Chapter 3
Single-Phase Flow and Numerical Solution

The basic differential equations that govern the flow of a single phase through a reservoir are described. They include a mass conservation equation, Darcy's law, and an equation of state relating the fluid pressure to its density. The cases of incompressible, slightly compressible, and compressible fluids are considered. Then an analytic solution for a 1D radial flow is obtained, which is usually used to estimate the pressure of a wellbore. As an example, a numerical solution of single-phase flow equations using finite difference methods is presented, for which these methods for transient (parabolic), stationary (elliptic), and wave (hyperbolic) problems are reviewed. For applications of other numerical methods such as finite volume and finite element methods to the numerical solution of the flow equations, the reader may refer to the books by Chen (2005) and Chen, Huan, and Ma (2006). Much attention in this chapter is paid to the treatment of practical issues in reservoir simulation, such as gridblock transmissibility, material balance, and the treatment of nonlinearity. The solution of linear systems of algebraic equations will not be discussed here. For more information on linear solvers, the reader should consult with reservoir simulation books by Aziz and Settari (1979), Ertekin, Abou-Kassem, and King (2001), and Chen, Huan, and Ma (2006). In particular, this last book contains all advanced solvers to date such as Krylov subspace linear solvers.

3.1 Basic Differential Equations

3.1.1 Mass Conservation

We briefly derive the governing differential equations for the flow and transport of a fluid in a porous medium in order to introduce the terminologies and notation used throughout this book.

The spatial and temporal variables will be represented by $\mathbf{x} = (x_1, x_2, x_3)$ and t, respectively. Denote by ϕ the *porosity* of the porous medium, by ρ 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. Consider a rectangular cube such that its faces are parallel to the coordinate axes (cf. Fig. 3.1). The centroid of this cube is denoted (x_1, x_2, x_3), and its

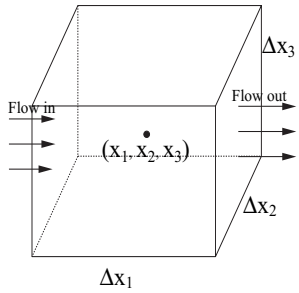

Figure 3.1. *A differential volume.*

length in the x_i-coordinate direction is Δx_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 ρu_i. Referring to Fig. 3.1, the mass inflow across the surface at $x_1 - \frac{\Delta x_1}{2}$ per unit time is

$$(\rho u_1)_{x_1-\frac{\Delta x_1}{2},x_2,x_3}\,\Delta x_2 \Delta x_3,$$

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

$$(\rho u_1)_{x_1+\frac{\Delta x_1}{2},x_2,x_3}\,\Delta x_2 \Delta x_3.$$

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

$$(\rho u_2)_{x_1,x_2-\frac{\Delta x_2}{2},x_3}\,\Delta x_1 \Delta x_3, \quad (\rho u_2)_{x_1,x_2+\frac{\Delta x_2}{2},x_3}\,\Delta x_1 \Delta x_3,$$

and

$$(\rho u_3)_{x_1,x_2,x_3-\frac{\Delta x_3}{2}}\,\Delta x_1 \Delta x_2, \quad (\rho u_3)_{x_1,x_2,x_3+\frac{\Delta x_3}{2}}\,\Delta x_1 \Delta x_2.$$

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 within this volume:

$$\begin{aligned}
&\left[(\rho u_1)_{x_1-\frac{\Delta x_1}{2},x_2,x_3} - (\rho u_1)_{x_1+\frac{\Delta x_1}{2},x_2,x_3}\right]\Delta x_2 \Delta x_3 \\
&\quad + \left[(\rho u_2)_{x_1,x_2-\frac{\Delta x_2}{2},x_3} - (\rho u_2)_{x_1,x_2+\frac{\Delta x_2}{2},x_3}\right]\Delta x_1 \Delta x_3 \\
&\quad + \left[(\rho u_3)_{x_1,x_2,x_3-\frac{\Delta x_3}{2}} - (\rho u_3)_{x_1,x_2,x_3+\frac{\Delta x_3}{2}}\right]\Delta x_1 \Delta x_2 \\
&\quad = \left(\frac{\partial(\phi\rho)}{\partial t} - q\right)\Delta x_1 \Delta x_2 \Delta x_3.
\end{aligned}$$

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

$$-\frac{(\rho u_1)_{x_1+\frac{\Delta x_1}{2},x_2,x_3} - (\rho u_1)_{x_1-\frac{\Delta x_1}{2},x_2,x_3}}{\Delta x_1}$$
$$-\frac{(\rho u_2)_{x_1,x_2+\frac{\Delta x_2}{2},x_3} - (\rho u_2)_{x_1,x_2-\frac{\Delta x_2}{2},x_3}}{\Delta x_2}$$
$$-\frac{(\rho u_3)_{x_1,x_2,x_3+\frac{\Delta x_3}{2}} - (\rho u_3)_{x_1,x_2,x_3-\frac{\Delta x_3}{2}}}{\Delta x_3} = \frac{\partial(\phi\rho)}{\partial t} - q.$$

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

$$\frac{\partial(\phi\rho)}{\partial t} = -\nabla \cdot (\rho \mathbf{u}) + q, \tag{3.1}$$

where $\nabla\cdot$ is the *divergence* operator:

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

Note that q is negative for sinks and positive for sources.

The *formation volume factor* B of the fluid is

$$\rho = \frac{\rho_s}{B},$$

where ρ_s is the fluid density at standard conditions. Substituting ρ into (3.1), we have

$$\frac{\partial}{\partial t}\left(\frac{\phi}{B}\right) = -\nabla \cdot \left(\frac{1}{B}\mathbf{u}\right) + \frac{q}{\rho_s}. \tag{3.2}$$

Equations (3.1) and (3.2) are equivalent; they are the most general forms of the single-phase equation.

3.1.2 Darcy's Law

Darcy's law (Darcy, 1856) was originally a law for single-phase flow that relates the total volumetric flow rate of a fluid through a porous medium to the pressure gradient and the properties of the fluid (viscosity, μ) and the medium (permeability, k, and a cross-sectional area, A). It can be used to define the permeability in one of the flow directions, for example, in the x_1-direction (cf. Fig. 3.2):

$$q = -\frac{kA}{\mu}\frac{\partial p}{\partial x_1}.$$

Darcy's velocity is calculated by $u = q/A$, so

$$u = -\frac{k}{\mu}\frac{\partial p}{\partial x_1}. \tag{3.3}$$

Note that the pore velocity v is the fluid velocity: $v = u/\phi$.

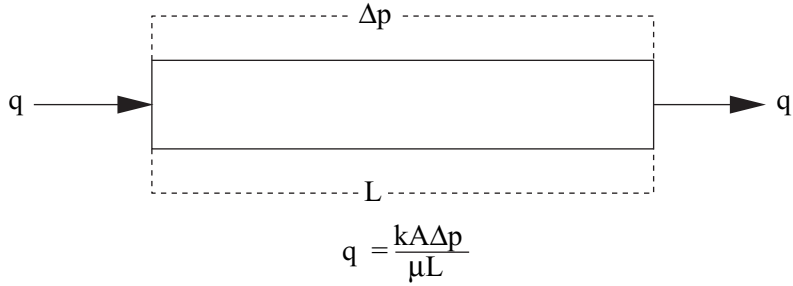

Figure 3.2. *Volumetric flow rate.*

For a 3D flow system with the gravitational force, the differential form of Darcy's law is

$$\mathbf{u} = -\frac{1}{\mu}\mathbf{k}\left(\nabla p - \rho g \nabla z\right), \tag{3.4}$$

where $\mathbf{k}$ is the *absolute permeability tensor* of the porous medium, g is the magnitude of the gravitational acceleration, z is the depth, and ∇ 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 equation (3.4) is in the vertical downward direction.

3.1.3 Units

In this book the basic units are customary (English) and metric. Their conversion factors are stated in the preceding chapter. Here we describe these units for the variables used in single-phase flow; multiphase flow uses similar variables and units. One multiplies a customary unit by a conversion factor to obtain the corresponding metric unit. STB (standard barrel) and SCF (standard cubic feet) are measured at 60°F and 14.696 psia, while std m^3 (at standard conditions) is measured at 15°C and 100 kPa. In Table 3.1, FVF stands for formation volume factor.

3.1.4 Different Forms of Flow Equations

Substituting (3.4) into (3.1) yields

$$\frac{\partial(\phi\rho)}{\partial t} = \nabla \cdot \left(\frac{\rho}{\mu}\mathbf{k}\left(\nabla p - \rho g \nabla z\right)\right) + q. \tag{3.5}$$

An equation of state is expressed in terms of the *fluid compressibility* c_f:

$$c_f = -\frac{1}{V}\frac{\partial V}{\partial p}\bigg|_T = \frac{1}{\rho}\frac{\partial \rho}{\partial p}\bigg|_T \tag{3.6}$$

Table 3.1. *Customary and metric units.*

Quantity	Symbol	Customary	Metric	Conversion factor
Time	t	day	day	1.0
Angle	θ	rad	rad	1.0
Length	x_i, z	ft	m	0.3048
Area	A	ft^2	m^2	0.09290304
Volume	V	ft^3	m^2	0.02831685
Porosity	ϕ	fraction	fraction	1.0
Permeability	$\mathbf{k}$	darcy	μm^2	0.9869233
Density	ρ	lbm/ft^3	kg/m^3	16.01846
Gravitational acceleration	$\wp$	$32.174 ft/s^2$	$9.8066352\ m/s^2$	0.3048
Fluid gravity	γ	psi/ft	kPa/m	22.62059
Pressure	p	psia	kPa	6.894757
Velocity	$\mathbf{u}$	ft/D	m/d	0.3048
Viscosity	μ	cp	Pa·s	0.001
Compressibility	c	psi^{-1}	kPa^{-1}	0.1450377
Compressibility factor	Z	dimensionless	dimensionless	1.0
Flow rate	q	$lbm/(ft^3 \cdot d)$	$kg/(m^3 \cdot d)$	16.018653
Liquid FVF	B_w, B_o	RB/STB	$m^3/std\ m^3$	1.0
Gas FVF	B_g	RB/SCF	$m^3/std\ m^3$	5.5519314
Solution gas/oil ratio	R_{so}	SCF/STB	$std\ m^3/std\ m^3$	0.1801175
Gravity conversion factor	γ_c	0.21584E-3	1.0E-3	

at a fixed temperature T, where V stands for the volume occupied by the fluid at reservoir conditions. Combining equations (3.5) and (3.6) gives a closed system for the main unknown p or ρ. Simplified expressions such as a linear relationship between p and ρ for a *slightly compressible fluid* can be used.

It is sometimes convenient in mathematical analysis to write equation (3.5) in a form without the explicit appearance of gravity by the introduction of a *pseudopotential* (Hubbert, 1956):

$$\Phi' = \int_{p^o}^{p} \frac{1}{\rho(\xi)\wp}\, d\xi - z, \tag{3.7}$$

where p^o is a reference pressure. Using (3.7), equation (3.5) reduces to

$$\frac{\partial(\phi\rho)}{\partial t} = \nabla \cdot \left(\frac{\rho^2 \wp}{\mu} \mathbf{k} \nabla \Phi' \right) + q. \tag{3.8}$$

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

$$\Phi = p - \rho \wp z,$$

which is related to Φ' (with, e.g., $p^o = 0$ and constant ρ) by

$$\Phi = \rho g \Phi'.$$

If we neglect the term $g z \nabla \rho$, in terms of Φ equation (3.5) becomes

$$\frac{\partial(\phi\rho)}{\partial t} = \nabla \cdot \left(\frac{\rho}{\mu} \mathbf{k} \nabla \Phi \right) + q. \tag{3.9}$$

Incompressible flow

When the rock and fluid are incompressible, the density ρ and porosity ϕ are assumed to be constant. In this case, equation (3.9) reduces to

$$\nabla \cdot \left(\frac{\rho}{\mu} \mathbf{k} \nabla \Phi \right) + q = 0, \tag{3.10}$$

which is an *elliptic equation* in Φ (cf. Section 5.1.3). For the flow of an incompressible fluid in a homogeneous and isotropic medium with a constant viscosity, equation (3.10) further becomes

$$\Delta \Phi = -\frac{\mu q}{\rho k}, \tag{3.11}$$

where the *Laplacian operator* Δ is defined by

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

Equation (3.11) is the *Poisson equation* in Φ. If there is no external source/sink term (well), it is called the *Laplace equation*.

Slightly compressible flow

It is sometimes possible to assume that the fluid compressibility c_f is constant over a certain range of pressures. Then, after integration, we write (3.6) as

$$\rho = \rho^o e^{c_f (p - p^o)}, \tag{3.12}$$

where ρ^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:

$$\rho \approx \rho^o \big(1 + c_f (p - p^o) \big). \tag{3.13}$$

The *rock compressibility* is defined by

$$c_R = \frac{1}{\phi} \frac{d\phi}{dp}. \tag{3.14}$$

After integration, it is given by

$$\phi = \phi^o e^{c_R(p-p^o)}, \tag{3.15}$$

where ϕ^o is the porosity at p^o. Similarly, it is approximated by

$$\phi \approx \phi^o\big(1 + c_R(p - p^o)\big). \tag{3.16}$$

Then it follows that

$$\frac{d\phi}{dp} = \phi^o c_R. \tag{3.17}$$

After carrying out the time differentiation on the left-hand side of equation (3.5), this equation becomes

$$\left(\phi\frac{\partial\rho}{\partial p} + \rho\frac{d\phi}{dp}\right)\frac{\partial p}{\partial t} = \nabla\cdot\left(\frac{\rho}{\mu}\mathbf{k}\left(\nabla p - \rho g\nabla z\right)\right) + q. \tag{3.18}$$

Substituting (3.6) and (3.17) into equation (3.18) gives

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

Defining the *total compressibility*

$$c_t = c_f + \frac{\phi^o}{\phi}c_R, \tag{3.19}$$

we see that

$$\phi\rho c_t\frac{\partial p}{\partial t} = \nabla\cdot\left(\frac{\rho}{\mu}\mathbf{k}\left(\nabla p - \rho g\nabla z\right)\right) + q, \tag{3.20}$$

which is a *parabolic equation* in p (cf. Section 5.1.3), with ρ given by (3.12).

Compressible flow

For gas flow, the compressibility c_g of gas is usually not assumed to be constant. In such a case, the general equation (3.18) applies; i.e.,

$$c(p)\frac{\partial p}{\partial t} = \nabla\cdot\left(\frac{\rho}{\mu}\mathbf{k}\left(\nabla p - \rho g\nabla z\right)\right) + q, \tag{3.21}$$

where

$$c(p) = \phi\frac{\partial\rho}{\partial p} + \rho\frac{d\phi}{dp}. \tag{3.22}$$

A different form of equation (3.21) can be derived if we use the real *gas law* (the pressure-volume-temperature (PVT) relation)

$$\rho = \frac{pW}{ZRT}, \tag{3.23}$$

where W is the molecular weight, Z is the gas compressibility factor, and R is the *universal gas constant*. For a pure gas reservoir, the gravitational constant is usually small and

neglected. We assume that the porous medium is isotropic; i.e., $\mathbf{k} = k\mathbf{I}$, where $\mathbf{I}$ is the identity tensor. Furthermore, we assume that ϕ and μ are constants. Then, substituting (3.23) into (3.5), we see that

$$\frac{\phi}{k}\frac{\partial}{\partial t}\left(\frac{p}{Z}\right) = \nabla\cdot\left(\frac{p}{\mu Z}\nabla p\right) + \frac{RT}{Wk}q. \tag{3.24}$$

Note that $2p\nabla p = \nabla p^2$, so (3.24) becomes

$$\frac{2\phi\mu Z}{k}\frac{\partial}{\partial t}\left(\frac{p}{Z}\right) = \Delta p^2 + 2pZ\frac{d}{dp}\left(\frac{1}{Z}\right)|\nabla p|^2 + \frac{2\mu ZRT}{Wk}q. \tag{3.25}$$

Because

$$c_g = \frac{1}{\rho}\frac{d\rho}{dp}\bigg|_T = \frac{1}{p} - \frac{1}{Z}\frac{dZ}{dp},$$

we have

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

Inserting this equation into (3.25) and neglecting the term involving $|\nabla p|^2$ (often smaller than other terms in (3.25)), we obtain

$$\frac{\phi\mu c_g}{k}\frac{\partial p^2}{\partial t} = \Delta p^2 + \frac{2ZRT\mu}{Wk}q, \tag{3.26}$$

which is a parabolic equation in p^2.

