ELEMENTS OF RESERVOIR SIMULATION

BY

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AND SUPPLEMENT BY

H. S. PRICE

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FORWARD

This volume was published in its present form for the general use of participants in INTERCOMP's RESERVOIR SIMULATION SCHOOLS. These Schools which are offered annually at international locations allow an individual the opportunity to learn the powerful techniques of reservoir simulation through a proper balance of formal lectures and case study practia. The material in this publication is particularly useful in the formal lecturing phase of that balance and, because of the depth of its treatment of some subjects, it also serves as a valuable reference for the participant after the School has been completed.

It should be added that the material contained herein is not considered to be a complete exposition of all aspects of reservoir simulation. A number of subjects, especially the analysis of specific recovery processes, have yet to be added. But that will come later - the fundamentals of mathematical modelling in the reservoir engineering context and the various ways of handling these models are all here and, with them, recommendations by an authority in the field on the most convenient routes to follow.

The volume is divided into two parts: the primary portion of the book - the first 163 pages - was written by K. H. Coats while the supplemental portion - the last 28 pages - was written by H. S. Price. Coats treats the development of the basic reservoir simulation mathematical models, the manner in which they are converted to finite difference form, and the various procedures which may be used for the direct solution of the finite difference models. Price, on the other hand, completes the exposition of solution techniques by pointing out the various iterative procedures which may be used to yield solutions to the finite difference equations.

Both of these authors have had extensive experience in both the mathematical development and practical application of reservoir simulation models. Keith Coats, with advanced degrees from Michigan in both mathematics and chemical engineering, has been employed in industry with ESSO research organizations and has taught on the faculties of the universities of Michigan and Texas. Since 1968 he has been Chairman of the

Board of INTERCOMP. Harvey Price, on the other hand, has degrees from Cornell and Case Western Reserve in engineering physics and numerical mathematics, respectively, was employed by the Gulf Oil research organization, has had teaching experience at both Carnegie Mellon and Pittsburgh universities and, at the present time, is Vice President (Marketing) of INTERCOMP. Both of these individuals have made valuable contributions to the literature of reservoir simulation during the past decade. Apart from carrying on their day-to-day functions with INTERCOMP, each is called upon to assist in the presentation of the Reservoir Simulation Schools.

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ELEMENTS OF RESERVOIR SIMULATION

K. H. Coats

1. INTRODUCTION

Webster defines "simulate" as "to assume the appearance of without reality". Simulation of petroleum reservoir performance refers to the construction and operation of a model whose behavior assumes the appearance of actual reservoir behavior. The model itself is either physical (e.g. laboratory sandpack) or mathematical. A mathematical model is simply a set of equations which, subject to certain assumptions, describes the physical processes active in the reservoir. While the model itself obviously lacks the reality of the oil or gas field, the behavior of valid model approximates (assumes the appearance of) that of the field.

The purpose of simulation is estimation of field performance (e.g. oil recovery) under a variety of producing schemes. While the field can be produced only once at considerable expense, a model can be produced or "run" many times at low expense over a short period of time. Observation of model performance under different producing conditions then aids in selecting an optimum set of producing conditions for the reservoir. More specifically, reservoir simulation allows estimation of: a) field performance under water injection and/or gas injection or under natural depletion, b) the advisability of flank as opposed to pattern waterflooding, c) the effects of well locations and spacing, and d) the effect of producing rate on recovery.

The mathematical models discussed herein consist of sets of partial differential equations which express conservation of mass and/or energy. In addition, the models entail various phemonenological "laws" describing the rate processes

active in the reservoir. Example laws are those due to Darcy (fluid flow), Fourier (heat conduction), and Fick (solute transport by diffusion or dispersion). Finally, various assumptions may be invoked such as those of one- or two-dimensional flow and single- or two-phase flow, negligible dispersion or gravity or capillary effects, etc.

The model equations are generally nonlinear and require numerical solution. A computer program is written to utilize some numerical technique in solving the equation. Required program input data include fluid PVT data (e.g. formation volume factors as functions of pressure), rock relative permeability and capillary pressure curves, and reservoir description data. The latter usually constitute the bulk of the input data and are the most difficult to accurately determine.

