Chapter 6 Conservation Equations for Multiphase-Multicomponent Flow Through Porous Media

The mass conservation equations will appear repeatedly in many different forms when different displacement processes are considered. The basic mass conservation principle is general and will be derived just once here and special cases will be considered as subsets of the general case. Only isothermal processes will be considered here. The material used here is extracted from the book by Larry W. Lake, Enhanced Oil Recovery, Prentice Hall, 1989. This book is a recommended reference for this class.

The Continuum Assumption

If we were to view the porous medium on a length scale on the order of the pore size, the pore space will appear extremely detailed and chaotic as in the electron micrographs we saw earlier. Also, the fluids in the pore space will be distributed in parts of the pore space that depends of the wettability and saturation history in addition to the saturation itself.

If we hope to model the flow and transport of phases and species on a macro or mega volume of the porous media, it is necessary to average the description of the system over a representative elementary volume (REV) that is large compared to the size of the pores but small compared to the macroscopic dimensions of the porous medium. The properties of the system will be described by continuum variables such as porosity, permeability, saturation, relative permeability, and capillary pressure.

Local Thermodynamic Equilibrium

It the following it is assumed that species within the REV is in local thermodynamic equilibrium. In means that the chemical potential of each species is the same in all phases within the REV. There are some cases when thermodynamic equilibration is not achieved and it is necessary to include kinetic or mass transfer terms to the mass balance. Examples are mineral dissolution and transformation in the presence of alkaline solution, laboratory experiments in short cores at high rates, and viscous fingering with solvent flooding.

Fluxes in Isothermal Flow

Volumetric Flux

We derived earlier Darcy's law from momentum conservation for the flow of a single phase in a representative elementary volume (REV) of the porous media. We will now generalize the definition of Darcy's law for the volumetric flux of phase $j$ in a system that can have $N_p$ phases.
\[ \ddot{u}_j = -\lambda_j \cdot k \cdot \left( \nabla p_j - \rho_j g \nabla D \right) \]

where the viscosity is now replaced by the relative mobility of phase \( j \),

\[ \lambda_{ij} = \frac{k_{ij}}{\mu_j} \]

The pressure is also identified with a phase. Two phases that are coexisting at the same place can have different pressures as a result of the curvature of the interface separating the phases. This pressure difference is identified as the capillary pressure, \( P_{cwo} \) and \( P_{cgo} \).

\[ P_{cwo} = p_o - p_w \]
\[ P_{cgo} = p_g - p_o \]

The driving forces for the volumetric flux of multiple phases can now be identified as due to: (1) pressure gradient, (2) capillary pressure gradient as a result of a gradient in the interfacial curvature which can result from a gradient in saturation or pore sizes, and (3) body forces or buoyancy that is different for phases with different densities.

**Dispersive Flux**

Within a single phase there is a diffusive flux due to a concentration gradient that can be described by Fick's law. In porous media there also is dispersion due to mixing of fluids passing through the multiple flow paths through the porous medium. The dispersive flux can be expressed as follows.

\[ N_{ij}^{\text{dispersion}} = -\phi \sum_{j=1}^{N_j} \rho_j S_j K_{ij} \cdot \nabla \omega_{ij} \]

where
- \( \rho_j \) density of phase \( j \)
- \( \omega_{ij} \) mass fraction of species \( i \) in phase \( j \)
- \( K_{ij} \) dispersion tensor of species \( i \) in phase \( j \)

The longitudinal and transverse components (i.e., parallel and perpendicular to the velocity vector) of the dispersion tensor in an isotropic medium are as follows.
\[
(K_i)_{ij} = \frac{D_{ij} \tau}{\phi S_j} + \alpha_{ij} [\bar{u}_j]
\]

where

- \(D_{ij}\) molecular dispersivity of species \(i\) in phase \(j\)
- \(\tau\) tortuosity
- \(\alpha_{ij}\) longitudinal dispersivity coefficient in phase \(j\)
- \(\alpha_{ij}\) transverse dispersivity coefficient in phase \(j\)

**Mass Balance**

Consider an arbitrary, fixed volume \(V\) embedded within a permeable medium through which is flowing \(i=1,2,...,N_c\) chemical species distributed among \(j=1,2,...,N_p\) phases. The volume \(V\) is greater than equal to the REV but smaller than or equal to the macroscopic porous medium dimensions. As Fig. 6.1 shows, the surface area of \(V\) is made up of elemental surface areas \(\Delta A\) from the center of which is pointing a unit outward normal vector \(n\) (bold type will be used for vectors in the text). The sum of all the surface elements \(\Delta A\) is the total surface area of \(V\). This sum becomes a surface integral as the largest \(\Delta A\) approaches zero.