There is another way to derive an equation similar to (3.26). Define a *pseudopressure* by

$$\psi = 2\int_{p^o}^{p}\frac{p}{Z\mu}\,dp.$$

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 (3.24) becomes

$$\frac{\phi\mu c_g}{k}\frac{\partial\psi}{\partial t} = \Delta\psi + \frac{2RT}{Wk}q. \tag{3.27}$$

The derivation of (3.27) does not require us to neglect the second term on the right-hand side of (3.25).

Boundary and initial 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 equation (3.5). We denote by Γ the external boundary or a boundary segment of the porous medium domain Ω under consideration.

Prescribed pressure. When the pressure is specified as a known function of position and time on Γ, 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 Γ, the boundary condition is

$$\rho \mathbf{u} \cdot \boldsymbol{\nu} = g_2 \quad \text{on } \Gamma,$$

where $\boldsymbol{\nu}$ indicates the outward unit normal to Γ. This condition is called a boundary condition of the *second kind*, or a *Neumann boundary condition*. For an *impervious boundary*, $g_2 = 0$ (i.e., a no-flow boundary condition).

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

$$g_p p + g_u \rho \mathbf{u} \cdot \boldsymbol{\nu} = g_3 \quad \text{on } \Gamma,$$

where g_p, g_u, and g_3 are given functions. This condition is referred to as a *Robin* or *Dankwerts boundary condition*. Such a condition occurs when Γ is a semipervious boundary.

Finally, the initial condition can be defined in terms of p:

$$p(\mathbf{x}, 0) = p^0(\mathbf{x}), \qquad \mathbf{x} \in \Omega.$$

In general, in reservoir simulation, an initial pressure is given only at a *datum level depth*. The pressure at other locations is determined by the *gravity equilibrium condition* (cf. Section 3.4.1).

3.2 An Analytic Solution

In this section, we obtain an *analytic solution* for equation (3.20) that can be used to check the approximation accuracy for a numerical method for fluid flow in porous media and find the pressure near a wellbore. We assume that Ω is an isotropic medium (cf. Section 2.1), so $\mathbf{k} = k\mathbf{I}$, where $\mathbf{I}$ is the identity tensor. In cylindrical coordinates (r, θ, x_3), equation (3.20) takes the form

$$\begin{aligned} \phi \rho c_t \frac{\partial p}{\partial t} = & \frac{1}{r} \frac{\partial}{\partial r} \left[\frac{r \rho k}{\mu} \left(\frac{\partial p}{\partial r} - \rho g \wp \frac{\partial z}{\partial r} \right) \right] \\ & + \frac{1}{r^2} \frac{\partial}{\partial \theta} \left[\frac{\rho k}{\mu} \left(\frac{\partial p}{\partial \theta} - \rho g \wp \frac{\partial z}{\partial \theta} \right) \right] \\ & + \frac{\partial}{\partial x_3} \left[\frac{\rho k}{\mu} \left(\frac{\partial p}{\partial x_3} - \rho g \wp \frac{\partial z}{\partial x_3} \right) \right]. \end{aligned} \tag{3.28}$$

We consider a reservoir Ω with an infinite extent in the horizontal direction. Assume that there is an isolated production well (located at $(0, 0, x_3)$) in this reservoir, all its properties are symmetric with respect to the axis of this well, and the reservoir is homogeneous in the vertical direction (cf. Fig. 3.3). In addition, if the gravity effect and density change are ignored, equation (3.28) reduces to

$$\frac{1}{\chi} \frac{\partial p}{\partial t} = \frac{\partial^2 p}{\partial r^2} + \frac{1}{r} \frac{\partial p}{\partial r}, \tag{3.29}$$

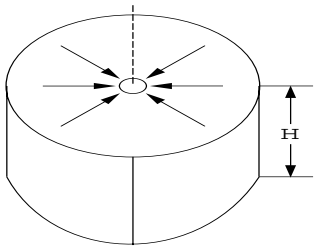

Figure 3.3. *1D radial flow.*

where

$$\chi = \frac{k}{\phi \mu c_t}.$$

Thus pressure p is a function of r and t only. That is, the flow is 1D in the radial direction. We find an analytic solution to this 1D equation. Initially, we assume that

$$p(r, 0) = p^0, \qquad 0 \le r < \infty, \tag{3.30}$$

where p^0 is constant. The boundary conditions are given by

$$\begin{aligned} p(r, t) &= p^0 && \text{as } r \to \infty,\ t \ge 0, \\ r\frac{\partial p}{\partial r} &= \frac{Q\mu}{2\pi k H} && \text{as } r \to 0, \quad t > 0, \end{aligned} \tag{3.31}$$

where Q is a fixed production rate of the well and H is the thickness of the reservoir.

To solve (3.29), we introduce the *Boltzmann change of variable*

$$y = \frac{r^2}{4t\chi}, \qquad t > 0.$$

Then we see that

$$\begin{aligned} \frac{\partial p}{\partial r} &= \frac{dp}{dy}\frac{\partial y}{\partial r} = \frac{dp}{dy}\frac{r}{2t\chi}, \\ \frac{\partial^2 p}{\partial r^2} &= \frac{\partial}{\partial r}\left(\frac{dp}{dy}\frac{r}{2t\chi}\right) = \frac{d^2 p}{dy^2}\left(\frac{r}{2t\chi}\right)^2 + \frac{dp}{dy}\frac{1}{2t\chi}, \\ \frac{\partial p}{\partial t} &= \frac{dp}{dy}\frac{\partial y}{\partial t} = -\frac{dp}{dy}\frac{r^2}{4t^2\chi}. \end{aligned} \tag{3.32}$$

Substituting (3.32) into (3.29) yields

$$y\frac{d^2 p}{dy^2} + (1 + y)\frac{dp}{dy} = 0. \tag{3.33}$$

Using the *method of separation of variables*, from (3.33) we obtain

$$\frac{dp}{dy} = \frac{C}{y}e^{-y}, \tag{3.34}$$

where C is an arbitrary constant. Applying the boundary condition (3.31) to (3.34) gives

$$\frac{dp}{dy} = \frac{Q\mu}{4\pi kH}\frac{e^{-y}}{y}. \tag{3.35}$$

Note that

$$p = p^0 \qquad \text{when } y = \infty, \qquad t = 0,$$
$$p = p(r,t) \qquad \text{when } y = \frac{r^2}{4t\chi}, \quad t > 0.$$

Integration of (3.35) from $t = 0$ to any t implies

$$p(r,t) = p^0 - \frac{Q\mu}{4\pi kH}\int_{r^2/(4t\chi)}^{\infty}\frac{e^{-y}}{y}\,dy. \tag{3.36}$$

The function $\int_{r^2/(4t\chi)}^{\infty}\frac{e^{-y}}{y}\,dy$ is the *exponential integral function* and is usually written as

$$\int_{r^2/(4t\chi)}^{\infty}\frac{e^{-y}}{y}\,dy = -Ei\left(-\frac{r^2}{4t\chi}\right) = -Ei(-y).$$

Consequently, it follows from (3.36) that pressure at any r is

$$p(r,t) = p^0 + \frac{Q\mu}{4\pi kH}Ei\left(-\frac{r^2}{4t\chi}\right), \qquad t > 0. \tag{3.37}$$

The graph of $-Ei(-y)$ in terms of y is displayed in Fig. 3.4, which shows that as y increases (r increases or t decreases), $-Ei(-y)$ decreases, so $p(r,t)$ increases and $p^0 - p$ decreases. That is, the farther we are from the well, the larger the pressure but the smaller the pressure drop. The same phenomenon can be observed as t decreases.

If the well starts to operate at $t = t_0$ instead of $t = 0$, the pressure becomes

$$p(r,t) = p^0 + \frac{Q\mu}{4\pi kH}Ei\left(-\frac{r^2}{4(t-t_0)\chi}\right), \qquad t > t_0. \tag{3.38}$$

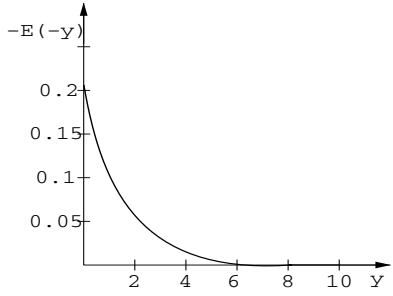

Figure 3.4. *The graph of* $-Ei(-y)$.

Similarly, if the well is located at $(x_{1,0}, x_{2,0})$ instead of $(0, 0)$, the pressure becomes

$$p(r,t) = p^0 + \frac{Q\mu}{4\pi kH} Ei\left(-\frac{(x_1 - x_{1,0})^2 + (x_2 - x_{2,0})^2}{4t\chi}\right), \qquad t > 0. \tag{3.39}$$

The exponential integral function can be expanded in the series

$$Ei\left(-\frac{r^2}{4t\chi}\right) = -\ln\left(\frac{4t\chi}{r^2}\right) + 0.5772 - \frac{r^2}{4t\chi} + \frac{1}{4}\left(\frac{r^2}{4t\chi}\right)^2 - \cdots, \quad t > 0.$$

When $r^2/(4t\chi) < 0.01$, this function can be approximated by

$$Ei\left(-\frac{r^2}{4t\chi}\right) \approx -\ln\left(\frac{4t\chi}{r^2}\right) + 0.5772 = -\ln\left(\frac{2.25t\chi}{r^2}\right),$$

and the resulting approximation error is less than 0.25%. The corresponding simplified analytic solution from (3.37) is

$$p(r,t) \approx p^0 - \frac{Q\mu}{4\pi kH} \ln\left(\frac{2.25t\chi}{r^2}\right). \tag{3.40}$$

At $r = r_w$ (the radius of the well), $r^2/(4t\chi)$ is small because r_w is small. Then, in a few seconds $r^2/(4t\chi) < 0.01$. Hence equation (3.40) can be used to find the pressure of the wellbore:

$$p_w(t) = p^0 - \frac{Q\mu}{4\pi kH} \ln\left(\frac{2.25t\chi}{r_w^2}\right). \tag{3.41}$$

3.3 Finite Difference Methods

As shown above, an analytic solution can be obtained only for a simplified reservoir system. In general, a numerical solution must be sought. For this, we very briefly touch on the finite difference methods. The books by Peaceman (1977a), Aziz and Settari (1979), and Ertekin, Abou-Kassem, and King (2001) gave detailed information on the use of these methods in reservoir simulation.

3.3.1 First Difference Quotients

We describe *first* and *second difference quotients* for functions of two space variables, x_1 and x_2, and of time, t. Reduction to functions of one space variable and extension to functions of three space variables are straightforward.

Consider a function $p(x_1, x_2, t)$ of x_1, x_2, and t. The first partial derivative of p with respect to x_1 can be defined in one of the following ways:

$$\frac{\partial p}{\partial x_1}(x_1, x_2, t) = \lim_{h_1 \to 0} \frac{p(x_1 + h_1, x_2, t) - p(x_1, x_2, t)}{h_1},$$

$$\frac{\partial p}{\partial x_1}(x_1, x_2, t) = \lim_{h_1 \to 0} \frac{p(x_1, x_2, t) - p(x_1 - h_1, x_2, t)}{h_1},$$

$$\frac{\partial p}{\partial x_1}(x_1, x_2, t) = \lim_{h_1 \to 0} \frac{p(x_1 + h_1, x_2, t) - p(x_1 - h_1, x_2, t)}{2h_1}.$$

We replace this derivative by a difference quotient. For this, we utilize the *Taylor series expansion*

$$p(x_1 + h_1, x_2, t) = p(x_1, x_2, t) + \frac{\partial p}{\partial x_1}(x_1, x_2, t)h_1 + \frac{\partial^2 p}{\partial x_1^2}(x_1^\star, x_2, t)\frac{h_1^2}{2},$$

where $x_1 \le x_1^\star \le x_1 + h_1$ and $h_1 > 0$ is a fixed number. The last term in this equation is a *remainder* that involves a second partial derivative of p. Then $\partial p/\partial x_1$ can be obtained:

$$\frac{\partial p}{\partial x_1}(x_1, x_2, t) = \frac{p(x_1 + h_1, x_2, t) - p(x_1, x_2, t)}{h_1} - \frac{\partial^2 p}{\partial x_1^2}(x_1^\star, x_2, t)\frac{h_1}{2}. \tag{3.42}$$

The expression

$$\frac{p(x_1 + h_1, x_2, t) - p(x_1, x_2, t)}{h_1}$$

is referred to as a *forward difference quotient*, and it approximates the derivative $\partial p/\partial x_1$ with an *error* of the first order in h_1.

Similarly, we have

$$\frac{\partial p}{\partial x_1}(x_1, x_2, t) = \frac{p(x_1, x_2, t) - p(x_1 - h_1, x_2, t)}{h_1} - \frac{\partial^2 p}{\partial x_1^2}(x_1^{\star\star}, x_2, t)\frac{h_1}{2}, \tag{3.43}$$

where $x_1 - h_1 \le x_1^{\star\star} \le x_1$, and the quantity

$$\frac{p(x_1, x_2, t) - p(x_1 - h_1, x_2, t)}{h_1}$$

is called a *backward difference quotient*. This quantity also gives a first order approximation to $\partial p/\partial x_1$.

Next, we use the Taylor series expansions with remainders involving a third partial derivative of p:

$$\begin{aligned} p(x_1 + h_1, x_2, t) &= p(x_1, x_2, t) + \frac{\partial p}{\partial x_1}(x_1, x_2, t)h_1 \\ &\quad + \frac{\partial^2 p}{\partial x_1^2}(x_1, x_2, t)\frac{h_1^2}{2!} + \frac{\partial^3 p}{\partial x_1^3}(x_1^\star, x_2, t)\frac{h_1^3}{3!}, \\ p(x_1 - h_1, x_2, t) &= p(x_1, x_2, t) - \frac{\partial p}{\partial x_1}(x_1, x_2, t)h_1 \\ &\quad + \frac{\partial^2 p}{\partial x_1^2}(x_1, x_2, t)\frac{h_1^2}{2!} - \frac{\partial^3 p}{\partial x_1^3}(x_1^{\star\star}, x_2, t)\frac{h_1^3}{3!}, \end{aligned}$$

where $x_1 \le x_1^\star \le x_1 + h_1$ and $x_1 - h_1 \le x_1^{\star\star} \le x_1$. Subtracting these two equations and solving for $\partial p/\partial x_1$ yields

$$\begin{aligned} \frac{\partial p}{\partial x_1}(x_1, x_2, t) &= \frac{p(x_1 + h_1, x_2, t) - p(x_1 - h_1, x_2, t)}{2h_1} \\ &\quad - \left(\frac{\partial^3 p}{\partial x_1^3}(x_1^\star, x_2, t) + \frac{\partial^3 p}{\partial x_1^3}(x_1^{\star\star}, x_2, t)\right)\frac{h_1^2}{12}. \end{aligned} \tag{3.44}$$

The quotient

$$\frac{p(x_1 + h_1, x_2, t) - p(x_1 - h_1, x_2, t)}{2h_1}$$

is termed a *centered difference quotient*, and it approximates $\partial p/\partial x_1$ with a higher order, i.e., second order in h_1.