Computed results generally consist of pressures and fluid saturations at each of (say) several hundred grid points throughout the reservoir. In problems involving heat or solute flow the model will also entail calculation of temperature or concentration at each grid point. These spatial distributions of pressure, etc., are determined at each of a sequence of time levels covering the producing period of interest.

There are several potential sources of error in computed results. First, the model itself is usually approximate since it involves certain assumptions which are only partially valid. Second, replacement of the model differential equations by difference equations introduces truncation error; that is, the exact solution of the difference equations differs somewhat from the solution to the original differential equations. Third, the exact solution of the difference equations is not obtained due to round-off error incurred by the finite word length of the computer. Finally, and perhaps most important, reservoir description data (e.g. permeability, porosity distributions) seldom are accurately known.

The level of truncation error in computed results may be estimated by repeating runs or portions of runs with smaller space and/or time increments. Significant sensitivity of computed results to changes in these increment sizes indicates a significant level of truncation error and the corresponding need for smaller spatial and/or time steps. Compared to the other error sources, round-off error is generally negligible.

Error caused by erroneous reservoir description data is difficult to determine since the true reservoir description is virtually never known. A combination of core analyses, well pressure tests and geological studies often gives valid insight into the nature of permeability and porosity distributions and reservoir geometry. The best method of obtaining a valid reservoir description is to determine (in some manner) that description which results in best agreement between calculated and observed field performance over a period of available reservoir history.

In some cases, the engineer is less concerned with the absolute accuracy of his reservoir description data and results than he is with the sensitivity of calculated results to variations in that data. This sensitivity can be determined by performing several runs with (say) 10 or 20% variation in description data. As a specific example, consider the question of estimating oil recovery from a field by waterflood as opposed to natural depletion. Assume that a computerized mathematical model using a certain reservoir description yielded recoveries of 55% for waterflood and 42% for natural depletion. Consider first the case where additional computer runs using variations in description data covering a reasonable range of uncertainty yield some spread of both figures but always a difference of 12-14% in recovery. This additional recovery by waterflood might then be accepted as meaningful. However if some reasonable descriptions result in calculated recoveries of (say) about 47% under both producing schemes then the

engineer must conclude that meaningful simulation results cannot be obtained until reservoir description is more accurately ascertained. If the engineer is interested in the absolute as well as relative levels of the two recoveries, then significant sensitivity of calculated recovery to description data variations would indicate the need for further effort on reservoir description.

The simulation model itself can be a useful tool in allocating effort and expense in determination of reservoir fluid and rock data. Computer runs may be performed at an early stage of the reservoir study to estimate sensitivity of calculated reservoir performance to variations in the various required input data. Effort should obviously be concentrated in obtaining those data which have the greatest effect on calculated performance. For example, in cases where the gravity drainage mechanism dominates oil recovery, the relative permeability curve to oil at low and middle-range oil saturations has a pronounced effect on calculated oil recovery. Gas viscosity and relative permeability and capillary pressure may play virtually no role whatsoever and effort expended in their determination is largely wasted.

Simulation model results frequently have considerable educational value, quite apart from their aid in reaching decisions regarding reservoir operation. The complex interactions of gravity, viscous and capillary forces in heterogeneous reservoirs often result in seemingly anomalous, or at least unexpected, calculated flow patterns. Verification of the validity of such patterns requires considerable insight into the physics of the situation. Such verification can often be attained by recourse to simpler models. For example, calculated water saturation profiles for a one-dimensional vertical water drive in a heterogeneous pinnacle reef reservoir exhibit pronounced oscillation with vertical distance. These calculated oscillations persist virtually unchanged despite considerable reduction of spatial and time increments, i.e. they are

not caused by truncation error. The oscillations are caused by the dependence of frontal water saturation upon both gravity and viscous forces. The ratio of these forces varies markedly with permeability of successive layers upward through the reservoir. The simpler Buckley-Leverett model, extended to heterogeneous one-dimensional systems, shows precisely the same oscillations. In high permeability layers, gravity forces dominate viscous forces and a high frontal water saturation develops. However, as this front passes upwards into a low permeability block, viscous forces are dominant and give a low frontal saturation. Upon leaving the tight layer and again entering a loose one, the frontal saturation again jumps to a high value, resulting in an oscillatory water saturation profile at any given time.