The mass conservation equation for species \(i\) in volume \(V\) is

\[
\left\{\begin{array}{c}
\text{rate of accumulation of } i \text{ in } V \\
\text{rate of transport of } i \text{ into } V \\
\text{rate of production of } i \text{ in } V \\
\end{array}\right\} = \left\{\begin{array}{c}
\text{Net rate of } i \\
\text{Net rate of } i \\
\text{Net rate of } i \\
\end{array}\right\}, \quad i = 1,2,...,N_c
\]

The mass conservation equation is usually stated as "accumulation equals net flux (or input minus output) plus net source (or generation)". These will be derived in the following.

The accumulation term for species \(i\) is
rate of accumulation of i in V

\[ \frac{\partial}{\partial t} \left\{ \int_V W_i \, dV \right\} = \frac{\partial}{\partial t} \left\{ \text{Total mass of } i \text{ in } V \right\} \]

where \( W_i \) is the overall concentration of \( i \) in units of mass of \( i \) per unit bulk volume. Since \( V \) is a fixed volume,

\[ \frac{\partial}{\partial t} \left\{ \int_V W_i \, dV \right\} = \int_V \frac{\partial W_i}{\partial t} \, dV \]

The net flux term follows from considering the rate of transport across a surface element as shown in Fig. 6.1. Let \( \mathbf{N}_i \) be the flux vector of species \( i \) evaluated at the center of \( \Delta A \) in units of mass of \( i \) per surface area-time. The transport of \( i \) across \( \Delta A \) is given by the negative of the normal component of \( \mathbf{N}_i \)

\[ \text{Net rate of transport of } i \text{ into } V = -\int_A \mathbf{n} \cdot \mathbf{N}_i \, dA \]

This equation can be transformed into a volume integral over \( V \) by applying the divergence theorem.

\[ \text{Net rate of transport of } i \text{ into } V = -\int_V \nabla \cdot \mathbf{N}_i \, dV \]

The net rate of production of \( i \) in \( V \) is

\[ \text{Net rate of production of } i \text{ in } V = \int_V \mathbf{R}_i \, dV \]

where \( \mathbf{R}_i \) is the mass rate of production of \( i \) in units of mass of \( i \) per unit bulk volume-time. This term can account for both production or generation (\( \mathbf{R}_i > 0 \)) and destruction (\( \mathbf{R}_i < 0 \)) of \( i \), either through one or more chemical reactions or through physical sources (wells) in \( V \).

Combining each term into the mass balance equations gives,

\[ \int_V \left( \frac{\partial W_i}{\partial t} + \nabla \cdot \mathbf{N}_i - \mathbf{R}_i \right) \, dV = 0, \quad i = 1, 2, \ldots N_c \]

But since \( V \) is arbitrary, the integrand must be zero.
\[
\frac{\partial W_i}{\partial t} + \nabla \cdot \vec{N}_i - R_i = 0, \quad i = 1, 2, \ldots, N_c
\]

This equation is the differential form for the species conservation equation. It applies to any point within the macroscopic dimensions of the permeable medium. In the next section we give specific expressions for the terms in the equation.

Definitions and Constitutive Equations for Isothermal Flow

Table 2.2 (Lake 1989) summarizes the equations needed for a complete description of isothermal, multiphase flow in permeable media. Column 1 in Table 2-2 gives the differential form of the equation named in column 2. Column 3 gives the number of scalar equations represented by the equation named in column 1. Columns 4 and 5 give the identity and number of independent variables added to the formulation by the equation in column 1. \( N_D \) is the number of spatial dimensions (\( N_D \leq 3 \)). The stationary phase is treated here as a single homogeneous phase though more than one solid phase can exist (e.g., dissolution and precipitation of minerals). A normally subscripted quantity (for example \( \omega_{ij} \)) appearing without subscripts in Table 2-2 indicates a relationship involving, at most, all members of the subscripted set. In the listing of dependent variables, the primary media properties, such as the porosity \( \phi \), and the permeability \( k \), are given functions of position \( x \) within the porous media. These functions are, to a slight degree, a function of the fluid pressure because of compaction.