From equations (3.42), (3.43), and (3.44), it would appear preferable to employ the centered difference approximation to $\partial p/\partial x_1$. This is not always the case. Which quotient is used depends on the particular problem (cf. Section 3.3.8).

It is sometimes necessary to use a difference quotient to approximate $\partial p/\partial x_1$ computed halfway between x_1 and $x_1 + h_1$. Analogously to (3.44), we can obtain

$$\begin{aligned}\frac{\partial p}{\partial x_1}\left(x_1 + \frac{h_1}{2}, x_2, t\right) = \frac{p(x_1 + h_1, x_2, t) - p(x_1, x_2, t)}{h_1} \\ - \left(\frac{\partial^3 p}{\partial x_1^3}(x_1^\star, x_2, t) + \frac{\partial^3 p}{\partial x_1^3}(x_1^{\star\star}, x_2, t)\right)\frac{h_1^2}{48},\end{aligned} \tag{3.45}$$

where $x_1 \le x_1^\star,\ x_1^{\star\star} \le x_1 + h_1$. In summary, we have defined three first difference quotients in x_1. The same quotients can be introduced in x_2 and t.

3.3.2 Second Difference Quotients

We exploit the Taylor series expansions with remainders involving a fourth partial derivative of p:

$$\begin{aligned}p(x_1 + h_1, x_2, t) &= p(x_1, x_2, t) + \frac{\partial p}{\partial x_1}(x_1, x_2, t)h_1 \\ &\quad + \frac{\partial^2 p}{\partial x_1^2}(x_1, x_2, t)\frac{h_1^2}{2!} + \frac{\partial^3 p}{\partial x_1^3}(x_1, x_2, t)\frac{h_1^3}{3!} + \frac{\partial^4 p}{\partial x_1^4}(x_1^\star, x_2, t)\frac{h_1^4}{4!}, \\ p(x_1 - h_1, x_2, t) &= p(x_1, x_2, t) - \frac{\partial p}{\partial x_1}(x_1, x_2, t)h_1 \\ &\quad + \frac{\partial^2 p}{\partial x_1^2}(x_1, x_2, t)\frac{h_1^2}{2!} - \frac{\partial^3 p}{\partial x_1^3}(x_1, x_2, t)\frac{h_1^3}{3!} + \frac{\partial^4 p}{\partial x_1^4}(x_1^{\star\star}, x_2, t)\frac{h_1^4}{4!},\end{aligned}$$

where $x_1 \le x_1^\star \le x_1 + h_1$ and $x_1 - h_1 \le x_1^{\star\star} \le x_1$. Adding these two equations and solving for $\partial^2 p/\partial x_1^2$ yields

$$\begin{aligned}\frac{\partial^2 p}{\partial x_1^2}(x_1, x_2, t) = \frac{p(x_1 + h_1, x_2, t) - 2p(x_1, x_2, t) + p(x_1 - h_1, x_2, t)}{h_1^2} \\ - \left(\frac{\partial^4 p}{\partial x_1^4}(x_1^\star, x_2, t) + \frac{\partial^4 p}{\partial x_1^4}(x_1^{\star\star}, x_2, t)\right)\frac{h_1^2}{24}.\end{aligned} \tag{3.46}$$

The expression

$$\Delta^2_{x_1} p(x_1, x_2, t) = \frac{p(x_1 + h_1, x_2, t) - 2p(x_1, x_2, t) + p(x_1 - h_1, x_2, t)}{h_1^2} \tag{3.47}$$

defines a *centered second difference quotient*, which approximates the partial derivative $\partial^2 p/\partial x_1^2$ with a second order accuracy in h_1.

Equation (3.46) is derived with the left and right intervals at x_1 of equal length. We now consider p on the intervals $(x_1 - h_1', x_1)$ and $(x_1, x_1 + h_1'')$, where h_1' and h_1'' are not necessarily the same, and introduce a difference quotient for the second derivative

$$\frac{\partial}{\partial x_1}\left(a(x_1, x_2, t)\frac{\partial p}{\partial x_1}\right),$$

where a is a given function. Using Taylor series expansions as above, the following approximations hold:

$$\begin{aligned}
\left(a\frac{\partial p}{\partial x_1}\right)\left(x_1 - \frac{h_1'}{2}, x_2, t\right) &\approx a\left(x_1 - \frac{h_1'}{2}, x_2, t\right)\frac{p(x_1, x_2, t) - p(x_1 - h_1', x_2, t)}{h_1'}, \\
\left(a\frac{\partial p}{\partial x_1}\right)\left(x_1 + \frac{h_1''}{2}, x_2, t\right) &\approx a\left(x_1 + \frac{h_1''}{2}, x_2, t\right)\frac{p(x_1 + h_1'', x_2, t) - p(x_1, x_2, t)}{h_1''}.
\end{aligned} \tag{3.48}$$

Note that

$$\begin{aligned}
\frac{\partial}{\partial x_1}\left(a\frac{\partial p}{\partial x_1}\right)(x_1, x_2, t) \approx \Bigg\{&\left(a\frac{\partial p}{\partial x_1}\right)\left(x_1 + \frac{h_1''}{2}, x_2, t\right) \\
&- \left(a\frac{\partial p}{\partial x_1}\right)\left(x_1 - \frac{h_1'}{2}, x_2, t\right)\Bigg\} \\
&\Bigg/\left(\left(x_1 + \frac{h_1''}{2}\right) - \left(x_1 - \frac{h_1'}{2}\right)\right).
\end{aligned}$$

Consequently, using (3.48), we see that

$$\begin{aligned}
&\frac{\partial}{\partial x_1}\left(a\frac{\partial p}{\partial x_1}\right)(x_1, x_2, t) \\
&\quad\approx \left\{a\left(x_1 + \frac{h_1''}{2}, x_2, t\right)\frac{p(x_1 + h_1'', x_2, t) - p(x_1, x_2, t)}{h_1''}\right. \\
&\qquad \left. - a\left(x_1 - \frac{h_1'}{2}, x_2, t\right)\frac{p(x_1, x_2, t) - p(x_1 - h_1', x_2, t)}{h_1'}\right\}\Bigg/\frac{h_1' + h''}{2},
\end{aligned}$$

which we write as

$$\Delta_{x_1}(a\Delta_{x_1} p). \tag{3.49}$$

This approximation to $\frac{\partial}{\partial x_1}(a\frac{\partial p}{\partial x_1})$ is of second order in h_1, where $h_1 = \max\{h_1', h_1''\}$. A similar definition can be given for $\Delta_{x_2}(a\Delta_{x_2} p)$.

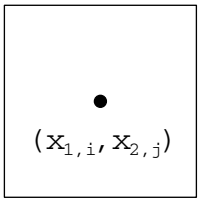

Figure 3.5. *A block-centered grid.*

3.3.3 Grid Systems

There are two types of *grid systems* commonly employed in reservoir simulation: *block-centered* and *point-distributed*. Let the integer i indicate the index in the x_1-direction, and the integer j denote the index in the x_2-direction. Furthermore, let $x_{1,i}$ and $x_{2,j}$ represent the ith and jth values of x_1 and x_2, respectively. Then we set

$$p_{ij} = p(x_{1,i}, x_{2,j}).$$

Block-centered grid

A rectangular solution domain Ω is divided into rectangles, and the point $(x_{1,i}, x_{2,j})$ is at the center of the rectangle (i, j), as in Fig. 3.5. The left side of the rectangle is at $x_{1,i-\frac{1}{2}}$, and the right side is at $x_{1,i+\frac{1}{2}}$. Similarly, $x_{2,j-\frac{1}{2}}$ and $x_{2,j+\frac{1}{2}}$ are the bottom and top sides of the rectangle (i, j). This type of grid is called a *block-centered grid*. It is specified by the sequences $0 = x_{1,\frac{1}{2}} < x_{1,\frac{3}{2}} < \cdots$ and $0 = x_{2,\frac{1}{2}} < x_{2,\frac{3}{2}} < \cdots$ if $\Omega = (0, 1)^2$ is the unit square, for example. Also, we see that

$$\begin{aligned} x_{1,i} &= \frac{1}{2}\left(x_{1,i-\frac{1}{2}} + x_{1,i+\frac{1}{2}}\right), \\ h_{1,i} &= x_{1,i+\frac{1}{2}} - x_{1,i-\frac{1}{2}}, \\ h_{1,i-\frac{1}{2}} &= x_{1,i} - x_{1,i-1}. \end{aligned}$$

Similar notation can be given for the x_2 variable.

Point-distributed grid

In the other type of grid, the point $(x_{1,i}, x_{2,j})$ is now a vertex of a rectangle, as in Fig. 3.6. This grid is referred to as a *point-distributed grid*. In this case, the grid is specified by the sequences $0 = x_{1,0} < x_{1,1} < \cdots$ and $0 = x_{2,0} < x_{2,1} < \cdots$ for $\Omega = (0, 1)^2$. Also, note that

$$\begin{aligned} x_{1,i-\frac{1}{2}} &= \frac{1}{2}\left(x_{1,i-1} + x_{1,i}\right), \\ h_{1,i} &= x_{1,i} - x_{1,i-1}. \end{aligned}$$

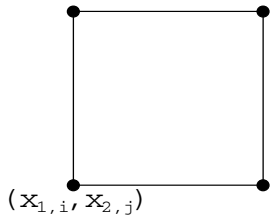

Figure 3.6. *A point-distributed grid.*

3.3.4 Treatment of Boundary Conditions

As we will see, the difference equations written for the two grid systems are the same in form. There are, however, significant differences between them. Specifically, when the grids are not uniform, the locations of points and block boundaries do not coincide. Also, the treatment of boundary conditions is different. Here we introduce difference equations to approximate the boundary conditions described in Section 3.1.4.

Boundary conditions of first kind

Suppose that we are given the boundary condition at $x_1 = 0$:

$$p(0, x_2, t) = g(x_2, t). \tag{3.50}$$

This is a boundary condition of the *first kind*, i.e., the Dirichlet kind. In reservoir simulation, Dirichlet boundary conditions arise when pressure on the reservoir boundary or at a well is specified. For a point-distributed grid (cf. Fig. 3.7), this boundary condition is given by

$$p_{0j} = g_j. \tag{3.51}$$

Equation (3.51) is utilized whenever p^n_{0j} is required in a difference equation.

For a block-centered grid, the closest point to the boundary is $(x_{1,1}, x_{2,j})$ (cf. Fig. 3.8). The value of p^n_{1j} must be *extrapolated* to this point. The simplest approach is

$$p_{1j} = g_j, \tag{3.52}$$

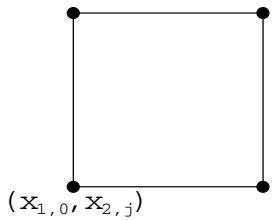

Figure 3.7. *The Dirichlet boundary condition for a point-distributed grid.*

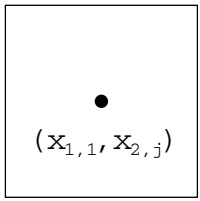

Figure 3.8. *The Dirichlet boundary condition for a block-centered grid.*

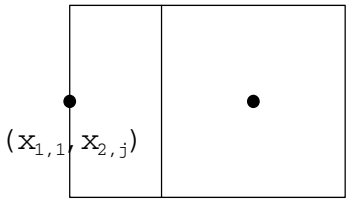

Figure 3.9. *The use of half blocks at the Dirichlet boundary.*

which is only of first order accuracy in space. A second order approximation uses

$$\frac{1}{2}\left(3p_{1j} - p_{2j}\right) = g_j. \tag{3.53}$$

Note that equation (3.53) must be included in the system of difference equations to be solved. For this reason, the block-centered grid is sometimes modified by use of half blocks at Dirichlet boundaries (cf. Fig. 3.9).

Boundary conditions of the second kind

Consider the following boundary condition at $x_1 = 0$:

$$\frac{\partial p}{\partial x_1}(0, x_2, t) = g(x_2, t). \tag{3.54}$$

This is a boundary condition of the *second kind*, i.e., the Neumann kind, and can be used to express a flow rate across a boundary or to specify an injection or production rate at a well. For a point-distributed grid, equation (3.54) can be approximated by

$$\frac{p_{1j} - p_{0j}}{h_{1,1}} = g_j, \tag{3.55}$$

which is a first order approximation. A second order accurate scheme uses a *reflection* (*ghost*) point; for each j, we introduce an auxiliary point $(x_{1,-1}, x_{2,j})$ (cf. Fig. 3.10). The boundary condition (3.54) is discretized using the centered difference at $x_1 = 0$:

$$\frac{p_{1j} - p_{-1j}}{2h_{1,1}} = g_j. \tag{3.56}$$

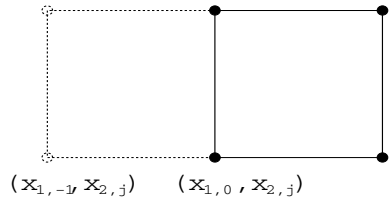

Figure 3.10. *A reflection point for a point-distributed grid.*

Equation (3.56) is exploited to eliminate $p^n_{-1\,j}$ from the difference equation for the differential equation at $x_1 = 0$. The first and second order approximations for (3.54) can also be defined for a block-centered grid, using a modification similar to that for (3.50).

Boundary conditions of the third kind

A boundary condition of the *third kind* has the form

$$\left(a\frac{\partial p}{\partial x_1} + bp\right)(0, x_2, t) = g(x_2, t), \tag{3.57}$$

where the functions a and b are given. Such a condition occurs when part of the external boundary is semipervious. For a point-distributed grid, this equation can be approximated by

$$a_{0j}\frac{p_{1j} - p_{-1j}}{2h_{1,1}} + b_{0j}p_{0j} = g_j, \tag{3.58}$$

where we recall that $(x_{1,-1}, x_{2,j})$ is a reflection point. It is difficult to approximate (3.57) for a block-centered grid.