The question often arises as to the circumstances under which simulation in three-dimensions is necessary as opposed to two or even one dimension. Inclusion of flow in the third (nearly vertical) direction is often recommended only if reservoir thickness is "large" in relation to areal extent or if pronounced heterogeneity exists in the vertical direction (e.g. high stratification). These rules may be sufficient in some cases but certainly are not necessary. The following example of a three-dimensional problem is a somewhat generalized and simplified version of an actual field study.

The problem was estimation of oil recovery by crestal gas injection in a steeply-dipping reservoir. The reservoir sand was only 40 feet thick and was clean and unusually isotropic. With the simplification just mentioned, Figure 1 shows the reservoir configuration. Permeability was low at the southern boundary and increased uniformly toward the northern boundary.

Neither gas injection nor oil production wells were equally spaced or symmetrically located. The areal heterogeneity along with nonuniform well spacing dictated the need for simulation of flow at least in the two areal (x-y)

directions. In spite of the small sand thickness and homogeneity in the vertical direction, simulation of flow in the vertical direction was also required. The reason was the low relative permeability to oil in the low and middle-oil saturation range - i.e. again, the gravity drainage problem. The injected gas overrode and bypassed the oil, leaving appreciable amounts of oil behind the gas front. This oil slowly drained down-dip and normal to the bedding planes ("vertically"). This vertical gravity drainage of oil was an important mechanism in the recovery and could not be accounted for in an areal, two-dimensional (x-y) calculation.

The most frequent misuse of reservoir models is a kind of "overkill". Just a few years ago we made decisions regarding reservoir performance using only the tools of judgment and the conventional (zero-dimensional) material balance or perhaps a one-dimensional Buckley-Leverett analysis. Now, almost overnight it seems, questions regarding reservoir performance can only be answered by performing several thousand-block two- or three-dimensional simulations of two or three phase flow.

Too often we automatically apply to a problem the most sophisticated and complex calculation tool available. Typically, grid sizes are used which are finer (smaller) than justified by available information concerning reservoir properties. Often the reasons given for fine grid structure have little basis in fact. In short, the overkill referred to here is the application of models accounting for m-phase flow using n grid blocks where the questions faced could be equally well answered using a model describing m-1 or even m-2 phase flow in a grid of n/2 or n/3 blocks.

These comments are not meant to imply the lack of a need for small-grid element, three-dimensional simulations. The writer has observed well founded three-dimensional studies and ill-conceived one-dimensional simulations.

However, the use of engineering judgment in many cases would dictate use of a less complex model. Equally valid answers would be obtained at appreciably lower man and machine cost and in a shorter time. A general rule that should be followed is "select the least complicated model and grossest reservoir description which will allow the desired estimation of reservoir performance".

Another misuse of reservoir models is their application under gross uncertainty regarding input data which critically affect computed results. The writer was involved in a study of oil recovery by gas injection in a dipping, cross-section (two-dimensional vertical slice). Initially, relative permeability and other reservoir data were rather crudely estimated and a considerable number of runs were performed investigating the effect of injection rate on recovery. Subsequent sensitivity studies showed these early computed results to be largely meaningless for the following reason. The answers obtained were virtually entirely dependent upon the oil relative permeability curve employed. And variations of this curve well within the range of uncertainty gave significantly different estimates of oil recovery. The computed recovery was almost totally insensitive to gas relative permeability and capillary pressure curves and reservoir porosity. Also, reservoir permeability had an insignificant effect within a reasonable range of uncertainty. Having isolated the particular data (oil relative permeability curve) that almost solely determined the answer, we expended an intensive effort in its determination. Subsequent computer runs were then believed to yield reliable estimates of oil recovery and the quantitative effect of rate on recovery. This overriding importance of the oil relative permeability curve is typical, of course, in problems where oil recovery is dominated by the gravity drainage mechanism.