The first four equations in Table 2-2 are the species conservation equation and definitions for the accumulation, flux, and source terms in this equation. The overall concentrations are formally defined here as an overall mass fraction. When we get to special cases, we will see that there are convenient ways for defining the overall concentration in terms of phase concentrations and pore volume.
<table>
<thead>
<tr>
<th>Equation (1)</th>
<th>Name (2)</th>
<th>Number independent scalar* equations (3)</th>
<th>Dependent variables (4)</th>
<th>Number (5)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2.1-9) $\frac{\partial \tilde{W}_i}{\partial t} = \vec{V} \cdot \tilde{N}_i - R_i$</td>
<td>Species i conservation</td>
<td>$N_C$</td>
<td>$\tilde{W}_i, R_i, \tilde{N}_i$</td>
<td>$2N_P + N_C N_D$</td>
</tr>
<tr>
<td>(2.2-1) $\tilde{W}<em>i = \phi \sum</em>{j=1}^{N_C} p_j s_j w_{ij} + (1 - \phi) p_i w_i$</td>
<td>Overall concentration</td>
<td>$N_C - 1$</td>
<td>$p_i, s_j, w_{ij}, w_i$</td>
<td>$2N_P + 2N_C N_P + N_C$</td>
</tr>
<tr>
<td>(2.2-2) $\tilde{N}<em>i = \sum</em>{j=1}^{N_C} (p_i w_i \tilde{u}_j - \phi p_j s_j \tilde{V}_j)$</td>
<td>Species i flux</td>
<td>$N_C N_D$</td>
<td>$\tilde{u}_j$</td>
<td>$N_P N_D$</td>
</tr>
<tr>
<td>(2.2-3) $R_i = \phi \sum_{j=1}^{N_C} s_j r_{ij} + (1 - \phi)r_{i}$</td>
<td>Species i source</td>
<td>$N_C - 1$</td>
<td>$r_{i}$, $r_{ij}$</td>
<td>$N_P N_C + N_C$</td>
</tr>
<tr>
<td>(2.2-4) $\sum_{i=1}^{N_C} R_i = 0$</td>
<td>Total reaction definition</td>
<td>1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(2.2-5) $\tilde{u}_i = -\lambda_i \tilde{V}_i \cdot (\nabla \tilde{p}_i + p_i \tilde{g})$</td>
<td>Darcy's law</td>
<td>$N_P N_D$</td>
<td>$\lambda_i, p_i$</td>
<td>$2N_P$</td>
</tr>
<tr>
<td>(2.2-6) $\lambda_i = \lambda_i(s_i, \omega_i, \tilde{u}_i, \tilde{x})$</td>
<td>Relative mobility</td>
<td>$N_P$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(2.2-7) $P_j - P_x = P_{ij}(s_i, \omega_i, \tilde{x})$</td>
<td>Capillary pressure definition</td>
<td>$N_P - 1$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*Total independent equations = $N_D(N_P + N_C) + 2N_P N_C + 4N_P + 4N_C$

