c} c_i = 1.
$$

Sources and sinks of a component can result from injection and production of this component by external means. They can also stem from various processes within the fluid phase, such as chemical reactions among components, radioactive decay, biodegradation, and growth due to bacterial activities, that cause the quantity of this component to increase or decrease, as noted earlier. In this section, we focus only on chemical reactions, i.e., a reactive flow problem.

When a component participates in chemical reactions that cause its concentration to increase or decrease, $q_i$ can be expressed as

$$
q_i = Q_i - L_i c_i, \tag{2.60}
$$

where $Q_i$ and $L_i$ represent the chemical production and loss rates, respectively, of the $i$th component. To see their expressions in terms of concentrations, we consider unimolecular,
bimolecular, and trimolecular reactions among the chemical components. These cases can be generally written as

\[
\begin{align*}
    s_1 & \rightleftharpoons s_2 + s_3, \\
    s_1 + s_2 & \rightleftharpoons s_3 + s_4, \\
    s_1 + s_2 + s_3 & \rightleftharpoons s_4 + s_5,
\end{align*}
\]

where the \( s_i \)'s denote generic chemical components. Corresponding to these reactions, \( Q_i \) and \( L_i \) can be expressed as

\[
\begin{align*}
    Q_i &= \sum_{j=1}^{N_c} k^f_{i,j} c_j + \sum_{j,l=1}^{N_c} k^f_{i,j,l} c_j c_l + \sum_{j,l,m=1}^{N_c} k^f_{i,j,l,m} c_j c_l c_m, \\
    L_i &= k^r_i + \sum_{j=1}^{N_c} k^r_{i,j} c_j + \sum_{j,l=1}^{N_c} k^r_{i,j,l} c_j c_l,
\end{align*}
\]

where \( k^f \) and \( k^r \) are forward and reverse chemical rates, respectively. These rates are functions of pressure and temperature (Oran and Boris, 2001).

Darcy’s law (2.56) and the overall mass balance equation (2.57) hold for the transport of multicomponents. Again, after Darcy’s velocity is eliminated, we have a coupled system of \( N_c + 1 \) equations for \( c_i \) and \( p_i, i = 1, 2, \ldots, N_c \) (cf. Exercise 2.4).

## 2.6 The Black Oil Model

We now develop basic equations for the simultaneous flow of three phases (e.g., water, oil, and gas) through a porous medium. Previously, we assumed that mass does not transfer between phases. The black oil model relaxes this assumption. It is now assumed that the hydrocarbon components are divided into a gas component and an oil component in a stock tank at standard pressure and temperature, and that no mass transfer occurs between the water phase and the other two phases (oil and gas). The gas component mainly consists of methane and ethane.

To reduce confusion, we carefully distinguish between phases and components. We use lowercase and uppercase letter subscripts to denote the phases and components, respectively. Note that the water phase is just the water component. The subscript \( s \) indicates standard conditions. The mass conservation equations stated in (2.36) apply here. However, because of mass interchange between the oil and gas phases, mass is not conserved within each phase, but rather the total mass of each component must be conserved:

\[
\frac{\partial}{\partial t} (\phi \rho_w S_w) = -\nabla \cdot (\rho_w \mathbf{u}_w) + q_w \tag{2.61}
\]

for the water component,

\[
\frac{\partial}{\partial t} (\phi \rho_o S_o) = -\nabla \cdot (\rho_o \mathbf{u}_o) + q_o \tag{2.62}
\]

for the oil component, and

\[
\frac{\partial}{\partial t} \left( \phi (\rho_o S_o + \rho_g S_g) \right) = -\nabla \cdot (\rho_o \mathbf{u}_o + \rho_g \mathbf{u}_g) + q_G \tag{2.63}
\]
for the gas component, where \( \rho_{Oo} \) and \( \rho_{Go} \) indicate the partial densities of the oil and gas components in the oil phase, respectively. Equation (2.63) implies that the gas component may exist in both the oil and gas phases.

Darcy’s law for each phase is written in the usual form

\[
\mathbf{u}_\alpha = -\frac{1}{\mu_\alpha} k_\alpha \left( \nabla p_\alpha - \rho_\alpha g \nabla z \right), \quad \alpha = w, o, g. \tag{2.64}
\]

The fact that the three phases jointly fill the void space is given by the equation

\[
S_w + S_o + S_g = 1. \tag{2.65}
\]

Finally, the phase pressures are related by capillary pressures

\[
p_{cow} = p_o - p_w, \quad p_{cgo} = p_g - p_o. \tag{2.66}
\]

It is not necessary to define a third capillary pressure since it can be defined in terms of \( p_{cow} \) and \( p_{cgo} \).

The alternative differential equations developed for two phases can be adapted for the three-phase black oil model in a similar fashion (Chen, 2000). That is, (2.61)–(2.66) can be rewritten in the three-pressure formulation (cf. Exercise 2.5), in a pressure and two-saturation formulation (cf. Exercise 2.6), or in a global pressure and two-saturation formulation (cf. Exercise 2.7). In the global formulation, the pressure equation is elliptic or parabolic depending on the effects of densities. The two saturation equations are parabolic if the capillary pressure effects exist; otherwise, they are hyperbolic (Chen, 2000).

For the black oil model, it is often convenient to work with the conservation equations on “standard volumes,” instead of the conservation equations on “mass” (2.61)–(2.63). The mass fractions of the oil and gas components in the oil phase can be determined by gas solubility, \( R_{so} \) (also called dissolved gas-oil ratio), which is the volume of gas (measured at standard conditions) dissolved at a given pressure and reservoir temperature in a unit volume of stock-tank oil:

\[
R_{so}(p, T) = \frac{V_{Gs}}{V_{Os}}. \tag{2.67}
\]

Note that

\[
V_{Os} = \frac{W_O}{\rho_{Os}}, \quad V_{Gs} = \frac{W_G}{\rho_{Gs}}, \tag{2.68}
\]

where \( W_O \) and \( W_G \) are the weights of the oil and gas components, respectively. Then (2.67) becomes

\[
R_{so} = \frac{W_G \rho_{Os}}{W_O \rho_{Gs}}. \tag{2.69}
\]

The oil formation volume factor \( B_o \) is the ratio of the volume \( V_o \) of the oil phase measured at reservoir conditions to the volume \( V_{Os} \) of the oil component measured at standard conditions:

\[
B_o(p, T) = \frac{V_o(p, T)}{V_{Os}}, \tag{2.70}
\]

where

\[
V_o = \frac{W_O + W_G}{\rho_o}. \tag{2.71}
\]
2.6. The Black Oil Model

Consequently, combining (2.68), (2.70), and (2.71), we have

\[ B_o = \frac{(W_O + W_G)\rho_o}{W_O \rho_o} \]  

(2.72)

Now, using (2.69) and (2.72), the mass fractions of the oil and gas components in the oil phase are, respectively,

\[
C_{O_o} = \frac{W_O}{W_O + W_G} = \frac{\rho_o}{B_o \rho_o},
\]

\[
C_{G_o} = \frac{W_G}{W_O + W_G} = \frac{R_{so} \rho_{G_s}}{B_o \rho_o},
\]

which, together with \( C_{O_o} + C_{G_o} = 1 \), yield

\[
\rho_o = \frac{R_{so} \rho_{G_s} + \rho_o}{B_o}. \]