3.3.5 Finite Differences for Stationary Problems

We consider the *stationary problem* in two dimensions on a rectangular domain Ω,

$$-\nabla \cdot (a\nabla p) = f(x_1, x_2), \quad (x_1, x_2) \in \Omega, \tag{3.59}$$

where the functions a and f are given. Function a is assumed to be positive on Ω. A pressure equation for incompressible flow is stationary, for example. As pointed out earlier, there are two types of grids widely used in reservoir simulation; the difference equations are the same in form for both grids. Equation (3.59) at grid point (i, j) can be approximated by

$$\begin{aligned} &-\frac{a_{i+\frac{1}{2},j}\dfrac{p_{i+1,j} - p_{i,j}}{h_{1,i+\frac{1}{2}}} - a_{i-\frac{1}{2},j}\dfrac{p_{i,j} - p_{i-1,j}}{h_{1,i-\frac{1}{2}}}}{h_{1,i}} \\ &-\frac{a_{i,j+\frac{1}{2}}\dfrac{p_{i,j+1} - p_{i,j}}{h_{2,j+\frac{1}{2}}} - a_{i,j-\frac{1}{2}}\dfrac{p_{i,j} - p_{i,j-1}}{h_{2,j-\frac{1}{2}}}}{h_{2,j}} = f_{ij}, \end{aligned} \tag{3.60}$$

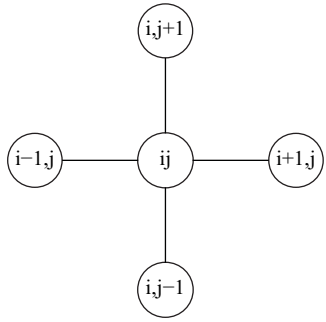

Figure 3.11. *A five-point stencil scheme.*

where $p_{ij} = p(x_{1,i}, x_{2,j})$ and $a_{i+\frac{1}{2},j} = a(x_{1,i+\frac{1}{2}}, x_{2,j})$. If we define

$$a_{1,i+\frac{1}{2},j} = \frac{a_{i+\frac{1}{2},j} h_{2,j}}{h_{1,i+\frac{1}{2}}},$$
$$a_{2,i,j+\frac{1}{2}} = \frac{a_{i,j+\frac{1}{2}} h_{1,i}}{h_{2,j+\frac{1}{2}}},$$

equation (3.60) can be then written as

$$\begin{aligned} &-a_{1,i+\frac{1}{2},j}(p_{i+1,j} - p_{i,j}) + a_{1,i-\frac{1}{2},j}(p_{i,j} - p_{i-1,j}) \\ &\quad - a_{2,i,j+\frac{1}{2}}(p_{i,j+1} - p_{i,j}) + a_{2,i,j-\frac{1}{2}}(p_{i,j} - p_{i,j-1}) = F_{ij}, \end{aligned} \tag{3.61}$$

where $F_{ij} = f_{ij} h_{1,i} h_{2,j}$. F_{ij} may be interpreted as the integral of $f(x_1, x_2)$ over a rectangle with area $h_{1,i} h_{2,j}$. The *truncation error* is the error incurred by replacing a differential equation by a difference equation. From the discussion in Section 3.3.2, the truncation error in the approximation of the difference scheme (3.61) to (3.59) is of second order in both h_1 and h_2. This scheme is the commonly used *five-point stencil* scheme for 2D problems (cf. Fig. 3.11). For some points near or on the boundary of the solution domain, it involves one or two fictitious points outside the domain. The values of p at these points are eliminated, depending on which type of grid and boundary condition is employed. Equation (3.61) can be written in matrix form involving unknowns $\{p_{i,j}\}$ and must be solved via a direct or iterative algorithm (Chen, Huan, and Ma, 2006).

3.3.6 Finite Differences for Parabolic Problems

We turn to the *transient* (*parabolic*) *problem* in two dimensions on a rectangular domain Ω,

$$\phi \frac{\partial p}{\partial t} - \nabla \cdot (a \nabla p) = f(x_1, x_2, t), \quad (x_1, x_2) \in \Omega, \ t > 0, \tag{3.62}$$

where a, f, and ϕ are given functions of x_1, x_2, and t. Functions a and ϕ are assumed to be positive and nonnegative on Ω, respectively. A pressure equation for slightly compressible

and compressible flow is parabolic. For a parabolic problem, in addition to a boundary condition, an initial condition is also needed:

$$p(x_1, x_2, 0) = p^0(x_1, x_2).$$

Let $\{t^n\}$ be a sequence of real numbers such that

$$0 = t^0 < t^1 < \cdots < t^n < t^{n+1} < \cdots .$$

For the transient problem, we proceed from the initial solution at t^0 to a solution at t^1; in general, we obtain a solution at t^{n+1} from solutions at the previous time levels. Thus the solution procedure advances through time. Set

$$\Delta t^n = t^{n+1} - t^n, \qquad n = 1, 2, \ldots,$$

and

$$p_{ij}^n = p(x_{1,i}, x_{2,j}, t^n).$$

Forward difference scheme

The simplest difference scheme for (3.62) is to replace the second partial derivatives in space by a second difference at t^n and $\partial p/\partial t$ by a forward difference. The resulting scheme is a centered second difference in space and a forward difference in time and is called the *forward difference* scheme (or *forward Euler* scheme):

$$\begin{aligned}\phi_{ij}^n \frac{p_{i,j}^{n+1} - p_{i,j}^n}{\Delta t^n} h_{1,i} h_{2,j} - a_{1,i+\frac{1}{2},j}^n (p_{i+1,j}^n - p_{i,j}^n) + a_{1,i-\frac{1}{2},j}^n (p_{i,j}^n - p_{i-1,j}^n) \\ - a_{2,i,j+\frac{1}{2}}^n (p_{i,j+1}^n - p_{i,j}^n) + a_{2,i,j-\frac{1}{2}}^n (p_{i,j}^n - p_{i,j-1}) = F_{ij}^n\end{aligned} \tag{3.63}$$

for $n = 0, 1, 2, \ldots$. Note that this equation can be solved *explicitly* for $p_{i,j}^{n+1}$. The use of an explicit scheme brings about a *stability* problem. For $a = \phi = 1$ and $f = 0$, for example, a stability analysis (cf. Section 3.3.7) shows that the time and space step sizes must satisfy the condition

$$\Delta t \left(\frac{1}{h_1^2} + \frac{1}{h_2^2} \right) \leq \frac{1}{2} \tag{3.64}$$

to obtain stability, where $\Delta t = \max\{\Delta t^n : n = 0, 1, \ldots\}$. Hence the forward difference scheme is *conditionally stable*.

Backward difference scheme

The stability condition (3.64) on the time steps is inherent in the forward difference scheme and can be removed by evaluating the second partial derivatives at t^{n+1}:

$$\begin{aligned}&\phi_{ij}^{n+1} \frac{p_{i,j}^{n+1} - p_{i,j}^n}{\Delta t^n} h_{1,i} h_{2,j} \\ &- a_{1,i+\frac{1}{2},j}^{n+1} (p_{i+1,j}^{n+1} - p_{i,j}^{n+1}) + a_{1,i-\frac{1}{2},j}^{n+1} (p_{i,j}^{n+1} - p_{i-1,j}^{n+1}) \\ &- a_{2,i,j+\frac{1}{2}}^{n+1} (p_{i,j+1}^{n+1} - p_{i,j}^{n+1}) + a_{2,i,j-\frac{1}{2}}^{n+1} (p_{i,j}^{n+1} - p_{i,j-1}^{n+1}) = F_{ij}^{n+1}.\end{aligned} \tag{3.65}$$

As we go from n to $n+1$, equation (3.65) defines $p_{i,j}^{n+1}$ *implicitly* and is termed the *backward difference* (or *backward Euler*) scheme. At each time level t^{n+1}, a linear system of algebraic equations must be solved. This system has the same form as that arising from the stationary problem. A stability analysis indicates that scheme (3.65) is *unconditionally stable*; that is, there is no restriction on the time step Δt that can be used (cf. Section 3.3.7).

The truncation errors for both the forward and backward difference schemes are of second order in h_1 and h_2 and of first order in Δt. To improve accuracy in time, the Crank–Nicolson difference scheme can be exploited, for example.

Crank–Nicolson difference scheme

Another implicit difference scheme for equation (3.62) is to replace the average $(\partial p(t^{n+1})/\partial t + \partial p(t^n)/\partial t)/2$ by the difference quotient $(p^{n+1} - p^n)/\Delta t^n$:

$$
\begin{aligned}
&\phi_{ij}^{n+1} \frac{p_{i,j}^{n+1} - p_{i,j}^{n}}{\Delta t^n} h_{1,i} h_{2,j} \\
&\quad - \frac{1}{2} \Big\{ a_{1,i+\frac{1}{2},j}^{n+1} (p_{i+1,j}^{n+1} - p_{i,j}^{n+1}) - a_{1,i-\frac{1}{2},j}^{n+1} (p_{i,j}^{n+1} - p_{i-1,j}^{n+1}) \\
&\qquad + a_{2,i,j+\frac{1}{2}}^{n+1} (p_{i,j+1}^{n+1} - p_{i,j}^{n+1}) - a_{2,i,j-\frac{1}{2}}^{n+1} (p_{i,j}^{n+1} - p_{i,j-1}^{n+1}) \\
&\qquad + a_{1,i+\frac{1}{2},j}^{n} (p_{i+1,j}^{n} - p_{i,j}^{n}) - a_{1,i-\frac{1}{2},j}^{n} (p_{i,j}^{n} - p_{i-1,j}^{n}) \\
&\qquad + a_{2,i,j+\frac{1}{2}}^{n} (p_{i,j+1}^{n} - p_{i,j}^{n}) - a_{2,i,j-\frac{1}{2}}^{n} (p_{i,j}^{n} - p_{i,j-1}^{n}) \Big\} \\
&\qquad = \frac{1}{2} \left(F_{ij}^{n+1} + F_{ij}^{n} \right).
\end{aligned}
\tag{3.66}
$$

The truncation error for this scheme is of second order in h_1, h_2, and Δt. This implicit scheme is also unconditionally stable. Moreover, it gives rise to a system of simultaneous equations that is of the same form as that arising from the backward difference scheme.

3.3.7 Consistency, Stability, and Convergence

We give the basic definitions of *consistency*, *stability*, and *convergence* of a finite difference scheme. We concentrate on pure initial value problems. When boundary conditions are included, the definitions must be extended to initial boundary value problems (Thomas, 1995). Furthermore, we focus on 1D transient problems, and the solution domain is the entire x_1-axis; i.e., $-\infty < x_1 < \infty$. Let $x_{1,i} = ih$, $i = 0, \pm 1, \pm 2, \ldots$, and $t^n = n\Delta t$, $n = 0, 1, 2, \ldots$

Consistency

For two real numbers ϵ and $h > 0$, we write

$$\epsilon = \mathcal{O}(h)$$

if there is a positive constant C such that

$$|\epsilon| \leq Ch.$$

A finite difference scheme $L_i^n P_i^n = G_i^n$ is (pointwise) *consistent* with the partial differential equation $\mathcal{L}p = \mathcal{F}$ at point (x, t) if for any smooth function $v = v(x, t)$

$$R_i^n \equiv (\mathcal{L}v - \mathcal{F})|_i^n - \left\{L_i^n v(ih, n\Delta t) - G_i^n\right\} \to 0 \tag{3.67}$$

as $h, \Delta t \to 0$ and $(ih, n\Delta t) \to (x, t)$. Note that the truncation errors for the forward difference scheme (3.63) and the backward difference scheme (3.65) take the form

$$R_i^n = \mathcal{O}(h^2) + \mathcal{O}(\Delta t),$$

whereas the truncation error for the Crank–Nicolson scheme (3.66) has the form

$$R_i^n = \mathcal{O}(h^2) + \mathcal{O}\big((\Delta t)^2\big).$$

Hence these schemes are consistent with equation (3.62).

Stability

A finite difference scheme is *stable* if the effect of an error (or perturbation) made in any stage of computation is not propagated into larger errors in later stages of the computation; i.e., if local errors are not magnified by further computation. A difference scheme can be examined for stability by substituting into it *perturbed values* of the solution.

We consider the 1D version of equation (3.62) (with $x = x_1$):

$$\frac{\partial p}{\partial t} = \frac{\partial^2 p}{\partial x^2}. \tag{3.68}$$

Let P_i^n be a solution of the corresponding forward difference scheme, and let its perturbation $P_i^n + \epsilon_i^n$ satisfy the same scheme:

$$\frac{(P_i^{n+1} + \epsilon_i^{n+1}) - (P_i^n + \epsilon_i^n)}{\Delta t} = \frac{(P_{i+1}^n + \epsilon_{i+1}^n) - 2(P_i^n + \epsilon_i^n) + (P_{i-1}^n + \epsilon_{i-1}^n)}{h^2}.$$

Because of the definition of P_i^n, we see that

$$\frac{\epsilon_i^{n+1} - \epsilon_i^n}{\Delta t} = \frac{\epsilon_{i+1}^n - 2\epsilon_i^n + \epsilon_{i-1}^n}{h^2}. \tag{3.69}$$

We expand the error ϵ_i^n in a Fourier series of the form

$$\epsilon_i^n = \sum_k \bar{\gamma}_k^n \exp(\bar{i}kx_i),$$

where $\bar{i} = \sqrt{-1}$. The analysis can be simplified somewhat if we assume that a solution to the error equation (3.69) has one term (dropping the subscript k in $\bar{\gamma}_k^n$),

$$\epsilon_i^n = \bar{\gamma}^n \exp(\bar{i}kx_i). \tag{3.70}$$

We substitute (3.70) into (3.69) and solve for the *amplification factor*

$$\bar{\gamma} = \bar{\gamma}^{n+1}/\bar{\gamma}^n.$$

The *von Neumann criterion* for stability is that the modulus of this factor must not be greater than 1 (Thomas, 1995). Using (3.69) and (3.70), we see that

$$\frac{\bar{\gamma}^{n+1} - \bar{\gamma}^n}{\Delta t} = \frac{\bar{\gamma}^n \exp(\bar{i}kh) - 2\bar{\gamma}^n + \bar{\gamma}^n \exp(-\bar{i}kh)}{h^2}. \tag{3.71}$$

Since

$$\exp(\bar{i}kh) - 2 + \exp(-\bar{i}kh) = 2\cos(kh) - 2 = -4\sin^2(kh/2),$$

it follows from (3.71) that

$$\bar{\gamma}^{n+1} = \left(1 - \frac{4\Delta t}{h^2}\sin^2(kh/2)\right)\bar{\gamma}^n.$$

Dividing this equation by $\bar{\gamma}^n$, we obtain

$$\bar{\gamma} = 1 - \frac{4\Delta t}{h^2}\sin^2(kh/2).$$

Thus the von Neumann criterion for stability is satisfied if

$$\left|1 - \frac{4\Delta t}{h^2}\sin^2(kh/2)\right| \leq 1. \tag{3.72}$$

Inequality (3.72) is satisfied when the *stability condition*

$$\frac{\Delta t}{h^2} \leq \frac{1}{2} \tag{3.73}$$

holds. Therefore, the forward difference scheme for equation (3.68) is stable under condition (3.73); i.e., this scheme is *conditionally stable*, as noted earlier.

We perform a similar von Neumann stability analysis for the backward difference scheme (3.65) for (3.68). In this case, the error equation takes the form

$$\frac{\epsilon_i^{n+1} - \epsilon_i^n}{\Delta t} = \frac{\epsilon_{i+1}^{n+1} - 2\epsilon_i^{n+1} + \epsilon_{i-1}^{n+1}}{h^2}. \tag{3.74}$$

Substituting (3.70) into (3.74) and performing simple algebraic calculations yields the equation for the amplification factor $\bar{\gamma}$,

$$\bar{\gamma} = \frac{1}{1 + (4\Delta t/h^2)\sin^2(kh/2)},$$

which is always less than or equal to 1 for any choice of k, Δt, and h. Hence the backward difference scheme is *unconditionally stable*. An analogous analysis shows that the Crank–Nicolson scheme is also unconditionally stable.

Convergence

Finite difference schemes are used because their solutions approximate the solutions to certain partial differential equations. What we really need is that the solutions of difference schemes can be made to approximate the solutions of the differential equations to any desired accuracy. Namely, we need *convergence* of the finite difference solutions to those of the differential equations. Specifically, a finite difference scheme $L_i^n P_i^n = G_i^n$ approximating the partial differential equation $\mathcal{L}p = \mathcal{F}$ is (pointwise) *convergent* if, for any (x, t), P_i^n converges to $p(x, t)$ as h, $\Delta t \to 0$ and $(ih, n\Delta t) \to (x, t)$.