| Table 2-2 Continued |

<table>
<thead>
<tr>
<th>Equation (1)</th>
<th>Name (2)</th>
<th>Number independent scalar* equations (3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2.2-8a) $\sum_{i=1}^{N_C} \omega_i = 1$</td>
<td>Mass fraction definition</td>
<td>$N_P$</td>
</tr>
<tr>
<td>(2.2-8b) $\sum_{i=1}^{N_C} \omega_i \nu_i = 1$</td>
<td>Stationary phase mass fraction definition</td>
<td>1</td>
</tr>
<tr>
<td>(2.2-9) $\sum_{i=1}^{N_C} s_i = 1$</td>
<td>Saturation definition</td>
<td>1</td>
</tr>
<tr>
<td>(2.2-10a) $r_{ij} = r_{ij}(\omega_i, s_j)$</td>
<td>Homogeneous kinetic reaction rates</td>
<td>$(N_C - 1)N_P$</td>
</tr>
<tr>
<td>(2.2-10b) $r_{ij} = r_{ij}(\omega_i)$</td>
<td>Stationary phase reaction rates</td>
<td>$N_C - 1$</td>
</tr>
<tr>
<td>(2.2-10c) $\sum_{i=1}^{N_C} r_{ij} = 0$</td>
<td>Total phase reaction definition</td>
<td>$N_P$</td>
</tr>
<tr>
<td>(2.2-10d) $\sum_{i=1}^{N_C} r_{ij} = 0$</td>
<td>Stationary phase total reaction rates</td>
<td>1</td>
</tr>
<tr>
<td>(2.2-11a) $\omega_{ij} = \omega_{ij}(\omega_i, s_j)$</td>
<td>Equilibrium relations (or phase balances)</td>
<td>$N_C(N_P - 1)$</td>
</tr>
<tr>
<td>(2.2-11b) $\omega_{ij} = \omega_{ij}(\omega_i)$</td>
<td>Stationary phase equilibrium relations (or phase balances)</td>
<td>$N_C$</td>
</tr>
<tr>
<td>(2.2-12) $p_i = p_i(T, P)$</td>
<td>Equations of state</td>
<td>$N_P$</td>
</tr>
</tbody>
</table>

*Total independent equations = $N_D(N_P + N_C) + 2N_P N_C + 4N_P + 4N_C$

*Total dependent variables = $N_D(N_P + N_C) + 2N_P N_C + 4N_P + 4N_C$
Continuity Equation

If we insert Eqs. 2.2-1 through 2.2-3 into 2.19 we arrive at

$$\frac{\partial}{\partial t} \left( \phi \sum_{j=1}^{N_p} \rho_j S_j \omega_j + (1 - \phi) \rho_s \omega_s \right) + \nabla \cdot \left( \sum_{j=1}^{N_p} \rho_j \omega_j \mathbf{u}_j - \phi \rho_j K_j \cdot \nabla \omega_j \right)$$

$$= \phi \sum_{j=1}^{N_p} S_j r_j + (1 - \phi) r_i$$

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

This is the overall mass conservation equation for species \(i\). We sum over the \(N_c\) components to obtain the equation of continuity or conservation of total mass.

$$\frac{\partial}{\partial t} \left( \phi \sum_{j=1}^{N_p} \rho_j S_j + (1 - \phi) \rho_s \right) + \nabla \cdot \left( \sum_{j=1}^{N_p} \rho_j \mathbf{u}_j \right) = 0$$

Concentration Variables

The concentrations were expressed here as a mass fraction. This choice of concentration is the most general. When we examine special cases we will find other concentration variables to be more convenient. In the case of incompressible, immiscible fluids the only changing parameter is the phase saturations. In the case of ion exchange, the concentration may be expressed in moles or equivalents per unit aqueous volume. Tracer quantities may be expressed as parts per million, ppm. Oil field practice expresses the quantity of oil as stock tank barrel (STB) and the quantity of gas as thousand cubic feet of gas at standard conditions (Mcf).
Special Cases

We will now consider special cases of the general mass conservation equations derived earlier.

One Dimensional Displacement - Fractional Flow Formulation

The classical equation for two phase displacement is the case of one dimensional, homogeneous, incompressible, immiscible, isothermal, displacement with no capillary pressure ($P_c=0$), sorption ($W_s=0$), reaction ($R_f=0$), or interphase mass transfer ($\omega_{ij}=\delta_{ij}$). The mass transfer equations reduce to,

$$\phi \frac{\partial S_j}{\partial t} + \frac{\partial u_j}{\partial x} = 0, \quad j = 1, 2, \ldots, N_p$$

The continuity equation and the saturation definition reduces to,

$$\frac{\partial u}{\partial x} = 0$$

where

$$u = \sum_{j=1}^{N_p} u_j$$

where $u$ is the **total volumetric flux**. The continuity equation reduces the number of independent species conservation equations by one. The pressure gradient can be eliminated from Darcy's law by expressing the fluxes in terms of the **fractional flow** function.