(2.73)

The gas formation volume factor \( B_g \) is the ratio of the volume of the gas phase measured at reservoir conditions to the volume of the gas component measured at standard conditions:

\[ B_g(p, T) = \frac{V_g(p, T)}{V_{G_s}}. \]

Let \( W_g = W_G \) be the weight of free gas. Because \( V_g = W_G/\rho_g \) and \( V_{G_s} = W_G/\rho_{G_s} \), we see that

\[
\rho_g = \frac{\rho_{G_s}}{B_g}. \]

(2.74)

For completeness, the water formation volume factor, \( B_w \), is defined by

\[
\rho_w = \frac{\rho_{W_s}}{B_w}. \]

(2.75)

Finally, substituting (2.73)–(2.75) into (2.61)–(2.63) yields the conservation equations on standard volumes:

\[
\frac{\partial}{\partial t} \left( \phi \rho_{W_s} S_w \frac{\rho_{W_s}}{B_w} u_w \right) = -\nabla \cdot \left( \rho_{W_s} \frac{\rho_{W_s}}{B_w} \mathbf{u}_w \right) + q_w
\]

(2.76)

for the water component,

\[
\frac{\partial}{\partial t} \left( \phi \rho_o S_o \frac{\rho_o}{B_o} u_o \right) = -\nabla \cdot \left( \rho_o \frac{\rho_o}{B_o} \mathbf{u}_o \right) + q_o
\]

(2.77)

for the oil component, and

\[
\frac{\partial}{\partial t} \left[ \phi \left( \frac{\rho_{G_s}}{B_g} S_g + \frac{R_{so} \rho_{G_s}}{B_o} S_o \right) \right] = -\nabla \cdot \left( \frac{\rho_{G_s}}{B_g} \mathbf{u}_g + \frac{R_{so} \rho_{G_s}}{B_o} \mathbf{u}_o \right) + q_G
\]

(2.78)
for the gas component. Equations (2.76)–(2.78) represent balances on standard volumes. The volumetric rates at standard conditions are

\[ q_W = \frac{q_{Ws} \rho_{Ws}}{B_w}, \quad q_O = \frac{q_{Os} \rho_{Os}}{B_o}, \quad q_G = \frac{q_{Gs} \rho_{Gs}}{B_g} + \frac{q_{Os} R_{so} \rho_{Gs}}{B_o}. \]  

(2.79)

Since \( \rho_{Ws} \), \( \rho_{Os} \), and \( \rho_{Gs} \) are constant, they can be eliminated after (2.79) is substituted into (2.76)–(2.78).

The basic equations for the black oil model consist of (2.64)–(2.66) and (2.76)–(2.78). The choice of main unknowns depends on the state of the reservoir, i.e., the saturated or undersaturated state, which will be discussed in Chapter 8.

### 2.7 A Volatile Oil Model

The black oil model developed above is not suitable for handling a volatile oil reservoir. A reservoir of volatile oil type is one that contains relatively large proportions of ethane through decane at a reservoir temperature near or above 250° F with a high formation volume factor and stock-tank oil gravity above 45° API (Jacoby and Berry, 1957). With a more elaborate two-component hydrocarbon model, a volatile oil model, the effect of oil volatility can be included. In this model, there are both oil and gas components, solubility of gas in both oil and gas phases is permitted, and vaporization of oil into the gas phase is allowed. Therefore, the two hydrocarbon components can exist in both oil and gas phases.

**Oil volatility** in the gas phase is

\[ R_v = \frac{V_{Os}}{V_{Gs}}. \]

Using a similar approach as for the black oil model, the conservation equations on standard volumes are

\[
\frac{\partial}{\partial t} \left( \phi \frac{\rho_{Ws} S_w}{B_w} \right) = -\nabla \cdot \left( \frac{\rho_{Ws}}{B_w} \mathbf{u}_w \right) + q_W
\]  

(2.80)

for the water component,

\[
\frac{\partial}{\partial t} \left[ \phi \left( \frac{\rho_{Os} S_o}{B_o} + \frac{R_v \rho_{Os}}{B_g} S_g \right) \right] = -\nabla \cdot \left( \frac{\rho_{Os}}{B_o} \mathbf{u}_o + \frac{R_v \rho_{Os}}{B_g} \mathbf{u}_g \right) + q_O
\]  

(2.81)

for the oil component, and

\[
\frac{\partial}{\partial t} \left[ \phi \left( \frac{\rho_{Gs} S_g}{B_g} + \frac{R_{so} \rho_{Gs}}{B_o} S_o \right) \right] = -\nabla \cdot \left( \frac{\rho_{Gs}}{B_g} \mathbf{u}_g + \frac{R_{so} \rho_{Gs}}{B_o} \mathbf{u}_o \right) + q_G
\]  

(2.82)

for the gas component. In general, the hydrocarbon components (i.e., oil and gas) can be defined using pseudocomponents obtained from the compositional flow described in the next section.
2.8 Compositional Flow

In the black oil and volatile oil models, two hydrocarbon components are involved. Here we consider *compositional flow* that involves many components and *mass transfer* between phases in a general fashion. In a *compositional model*, a finite number of hydrocarbon components are used to represent the composition of reservoir fluids. These components associate as phases in a reservoir. We describe the model under the assumptions that the flow process is isothermal (i.e., at constant temperature), the components form at most three phases (e.g., vapor, liquid, and water), and there is no mass interchange between the water phase and the hydrocarbon phases (i.e., the vapor and liquid phases). We could state a general compositional model that involves any number of phases and components, each of which may exist in any or all of these phases (cf. Section 2.10). While the governing differential equations for this type of model are easy to set up, they are extremely complex to solve. Therefore, we describe the compositional model that has been widely used in the petroleum industry.

Instead of using the concentration, it is more convenient to employ the *mole fraction* for each component in the compositional flow, since the phase equilibrium relations are usually defined in terms of mole fractions (cf. (2.91)). Let $\xi_{io}$ and $\xi_{ig}$ be the molar densities of component $i$ in the liquid (e.g., oil) and vapor (e.g., gas) phases, respectively, $i = 1, 2, \ldots, N_c$, where $N_c$ is the number of components. Their physical dimensions are moles per pore volume. If $W_i$ is the *molar mass* of component $i$, with dimensions mass of component $i$ / mole of component $i$, then $\xi_{i\alpha}$ is related to the mass density $\rho_{i\alpha}$ by $\xi_{i\alpha} = \rho_{i\alpha} / W_i$. The molar density of phase $\alpha$ is

$$\xi_{\alpha} = \sum_{i=1}^{N_c} \xi_{i\alpha}, \quad \alpha = o, g. \tag{2.83}$$

The mole fraction of component $i$ in phase $\alpha$ is then

$$x_{i\alpha} = \frac{\xi_{i\alpha}}{\xi_{\alpha}}, \quad i = 1, 2, \ldots, N_c, \quad \alpha = o, g. \tag{2.84}$$