As an example, we consider the forward difference scheme (3.63) for equation (3.68):

$$\frac{P_i^{n+1} - P_i^n}{\Delta t} = \frac{P_{i+1}^n - 2P_i^n + P_{i-1}^n}{h^2}. \tag{3.75}$$

Using the analysis in Section 3.3.7, it follows from (3.68) that

$$\frac{p_i^{n+1} - p_i^n}{\Delta t} = \frac{p_{i+1}^n - 2p_i^n + p_{i-1}^n}{h^2} + \mathcal{O}(h^2) + \mathcal{O}(\Delta t). \tag{3.76}$$

Define the error

$$z_i^n = P_i^n - p_i^n,$$

and subtract (3.76) from (3.75) to yield

$$z_i^{n+1} = (1 - 2\mathcal{R})z_i^n + \mathcal{R}(z_{i+1}^n + z_{i-1}^n) + \mathcal{O}(h^2\Delta t) + \mathcal{O}\big((\Delta t)^2\big),$$

where $\mathcal{R} = \Delta t/h^2$. If $0 < \mathcal{R} \le 1/2$, the coefficients on the right-hand side of this equation are nonnegative. Thus we see that

$$\begin{aligned} \left|z_i^{n+1}\right| &\le (1 - 2\mathcal{R})\left|z_i^n\right| + \mathcal{R}\left(\left|z_{i+1}^n\right| + \left|z_{i-1}^n\right|\right) + C\Delta t\left(h^2 + \Delta t\right) \\ &\le z^n + C\Delta t\left(h^2 + \Delta t\right), \end{aligned} \tag{3.77}$$

where $z^n = \sup_i\{\left|z_i^n\right|\}$ and the constant C is a uniform constant used to bound the "big $\mathcal{O}$" terms. Taking the supremum over i on the left-hand side of (3.77), we obtain

$$z^{n+1} \le z^n + C\Delta t\left(h^2 + \Delta t\right). \tag{3.78}$$

Applying inequality (3.78) repeatedly implies

$$z^{n+1} \le z^0 + C(n+1)\Delta t\left(h^2 + \Delta t\right).$$

Initially, let $z^0 = 0$. Then we have

$$\begin{aligned} \left|P_i^{n+1} - p(ih, (n+1)\Delta t)\right| &\le z^{n+1} \\ &\le C(n+1)\Delta t\left(h^2 + \Delta t\right) \\ &\to 0, \end{aligned}$$

as $(n+1)\Delta t \to t$ and $h,\ \Delta t \to 0$. Therefore, we have proven convergence of the forward difference scheme for (3.68) under condition (3.73). Convergence of the backward and Crank–Nicolson difference schemes can be shown without such a condition.

There is a connection between stability and convergence. In fact, a consistent, two-level difference scheme (i.e., it involves two time levels) for a well-posed linear initial value problem is stable if and only if it is convergent. This is the *Lax equivalence theorem* (Thomas, 1995).

3.3.8 Finite Differences for Hyperbolic Problems

For the introduction of finite differences for hyperbolic problems, we consider the model problem

$$\frac{\partial p}{\partial t} + b\frac{\partial p}{\partial x} = 0, \tag{3.79}$$

where b is a constant and $x = x_1$. This problem is a *one-way wave problem*. The 1D Buckley–Leverett equation is of this form (cf. Section 5.1.3). A boundary condition for (3.79) depends on the sign of b. If this problem is imposed on a bounded interval (l_1, l_2), for example, only an *inflow boundary condition* is needed. That is, p is given at l_1 if $b > 0$, and it is given at l_2 if $b < 0$. For brevity of presentation, we consider problem (3.79) over the entire real line $\mathbb{R}$. Of course, in any case, an initial condition must be given:

$$p(x, 0) = p^0(x).$$

Explicit schemes

We consider an *explicit scheme* for problem (3.79):

$$\frac{p_i^{n+1} - p_i^n}{\Delta t} + b\frac{p_{i+1}^n - p_i^n}{h} = 0, \tag{3.80}$$

which is consistent with (3.79). The amplification factor $\bar{\gamma}$ for (3.80) satisfies

$$\bar{\gamma} = 1 + \frac{b\Delta t}{h}(1 - \cos(kh)) - i\frac{b\Delta t}{h}\sin(kh).$$

In the case $b > 0$, $|\bar{\gamma}| > 1$. Thus, by the von Neumann criterion for stability, the difference scheme (3.80) is always *unstable*. In the case $b < 0$, it can be checked that scheme (3.80) is stable, provided that

$$\frac{|b|\Delta t}{h} \leq 1. \tag{3.81}$$

This is the Courant–Friedrichs–Lewy (CFL) condition. That is, scheme (3.80) is conditionally stable if $b < 0$.

It is not surprising that scheme (3.80) is a good choice for problem (3.79) when $b < 0$, and a bad choice when $b > 0$. When $b < 0$, the characteristic for (3.80) through any point runs down to the right towards the x-axis (cf. Fig. 3.12). Scheme (3.80) must then follow back in the same direction. For this reason, when $b > 0$, a good choice for (3.79) is

$$\frac{p_i^{n+1} - p_i^n}{\Delta t} + b\frac{p_i^n - p_{i-1}^n}{h} = 0. \tag{3.82}$$

In fact, when $b > 0$, it can be seen that scheme (3.82) is stable under condition (3.81). (It is always unstable for $b < 0$.)

The explicit difference schemes (3.80) and (3.82) are *one-sided*. Based on the stability analysis above, only the *upwind* versions are conditionally stable.

There are other difference schemes for solving problem (3.79). The centered scheme in space is

$$\frac{p_i^{n+1} - p_i^n}{\Delta t} + b\frac{p_{i+1}^n - p_{i-1}^n}{2h} = 0. \tag{3.83}$$

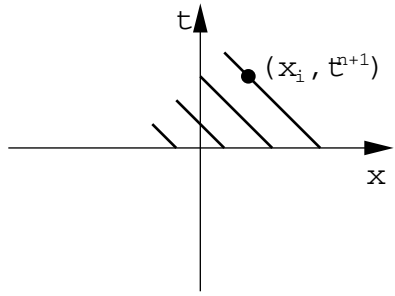

Figure 3.12. *Characteristics for problem* (3.79) *when* $b < 0$.

This scheme yields the amplification factor $\bar{\gamma}$:

$$\bar{\gamma} = 1 - \bar{i}\frac{b\Delta t}{h}\sin(kh).$$

Since $|\bar{\gamma}|^2 = 1 + b^2(\Delta t)^2 \sin^2(kh)/h^2 \geq 1$, we see that scheme (3.83) is always unstable.

Implicit schemes

A stability analysis analogous to that in the explicit case shows that one-sided, stable, fully implicit difference schemes must be upwind. When $b < 0$, the *upwind implicit scheme* is

$$\frac{p_i^{n+1} - p_i^n}{\Delta t} + b\frac{p_{i+1}^{n+1} - p_i^{n+1}}{h} = 0, \tag{3.84}$$

and when $b > 0$,

$$\frac{p_i^{n+1} - p_i^n}{\Delta t} + b\frac{p_i^{n+1} - p_{i-1}^{n+1}}{h} = 0. \tag{3.85}$$

Scheme (3.84) has the amplification factor $\bar{\gamma}$,

$$\bar{\gamma} = \left(1 - \frac{b\Delta t}{h}(1 - \cos(kh)) + \bar{i}\frac{b\Delta t}{h}\sin(kh)\right)^{-1},$$

so

$$|\bar{\gamma}|^2 = \left(1 - 4\frac{b\Delta t}{h}\sin^2\left(\frac{kh}{2}\right)\left(1 - \frac{b\Delta t}{h}\right)\right)^{-1} \leq 1 \quad \text{if } b < 0.$$

Hence scheme (3.84) is unconditionally stable when $b < 0$. A similar argument can be used to prove that scheme (3.85) has the same stability property when $b > 0$.

Now, we consider a fully implicit analogue to scheme (3.83):

$$\frac{p_i^{n+1} - p_i^n}{\Delta t} + b\frac{p_{i+1}^{n+1} - p_{i-1}^{n+1}}{2h} = 0. \tag{3.86}$$

The amplification factor $\bar{\gamma}$ of this scheme is

$$\bar{\gamma} = \left(1 + \bar{i}\frac{b\Delta t}{h}\sin(kh)\right)^{-1},$$

which satisfies $|\bar{\gamma}| \leq 1$. Therefore, scheme (3.86) is unconditionally stable, in contrast with the always unstable (3.83). A centered scheme in time (e.g., the Crank–Nicolson scheme) can be also defined for the solution of problem (3.79).

Numerical dispersion

The local *truncation error* associated with the upwind version of the difference scheme (3.80) for problem (3.79) with $b < 0$ is

$$R_i^n = -\frac{bh}{2}\frac{\partial^2 p}{\partial x^2}(x_i, t^n) - \frac{\Delta t}{2}\frac{\partial^2 p}{\partial t^2}(x_i, t^n) + \mathcal{O}(h^2) + \mathcal{O}\big((\Delta t)^2\big). \tag{3.87}$$

Differentiation of equation (3.79) with respect to t gives

$$\frac{\partial^2 p}{\partial t^2} = -b\frac{\partial^2 p}{\partial x \partial t},$$

and differentiation with respect to x yields

$$\frac{\partial^2 p}{\partial x \partial t} = -b\frac{\partial^2 p}{\partial x^2}.$$

Consequently,

$$\frac{\partial^2 p}{\partial t^2} = b^2\frac{\partial^2 p}{\partial x^2},$$

which is substituted into (3.87) to give

$$R_i^n = -\frac{bh}{2}\left(1 + \frac{b\Delta t}{h}\right)\frac{\partial^2 p}{\partial x^2}(x_i, t^n) + \mathcal{O}(h^2) + \mathcal{O}\big((\Delta t)^2\big). \tag{3.88}$$

This is the local truncation error associated with scheme (3.80).

By the definition (3.67) of the local truncation error, equation (3.88) can be written as

$$\begin{aligned}\frac{p_i^{n+1} - p_i^n}{\Delta t} + b\frac{p_{i+1}^n - p_i^n}{h} = &\left\{\frac{\partial p}{\partial t} + b\frac{\partial p}{\partial x} + a_{num}\frac{\partial^2 p}{\partial x^2}\right\}(x_i, t^n) \\ &+ \mathcal{O}(h^2) + \mathcal{O}\big((\Delta t)^2\big),\end{aligned} \tag{3.89}$$

where

$$a_{num} = \frac{bh}{2}\left(1 + \frac{b\Delta t}{h}\right). \tag{3.90}$$

Therefore, we are, in fact, solving the difference equation (3.80) for the diffusion-convection problem

$$\frac{\partial p}{\partial t} + b\frac{\partial p}{\partial x} + a_{num}\frac{\partial^2 p}{\partial x^2} = 0,$$

rather than for the pure hyperbolic problem (3.79). That is, the truncation error of (3.80) includes the *numerical dispersion* term a_{num}.

If we consider the diffusion-convection problem

$$\frac{\partial p}{\partial t} + b\frac{\partial p}{\partial x} - a\frac{\partial^2 p}{\partial x^2} = 0, \quad a > 0,$$

and develop a difference scheme similar to (3.80), then the above truncation error analysis indicates that the solution of the resulting difference equation will be associated with the problem

$$\frac{\partial p}{\partial t} + b\frac{\partial p}{\partial x} - (a - a_{num})\frac{\partial^2 p}{\partial x^2} = 0.$$

When the physical diffusion coefficient a is small, a serious problem arises. If numerical dispersion is severe (it is frequently so), a_{num} can easily dominate a. Consequently, the numerical dispersion swamps the physical dispersion, leading to a sharp front being severely smeared.

Grid orientation effects

Another drawback of finite difference methods is that the solution of a partial differential problem using these methods heavily depends on spatial orientations of a computational grid, known as *grid orientation effects*. In petroleum reservoir simulation, this means that drastically different predictions from simulators can be obtained from different grid orientations.

If an upwind technique is used as in (3.80) for a 2D counterpart, the resulting numerical dispersion is related to the quantity (cf. equation (3.90))

$$\frac{h_1}{2}\frac{\partial^2 p}{\partial x_1^2} + \frac{h_2}{2}\frac{\partial^2 p}{\partial x_2^2},$$

which is not rotationally invariant and is thus directionally dependent. When modeling multiphase flow with a high mobility ratio (mainly due to a large viscosity ratio), once a preferential flow pattern has been established, the greater mobility of the less viscous fluid causes this flow path to dominate the flow pattern. With the five-point in 2D or seven-point in 3D finite difference stencil schemes, preferred flow paths are established along the coordinate directions. Then the use of an upwind stabilizing technique greatly enhances flow in these preferred directions. This grid orientation effect is dramatic in cases with very high mobility ratios.

3.4 Numerical Solution of Single-Phase Flow

The development of finite difference methods will be carried out for the general single-phase flow equation (3.21), which applies to all the cases: incompressible, slightly compressible, and compressible. The discretization of these cases will be different, particularly in the treatment of transmissibility terms, and the difference will be pointed out as appropriate. Most noticeably, the flow equation in the incompressible case is linear and does not contain

the accumulation term, while the equations in the other two cases are nonlinear and involve the accumulation term; nonlinearity in the slightly compressible case is weaker than that in the compressible case.

Assume that the permeability tensor $\mathbf{k}$ is diagonal: $\mathbf{k} = \text{diag}(k_{11}, k_{22}, k_{33})$. Then equation (3.21) is expanded as follows:

$$\begin{aligned} c(p)\frac{\partial p}{\partial t} = &\frac{\partial}{\partial x_1}\left(\frac{\rho k_{11}}{\mu}\left(\frac{\partial p}{\partial x_1} - \gamma\frac{\partial z}{\partial x_1}\right)\right) + \frac{\partial}{\partial x_2}\left(\frac{\rho k_{22}}{\mu}\left(\frac{\partial p}{\partial x_2} - \gamma\frac{\partial z}{\partial x_2}\right)\right) \\ &+\frac{\partial}{\partial x_3}\left(\frac{\rho k_{33}}{\mu}\left(\frac{\partial p}{\partial x_3} - \gamma\frac{\partial z}{\partial x_3}\right)\right) + q, \end{aligned} \tag{3.91}$$

where $\gamma = \rho_{\mathscr{D}}$ is the fluid density in terms of pressure per distance (usually called *fluid gravity*). The grid point $(x_{1,i}, x_{2,j}, x_{3,k})$ and spatial steps $h_{1,i}$, $h_{2,j}$, and $h_{3,k}$ will be simply written as (i, j, k) and h_1, h_2, h_3, respectively. In addition, Δt will simply indicate Δt^n. Because the difference equations are the same in form for both types of grid systems, the block-centered grid structure is used as an example.

3.4.1 Treatment of Initial Conditions

In reservoir simulation, in general, an initial pressure p_d^0 is given at a *datum level depth* z_d. The pressure at other grid points (i, j, k) is determined by the *gravity equilibrium break condition*:

$$p_{i,j,k}^0 = p_d^0 + \gamma\left(z_{i,j,k} - z_d\right). \tag{3.92}$$

For slightly compressible and compressible flow, the fluid density γ depends on p. Hence an iteration procedure may be required in the application of equation (3.92).