Erroneous use of reservoir models occasionally occurs in two-dimensional areal studies. The error involves inadequate representation of fluid saturation

distributions through the thickness of the reservoir. An areal, as opposed to full three-dimensional, calculation is justified in the two limiting cases of 1) fluids are completely segregated (i.e. gravitational-capillary equilibrium exists) throughout the thickness and 2) no segregation exists - i.e. fluid saturations are uniform throughout the thickness. In the latter case, rock (laboratory) relative permeability and capillary pressure curves should be used in the areal calculation. In the former case, pseudo relative permeability and curves, reflecting the state of segregation, should be employed [1]. In most cases, the assumption of segregation is more nearly correct than the assumption of uniform saturations but in many cases neither assumption is valid. If neither assumption is valid, a three-dimensional calculation should be performed or totally empirical pseudo curves for areal calculations should be determined, if possible, as those which, when used in one-dimensional areal calculations, result in agreement with two-dimensional cross-sectional calculations using laboratory curves.

A somewhat widely held misconception concerning simulation models is that they serve to eliminate the need for engineering judgment, indeed eliminate the need for engineers. Actually, the model results serve only as an aid to the engineer and management in making intelligent decisions regarding future reservoir operation. Second, an engineer using a computerized simulation model in studying a reservoir must excercise considerably more judgment than he would if no such model were employed. He must decide what type of model his questions and the reservoir warrant. The question is not <u>whether</u> to simulate but rather what tools to use in performing the simulation. In selecting the model he faces the question of what assumptions are valid for his reservoir. He must also exercise judgment in obtaining and interpreting reservoir data necessary for the model calculations.

2. NOTATION AND BASIC MATHEMATICAL OPERATIONS

2.1. Reservoir Grids and Finite Difference Notation

Reservoir simulation problems involve one or more dependent variables, typical pressure (p), temperature (T), concentration (C), saturation (S). In general, any variable U is a function of the independent spatial variables x, y, z and time t,

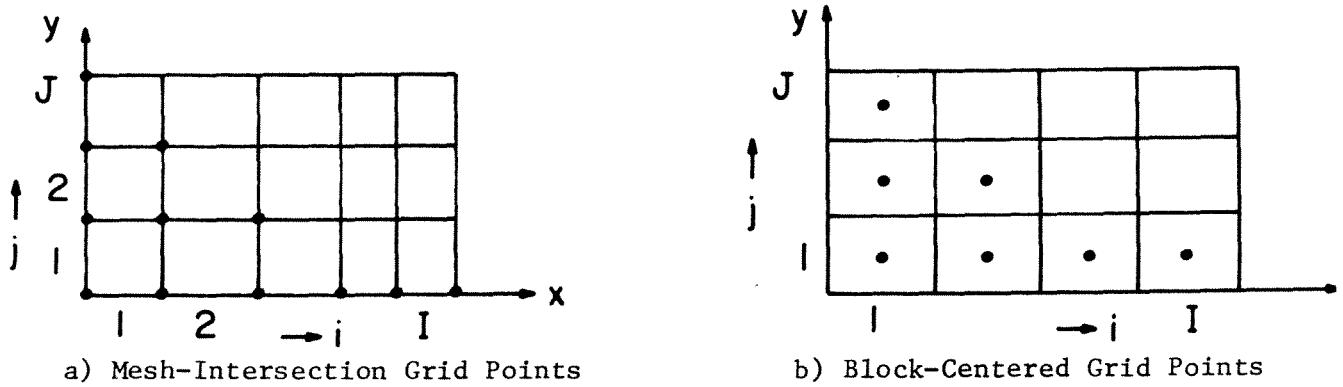
$$U = U(x,y,z,t)$$

The mathematical models are sets of partial differential equations involving partia derivatives of the dependent variables with respect to the independent variables. We approximate these derivatives by finite differences and numerically solve the resulting finite-difference equations. These difference equations involve values of the dependent variables at discrete points in space and time,

$$U_{i,j,k,n} \cong U(x_i, y_j, z_k, t_n)$$

The spatial position or point (x_i, y_j, z_k) is a grid point in the reservoir.