Because of mass interchange between the phases, mass is not conserved within each phase; the total mass is conserved for each component:

$$\frac{\partial (\phi \xi_{w} S_w)}{\partial t} + \nabla \cdot (\xi_{w} u_w) = q_w,$$

$$\frac{\partial (\phi [x_{io} \xi_{o} S_o + x_{ig} \xi_{g} S_g] + \nabla \cdot (x_{io} \xi_{o} u_o + x_{ig} \xi_{g} u_g) + \nabla \cdot (d_{io} + d_{ig}) = q_i, \quad i = 1, 2, \ldots, N_c, \tag{2.85}$$

where $\xi_{w}$ is the molar density of water, $q_{w}$ and $q_{i}$ are the molar flow rates of water and the $i$th component, respectively, and $d_{io}$ denotes the *diffusive flux* of the $i$th component in the $\alpha$-phase, $\alpha = o, g$. In (2.85), the volumetric velocity $u_{\alpha}$ is given by Darcy’s law as in (2.64):

$$u_{\alpha} = -\frac{1}{\mu_{\alpha}} k_{\alpha} (\nabla p_{\alpha} - \rho_{\alpha} \phi \nabla z), \quad \alpha = w, o, g. \tag{2.86}$$

From "Computational Methods for Multiphase Flows in Porous Media" by Zhangxin Chen, Guanren Huan and Yuanle Ma

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In addition to the differential equations (2.85) and (2.86), there are also algebraic constraints. The mole fraction balance implies that

\[ \sum_{i=1}^{N_c} x_{i,o} = 1, \quad \sum_{i=1}^{N_c} x_{i,g} = 1. \]  

(2.87)

In the transport process, the porous medium is saturated with fluids:

\[ S_w + S_o + S_g = 1. \]

(2.88)

The phase pressures are related by capillary pressures:

\[ p_{cow} = p_o - p_w, \quad p_{cgo} = p_g - p_o. \]

(2.89)

These capillary pressures are assumed to be known functions of the saturations. The relative permeabilities \( k_{\alpha} \) are also assumed to be known in terms of the saturations, and the viscosities \( \mu_{\alpha} \), molar densities \( \xi_{\alpha} \), and mass densities \( \rho_{\alpha} \) are functions of their respective phase pressure and compositions, \( \alpha = w, o, g \).

The least well understood term in (2.85) is that involving the diffusive fluxes \( d_{i\alpha} \). The precise constitutive relations for these quantities still need to be derived; however, from a practical point of view the following straightforward extension of the single phase Fick's law to multiphase flow is in widespread use:

\[ d_{i\alpha} = -\xi_{\alpha} D_{i\alpha} \nabla x_{i\alpha}, \quad i = 1, 2, \ldots, N_c, \quad \alpha = o, g, \]

(2.90)

where \( D_{i\alpha} \) is the diffusion coefficient of component \( i \) in phase \( \alpha \) (cf. (2.58) or Section 2.10). The diffusive fluxes must satisfy

\[ \sum_{i=1}^{N_c} d_{i\alpha} = 0, \quad \alpha = o, g. \]

Note that there are more dependent variables than there are differential and algebraic relations combined; there are formally \( 2N_c + 9 \) dependent variables: \( x_{i,o}, x_{i,g}, u_{\alpha}, p_{\alpha} \), and \( S_{\alpha}, \alpha = w, o, g, i = 1, 2, \ldots, N_c \). It is then necessary to have \( 2N_c + 9 \) independent relations to determine a solution of the system. Equations (2.85)–(2.89) provide \( N_c + 9 \) independent relations, differential or algebraic; the additional \( N_c \) relations are provided by the equilibrium relations that relate the numbers of moles.

Mass interchange between phases is characterized by the variation of mass distribution of each component in the vapor and liquid phases. As usual, these two phases are assumed to be in the phase equilibrium state. This is physically reasonable since the mass interchange between phases occurs much faster than the flow of porous media fluids. Consequently, the distribution of each hydrocarbon component into the two phases is subject to the condition of stable thermodynamic equilibrium, which is given by minimizing the Gibbs free energy of the compositional system (Bear, 1972; Chen et al., 2000C):

\[ f_{i,o}(p_o, x_{1,o}, x_{2,o}, \ldots, x_{N_c,o}) = f_{i,g}(p_g, x_{1,g}, x_{2,g}, \ldots, x_{N_c,g}), \]

(2.91)
where \( f_{i,o} \) and \( f_{i,g} \) are the fugacity functions of the \( i \)th component in the liquid and vapor phases, respectively, \( i = 1, 2, \ldots, N_c \). More details will be given on these fugacity functions in Chapters 3 and 9.

We end with a remark on the calculation of mass fractions \( c_{i\alpha} \) of component \( i \) in phase \( \alpha \) from the mole fractions \( x_{i\alpha} \) (cf. Exercise 2.8)

\[
c_{i\alpha} = \frac{W_i x_{i\alpha}}{\sum_{j=1}^{N_c} W_j x_{j\alpha}}, \quad i = 1, 2, \ldots, N_c, \quad \alpha = o, g, \tag{2.92}
\]

and the calculation of mass densities \( \rho_{\alpha} \) from the molar densities \( \xi_{\alpha} \)

\[
\rho_{\alpha} = \xi_{\alpha} \sum_{i=1}^{N_c} W_i x_{i\alpha}. \tag{2.93}
\]

### 2.9 Nonisothermal Flow

The differential equations so far have been developed under the condition that flow is isothermal. This condition can be removed by adding a conservation of energy equation. This equation introduces an additional dependent variable, temperature, to the system. Unlike the case of mass transport, where the solid itself is assumed impervious to mass flux, the solid matrix does conduct heat. The average temperature of the solid and fluids in a porous medium may not be the same. Furthermore, heat may be exchanged between the phases. For simplicity, we invoke the requirement of local thermal equilibrium that the temperature be the same in all phases.

For multicomponent, multiphase flow in a porous medium, the mass balance and other equations are presented as in (2.85)–(2.91). Under the nonisothermal condition, some variables such as porosity, density, and viscosity may depend on temperature (cf. Chapter 3). The conservation of energy equation can be derived as in Section 2.2 for the mass conservation. A statement of the energy balance or first law of thermodynamics in a differential volume \( V \) is

\[
\begin{align*}
\frac{\partial}{\partial t} \left( \rho_{t} U + \frac{1}{2} \sum_{\alpha=1}^{g} \rho_{\alpha} |u_{\alpha}|^2 \right) + \nabla \cdot \mathbf{E} \\
+ \sum_{\alpha=1}^{g} (\nabla \cdot (p_{\alpha} u_{\alpha}) - \rho_{\alpha} u_{\alpha} \cdot \rho_{\alpha} \nabla z) = q_{H} - q_{L},
\end{align*}
\tag{2.94}
\]

where \( \rho_{t} \) is the overall density, \( \rho_{t} U \) is the total internal energy, the term \( \sum_{\alpha=1}^{g} \rho_{\alpha} |u_{\alpha}|^2 / 2 \) represents kinetic energy per unit bulk volume, \( \mathbf{E} \) is the energy flux, the term

\[
\sum_{\alpha=1}^{g} (\nabla \cdot (p_{\alpha} u_{\alpha}) - \rho_{\alpha} u_{\alpha} \cdot \rho_{\alpha} \nabla z)
\]

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is the rate of work done against the pressure field and gravity, \( q_H \) indicates the enthalpy source term per bulk volume, and \( q_L \) is heat loss.