3.4.2 Time Discretization

The time discretization of equation (3.91) is similar to that given in (3.65) for a linear parabolic problem:

$$\left(Vc(p)\frac{\partial p}{\partial t}\right)_{i,j,k}^n \approx \left(Vc\left(p^{n+1}\right)\frac{p^{n+1} - p^n}{\Delta t}\right)_{i,j,k}, \tag{3.93}$$

where $V_{i,j,k}$ is the volume of the gridblock at (i, j, k). For incompressible flow, c is zero. In slightly compressible case, $c(p) = \phi\rho c_t$, with ρ, ϕ, and c_t given by (3.13), (3.16), and (3.19), respectively. For compressible flow, $c(p)$ is defined by (3.22); particularly, for gas flow, the real gas law (3.23) can be applied.

3.4.3 Spatial Discretization

An extension of the difference equation (3.61) to equation (3.91) in three dimensions gives

$$\begin{aligned}
&\left(\frac{A_1\rho k_{11}}{\mu h_1}\right)_{i+1/2,j,k}\left(p_{i+1,j,k}-p_{i,j,k}\right)-\left(\frac{A_1\rho k_{11}}{\mu h_1}\right)_{i-1/2,j,k}\left(p_{i,j,k}-p_{i-1,j,k}\right)\\
&+\left(\frac{A_2\rho k_{22}}{\mu h_2}\right)_{i,j+1/2,k}\left(p_{i,j+1,k}-p_{i,j,k}\right)-\left(\frac{A_2\rho k_{22}}{\mu h_2}\right)_{i,j-1/2,k}\left(p_{i,j,k}-p_{i,j-1,k}\right)\\
&+\left(\frac{A_3\rho k_{33}}{\mu h_3}\right)_{i,j,k+1/2}\left(p_{i,j,k+1}-p_{i,j,k}\right)-\left(\frac{A_3\rho k_{33}}{\mu h_3}\right)_{i,j,k-1/2}\left(p_{i,j,k}-p_{i,j,k-1}\right)\\
&-\left(\frac{A_1\rho k_{11}\gamma}{\mu h_1}\right)_{i+1/2,j,k}\left(z_{i+1,j,k}-z_{i,j,k}\right)+\left(\frac{A_1\rho k_{11}\gamma}{\mu h_1}\right)_{i-1/2,j,k}\left(z_{i,j,k}-z_{i-1,j,k}\right)\\
&-\left(\frac{A_2\rho k_{22}\gamma}{\mu h_2}\right)_{i,j+1/2,k}\left(z_{i,j+1,k}-z_{i,j,k}\right)+\left(\frac{A_2\rho k_{22}\gamma}{\mu h_2}\right)_{i,j-1/2,k}\left(z_{i,j,k}-z_{i,j-1,k}\right)\\
&-\left(\frac{A_3\rho k_{33}\gamma}{\mu h_3}\right)_{i,j,k+1/2}\left(z_{i,j,k+1}-z_{i,j,k}\right)+\left(\frac{A_3\rho k_{33}\gamma}{\mu h_3}\right)_{i,j,k-1/2}\left(z_{i,j,k}-z_{i,j,k-1}\right)\\
&+Q_{i,j,k},
\end{aligned}\tag{3.94}$$

where $Q_{i,j,k}=q_{i,j,k}V_{i,j,k}$ is the injection/production and A_i is the cross-sectional area normal to the x_i-direction, $i=1,2,3$.

3.4.4 Treatment of Block Transmissibility

The transmissibilities

$$T_{1,i\pm1/2,j,k}=\left(\frac{A_1\rho k_{11}}{\mu h_1}\right)_{i\pm1/2,j,k}\tag{3.95}$$

(and analogously in the x_2- and x_3-directions) are evaluated at gridblock boundaries (as shown by the subscripts $i\pm1/2$, $j\pm1/2$, and $k\pm1/2$). The gridblock dimensions and labeling are displayed in Fig. 3.13. The grid dimension in each direction and other properties, such as formation thickness, permeability, and porosity, can significantly differ from one block to another. The rock and fluid properties are often given only at the block centers, but the transmissibilities are computed at the gridblock boundaries. Hence some sort of averaging techniques must be utilized to estimate these properties between two adjacent gridblocks.

Several averaging techniques are available for a set of real numbers $\{a_1, a_2, \ldots, a_m\}$:

- Arithmetic averaging,
$$A_A=\frac{a_1+a_2+\cdots+a_m}{m}.$$
- Geometric averaging,
$$A_G=(a_1a_2\ldots a_m)^{1/m}.$$

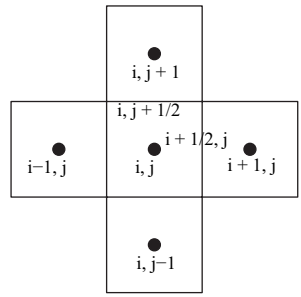

Figure 3.13. *Grid labeling.*

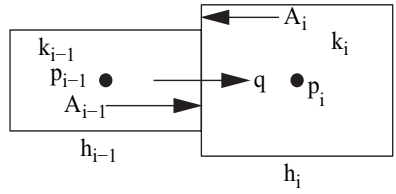

Figure 3.14. *Two cells.*

- Weighted averaging, with weights $w_1, w_2, \ldots, w_m$,

$$A_W = \frac{w_1 a_1 + w_2 a_2 + \cdots + w_m a_m}{w_1 + w_2 + \cdots + w_m}.$$

- Harmonic averaging,

$$\frac{1}{A_H} = \frac{1}{m}\left(\frac{1}{a_1} + \frac{1}{a_2} + \cdots + \frac{1}{a_m}\right).$$

Note that $A_H \le A_G \le A_A$. These averages are equal if $a_1 = a_2 = \cdots = a_m$.

The transmissibilities in equations (3.95) have two distinct quantities: $A_1 k_{11}/h_1$ represents the rock and grid properties and ρ/μ represents the fluid properties. What average should be used for these quantities?

Consider a 1D example with two cells (cf. Fig. 3.14) and a constant viscosity, without gravity. The flow rate q in the left and right cells is, respectively,

$$q = -\frac{k_{i-1}A_{i-1}}{\mu}\frac{p_{i-1/2} - p_{i-1}}{h_{i-1}/2}, \quad q = -\frac{k_i A_i}{\mu}\frac{p_i - p_{i-1/2}}{h_i/2}.$$

Consequently,

$$p_{i-1/2} - p_{i-1} = -q\mu\frac{h_{i-1}}{2}\frac{1}{(kA)_{i-1}}, \quad p_i - p_{i-1/2} = -q\mu\frac{h_i}{2}\frac{1}{(kA)_i}.$$

Adding these two equations yields

$$p_i - p_{i-1} = -\frac{q\mu}{2}\left(\frac{h_{i-1}}{(kA)_{i-1}} + \frac{h_i}{(kA)_i}\right). \tag{3.96}$$

On the other hand, the single-phase Darcy law is

$$q = -\frac{\overline{kA}}{\mu}\frac{p_i - p_{i-1}}{(h_{i-1}+h_i)/2}, \tag{3.97}$$

where $\overline{kA}$ is some average of kA at the two cell interface. Comparing equations (3.96) and (3.97), we see that

$$\overline{kA} = \frac{h_{i-1}+h_i}{\dfrac{h_{i-1}}{(kA)_{i-1}} + \dfrac{h_i}{(kA)_i}}, \tag{3.98}$$

which is the (weighted) harmonic average for kA. This average weights the effect of a lower permeability. To see this, letting $h_{i-1} = h_i$, $A_{i-1} = A_i$, $k_{i-1} = 200$ md, and $k_i = 2$ md, then we have

$$\frac{1}{k_H} = \frac{1}{2}\left(\frac{1}{k_{i-1}} + \frac{1}{k_i}\right),$$

i.e., $k_H = 3.9$ md. As a result, the flow between gridblocks is affected more by lower permeability blocks. The same argument carries over to the multiphase flow to be studied in the subsequent chapters.

From the above argument, the harmonic average is used for the rock and grid properties in the transmissibility $T_{1,i\pm1/2,j,k}$:

$$\left(\frac{A_1 k_{11}}{h_1}\right)_{i\pm1/2,j,k} = \frac{2(A_1k_{11})_{i,j,k}(A_1k_{11})_{i\pm1,j,k}}{(A_1k_{11})_{i,j,k}(h_1)_{i\pm1,j,k} + (A_1k_{11})_{i\pm1,j,k}(h_1)_{i,j,k}}; \tag{3.99}$$

similar quantities can be defined in the x_2- and x_3-directions.

Since the fluid properties in the transmissibility term for the single-phase flow do not change much from block to block (they are slowly varying functions of pressure only), the usual arithmetic average can be used for them. Two of the common methods are used in petroleum industry practices: The first one averages the pressure before the properties are computed:

$$\begin{aligned} p_{i\pm1/2,j,k} &= \beta p_{i,j,k} + (1-\beta)p_{i\pm1,j,k}, \\ \left(\frac{\rho}{\mu}\right)_{i\pm1/2,j,k} &= \left(\frac{\rho}{\mu}\right)\left(p_{i\pm1/2,j,k}\right), \end{aligned} \tag{3.100}$$

where β is a weighting factor of either 0.5 for the standard arithmetic average or the fraction of the pore volumes for the pore-volume weighted average. The second method uses the block-centered pressures and then averages the properties:

$$\left(\frac{\rho}{\mu}\right)_{i\pm1/2,j,k} = \beta\left(\frac{\rho}{\mu}\right)\left(p_{i,j,k}\right) + (1-\beta)\left(\frac{\rho}{\mu}\right)\left(p_{i\pm1,j,k}\right). \tag{3.101}$$

We end with a remark that the transmissibilities are constant for incompressible flow. It is in the slightly compressible and compressible cases that they must be carefully evaluated. For multiphase flow, the relative permeabilities can change a great deal from block to block, which will require use of a different averaging (cf. Chapter 5).

3.4.5 Solution Approaches in Time

Note that the above definition of transmissibilities has not involved time. To obtain the pressure at a certain time level t^{n+1}, the pressure equation must be advanced from an initial datum. For the discretization of linear parabolic problems in Section 3.3.6, there are essentially three different solution approaches: forward, backward, and Crank–Nicolson. The flow equation under consideration raises another difficulty: nonlinearity; i.e., the coefficients in this equation depend on the pressure. Four approaches for linearizing the coefficients are discussed: explicit, linearization, extrapolation, and fully implicit.

Explicit approach

In the explicit solution approach, which is also called the forward difference scheme in Section 3.3.6, all the coefficients and pressure in spatial derivatives are evaluated at the previous time:

$$
\begin{aligned}
&\left(Vc\left(p^{n+1}\right)\frac{p^{n+1}-p^{n}}{\Delta t}\right)_{i,j,k}\\
&\quad= T^{n}_{1,i+1/2,j,k}\left(p^{n}_{i+1,j,k}-p^{n}_{i,j,k}\right)-T^{n}_{1,i-1/2,j,k}\left(p^{n}_{i,j,k}-p^{n}_{i-1,j,k}\right)\\
&\qquad+T^{n}_{2,i,j+1/2,k}\left(p^{n}_{i,j+1,k}-p^{n}_{i,j,k}\right)-T^{n}_{2,i,j-1/2,k}\left(p^{n}_{i,j,k}-p^{n}_{i,j-1,k}\right)\\
&\qquad+T^{n}_{3,i,j,k+1/2}\left(p^{n}_{i,j,k+1}-p^{n}_{i,j,k}\right)-T^{n}_{3,i,j,k-1/2}\left(p^{n}_{i,j,k}-p^{n}_{i,j,k-1}\right)\\
&\qquad-(T\gamma)^{n}_{1,i+1/2,j,k}\left(z_{i+1,j,k}-z_{i,j,k}\right)+(T\gamma)^{n}_{1,i-1/2,j,k}\left(z_{i,j,k}-z_{i-1,j,k}\right)\\
&\qquad-(T\gamma)^{n}_{2,i,j+1/2,k}\left(z_{i,j+1,k}-z_{i,j,k}\right)+(T\gamma)^{n}_{2,i,j-1/2,k}\left(z_{i,j,k}-z_{i,j-1,k}\right)\\
&\qquad-(T\gamma)^{n}_{3,i,j,k+1/2}\left(z_{i,j,k+1}-z_{i,j,k}\right)+(T\gamma)^{n}_{3,i,j,k-1/2}\left(z_{i,j,k}-z_{i,j,k-1}\right)\\
&\qquad+Q^{n}_{i,j,k}.
\end{aligned}
\tag{3.102}
$$

Each gridblock (i, j, k) contributes only one equation in one unknown $p^{n+1}_{i,j,k}$. Advancing the pressure from n to $n+1$ is achieved by moving through all blocks in a systematic fashion and solving equation (3.102) for $p^{n+1}_{i,j,k}$. To preserve material balance, some iteration may be needed in the evaluation of the compressibility coefficient c^{n+1}. For slightly compressible flow, an iteration may be not required in practice; this coefficient can be computed just at time level t^n, and equation (3.102) is solved in a noniterative manner. However, for compressible flow, this iteration is required.

As discussed in Section 3.3.6, the forward difference scheme is conditionally stable. That is, the time step must satisfy the stability condition for (3.102) to be stable:

$$
\Delta t \le \min_{i,j,k}\left(\frac{\left(Vc(p)\right)_{(i,j,k)}}{D_{i,j,k}}\right), \tag{3.103}
$$

where the minimum is taken over all gridblocks and

$$
D_{i,j,k}=T_{1,i+1/2,j,k}+T_{1,i-1/2,j,k}+T_{2,i,j+1/2,k}+T_{2,i,j-1/2,k}+T_{3,i,j,k+1/2}+T_{3,i,j,k-1/2}.
$$

Consequently, the explicit solution approach suffers from severe restrictions on time step sizes and is not used in numerical simulation of the single-phase flow.

Linearization approach

A way to avoid the stability problem in the explicit approach is to use the explicit treatment only in the transmissibilities:

$$
\begin{aligned}
&\left(Vc\left(p^{n+1}\right)\frac{p^{n+1}-p^{n}}{\Delta t}\right)_{i,j,k}\\
&\quad= T^{n}_{1,i+1/2,j,k}\left(p^{n+1}_{i+1,j,k}-p^{n+1}_{i,j,k}\right)-T^{n}_{1,i-1/2,j,k}\left(p^{n+1}_{i,j,k}-p^{n+1}_{i-1,j,k}\right)\\
&\qquad+T^{n}_{2,i,j+1/2,k}\left(p^{n+1}_{i,j+1,k}-p^{n+1}_{i,j,k}\right)-T^{n}_{2,i,j-1/2,k}\left(p^{n+1}_{i,j,k}-p^{n+1}_{i,j-1,k}\right)\\
&\qquad+T^{n}_{3,i,j,k+1/2}\left(p^{n+1}_{i,j,k+1}-p^{n+1}_{i,j,k}\right)-T^{n}_{3,i,j,k-1/2}\left(p^{n+1}_{i,j,k}-p^{n+1}_{i,j,k-1}\right)\\
&\qquad-(T\gamma)^{n}_{1,i+1/2,j,k}\left(z_{i+1,j,k}-z_{i,j,k}\right)+(T\gamma)^{n}_{1,i-1/2,j,k}\left(z_{i,j,k}-z_{i-1,j,k}\right)\\
&\qquad-(T\gamma)^{n}_{2,i,j+1/2,k}\left(z_{i,j+1,k}-z_{i,j,k}\right)+(T\gamma)^{n}_{2,i,j-1/2,k}\left(z_{i,j,k}-z_{i,j-1,k}\right)\\
&\qquad-(T\gamma)^{n}_{3,i,j,k+1/2}\left(z_{i,j,k+1}-z_{i,j,k}\right)+(T\gamma)^{n}_{3,i,j,k-1/2}\left(z_{i,j,k}-z_{i,j,k-1}\right)\\
&\qquad+Q^{n+1}_{i,j,k}.
\end{aligned}
\tag{3.104}
$$

For slightly compressible flow, the pressure-dependent fluid properties, ρ (or B) and μ, are weakly nonlinear and can be evaluated at the previous time level. Fig. 3.15 shows the value of transmissibility used in the explicit treatment of the linearization approach. The source/sink term $Q^{n+1}_{i,j,k}$ needs special consideration, depending on the type of the constraint of the well (cf. Chapter 4).