The two common types of grids involve mesh-intersection or block-centered grid points as illustrated in Fig. 2.1. The choice of grid type for a given problem depends largely upon the form of the boundary conditions.



a) Mesh-Intersection Grid Points b) Block-Centered Grid Points

Fig. 2.1 TWO GRID TYPES

The mesh-intersection grid of Fig. 2.1a is employed in Dirichlet-type problems where boundary conditions specify values of pressure on the reservoir boundaries. The block-centered grid has an advantage in the Neumann problem where boundary conditions specify flux or flow across the reservoir boundaries. For example, the Neumann condition of zero flow across the boundary is expressible for the block-centered grid as

$$p_{i,0} = p_{i,1} \qquad i = 1, 2, ---, I$$

The equation reflects pressure $p_{i,1}$ symmetrically across the boundary to an imaginary row of blocks having centers located $\Delta y/2$ outside the reservoir.

Throughout this text we will employ the block-centered grid. In cases of Dirichlet boundary conditions, we will utilize half-blocks on the boundary and quarter-blocks on the corners. Fig. 2.2 illustrates a block-centered grid representing the same reservoir as Fig. 2.1b. The grids of Figs. 2.1b

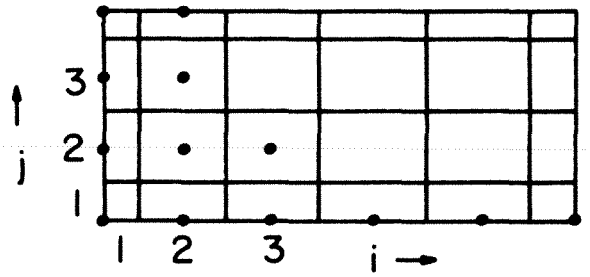


Fig. 2.2 BLOCK-CENTERED GRID FOR PRESSURE BOUNDARY CONDITION

and 2.2 would be employed for the Neumann and Dirichlet problems, respectively. Note the half-blocks on the boundaries and quarter-blocks on the corners in Fig. 2.2. The grids of Figs. 2.1 and 2.2 are referred to as "regular" grids in that regular or equal spacing is employed; Δx and Δy are constants.

Irregular grids are employed to represent reservoirs where more definition is required in certain regions due to heterogeneity or concentrations of wells. Fig. 2.3 illustrates an irregular grid. Point (x_i, y_j) is located

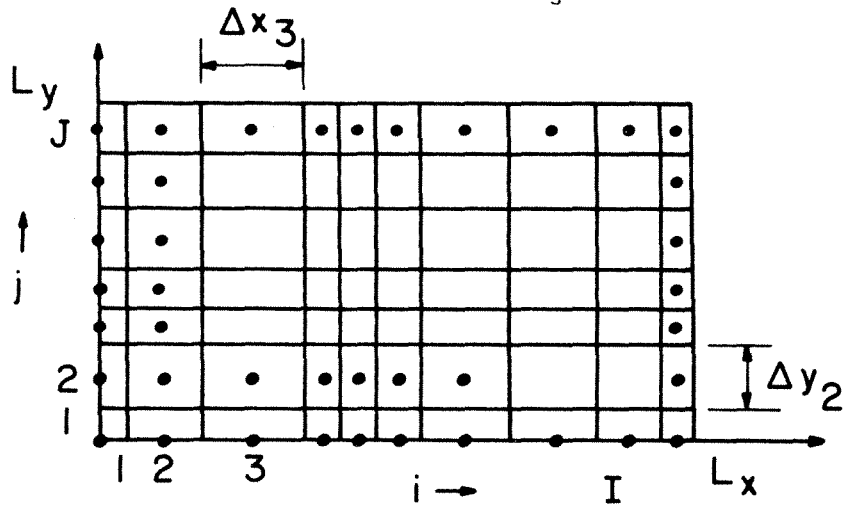


Fig. 2.3 IRREGULAR, BLOCK-CENTERED GRID

in the center of a block of dimension Δx_i, Δy_j. Fig. 2.3 also illustrates a grid for handling a problem having mixed boundary conditions. Thus, the half-blocks along the sides x = 0 and y = 0 accomodate the Diriehlet boundary condition of specified pressure. The full blocks along the sides $x = L_x$ and $y = L_y$ reflect the Neumann boundary condition of specified flux.