The total internal energy is

\[
\rho_t U = \phi \sum_{\alpha=w}^g \rho_o S_o U_o + (1 - \phi) \rho_s C_s T, \tag{2.95}
\]

where \( U_o \) and \( C_s \) are the specific internal energy per unit mass of phase \( \alpha \) and the specific heat capacity of the solid, respectively, and \( \rho_t \) is the density of the solid. The overall density \( \rho_t \) is determined by

\[
\rho_t = \phi \sum_{\alpha=w}^g \rho_o S_o + (1 - \phi) \rho_s. \tag{2.96}
\]

The energy flux is made up of convective contributions from the flowing phases, conduction, and radiation (with all other contributions being ignored):

\[
E = \sum_{\alpha=w}^g \rho_o u_o \left( U_o + \frac{1}{2} |u_o|^2 \right) + q_c + q_r, \tag{2.97}
\]

where \( q_c \) and \( q_r \) are the conduction and radiation fluxes, respectively. For multiphase flow, the conductive heat flux is given by Fourier's law:

\[
q_c = -k_T \nabla T, \tag{2.98}
\]

where \( k_T \) represents the total thermal conductivity. For brevity, we ignore radiation, though it can be important in estimating heat losses from wellbores. Inserting (2.95)–(2.97) into (2.94) and combining the first term in the right-hand side of (2.96) with the work done by pressure, we see that

\[
\frac{\partial}{\partial t} \left( \phi \sum_{\alpha=w}^g \rho_o S_o U_o + (1 - \phi) \rho_s C_s T + \frac{1}{2} \sum_{\alpha=w}^g \rho_o |u_o|^2 \right)
+ \nabla \cdot \left( \sum_{\alpha=w}^g \rho_o u_o \left( H_o + \frac{1}{2} |u_o|^2 \right) \right)
- \nabla \cdot (k_T \nabla T) + \sum_{\alpha=w}^g \rho_o u_o \cdot \rho \nabla z = q_H - q_L. \tag{2.99}
\]

where \( H_o \) is the enthalpy of the \( \alpha \)-phase (per unit mass) given by

\[
H_o = U_o + \frac{p_o}{\rho_o} \quad \alpha = w, o, g.
\]

As usual (Lake, 1989), if we neglect the kinetic energy and the last term in the left-hand side of (2.98), we obtain the energy equation for temperature \( T \)

\[
\frac{\partial}{\partial t} \left( \phi \sum_{\alpha=w}^g \rho_o S_o U_o + (1 - \phi) \rho_s C_s T \right)
+ \nabla \cdot \sum_{\alpha=w}^g \rho_o u_o H_o - \nabla \cdot (k_T \nabla T) = q_H - q_L. \tag{2.99}
\]
2.9. Nonisothermal Flow

Figure 2.5. Reservoir, overburden, and underburden.

If desired, diffusive fluxes can be added to the left-hand side of (2.99) as in (2.85). Namely, using (2.90), the term

\[- \sum_{i=1}^{N_r} \sum_{a=w}^{g} \mathbf{\nabla} \cdot (\xi_{a} H_{a} W_{i} D_{i} \mathbf{\nabla} x_{i a})\]

can be inserted, where \(W_{i}\) is the molecular weight of component \(i\) and \(H_{i a}\) represents the enthalpy of component \(i\) in phase \(\alpha\).

In thermal methods heat is lost to the adjacent strata of a reservoir or the overburden and underburden, which is included in \(q_{L}\) of (2.99). We assume that the overburden and underburden extend to infinity along both the positive and negative \(x_3\)-axis (the vertical direction); see Figure 2.5. If the overburden and underburden are impermeable, heat is transferred entirely through conduction. With all fluid velocities and convective fluxes being zero, the energy conservation equation (2.99) reduces to

\[
\frac{\partial}{\partial t} \left( \rho_{ob} C_{p,ob} T_{ob} \right) = \mathbf{\nabla} \cdot (k_{ob} \mathbf{\nabla} T_{ob}),
\]

(2.100)

where the subscript \(ob\) indicates that the variables are associated with the overburden and \(C_{p,ob}\) is the heat capacity at constant pressure. The initial condition is the original temperature \(T_{ob,0}\) of the overburden:

\[T_{ob}(\mathbf{x}, 0) = T_{ob,0}(\mathbf{x}).\]

The boundary condition at the top of the reservoir is

\[T_{ob}(\mathbf{x}, t) = T(\mathbf{x}, t),\]

where we recall that \(T\) is the reservoir temperature. At infinity, \(T_{ob}\) is fixed:

\[T_{ob}(x_1, x_2, \infty, t) = T_{\infty}.\]

On other boundaries, we can use the impervious boundary condition

\[k_{ob} \mathbf{\nabla} T_{ob} \cdot \mathbf{n} = 0,\]

where \(\mathbf{n}\) represents the outward unit normal to these boundaries. Now, the rate of heat loss to the overburden is calculated by \(k_{ob} \mathbf{\nabla} T_{ob} \cdot \mathbf{n}\), where \(\mathbf{n}\) is the unit normal to the interface between the overburden and reservoir (pointing to the overburden). Similar differential equations and initial and boundary conditions can be developed for the underburden.

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2.10 Chemical Compositional Flow

An important method in enhanced oil recovery is chemical flooding, such as alkaline, surfactant, polymer, and foam (ASP+foam) flooding. The injection of these chemical components reduces fluid mobility to improve the sweep efficiency of a reservoir, i.e., increases the volume of the permeable medium contacted at any given time. For a chemical flooding compositional model, the governing differential equations consist of a mass conservation equation for each component, an energy equation, and an overall mass conservation or continuity equation for pressure. These equations are developed under the following assumptions: local thermodynamic equilibrium, immobile solid phase, Fickian dispersion, ideal mixing, slightly compressible soil and fluids, and Darcy’s law.

For this model, it is more convenient to use the concentration for each component in the mass conservation equation, as in Sections 2.4 and 2.5, since chemical reactions are involved. The mass conservation for component $i$ is expressed in terms of the overall concentration of this component per unit pore volume:

$$\frac{\partial}{\partial t} (\phi \tilde{c}_i \rho_i) = -\nabla \cdot \left( \sum_{a=1}^{N_p} \rho_i [c_{ia} \mathbf{u}_a - \mathbf{D}_{ia} \nabla c_{ia}] \right) + q_i, \quad i = 1, 2, \ldots, N_c. \tag{2.101}$$

where the overall concentration $\tilde{c}_i$ is the sum over all phases, including the adsorbed phases,

$$\tilde{c}_i = \left( 1 - \sum_{j=1}^{N_{c,i}} \hat{c}_j \right) \sum_{a=1}^{N_p} S_a c_{ia} + \hat{c}_i, \quad i = 1, 2, \ldots, N_c; \tag{2.102}$$

$N_{c,i}$ is the total number of volume-occupying components (such as water, oil, surfactant, and air); $N_p$ is the number of phases; $\hat{c}_i$, $\rho_i$, and $q_i$ are the adsorbed concentration, mass density, and source/sink term of component $i$; and $c_{ia}$ and $\mathbf{D}_{ia}$ are the concentration and diffusion-dispersion tensor, respectively, of component $i$ in phase $a$. The term $1 - \sum_{j=1}^{N_{c,i}} \hat{c}_j$ represents the reduction in pore volume due to adsorption.