Equation (3.104) can be rearranged in the *seven-point stencil scheme* (cf. Fig. 3.16):

$$
\begin{aligned}
&T^{n}_{3,i,j,k-1/2}p^{n+1}_{i,j,k-1}+T^{n}_{2,i,j-1/2,k}p^{n+1}_{i,j-1,k}+T^{n}_{1,i-1/2,j,k}p^{n+1}_{i-1,j,k}\\
&\quad-\left\{\frac{1}{\Delta t}\left(Vc\left(p^{n+1}\right)\right)_{i,j,k}+T^{n}_{3,i,j,k-1/2}+T^{n}_{2,i,j-1/2,k}+T^{n}_{1,i-1/2,j,k}\right.\\
&\qquad\left.+T^{n}_{1,i+1/2,j,k}+T^{n}_{2,i,j+1/2,k}+T^{n}_{3,i,j,k+1/2}\right\}p^{n+1}_{i,j,k}\\
&\quad+T^{n}_{1,i+1/2,j,k}p^{n+1}_{i+1,j,k}+T^{n}_{2,i,j+1/2,k}p^{n+1}_{i,j+1,k}+T^{n}_{3,i,j,k+1/2}p^{n+1}_{i,j,k+1}\\
&\quad=-\frac{1}{\Delta t}\left(Vc\left(p^{n+1}\right)\right)_{i,j,k}p^{n}_{i,j,k}\\
&\qquad+(T\gamma)^{n}_{1,i+1/2,j,k}\left(z_{i+1,j,k}-z_{i,j,k}\right)-(T\gamma)^{n}_{1,i-1/2,j,k}\left(z_{i,j,k}-z_{i-1,j,k}\right)\\
&\qquad+(T\gamma)^{n}_{2,i,j+1/2,k}\left(z_{i,j+1,k}-z_{i,j,k}\right)-(T\gamma)^{n}_{2,i,j-1/2,k}\left(z_{i,j,k}-z_{i,j-1,k}\right)\\
&\qquad+(T\gamma)^{n}_{3,i,j,k+1/2}\left(z_{i,j,k+1}-z_{i,j,k}\right)-(T\gamma)^{n}_{3,i,j,k-1/2}\left(z_{i,j,k}-z_{i,j,k-1}\right)\\
&\qquad-Q^{n+1}_{i,j,k}.
\end{aligned}
\tag{3.105}
$$

Again, some iteration may be needed for the compressibility coefficient $c(p)$. Unlike the explicit solution approach, equation (3.105) is now a system of equations, which must be solved by either a direct algorithm or an iterative algorithm. When the entire grid system is written in *natural ordering* (i.e., when the unknowns are ordered by lines vertically or horizontally, in increasing orders of i, j, and k in a nested manner, where i is the innermost index, j is the intermediate index, and k is the outermost index) (Chen, Huan, and Ma, 2006),

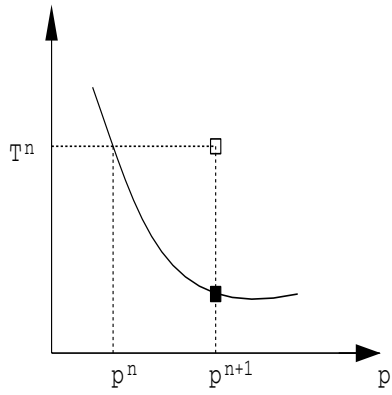

Figure 3.15. *Value of transmissibility in linearization.*

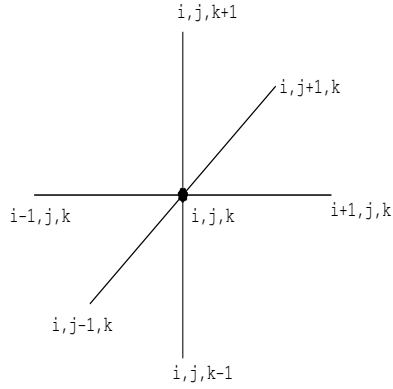

Figure 3.16. *Seven-point stencil.*

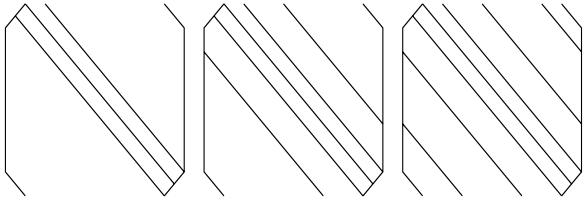

Figure 3.17. *Tridiagonal, pentadiagonal, and heptadiagonal matrices.*

the coefficient matrix associated with (3.105) is *heptadiagonal* (cf. Fig. 3.17). For 1D and 2D flow, the coefficient matrix will become *tridiagonal* and *pentadiagonal*, respectively (cf. Fig. 3.17). If there is no irregularity on the outer boundary of the reservoir, this matrix always exhibits a well-structured manner. However, this well-defined structure is usually spoiled by wells that perforate into many gridblocks and/or by irregular gridblocks.

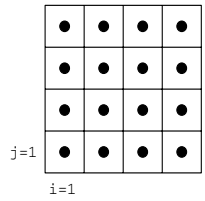

Figure 3.18. *Boundary of a domain.*

Treatment of boundary conditions

If a Dirichlet boundary condition is imposed on the external boundary of the reservoir domain, the pressures on the boundary are given. Thus, after the transmissibilities are properly evaluated on the boundary, the known pressures are moved to the right-hand side of equation (3.105).

When a Neumann boundary condition is given, for example, at the left boundary (cf. Fig. 3.18),

$$\frac{\partial p}{\partial x_1} = g,$$

the *reflection point* method (cf. Section 3.3.4) is used:

$$\frac{p_{1,j,k} - p_{0,j,k}}{h_1} = g_{j,k}. \tag{3.106}$$

A no-flow boundary condition (i.e., $g = 0$) is the most commonly used in reservoir simulation. This type of boundary condition can be alternatively modeled by assigning a zero value to the boundary transmissibility.

Extrapolation approach

The explicit handling of the transmissibility terms may result in a stability problem, especially for multiphase problems. Furthermore, the linearization will reduce the accuracy of time discretization if a more accurate discretization method in time, such as Crank–Nicolson (cf. Section 3.3.6), is used. That is true for any higher order time discretization method with the present linearization technique. This drawback can be overcome by using *extrapolation techniques* in the linearization of the transmissibility coefficients.

In the *extrapolation approach*, the pressure at the new time level is obtained from the previous two time levels,

$$p_{i,j,k}^{(n+1)^*} = p_{i,j,k}^{n} + \frac{\Delta t^{n+1}}{\Delta t^{n}}(p_{i,j,k}^{n} - p_{i,j,k}^{n-1}), \tag{3.107}$$

and the corresponding transmissibilities are evaluated at the extrapolated time level,

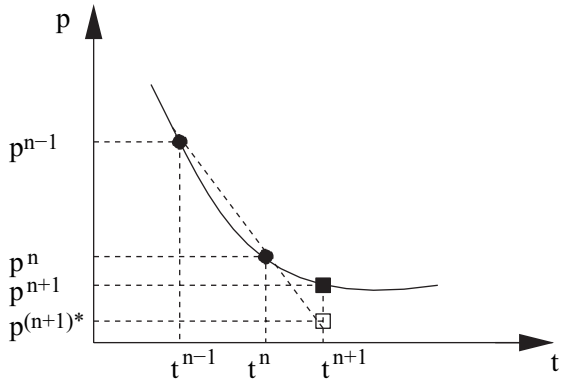

Figure 3.19. *Transmissibility in the extrapolation approach.*

$$
\begin{aligned}
&\left(Vc\left(p^{n+1}\right)\frac{p^{n+1}-p^{n}}{\Delta t}\right)_{i,j,k} \\
&\quad = T^{(n+1)^*}_{1,i+1/2,j,k}\left(p^{n+1}_{i+1,j,k}-p^{n+1}_{i,j,k}\right)-T^{(n+1)^*}_{1,i-1/2,j,k}\left(p^{n+1}_{i,j,k}-p^{n+1}_{i-1,j,k}\right) \\
&\qquad + T^{(n+1)^*}_{2,i,j+1/2,k}\left(p^{n+1}_{i,j+1,k}-p^{n+1}_{i,j,k}\right)-T^{(n+1)^*}_{2,i,j-1/2,k}\left(p^{n+1}_{i,j,k}-p^{n+1}_{i,j-1,k}\right) \\
&\qquad + T^{(n+1)^*}_{3,i,j,k+1/2}\left(p^{n+1}_{i,j,k+1}-p^{n+1}_{i,j,k}\right)-T^{(n+1)^*}_{3,i,j,k-1/2}\left(p^{n+1}_{i,j,k}-p^{n+1}_{i,j,k-1}\right) \\
&\qquad - (T\gamma)^{(n+1)^*}_{1,i+1/2,j,k}\left(z_{i+1,j,k}-z_{i,j,k}\right)+(T\gamma)^{(n+1)^*}_{1,i-1/2,j,k}\left(z_{i,j,k}-z_{i-1,j,k}\right) \\
&\qquad - (T\gamma)^{(n+1)^*}_{2,i,j+1/2,k}\left(z_{i,j+1,k}-z_{i,j,k}\right)+(T\gamma)^{(n+1)^*}_{2,i,j-1/2,k}\left(z_{i,j,k}-z_{i,j-1,k}\right) \\
&\qquad - (T\gamma)^{(n+1)^*}_{3,i,j,k+1/2}\left(z_{i,j,k+1}-z_{i,j,k}\right)+(T\gamma)^{(n+1)^*}_{3,i,j,k-1/2}\left(z_{i,j,k}-z_{i,j,k-1}\right)+Q^{n+1}_{i,j,k},
\end{aligned}
\tag{3.108}
$$

which can be also rewritten in system form as in (3.105). Fig. 3.19 indicates the pressure value used to compute the transmissibility coefficients in this approach. It shows that the closer the pressure depletion to a linear function, the more accurate the approximation $p^{(n+1)^*}$ to $p^{(n+1)}$. Note that p^{-1} is required at the first time level t^1, which is generally not given and needs special care in the first iteration.

Fully implicit approach

In the previous three approaches, all the transmissibilities have been linearized before an iterative procedure is used to obtain the pressure at the new time level. The resulting convergence of the iterative procedure is very slow because of the poor approximation of these nonlinear coefficients. Figs. 3.15 and 3.19 illustrate the approximations in these approaches. To speed up convergence, a *fully implicit approach* is used in the solution of the single-phase flow equation:

$$
\begin{aligned}
&\left(Vc\left(p^{n+1}\right)\frac{p^{n+1}-p^{n}}{\Delta t}\right)_{i,j,k}\\
&\quad= T^{n+1}_{1,i+1/2,j,k}\left(p^{n+1}_{i+1,j,k}-p^{n+1}_{i,j,k}\right)-T^{n+1}_{1,i-1/2,j,k}\left(p^{n+1}_{i,j,k}-p^{n+1}_{i-1,j,k}\right)\\
&\qquad+T^{n+1}_{2,i,j+1/2,k}\left(p^{n+1}_{i,j+1,k}-p^{n+1}_{i,j,k}\right)-T^{n+1}_{2,i,j-1/2,k}\left(p^{n+1}_{i,j,k}-p^{n+1}_{i,j-1,k}\right)\\
&\qquad+T^{n+1}_{3,i,j,k+1/2}\left(p^{n+1}_{i,j,k+1}-p^{n+1}_{i,j,k}\right)-T^{n+1}_{3,i,j,k-1/2}\left(p^{n+1}_{i,j,k}-p^{n+1}_{i,j,k-1}\right)\\
&\qquad-(T\gamma)^{n+1}_{1,i+1/2,j,k}\left(z_{i+1,j,k}-z_{i,j,k}\right)+(T\gamma)^{n+1}_{1,i-1/2,j,k}\left(z_{i,j,k}-z_{i-1,j,k}\right)\\
&\qquad-(T\gamma)^{n+1}_{2,i,j+1/2,k}\left(z_{i,j+1,k}-z_{i,j,k}\right)+(T\gamma)^{n+1}_{2,i,j-1/2,k}\left(z_{i,j,k}-z_{i,j-1,k}\right)\\
&\qquad-(T\gamma)^{n+1}_{3,i,j,k+1/2}\left(z_{i,j,k+1}-z_{i,j,k}\right)+(T\gamma)^{n+1}_{3,i,j,k-1/2}\left(z_{i,j,k}-z_{i,j,k-1}\right)\\
&\qquad+Q^{n+1}_{i,j,k}.
\end{aligned}
\tag{3.109}
$$

Now, system (3.109) is a system of nonlinear equations in p^{n+1}, which must be solved at each time step via an iteration method. Here the classic *Newton–Raphson method* is applied.

The Newton–Raphson method. Consider a general system of nonlinear differential equations:

$$
\pounds_m\{F_m\left[\mathbf{p}(\mathbf{x})\right]\}=f_m(\mathbf{x}),\quad m=1,2,\ldots,M,\quad \mathbf{x}\in\Omega,
\tag{3.110}
$$

where $\pounds_m$ denotes a linear differential operator, $F_m(\cdot)$ is a nonlinear function, $\mathbf{p}=(p_1,\,p_2,\,\ldots,\,p_M)^T$ is the vector of dependent variables, $\mathbf{f}=(f_1,\,f_2,\,\ldots,\,f_M)^T$ is a given vector, M is the total number of equations, and the superscript T denotes the transpose. The *Newton–Raphson iteration* for solving (3.110) establishes an iterative equation system. Taylor's series expansion for $F_m(\mathbf{p}+\delta\mathbf{p})$ is

$$
F_m(\mathbf{p}+\delta\mathbf{p})=F_m(\mathbf{p})+\nabla F_m(\mathbf{p})\cdot\delta\mathbf{p}+\mathcal{O}(|\delta\mathbf{p}|^2),
\tag{3.111}
$$

where $|\delta\mathbf{p}|$ is the Euclidean norm of $\delta\mathbf{p}$. If the higher order term $\mathcal{O}(|\delta\mathbf{p}|^2)$ (relative to $|\delta\mathbf{p}|$) is truncated, $F_m(\mathbf{p}+\delta\mathbf{p})$ can be approximated:

$$
F_m(\mathbf{p}+\delta\mathbf{p})\approx F_m(\mathbf{p})+\nabla F_m(\mathbf{p})\cdot\delta\mathbf{p}.
\tag{3.112}
$$

If we substitute (3.112) into (3.110), we obtain the iterative equations

$$
\begin{aligned}
\pounds_m\left[F_m(\mathbf{p}^l)+\nabla F_m(\mathbf{p}^l)\cdot\delta\mathbf{p}^{l+1}\right]&=f_m(\mathbf{x}),\\
m=1,2,\ldots,M,\quad \mathbf{x}\in\Omega,&
\end{aligned}
\tag{3.113}
$$

where $\mathbf{p}^l$ is the lth iterative solution of $\mathbf{p}$ and $\nabla F_m(\mathbf{p}^l)$ is $\nabla F_m(\mathbf{p})$ at $\mathbf{p}=\mathbf{p}^l$, with an initial solution $\mathbf{p}^0$. In the iterative equation system (3.113), the correction vector $\delta\mathbf{p}^{l+1}$ is the unknown. This system can be rewritten:

$$
\pounds_m\left[\nabla F_m(\mathbf{p}^l)\cdot\delta\mathbf{p}^{l+1}\right]=g_m(\mathbf{x}),\quad m=1,2,\ldots,M,\quad \mathbf{x}\in\Omega,
\tag{3.114}
$$

where $g_m(\mathbf{x})=f_m(\mathbf{x})-\pounds_m\left[F_m(\mathbf{p}^l)\right]$, and $F_m(\mathbf{p}^l)$ and $\nabla F_m(\mathbf{p}^l)$ are treated as fixed. Now, (3.114) is a linear system for $\delta\mathbf{p}^{l+1}$. Note that $\nabla F_m(\mathbf{p}^l)$ is the Jacobian matrix of F_m and that g_m is the *residual* of equation (3.110) at $\mathbf{p}^l$.