Fig. 2.4 shows the grid most commonly employed in a reservoir simulation. The irregular exterior boundary approximates the non-rectangular reservoir shape. The exterior boundary is closed; the Neumann boundary condition therefore applies and all boundary blocks are full blocks. A flow across a portion of the boundary can be represented by a source term ("well") in the reservoir simulation equations for the boundary blocks.

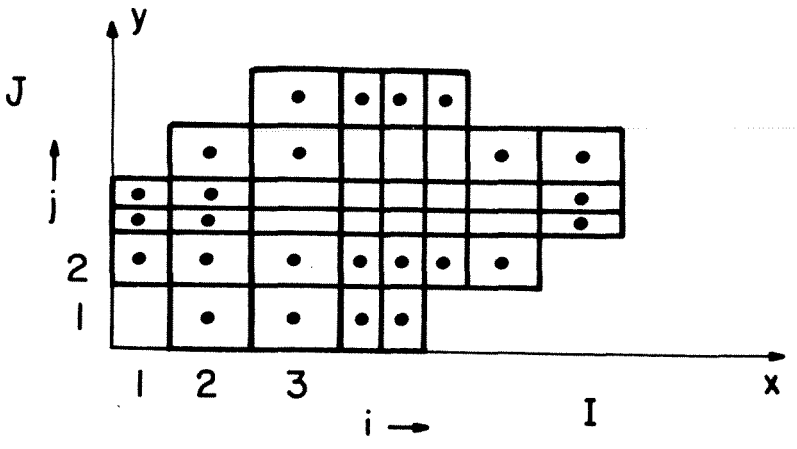


Fig. 2.4 TYPICAL RESERVOIR GRID

In general, $U_{i,j,k,n}$ is the <u>average</u> value of U(x,y,z,t) at time t_n in the block associated with the grid point. In the interest of clarity we typically suppress all subscripts which are at the "center" point i or j or k or n. Thus, for example,

$$U \equiv U_{i,j,k,n}$$

$$U_{k-1} \equiv U_{i,j,k-1,n}$$

The difference notation to be employed is

$$\Delta_x U \equiv U_{i+1} - U_i \tag{2.1}$$

That is, Δ denotes the forward difference; note that we would denote the difference $U_i - U_{i-1}$ by $\Delta_x U_{i-1}$. Second order differences are

$$\Delta_x^2 U \equiv (U_{i+1} - 2U + U_{i-1})/\Delta x^2$$

$$\Delta_y^2 U \equiv (U_{j+1} - 2U + U_{j-1})/\Delta y^2$$

$$\Delta^2 U \equiv \Delta_x^2 U + \Delta_y^2 U + \Delta_z^2 U \tag{2.2}$$

If T is a scalar function of x, y, z then

$$\Delta(T\Delta U) = \Delta_x (T \Delta_x U) + \Delta_y (T \Delta_y U) + \Delta_z (T \Delta_z U) \tag{2.3a}$$

$$\Delta_x (T \Delta_x U) = T_{i+\frac{1}{2}} (U_{i+1} - U_i) - T_{i-\frac{1}{2}} (U_i - U_{i-1}) \tag{2.3b}$$

2.2. Vector Calculus Notation

The divergence vector ∇ is defined by

$$\nabla \equiv \frac{\partial}{\partial x} \vec{i} + \frac{\partial}{\partial y} \vec{j} + \frac{\partial}{\partial z} \vec{k}$$