The density $\rho_i$ is related to pressure by (2.6). For slightly compressible fluids, it is given by (2.12); i.e., at a reference phase pressure $p_r$, it equals

$$\rho_i = \rho_i^r \left( 1 + \zeta^r_i (p_r - p_{cr}) \right), \tag{2.103}$$

where $\zeta^r_i$ is the constant compressibility and $\rho_i^r$ is the density at the reference pressure $p_{cr}$.

The diffusion-dispersion tensor $\mathbf{D}_{ia}$ is an extension of (2.58) to multiphase flow:

$$\mathbf{D}_{ia} (\mathbf{u}_a) = \phi \left[ S_a d_{ia} \mathbf{I} + | \mathbf{u}_a | \left( d_{ia} \mathbf{E}(\mathbf{u}_a) + d_{ia} \mathbf{E}^\perp(\mathbf{u}_a) \right) \right], \tag{2.104}$$

where $d_{ia}$ is the molecular diffusion coefficient of component $i$ in phase $a$; $d_{ia}$ and $d_{ia}$ are, respectively, the longitudinal and transverse dispersion coefficients of phase $a$; $| \mathbf{u}_a |$ is the Euclidean norm of $\mathbf{u}_a = (u_{1a}, u_{2a}, u_{3a})$, $| \mathbf{u}_a | = \sqrt{u_{1a}^2 + u_{2a}^2 + u_{3a}^2}$; $\mathbf{E}(\mathbf{u}_a)$ is the orthogonal projection along the velocity,

$$\mathbf{E}(\mathbf{u}_a) = \frac{1}{| \mathbf{u}_a |^2} \begin{pmatrix} u_{1a}^2 & u_{1a} u_{2a} & u_{1a} u_{3a} \\ u_{2a} u_{1a} & u_{2a}^2 & u_{2a} u_{3a} \\ u_{3a} u_{1a} & u_{3a} u_{2a} & u_{3a}^2 \end{pmatrix}.$$
2.10. Chemical Compositional Flow

and $E^\perp(u_i) = I - E(u_i), i = 1, 2, \ldots, N_c, \alpha = 1, 2, \ldots, N_p$. The source/sink term $q_i$ combines all rates for component $i$ and is expressed as

$$q_i = \phi \sum_{\alpha=1}^{N_p} S_{\alpha} r_{i\alpha} + (1 - \phi) r_{is} + \tilde{q}_i,$$

(2.105)

where $r_{i\alpha}$ and $r_{is}$ are the reaction rates of component $i$ in the $\alpha$ fluid phase and rock phase, respectively, and $\tilde{q}_i$ is the injection/production rate of the same component per bulk volume. The volumetric velocity $u_\alpha$ is given by Darcy's law as in (2.86):

$$u_\alpha = -\frac{1}{\mu_{\alpha}} k_{\alpha}(\nabla p_{\alpha} - \rho_{\alpha} \rho_{\alpha}^g \nabla z), \quad \alpha = 1, 2, \ldots, N_p.$$

(2.106)

The energy conservation equation is given as in (2.99):

$$\frac{\partial}{\partial t} \left( \phi \sum_{\alpha=1}^{N_p} \rho_{\alpha} S_{\alpha} U_{\alpha} + (1 - \phi) \rho_s c_1 T \right) + \nabla \cdot \sum_{\alpha=1}^{N_p} \rho_{\alpha} u_{\alpha} H_{\alpha} - \nabla \cdot (k_T \nabla T) = q_H - q_L.$$

(2.107)

The heat loss to the overburden and underburden can be calculated as in Section 2.9.

In the simulation of chemical flooding, a pressure equation for the aqueous phase (e.g., phase 1) is obtained by an overall mass balance on volume-occupying components. Other phase pressures are evaluated using the capillary pressure functions, as in (2.89):

$$p_{\alpha 1} = p_{\alpha} - p_1, \quad \alpha = 1, 2, \ldots, N_p,$$

(2.108)

where $p_{1 1} = 0$ for convenience. Introduce the phase mobility

$$\lambda_{\alpha} = \frac{k_{\alpha}}{\mu_{\alpha}} \sum_{i=1}^{N_c} \rho_{ci} c_{i\alpha}, \quad \alpha = 1, 2, \ldots, N_p,$$

and the total mobility

$$\lambda = \sum_{\alpha=1}^{N_p} \lambda_{\alpha}.$$

Note that

$$\sum_{i=1}^{N_c} \rho_{D_{ci}} \nabla c_{i\alpha} = 0,$$

$$\sum_{\alpha=1}^{N_p} r_{i\alpha} = \sum_{\alpha=1}^{N_p} r_{is} = 0, \quad \alpha = 1, 2, \ldots, N_p.$$

Now, by adding (2.101) over $i, i = 1, 2, \ldots, N_c$, we obtain the pressure equation (cf. Exercise 2.9)

$$\phi c_1 \frac{\partial p_1}{\partial t} - \nabla \cdot (\lambda k \nabla p_1) = \nabla \cdot \sum_{\alpha=1}^{N_p} \lambda_{\alpha} k (\nabla p_{\alpha 1} - \rho_{\alpha} \rho_{\alpha}^g \nabla z) + \sum_{i=1}^{N_c} \tilde{q}_i,$$

(2.109)

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where the total compressibility \( c_t \) is defined by

\[
c_t = \frac{1}{\phi} \frac{\partial}{\partial p} \sum_{i=1}^{N_c} \phi \tilde{c}_i \rho_i.
\]

Assume that the rock compressibility is given by (2.16); i.e., at the reference pressure \( p_0^r \),

\[
\phi = \phi^o \left( 1 + c_R (p_r - p_0^r) \right).
\] (2.110)

With \( p_r = p_1 \) and using (2.103) and (2.110), we have

\[
\phi \tilde{c}_i \rho_i = \phi^o \tilde{c}_i \rho_i^o \left( 1 + (c_R + C_0^i)(p_1 - p_0^r) \right) + c_R C_0^i (p_1 - p_0^r)^2.
\]

Neglecting the higher-order term in this equation, it becomes

\[
\phi \tilde{c}_i \rho_i \approx \phi^o \tilde{c}_i \rho_i^o \left( 1 + (c_R + C_0^i)(p_1 - p_0^r) \right).
\] (2.111)

Applying (2.111), the total compressibility \( c_t \) is simplified to

\[
c_t = \frac{\phi^o}{\phi} \sum_{i=1}^{N_c} \tilde{c}_i \rho_i^o \left( c_R + C_0^i \right).
\] (2.112)

Note that there are more dependent variables than there are differential and algebraic relations; there are formally \( N_c + N_c + N_p + 3N_p + 1 \) dependent variables: \( c_i, \tilde{c}_j, c_{ia}, T, u_a, p_a, \) and \( S_a, \alpha = 1, 2, \ldots, N_p, i = 1, 2, \ldots, N_c, j = 1, 2, \ldots, N_c, \) \( c_{ia} \). Equations (2.101) and (2.106)–(2.109) provide \( N_c + 2N_p \) independent relations, differential or algebraic; the additional \( N_c + N_c + N_p + 1 \) relations are given by the constraints

\[
\sum_{a=1}^{N_c} S_a = 1 \quad \text{(a saturation constraint)},
\]

\[
\sum_{i=1}^{N_c} c_{ia} = 1 \quad \text{\( N_p \) phase concentration constraints),}
\]

\[
c_i = \sum_{a=1}^{N_c} S_a c_{ia} \quad \text{\( N_c \) component concentration constraints),}
\]

\[
\tilde{c}_j = \tilde{c}_j \left( c_1, c_2, \ldots, c_{N_c} \right) \quad \text{\( N_c \) adsorption constraints),}
\]

\[
f_{ia}(p_a, T, c_{1a}, \ldots, c_{N,a}) = f_{i\beta}(p_\beta, T, c_{1\beta}, \ldots, c_{N,\beta}) \quad \text{\( N_c \) phase equilibrium relations),}
\]

where \( f_{ia} \) is the fugacity function of the \( i \)th component in the \( \alpha \)-phase.