$$f_j = \frac{u_j}{u} = \frac{\lambda_{nj}}{\sum_{k=1}^{N_p} \lambda_{rk}} \left[1 - \frac{kg \sin \alpha}{\sum_{k=1}^{N_p} \lambda_{rk}} \left(\rho_j - \rho_k\right)\right]$$

where

$$\sin \alpha = -\frac{dD}{dx}$$

where $\alpha$ is the dip angle, i.e., the inclination of the direction of the displacement relative to the horizon, measured positive in the counter clockwise direction. The flux expressed as a function of the fractional flow can be substituted into the conservation equation and the total flux factored out to give the conservation equation in terms of the fractional flow.
The initial conditions is usually a uniform saturation with only one phase mobile. The boundary conditions are a specified total flux and fractional flow at the inlet end. There is no down stream boundary conditions. Buckley and Leverett (1942) first solved this equation for two-phase flow, and the water flood or gas flood calculations using this equation is called the Buckley-Leverett theory. This theory has been extended to much more complex systems (Larson 1982; Pope 1980).

**Assignment 6.1 Buckley-Leverett Equation**

Derive the preceding equations (including the fractional flow function) starting from the equations in Table 2.2. State your assumptions at each step.

**Multi - Dimensional, Immiscible, Incompressible Displacement**

The fractional flow formulation is not useful in multidimensional displacement because the total volumetric flux is not independent of position as in one dimensional displacement. However, the equations still simplify in the case of immiscible, incompressible displacement in multidimensions. Rather than deriving the continuity equation as a condition of conservation of total mass, the density can be factored out of the species conservation equations and the sum of the equations is then a statement of the conservation phase volumes. Since the sum of the saturations is equal to unity and thus independent of time, the continuity equation reduces to the statement that the divergence of the total flux is zero.

\[
\nabla \cdot \left( \sum_{j=1}^{N_p} \bar{u}_j \right) = 0
\]

When Darcy's law is substituted into the above equation the result is an elliptic partial differential equation for pressure of one of the phases. The pressures of the other phases are related through the capillary pressure relations. The phase saturations can be calculated from the \(N_p-1\) species conservation equations. A condition for the existence of a solution to the system of equations is that the net sum of the volumetric sources and sinks must be zero if there is no flow out of the boundaries of the system.
Miscible Displacement

We now treat the isothermal case of many components flowing simultaneously in a single fluid phase. Thus only one phase flows regardless of composition, but both convection and dispersion of these components must be included. Miscible processes of interest include (1) truly miscible displacement of oil by a solvent; (2) chromatographic processes such as analytical chromatography, separation chromatography, ion exchange process, and adsorption of chemicals as they percolate through soils or other permeable media; (3) leaching processes such as the in situ mining of uranium; and (4) chemical reaction processes of many types in fixed bed reactors.

The species mass conservation equation for single phase miscible displacement is

$$\frac{\partial (\rho \phi \omega_i)}{\partial t} + \nabla \cdot \left[ \rho \omega_i \vec{u} - \phi \rho \mathbf{K} \cdot \nabla \omega_i \right] = R_i$$

$$i = 1, 2, \ldots, N_c$$

The second subscript $j$ for the phase number is now superfluous and has been dropped. The auxiliary Eqs. (2.2-5), (2.2-6), (2.2-8), and (2.2-10) through (2.2-12) are still needed, but the others are no longer pertinent. Eq (2.2-5) or Darcy's law has a considerably simpler form,

$$\vec{u} = -\frac{k}{\mu} (\nabla p - \rho g \nabla D)$$

If density is constant, the pressure and depth gradients can be replaced with a flow potential gradient. Since the relative permeability is constant, it is lumped with the absolute permeability. However, the viscosity may be strongly dependent on the composition. If the saturation of the flowing phase is not unity (i.e., there is an immobile phase) it can be lumped with the porosity.