A new solution vector $\mathbf{p}^{l+1}$ is obtained by adding the correction vector $\delta\mathbf{p}^{l+1}$ to the previous iterative solution vector $\mathbf{p}^{l}$; i.e.,

$$\mathbf{p}^{l+1} = \mathbf{p}^{l} + \delta\mathbf{p}^{l+1}.$$

This iteration proceeds until the Euclidean norm of $\delta\mathbf{p}^{l+1}$ is smaller than a prescribed value.

The Newton–Raphson method is now applied for linearization of equation (3.109). Below we write

$$p^{n+1,l+1} = p^{n+1,l} + \delta p^{n+1,l+1} \text{ simply by } p^{l+1} = p^{l} + \delta p^{l+1}.$$

The residual of equation (3.109) at the Newton–Raphson iteration level l is

$$\begin{aligned}
R^l_{i,j,k} = &\left(Vc\left(p^l\right) \frac{p^l - p^n}{\Delta t} \right)_{i,j,k} \\
&- T^l_{1,i+1/2,j,k}\left(p^l_{i+1,j,k} - p^l_{i,j,k}\right) + T^l_{1,i-1/2,j,k}\left(p^l_{i,j,k} - p^l_{i-1,j,k}\right) \\
&- T^l_{2,i,j+1/2,k}\left(p^l_{i,j+1,k} - p^l_{i,j,k}\right) + T^l_{2,i,j-1/2,k}\left(p^l_{i,j,k} - p^l_{i,j-1,k}\right) \\
&- T^l_{3,i,j,k+1/2}\left(p^l_{i,j,k+1} - p^l_{i,j,k}\right) + T^l_{3,i,j,k-1/2}\left(p^l_{i,j,k} - p^l_{i,j,k-1}\right) \\
&+ (T\gamma)^l_{1,i+1/2,j,k}\left(z_{i+1,j,k} - z_{i,j,k}\right) - (T\gamma)^l_{1,i-1/2,j,k}\left(z_{i,j,k} - z_{i-1,j,k}\right) \\
&+ (T\gamma)^l_{2,i,j+1/2,k}\left(z_{i,j+1,k} - z_{i,j,k}\right) - (T\gamma)^l_{2,i,j-1/2,k}\left(z_{i,j,k} - z_{i,j-1,k}\right) \\
&+ (T\gamma)^l_{3,i,j,k+1/2}\left(z_{i,j,k+1} - z_{i,j,k}\right) - (T\gamma)^l_{3,i,j,k-1/2}\left(z_{i,j,k} - z_{i,j,k-1}\right) \\
&- Q^l_{i,j,k},
\end{aligned}$$

where the source/sink term $Q^l_{i,j,k}$ requires special consideration (cf. Chapter 4). Then application of the Newton–Raphson iteration yields a linear system of equations in terms of δp^{l+1}:

$$\begin{aligned}
&\frac{\partial R^l_{i,j,k}}{\partial p_{i,j,k-1}}\delta p^{l+1}_{i,j,k-1} + \frac{\partial R^l_{i,j,k}}{\partial p_{i,j-1,k}}\delta p^{l+1}_{i,j-1,k} + \frac{\partial R^l_{i,j,k}}{\partial p_{i-1,j,k}}\delta p^{l+1}_{i-1,j,k} \\
&\quad + \frac{\partial R^l_{i,j,k}}{\partial p_{i,j,k}}\delta p^{l+1}_{i,j,k} + \frac{\partial R^l_{i,j,k}}{\partial p_{i+1,j,k}}\delta p^{l+1}_{i+1,j,k} + \frac{\partial R^l_{i,j,k}}{\partial p_{i,j+1,k}}\delta p^{l+1}_{i,j+1,k} \\
&\quad + \frac{\partial R^l_{i,j,k}}{\partial p_{i,j,k+1}}\delta p^{l+1}_{i,j,k+1} = -R^l_{i,j,k},
\end{aligned} \tag{3.115}$$

which is the seven-point stencil in the increment δp^{l+1}.

In system (3.115), the derivative of the residual R in pressure p can be computed either numerically or analytically. When the numerical approach is used, the following approximation can be adopted, for example:

$$\frac{\partial T_1}{\partial p} \approx \frac{T_1(p+\epsilon) - T_1(p)}{\epsilon}.$$

The parameter ϵ should be chosen in such a way that it is small enough to produce a reasonable approximation to the derivative but large enough that a machine roundoff error does

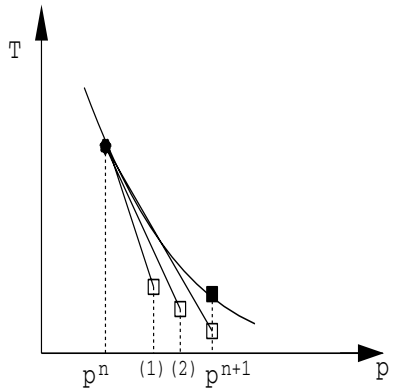

Figure 3.20. *Transmissibility in the fully implicit approach.*

not dominate the approximation. The convergence behavior of the fully implicit approach is indicated in Fig. 3.20.

In summary, we have developed explicit, linearization, and implicit time approximation approaches for numerically solving equation (3.21). In terms of computational efforts, the explicit approach is the simplest at each time step; however, it requires an impractical stability restriction. The linearization approach is more practical, but it reduces the order of accuracy in time for high order time discretization methods (unless extrapolations are exploited) and introduces stability problems. An efficient and accurate method is the fully implicit approach; the extra cost involved at each time step for this implicit method is usually more than compensated for by the fact that larger time steps may be taken. Modified implicit methods such as *semi-implicit methods* (Aziz and Settari, 1979) can be applied; for a given physical problem, the linearization approach should be applied for weak nonlinearity (e.g., the dependence of viscosity μ and density ρ on pressure p for slightly compressible flow), while the implicit one should be used for strong nonlinearity (e.g., the dependence of density ρ on p for compressible flow).

3.4.6 Material Balance Analysis

Material balance is engineering terminology for mass conservation over a fixed volume, which is the hydrocarbon reservoir. To ensure the accuracy of the numerical solution, the material balance must be checked over the entire reservoir: For a closed reservoir (no-flow boundary), the accumulation of mass must be equal to the net mass entering and leaving the boundary. That is, over each time step, it holds that

$$\sum_{i,j,k} \left(Vc\left(p^{n+1}\right) \frac{p^{n+1} - p^n}{\Delta t} \right)_{i,j,k} = \sum_{i,j,k} Q^{n+1}_{i,j,k}. \tag{3.116}$$

This material balance can also be checked over the whole time period:

$$\sum_n \sum_{i,j,k} \left(Vc\left(p^{n+1}\right) \left(p^{n+1} - p^n\right) \right)_{i,j,k} = \sum_n \sum_{i,j,k} Q^{n+1}_{i,j,k} \Delta t^n. \tag{3.117}$$

If the external boundary contains other types of boundary conditions (e.g., mass transport), equations (3.116) and (3.117) must be changed to account for these conditions. Because approximations occur in the solution process, a perfect material balance relation is seldom achieved.

Note that for an incompressible flow problem with a no-flow boundary, equation (3.116) reduces to

$$\sum_{i,j,k} Q^{n+1}_{i,j,k} = 0,$$

which is the incompressibility condition.

It follows from an addition of equation (3.109) over (i, j, k) that

$$\begin{aligned}
&\sum_{i,j,k}\left(Vc\left(p^{n+1}\right)\frac{p^{n+1}-p^{n}}{\Delta t}\right)_{i,j,k}\\
&\quad=\sum_{i,j,k}\Big\{T^{n+1}_{1,i+1/2,j,k}\left(p^{n+1}_{i+1,j,k}-p^{n+1}_{i,j,k}\right)-T^{n+1}_{1,i-1/2,j,k}\left(p^{n+1}_{i,j,k}-p^{n+1}_{i-1,j,k}\right)\\
&\qquad+T^{n+1}_{2,i,j+1/2,k}\left(p^{n+1}_{i,j+1,k}-p^{n+1}_{i,j,k}\right)-T^{n+1}_{2,i,j-1/2,k}\left(p^{n+1}_{i,j,k}-p^{n+1}_{i,j-1,k}\right)\\
&\qquad+T^{n+1}_{3,i,j,k+1/2}\left(p^{n+1}_{i,j,k+1}-p^{n+1}_{i,j,k}\right)-T^{n+1}_{3,i,j,k-1/2}\left(p^{n+1}_{i,j,k}-p^{n+1}_{i,j,k-1}\right)\\
&\qquad-(T\gamma)^{n+1}_{1,i+1/2,j,k}\left(z_{i+1,j,k}-z_{i,j,k}\right)+(T\gamma)^{n+1}_{1,i-1/2,j,k}\left(z_{i,j,k}-z_{i-1,j,k}\right)\\
&\qquad-(T\gamma)^{n+1}_{2,i,j+1/2,k}\left(z_{i,j+1,k}-z_{i,j,k}\right)+(T\gamma)^{n+1}_{2,i,j-1/2,k}\left(z_{i,j,k}-z_{i,j-1,k}\right)\\
&\qquad-(T\gamma)^{n+1}_{3,i,j,k+1/2}\left(z_{i,j,k+1}-z_{i,j,k}\right)+(T\gamma)^{n+1}_{3,i,j,k-1/2}\left(z_{i,j,k}-z_{i,j,k-1}\right)\Big\}\\
&\qquad+\sum_{i,j,k}Q^{n+1}_{i,j,k}.
\end{aligned}\tag{3.118}$$

By the material balance equation (3.116), this equation becomes

$$\begin{aligned}
&\sum_{i,j,k}\Big\{T^{n+1}_{1,i+1/2,j,k}\left(p^{n+1}_{i+1,j,k}-p^{n+1}_{i,j,k}\right)-T^{n+1}_{1,i-1/2,j,k}\left(p^{n+1}_{i,j,k}-p^{n+1}_{i-1,j,k}\right)\\
&\qquad+T^{n+1}_{2,i,j+1/2,k}\left(p^{n+1}_{i,j+1,k}-p^{n+1}_{i,j,k}\right)-T^{n+1}_{2,i,j-1/2,k}\left(p^{n+1}_{i,j,k}-p^{n+1}_{i,j-1,k}\right)\\
&\qquad+T^{n+1}_{3,i,j,k+1/2}\left(p^{n+1}_{i,j,k+1}-p^{n+1}_{i,j,k}\right)-T^{n+1}_{3,i,j,k-1/2}\left(p^{n+1}_{i,j,k}-p^{n+1}_{i,j,k-1}\right)\\
&\qquad-(T\gamma)^{n+1}_{1,i+1/2,j,k}\left(z^{n+1}_{i+1,j,k}-z^{n+1}_{i,j,k}\right)+(T\gamma)^{n+1}_{1,i-1/2,j,k}\left(z_{i,j,k}-z_{i-1,j,k}\right)\\
&\qquad-(T\gamma)^{n+1}_{2,i,j+1/2,k}\left(z_{i,j+1,k}-z_{i,j,k}\right)+(T\gamma)^{n+1}_{2,i,j-1/2,k}\left(z_{i,j,k}-z_{i,j-1,k}\right)\\
&\qquad-(T\gamma)^{n+1}_{3,i,j,k+1/2}\left(z_{i,j,k+1}-z_{i,j,k}\right)+(T\gamma)^{n+1}_{3,i,j,k-1/2}\left(z_{i,j,k}-z_{i,j,k-1}\right)\Big\}\\
&\qquad=0.
\end{aligned}\tag{3.119}$$

At any interior gridblock boundary, the flow rate across the boundary is evaluated six times: once for each adjacent block that shares the boundary. Namely, these two terms,

$T_{1,i+1/2,j,k}\left(p_{i+1,j,k}-p_{i,j,k}\right)$ and $T_{1,i-1/2,j,k}\left(p_{i,j,k}-p_{i-1,j,k}\right)$, occur in the x_1-direction; analogous terms are present in the x_2- and x_3-directions. For a closed reservoir system, the transmissibilities on the boundary can be set to zero. Then, by changing the indices in the summation of equation (3.119), we obtain (with $n+1$ omitted)

$$\begin{aligned}\sum_{i,j,k}\Bigg\{&\left(T^{+}_{1,i-1/2,j,k}-T^{-}_{1,i-1/2,j,k}\right)\left(p_{i,j,k}-p_{i-1,j,k}\right)\\&+\left(T^{+}_{2,i,j-1/2,k}-T^{-}_{2,i,j-1/2,k}\right)\left(p_{i,j,k}-p_{i,j-1,k}\right)\\&+\left(T^{+}_{3,i,j,k-1/2}-T^{-}_{3,i,j,k-1/2}\right)\left(p_{i,j,k}-p_{i,j,k-1}\right)\\&-\left((T\gamma)^{+}_{1,i-1/2,j,k}-(T\gamma)^{-}_{1,i-1/2,j,k}\right)\left(z_{i,j,k}-z_{i-1,j,k}\right)\\&-\left((T\gamma)^{+}_{2,i,j-1/2,k}-(T\gamma)^{-}_{2,i,j-1/2,k}\right)\left(z_{i,j,k}-z_{i,j-1,k}\right)\\&-\left((T\gamma)^{+}_{3,i,j,k-1/2}-(T\gamma)^{-}_{3,i,j,k-1/2}\right)\left(z_{i,j,k}-z_{i,j,k-1}\right)\Bigg\}=0,\end{aligned}\tag{3.120}$$

where the summation is taken over all the interior gridblocks and $T^{+}_{1,i-1/2,j,k}$ and $T^{-}_{1,i-1/2,j,k}$ denote the transmissibility at an internal boundary evaluated from the positive and negative directions. In the presence of a pressure and depth gradient (i.e., $p_{i,j,k}\neq p_{i-1,j,k}$ and $z_{i,j,k}\neq z_{i-1,j,k}$), equation (3.120) holds only if

$$T^{+}_{1,i-1/2,j,k}=T^{-}_{1,i-1/2,j,k}\quad\text{and}\quad(T\gamma)^{+}_{1,i-1/2,j,k}=(T\gamma)^{-}_{1,i-1/2,j,k};\tag{3.121}$$

similar equations hold in the other two coordinate directions. The physical implication of equation (3.121) is that the flow rates at any internal gridblock boundary evaluated from the positive and negative directions must be equal.