If p is a scalar function of x, y, z, t then

$$\nabla p = \text{grad } p = \frac{\partial p}{\partial x} \vec{i} + \frac{\partial p}{\partial y} \vec{j} + \frac{\partial p}{\partial z} \vec{k} \tag{2.4}$$

where i, j, k are unit vectors along the (orthogonal) x, y, z axes. If $\vec{v}$ is a vector function of x, y, z, t then

$$\text{div } \vec{v} = \nabla \cdot \vec{v} = (\frac{\partial}{\partial x} \vec{i} + \frac{\partial}{\partial y} \vec{j} + \frac{\partial}{\partial z} \vec{k}) \cdot (v_x \vec{i} + v_y \vec{j} + v_z \vec{k})$$

$$= \frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z} \tag{2.5}$$

If k is a scalar function of x, y, z, t then

$$k\nabla p = k \frac{\partial p}{\partial x} \vec{i} + k \frac{\partial p}{\partial y} \vec{j} + k \frac{\partial p}{\partial z} \vec{k}$$

$$\nabla \cdot (k\nabla p) = \frac{\partial}{\partial x} \left(k \frac{\partial p}{\partial x}\right) + \frac{\partial}{\partial y} \left(k \frac{\partial p}{\partial y}\right) + \frac{\partial}{\partial z} \left(k \frac{\partial p}{\partial z}\right)$$

2.3. Matrix Notation and Operations

A row vector is an ordered set of numbers $\{c_1, c_2, ----, c_n\}$, denoted here by $\underline{c}$. The transpose of this row vector is a column vector:

$$\{c_1, c_2, ----, c_n\}^T = \begin{Bmatrix} c_1 \\ c_2 \\ \cdot \\ \cdot \\ \cdot \\ c_n \end{Bmatrix}$$

Whether $\underline{c}$ is a row or column vector will either be immaterial or clear from the context. Two vectors (of the same length or order, n) are equal if their corresponding entries are equal. Thus $\underline{c} = \underline{d}$ implies $c_1 = d_1$, $c_2 = d_2$. The scalar product of two vectors of equal length is defined by

$$\underline{c} \cdot \underline{d} = c_1 d_1 + c_2 d_2 + ---- + c_n d_n \qquad (2.6)$$

The m x n matrix A has m rows and n columns:

$$A = \{a_{ij}\} = \begin{Bmatrix} a_{11} & a_{12} & ---- & a_{1n} \\ a_{21} & a_{22} & ---- & a_{2n} \\ \cdot & & & \\ \cdot & & & \\ \cdot & & & \\ a_{m1} & a_{m2} & ---- & a_{mn} \end{Bmatrix}$$

The terms $a_{i,j}$ are the matrix elements or entries and, in this text, are real

numbers. The matrix can be viewed as a set of m row vectors $\{a_{i,1}, a_{i,2}, ----, a$ or as a set of n column vectors

$$\begin{Bmatrix} a_{1,j} \\ a_{2,j} \\ \cdot \\ \cdot \\ a_{m,j} \end{Bmatrix}$$

A column vector is an m x 1 matrix while a row vector is a 1 x n matrix.

The matrix product of the m_a x n_a matrix A and the m_b x n_b matrix B is define by

$$AB = C$$

where the elements $c_{i,j}$ of the m_a x n_b C matrix are defined by

$$c_{ij} = \underline{a}_i \cdot \underline{b}_j = a_{i,1}\, b_{1,j} + a_{i,2}\, b_{2,j} + ---- + a_{i,n_a}\, b_{m_b,j}$$

$\underline{a}_i$ is the i^{th} row vector of A and $\underline{b}_j$ is the j^{th} column vector of B. The matrix product is defined only if $n_a = m_b$, i.e. A must have as many colums as B has rows. Included in this definition is the product of an m x n matrix A and a column vecto $\underline{x}$ of length n. The product $A\underline{x}$ is an m x 1 matrix or column vector where the i^{th} element is $a_{i,1}\, x_1 + a_{i,2}\, x_2 + ---- a_{i,n}\, x_n$. The matrix equation

$$A\underline{x} = \underline{b}, \tag{2.7}$$

where A is an n x n square matrix and $\underline{x}$ and $\underline{b}$ are column vectors of order n, then represents the set of equations

$$
\begin{aligned}
a_{11}\, x_1 + a_{12}\, x_2 + \text{----} + a_{1n}\, x_n &= b_1 \\
a_{21}\, x_1 + a_{22}\, x_2 + \text{----} + a_{2n}\, x_n &= b_2 \\
&\vdots \\
a_{n1}\, x_1 + a_{n2}\, x_2 + \text{----} + a_{nn}\, x_n &= b_n
\end{aligned}
\qquad (2.8)
$$

Gaussian elimination is a standard method for solution of eqs. (2.8). This elimination procedure is a series of operations on the matrix of coefficients $\{a_{ij}\}$ which reduces the matrix to <u>triangular</u> form. An <u>upper</u> triangular matrix is one in which all entries below the main diagonal are zero (i.e. $a_{ij} = 0$ if $i > j$); a <u>lower triangular</u> matrix has all entries zero above the main diagonal.