### 2.11 Flows in Fractured Porous Media

A dual porosity model has been developed for single phase flow in Section 2.2.6. This concept can be generalized to flows of other types. As an example, we consider the compositional flow in fractured porous media. For brevity of presentation, we neglect the diffusive effects.
2.11. Flows in Fractured Porous Media

2.11.1 Dual porosity/permeability models

In the development of the dual porosity model for single phase flow in Section 2.2.6, the fluid was assumed to flow only from the matrix into the fractures, not vice versa. Also, there was no connection between matrix blocks. Now, we consider a more general case without these two assumptions. In this general case, the mass balance equations in the matrix also contain the matrix-fracture transfer terms, \( i = 1, 2, \ldots, N_c \):

\[
\frac{\partial (\phi_x w S_w)}{\partial t} + \nabla \cdot (\xi_w u_w) = -q_{w,mf},
\]

\[
\frac{\partial (\phi [x_{io} \xi_o S_o + x_{ig} \xi_g S_g])}{\partial t} + \nabla \cdot (x_{io} \xi_o u_o + x_{ig} \xi_g u_g) = -q_{i,mf},
\]

(2.114)

where it is assumed that the external source/sink terms do not interact with this system. In the fracture system, the mass balance equations are

\[
\frac{\partial (\phi_x w S_w)_f}{\partial t} + \nabla \cdot (\xi_w u_w)_f = q_{w,mf} + q_w,
\]

\[
\frac{\partial (\phi [x_{io} \xi_o S_o + x_{ig} \xi_g S_g])_f}{\partial t} + \nabla \cdot (x_{io} \xi_o u_o + x_{ig} \xi_g u_g)_f = q_{i,mf} + q_i,
\]

(2.115)

where the subscript \( f \) represents the fracture quantities. Equations (2.86)–(2.91) remain valid for both the matrix and the fractures.

The matrix-fracture transfer terms for the dual porosity/permeability model, \( q_{w,mf} \) and \( q_{i,mf} \), are defined following Warren and Root (1963) and Kazemi (1969). The transfer term for a particular component is directly related to the matrix shape factor \( \sigma \), the fluid mobility, and the potential difference between the fracture and matrix systems. The capillary pressure, gravity, and viscous forces must be properly incorporated into this term. Furthermore, the contribution from a pressure gradient across each matrix block (and the molecular diffusion rate for each component) must be also included. For brevity of presentation, we neglect the diffusion rate.

The treatment of a pressure gradient across a block is based on the following observation: for an oil matrix block surrounded with water in the fractures, the pressure differences are

\[ \Delta p_w = 0, \quad \Delta p_o = \varphi (\rho_w - \rho_o). \]

Analogously, for an oil block surrounded with gas fractures and a gas block surrounded with water fractures, respectively,

\[ \Delta p_g = 0, \quad \Delta p_o = \varphi (\rho_o - \rho_g) \]

and

\[ \Delta p_w = 0, \quad \Delta p_g = \varphi (\rho_w - \rho_g). \]

We introduce the global fluid density in the fractures

\[ \rho_f = S_{w,f} \rho_w + S_{o,f} \rho_o + S_{g,f} \rho_g, \]
and define the pressure gradient effect
\[ \Delta p_\alpha = \mathcal{D} \left| \rho_f - \rho_\alpha \right|, \quad \alpha = w, o, g. \]

Now, the transfer terms that include the contributions from the capillary pressure, gravity, and viscous forces, and the pressure gradients across matrix blocks are
\begin{align*}
q_{w,mf} &= T_m \frac{k_{rw} \xi_w}{\mu_w} \left( \Phi_w - \Phi_{w,f} + L_c \Delta p_w \right), \\
q_{i,mf} &= T_m \left\{ \frac{k_{ri} x_{i0} \xi_o}{\mu_o} \left( \Phi_o - \Phi_{o,f} + L_c \Delta p_o \right) \\
&\quad + \frac{k_{rg} x_{iG} \xi_g}{\mu_g} \left( \Phi_g - \Phi_{g,f} + L_c \Delta p_g \right) \right\}, \quad (2.116)
\end{align*}

where \( \Phi_\alpha \) is the phase potential,
\[ \Phi_\alpha = p_\alpha - \rho_\alpha \mathcal{D} z, \quad \alpha = w, o, g, \]
\( L_c \) is the characteristic length for the matrix-fracture flow, and
\[ T_m = k \sigma \left( \frac{1}{l_{1z}^2} + \frac{1}{l_{2z}^2} + \frac{1}{l_{3z}^2} \right) \]

is the matrix-fracture transmissibility with \( \sigma \) the shape factor and \( l_{1z}, l_{2z}, \) and \( l_{3z} \) the matrix block dimensions. When the matrix permeability \( k \) is a tensor and different in the three coordinate directions, the matrix-fracture transmissibility is modified to
\[ T_m = \sigma \left( \frac{k_{11}}{l_{1z}^2} + \frac{k_{22}}{l_{2z}^2} + \frac{k_{33}}{l_{3z}^2} \right), \quad k = \text{diag}(k_{11}, k_{22}, k_{33}). \]

### 2.11.2 Dual porosity models

For the development of a dual porosity model, the matrix blocks act as a source term to the fracture system. In this case, there are two approaches for deriving this model: the Warren–Root approach as in Section 2.11.1 and the approach based on boundary conditions imposed explicitly on matrix blocks as in Section 2.2.6.