For miscible solvents, the sorption and reaction terms are zero, giving

$$\frac{\partial (\rho \phi \omega_i)}{\partial t} + \nabla \cdot \left[ \rho \omega_i \vec{u} - \phi \rho \mathbf{K} \cdot \nabla \omega_i \right] = 0, \quad i = 1, 2, \ldots, N_c$$

A special one dimensional case of the above equation is obtained when the effect of composition and pressure on density is neglected and the dispersivity is constant. Letting $C_i = \omega_i \rho$ be the mass concentration of component $i$, it follows that

$$\phi \frac{\partial C_i}{\partial t} + u \frac{\partial C_i}{\partial x} = \phi K_{ri} \frac{\partial^2 C_i}{\partial x^2}, \quad i = 1, 2, \ldots, N_c$$
where \( K_{ij} \), the longitudinal dispersion coefficient, is now a scalar,

\[
K_{ij} = \frac{D_i}{\tau} + \frac{\alpha_i |u|}{\phi}
\]

Because of the continuity equation, \( u \) is independent of \( x \). If \( D_i \) is taken as a constant, the above equation reduces to the linear convective-diffusion equation.

### Chromatographic Transport

The equations for chromatographic transport are special cases of the convective diffusion equation except that the sorption terms, \( C_{is} \), must be retained. The basis for chromatographic transport is the separation of components due to the difference in \( C_{is} \). These sorption reactions may be adsorption, the exchange of one ion for another on the stationary substrate, or precipitation-dissolution reactions. Dispersion may smear displacement fronts and reduce peak concentrations but will not alter the relative transport of the species. Thus the dispersion term will be neglected so that the equations can be investigated with the insightful methods available for hyperbolic partial differential equations, e.g., method of characteristics and coherence theory. These first order partial differential equations are sometimes called the chromatographic equations.

\[
\phi \frac{\partial C_i}{\partial t} + (1-\phi) \frac{\partial C_{is}}{\partial t} + u \frac{\partial C_i}{\partial x} = 0, \quad i = 1, 2, ..., N_c
\]

### Semimiscible, Incompressible, One Dimensional Displacement with Ideal Mixing

Helfferich (1981) has shown that the highly developed theory for chromatographic displacement can be also applied to multiphase, multicomponent systems. The components can partition between the phase with known equilibrium relationships. However, an assumption of ideal mixing is needed for the total volumetric flux to be independent of position. Also, the concentrations are expressed as volume fractions.
If we assume incompressible fluids, constant porosity, and ideal mixing and divide the species conservation equation by the respective pure component density, we have

\[
\frac{1}{\rho_j} = \sum_{i=1}^{N_p} \frac{\omega_{ij}}{\rho_i^o}, \quad j = 1, 2, ..., N_p
\]

\[
C_{ij} = \frac{\omega_{ij} \rho_j}{\rho_i^o}
\]

\[
\sum_{i=1}^{N_p} C_{ij} = \rho_j \sum_{i=1}^{N_p} \frac{\omega_{ij}}{\rho_i^o} = 1
\]

If we further assume the phase density can be included in the gradient, the equation can be expressed in terms of \( C_{ij} \). If we also assume that the divergence of the sum of the diffusive fluxes is zero, the sum of the species balances gives

\[
\nabla \cdot \left( \sum_{j=1}^{N_p} \phi S_j \frac{\rho_j \rho_i^o}{\rho_i} \nabla \omega_{ij} \right) = 0
\]

\( i = 1, 2, ..., N_C \)

This means that in one dimension the total volumetric flux is independent of position. With these assumptions, the equations reduce to

\[
\frac{\partial}{\partial t} \left[ \phi \sum_{j=1}^{N_p} C_{ij} S_j + (1 - \phi) C_{is} \right] + \nabla \cdot \left( \sum_{j=1}^{N_p} C_{ij} \vec{u}_j \right) - \frac{\partial}{\partial x} \left( \phi S_j K_{ij} \frac{\partial C_{ij}}{\partial x} \right) = 0
\]

\( i = 1, 2, ..., N_C \)

If we neglect the dispersion terms, these equations are mathematically equivalent to the chromatographic equations. However, phase saturations and fractional flows are now additional dependent variables.

**Single Phase, Constant Compressibility**

When only one phase is flowing and only small perturbations in pressure is considered, the dependence of densities and porosity can be linearized in pressure and analytical solutions can be derived from the resulting linear
parabolic partial differential equations. These solutions are used to interpret transient pressure analysis for reservoir characterization.