**The Warren–Root approach**

In this approach, the mass balance equations in the matrix become
\begin{align*}
\frac{\partial (\phi \xi_w S_w)}{\partial t} &= -q_{w,mf}, \\
\frac{\partial (\phi [x_{i0} \xi_o S_o + x_{iG} \xi_g S_g])}{\partial t} &= -q_{i,mf}, \quad i = 1, 2, \ldots, N_c, \quad (2.117)
\end{align*}

where \( q_{w,mf} \) and \( q_{i,mf} \) are defined by (2.116). The balance equations (2.115) in the fractures remain unchanged.
2.11. Flows in Fractured Porous Media

The boundary conditions approach

For a dual porosity model of the compositional flow under consideration, the fluid flow in the matrix system can be modeled in the same way as in (2.31) for single phase flow. Let the matrix system be composed of disjoint blocks \( \{ \Omega_i \} \). On each block \( \{ \Omega_i \} \) the mass balance equations hold, \( i = 1, 2, \ldots, N_c \):

\[
\begin{align*}
\frac{\partial (\phi \xi_w S_w)}{\partial t} + \nabla \cdot (\xi_w u_w) &= 0, \\
\frac{\partial (\phi [x_{i0} \xi_o S_o + x_{ig} \xi_g S_g])}{\partial t} + \nabla \cdot (x_{i0} \xi_o u_o + x_{ig} \xi_g u_g) &= 0.
\end{align*}
\]

The mass balance equations in the fractures are defined as in (2.115) with \( q_{w,mf} \) and \( q_{i,mf} \) given by (cf. Exercise 2.10)

\[
\begin{align*}
q_{w,mf} &= -\sum_j \chi_j \left( \frac{1}{|\Omega_j|} \int_{\Omega_i} \frac{\partial (\phi \xi_w S_w)}{\partial t} d\mathbf{x} \right), \\
q_{i,mf} &= -\sum_j \chi_j \left( \frac{1}{|\Omega_j|} \int_{\Omega_i} \frac{\partial (\phi [x_{i0} \xi_o S_o + x_{ig} \xi_g S_g])}{\partial t} d\mathbf{x} \right)
\end{align*}
\]

(2.119)

for \( i = 1, 2, \ldots, N_c \).

We impose boundary conditions for the matrix equations (2.118) as in Section 2.2.6. For \( \xi_1, \xi_2, \ldots, \xi_N \) fixed, we define the phase pseudopotential

\[
\Phi'_\alpha (p_\alpha, \xi_1, \xi_2, \ldots, \xi_N) = \int_{p_\alpha}^{p_0} \frac{1}{\rho_\alpha (\xi, \xi_1, \xi_2, \ldots, \xi_N)} d\xi - z,
\]

(2.120)

where \( p_0 \) is some reference pressure, \( \alpha = o, g \). The inverse of this integral is denoted \( \psi'_\alpha (\cdot, \xi_1, \xi_2, \ldots, \xi_N) \), again for \( \xi_1, \ldots, \xi_N \) fixed.

Now, the boundary conditions for (2.118) on the surface \( \partial \Omega_i \) of each matrix block \( \Omega_i \) are, for \( i = 1, 2, \ldots, N_c, \alpha = o, g \),

\[
\begin{align*}
x_{i\alpha} &= x_{i\alpha,f}, \\
\Phi'_\alpha (p_\alpha, x_{i\alpha}, x_{i\alpha}, \ldots, x_{iN\alpha}) &= \Phi'_\alpha (p_{\alpha,f}, x_{i\alpha,f}, x_{i\alpha,f}, \ldots, x_{iN\alpha,f}) = \Phi'_{\alpha,f}.
\end{align*}
\]

(2.121)

where, for a given \( \Phi'_{\alpha,f}, \Phi'_o \) is a pseudopotential reference value on each block \( \Omega_i \) determined by

\[
\frac{1}{|\Omega_i|} \int_{\Omega_i} \left( \phi \rho_\alpha \left( \psi'_\alpha (\Phi'_\alpha - \Phi'_o + x_3, x_{i\alpha,f}, x_{i\alpha,f}, \ldots, x_{iN\alpha,f}) \right) \right) d\mathbf{x} = (\phi \rho_\alpha) (p_{\alpha,f}, x_{i\alpha,f}, x_{i\alpha,f}, \ldots, x_{iN\alpha,f})
\]

(2.122)

If we assume that \( \partial \rho_\alpha / \partial p_\alpha \geq 0 \) (for \( x_{i3}, x_{i2}, \ldots, x_{iN\alpha} \) fixed), (2.122) is solvable for \( \Phi'_o \) (for incompressible \( \alpha \)-phase fluid, set \( \Phi'_o = 0 \)). The second equation in (2.121) applies to the first equation in (2.118); for the water component, the pseudopotential depends only on pressure.

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This model implies that the fracture system, being highly permeable, quickly comes into chemical and mechanical equilibrium locally on the fracture spacing scale. This equilibrium is defined in terms of the mole fractions and the chemical equilibrium pseudopotentials, and is reflected in the matrix equations through the boundary conditions in (2.121).

2.12 Concluding Remarks

In this chapter, the basic fluid flow and transport equations have been developed for a hierarchy of models: single phase, two-phase, black oil, volatile oil, compositional, thermal, and chemical. This hierarchy of models correspond to different oil production stages. Their governing differential equations consist of the mass and energy conservation equations and Darcy’s law. We have chosen to start with the simplest model for single phase flow and to end with the most complex model for chemical flooding. This approach can be reversed; that is, we can start with the chemical model, and in turn derive the thermal, compositional, volatile oil, black oil, two-phase, and single phase models.

In the chemical model, we have considered the general case where there are $N_c$ chemical components, each of which may exist in any or all of the $N_p$ phases. The basic equations consist of a mass conservation equation for each component (2.101), an energy equation for temperature (2.107), Darcy’s law for the volumetric velocity of each fluid phase (2.106), an overall mass conservation for a phase pressure (2.109), and algebraic constraints (2.113) that describe physical and chemical phenomena peculiar to chemical flooding. The flow equations allow for compressibility of soil and fluids, dispersion and molecular diffusion, chemical reactions, and phase behavior. Even though the displacement mechanisms are different in the thermal and chemical methods, there is not much difference between the corresponding models, both of which include mass and energy conservation and Darcy’s law. The mass equation is usually solved in terms of the mole fraction for each component in the thermal case (cf. (2.85)), while it is solved in terms of the volumetric concentration in the chemical case. In addition, the emphasis is placed on the solution of compositions and temperature in the former case, while it is on the solution of compositions and reactions for the components involved in the latter.

When flow is isothermal, the model equations in the chemical and thermal methods become the basic equations for compositional flow. An energy equation is not required in the compositional model, which now consists of a mass conservation equation in terms of the mole fraction for each component (2.85), Darcy’s law for the phase volumetric velocity (2.86), and phase equilibrium relations for the computation of compositions (2.91). In this model, $N_c$ components form at most three phases (e.g., vapor, liquid, and water), and mass interchanges only between the hydrocarbon phases (i.e., the vapor and liquid phases).

Instead of three fluid phases, if only a single phase is present in an entire porous medium, the mass conservation equation for each component in the compositional model becomes the transport equation of multicomponents in the fluid phase (2.59). When at most two components are involved, this equation reduces to the transport equation (2.55) for a component.

The black oil and volatile oil models can be treated as simplified, two-component compositional models. In these models, the hydrocarbon system is composed of the gas (mainly methane and ethane) and oil components at stock-tank conditions. There is no mass
transfer between the water phase and the oil and gas phases. In the black oil model, the gas component can exist in the oil and gas phases. In the volatile oil model, both hydrocarbon components can exist in these two phases. The black oil model is not suitable for handling a volatile oil reservoir. The governing differential equations of these two models are generally written in terms of volumetric rates at standard conditions; see (2.76)–(2.78) and (2.80)–(2.82).

The model for two-phase immiscible flow is a special case of the black oil model; when two phases are considered and there is no mass transfer between them, the two-phase immiscible flow model results, which consists of a mass conservation equation (2.36) and Darcy’s law for each phase (2.37). Finally, when only a single phase is present, the model for two-phase flow reduces to that for single phase flow (cf. (2.1) and (2.4)).

The relationship among the models is presented for ordinary porous media. For a fractured porous medium, the concept of dual porosity and dual porosity/permeability can be incorporated. Examples for single phase and compositional flows in fractured media have been discussed in Sections 2.2.6 and 2.11, respectively.

Limitations of the basic fluid flow equations for all the models presented in this chapter have not been fully discussed. Non-Newtonian fluids are not considered in subsequent chapters. Also, all considerations will be based on Darcy’s law in place of the momentum balance equation. Non-Darcy’s law and non-Newtonian phenomena have been briefly described in Sections 2.2.7 and 2.2.8 for single phase flow.

### 2.13 Bibliographical Information

The book by Aziz and Settari (1979) covered the single phase flow model through the black oil model, while the models covered in Peaceman’s book (1977) included the compositional flow model. The nonisothermal and chemical compositional flow models are presented in a quite condensed fashion in this chapter. For more information on the physics of these two models, the reader should refer to the book by Lake (1989) and to the technical documentation by Delshad et al. (2000) (also see Chapters 10 and 11).

### Exercises

2.1. Derive equation (2.12) from equation (2.6).

2.2. Derive the equation of mass conservation (2.36) for the simultaneous flow of two fluids in a porous medium.

2.3. Derive system (2.47) in detail.

2.4. Consider the transport equation of multicomponents in a fluid phase in a porous medium (cf. (2.59)),

\[
\frac{\partial (c_i \rho)}{\partial t} = -\nabla \cdot \left( c_i \rho \mathbf{u} - \rho D \nabla c_i \right) + \rho q_i, \quad i = 1, 2, \ldots, N_c, \quad (2.123)
\]

and Darcy’s law for the fluid

\[
\mathbf{u} = -\frac{1}{\mu} \mathbf{k} \nabla \rho. \quad (2.124)
\]
Recall the equation of state (cf. (2.6))

\[ \frac{d\rho}{\rho} = c_f dp, \]  

(2.125)

where we assume that the compressibility factor \( c_f \) is constant. Based on (2.123)–(2.125) and the concentration constraint

\[ \sum_{i=1}^{N_c} c_i = 1, \]

prove that the pressure equation

\[ \phi c_f \frac{\partial p}{\partial t} - \nabla \cdot \left( \frac{1}{\mu_k} \nabla p \right) = \sum_{i=1}^{N_c} q_i \]  

(2.126)

holds, provided that the “higher-order” quadratic term \( c_f u \cdot \nabla p \) is neglected. Equation (2.126) can be utilized along with \( N_c - 1 \) equations of form (2.123) to describe the transport of multicomponents in a fluid or the compressible miscible displacement process.

2.5. Assume that the capillary pressures \( p_{cow} \) and \( p_{cgo} \) take the forms \( p_{cow} = p_{cow}(S_w) \) and \( p_{cgo} = p_{cgo}(S_g) \) and have respective inverse functions \( p_{cow}^{-1} \) and \( p_{cgo}^{-1} \). Express equations (2.61)–(2.66) in a three-pressure \((p_w, p_o, p_g)\) formulation.

2.6. Under the same assumptions as in Exercise 2.5, express equations (2.61)–(2.66) in a pressure \((p_o)\) and two-saturation \((S_w, S_g)\) formulation.

2.7. Consider three-phase immiscible flow

\[ \frac{\partial (\phi \rho \alpha S_\alpha)}{\partial t} = - \nabla \cdot (\rho \alpha u_\alpha) + q_\alpha, \]  

(2.127)

and the additional constraints

\[ S_w + S_o + S_g = 1, \]

\[ p_{cw}(S_w, S_g) = p_w - p_o, \quad p_{cg}(S_w, S_g) = p_g - p_o, \]  

(2.128)

where \( p_{cow} = -p_{cow} \) and \( p_{cgo} = p_{cgo} \). The phase and total mobilities and the fractional flow functions are defined in the same manner as in Section 2.3:

\[ \lambda_\alpha = \frac{k_{rw}}{\mu_a}, \quad \lambda = \sum_{\alpha=w,o,g} \lambda_\alpha, \quad f_\alpha = \frac{\lambda_\alpha}{\lambda}, \quad \alpha = w, o, g, \]

where \( f_\alpha \) depends on the saturations \( S_w \) and \( S_g \).

(i) Prove that there exists a function \((S_w, S_g) \mapsto p_c(S_w, S_g)\) such that

\[ \nabla p_c = f_w \nabla p_{cw} + f_g \nabla p_{cg} \]  

(2.129)
if and only if the following equations are satisfied:

\[
\frac{\partial p_c}{\partial S_w} = f_w \frac{\partial p_{cw}}{\partial S_w} + f_g \frac{\partial p_{cg}}{\partial S_w} \quad \frac{\partial p_c}{\partial S_g} = f_w \frac{\partial p_{cw}}{\partial S_g} + f_g \frac{\partial p_{cg}}{\partial S_g} \tag{2.130}
\]

(ii) Show that a necessary and sufficient condition for existence of a function \( p_c \) satisfying (2.130) is

\[
\frac{\partial f_w}{\partial S_g} \frac{\partial p_{cw}}{\partial S_w} + \frac{\partial f_g}{\partial S_g} \frac{\partial p_{cg}}{\partial S_w} = \frac{\partial f_w}{\partial S_w} \frac{\partial p_{cw}}{\partial S_g} + \frac{\partial f_g}{\partial S_w} \frac{\partial p_{cg}}{\partial S_g}. \tag{2.131}
\]

This condition is referred to as the total differential condition.

(iii) When condition (2.131) is satisfied, the function \( p_c \) is

\[
p_c(S_w, S_g) = \int_1^{S_w} \left\{ f_w(\xi, 0) \frac{\partial p_{cw}}{\partial S_w}(\xi, 0) + f_g(\xi, 0) \frac{\partial p_{cg}}{\partial S_w}(\xi, 0) \right\} d\xi
+ \int_0^{S_g} \left\{ f_w(S_w, \xi) \frac{\partial p_{cw}}{\partial S_g}(S_w, \xi) + f_g(S_w, \xi) \frac{\partial p_{cg}}{\partial S_g}(S_w, \xi) \right\} d\xi, \tag{2.132}
\]

where we assume that the integrals are well defined. We introduce the global pressure and the total velocity

\[
p = p_o + p_c, \quad \mathbf{u} = \mathbf{u}_w + \mathbf{u}_o + \mathbf{u}_g. \tag{2.133}
\]

Write equations (2.127) and (2.128) in terms of the main unknowns \( p, S_w, \) and \( S_g \).

2.8. Let the mass and molar densities, \( \rho_{i\alpha} \) and \( \xi_{i\alpha} \), of component \( i \) in phase \( \alpha \) be related by \( \xi_{i\alpha} = \rho_{i\alpha} / W_i \), where \( W_i \) is the molar mass of component \( i \), \( i = 1, 2, \ldots, N_c \), \( \alpha = o, g \). Prove equations (2.92) and (2.93).

2.9. Derive the pressure equation (2.109) in detail.

2.10. Derive the matrix-fracture transfer terms \( q_{w,mf} \) and \( q_{c,mf} \) in equation (2.119) for the dual porosity model of compositional flow.