The compressibility of a phase is defined as the relative change in fluid volume per unit change in pressure.

\[
c = -\frac{1}{\rho} \frac{\partial v}{\partial p} = \frac{1}{\rho} \frac{\partial \rho}{\partial p}
\]

The formation compressibility is defined as the relative change in porosity per unit change in pressure.

\[
c_f = \frac{1}{\phi} \frac{\partial \phi}{\partial p}
\]

A change in porosity with reduction in pressure is usually associated with compaction of the bulk volume. Rather than rigorously defining a coordinate system that follows the compaction, we will just assume that the rock mass per unit volume remains constant as the porosity changes. It is assumed that the changes in saturation with change in pressure can be neglected. The small changes in saturation that occur with compaction and difference in the phase compressibilities may be neglected for small perturbations in pressure but dissolution or resolution of gas can not be neglected. The accumulation term of the continuity equation will be expressed as a function of pressure.

\[
\frac{\partial}{\partial t} \left( \sum_{j=1}^{N_p} \phi \rho_j S_j \right) = \left( \sum_{j=1}^{N_p} \rho_j c_j S_j \right) \frac{\partial p}{\partial t} + \nabla \cdot \vec{u}_i
\]

There will only one term in the divergence of the continuity equation, the flux of the one phase that is flowing. Denote the phase index of this phase as 1. Assume that the change in density of this phase can be neglected in the divergence. The continuity equation then reduces to the following equation.

\[
\phi \left( \sum_{j=1}^{N_p} \frac{\rho_j c_j S_j}{\rho_1} \right) \frac{\partial p}{\partial t} + \nabla \cdot \vec{u}_i = 0
\]

The factor inside the bracket is the total compressibility of the formation and its fluids. It is often presented without the ratio of densities. This ratio results from the rigorous derivation.
\[
c_i = \left( \sum_{j=1}^{N_p} \frac{\rho_j c_j S_j}{\rho_1} + c_f \sum_{j=1}^{N_p} \frac{\rho_j S_j}{\rho_1} \right)
\]

It is convenient to express the pressures relative to a datum, i.e., express as a flow potential.

\[
\Phi = p - \rho g (D - D_0)
\]

where \(D_0\) is a datum depth to which all pressures will be referred. In the following equation the symbol \(p\) will be used in place of \(\Phi\). Assume that the permeability and viscosity are constant and can be factored out the divergence.

\[
\phi c_i \frac{\partial}{\partial t} \left( \frac{k_{ri}}{\mu} \right) - \nabla^2 p = 0
\]

\[
\frac{1}{\eta} \frac{\partial}{\partial t} p = \nabla^2 p
\]

where

\[
\eta = \frac{k_{ri}}{\phi \mu c_i}
\]

This equation is the **heat or diffusion equation** and many classical solutions exist. The parameter \(\eta\) is called the **hydraulic diffusivity**.
Overall Material Balance

An overall mass balance is useful because (1) it summarizes the behavior of the system with a few "lumped" parameters, and (2) the finite difference solution of the differential equations should be consistent with the overall material balance. The overall mass balance is done by integrating the differential species balance (Eq. 2.1-9 in Table 2-2) over the volume of the system and from an initial time to a time \( t \). It is assumed that there are no reactions, i.e., \( R_i = 0 \). The integral of the accumulation term is as follows.

\[
\int_0^t \int_V \frac{\partial \bar{W}_i}{\partial t} dV dt = \int_0^t V \frac{\partial \bar{W}_i}{\partial t} dt = V \left[ \bar{W}_i(t) - \bar{W}_i(0) \right]
\]

The integral of the divergence term is determined from the divergence theorem for fluxes at boundaries and sum of the sinks and sources.

\[
\int_0^t \int_V \nabla \cdot \vec{N}_i dV dt = \int_0^t \int_{\partial V} \vec{n} \cdot \vec{N}_i dA + \sum (q_p - q_I) dt = \int_0^t \left[ \sum (q_s + q_p - q_I) \right] dt = \sum (Q_s + Q_p - Q_I)
\]

where \( q \) is a mass flow rate and \( Q \) is the cumulative flux, production or injection. The statement of the overall mass balance of species \( i \) is now

\[
V \left[ \bar{W}_i(t) - \bar{W}_i(0) \right] = \sum (Q_I - Q_B - Q_p)
\]

These overall material balance equations are very useful in estimating the volume of a reservoir and/or the parameters for the influx from an aquifer. Also, these material balances should always be used to validate numerical simulation results.