<u>EXAMPLE 2.1</u>

Solve the set of equations

$$
\begin{aligned}
x_1 - 2x_2 + x_3 - 3x_4 &= -12 \\
2x_1 - 2x_2 + 2x_3 + x_4 &= 8 \\
3x_1 - x_2 + 2x_3 - x_4 &= 3 \\
x_1 - x_2 - x_3 + 2x_4 &= 4
\end{aligned}
\qquad (2.9)
$$

<u>Solution</u>:

The <u>augmented</u> matrix B of coefficients is the 4 x 5 matrix obtained by inserting the right-hand side as the fifth column in A:

$$
B = \left\{ \begin{array}{ccccc}
\textcircled{1} & -2 & 1 & -3 & -12 \\
2 & -2 & 2 & 1 & 8 \\
3 & -1 & 2 & -1 & 3 \\
1 & -1 & -1 & 2 & 4
\end{array} \right\} = \{b_{ij}\}
$$

The upper triangular form we seek will have all entries zero below the dotted line. The first series of operations obtains zero for the entries in column 1 below the circled, diagonal, pivot element $b_{1,1}$. Multiplying each entry in the first row by $b_{2,1}$ (i.e. 2), each element in the second row by $b_{1,1}$ (i.e. 1) and then subtracting the second row (term by term) from the first yields the modified matrix

$$B_1 = \begin{Bmatrix} 1 & -2 & 1 & -3 & -12 \\ 0 & -2 & 0 & -7 & -32 \\ 3 & -1 & 2 & -1 & 3 \\ 1 & -1 & -1 & 2 & 4 \end{Bmatrix}$$

Multiplying each entry in the first row by $b_{3,1}$ (i.e. 3), each entry in the third row by $b_{1,1}$ and subtracting the third row from the first gives

$$B_2 = \begin{Bmatrix} 1 & -2 & 1 & -3 & -12 \\ 0 & -2 & 0 & -7 & -32 \\ 0 & -5 & 1 & -8 & -39 \\ 1 & -1 & -1 & 2 & 4 \end{Bmatrix}$$

Finally, multiplying the fourth row by $b_{1,1}$, the first by $b_{4,1}$, and subtracting gives

$$B_3 = \begin{Bmatrix} 1 & -2 & 1 & -3 & -12 \\ 0 & -2 & 0 & -7 & -32 \\ 0 & -5 & 1 & -8 & -39 \\ 0 & -1 & 2 & -5 & -16 \end{Bmatrix}$$

The procedure just followed to zero out the first column is now repeated, using $b_{2,2}$ as the pivot element, to obtain zeroes in the second column below the diagonal. The second row entries are first divided by the pivot element $b_{2,2}$ to obtain a pivot element of unity:

$$B_4 = \begin{Bmatrix} 1 & -2 & 1 & -3 & -12 \\ 0 & 1 & 0 & 7/2 & 16 \\ 0 & -5 & 1 & -8 & -39 \\ 0 & -1 & 2 & -5 & -16 \end{Bmatrix}$$

Multiplying the second row by -5 and subtracting the third from the second row gives

$$B_5 = \begin{Bmatrix} 1 & -2 & 1 & -3 & -12 \\ 0 & 1 & 0 & 7/2 & 16 \\ 0 & 0 & -1 & -19/2 & -41 \\ 0 & -1 & 2 & -5 & -16 \end{Bmatrix}$$

Omitting remaining steps, we finally obtain the upper triangular matrix

$$B_8 = \begin{Bmatrix} 1 & -2 & 1 & -3 & -12 \\ 0 & 1 & 0 & 7/2 & 16 \\ 0 & 0 & 1 & 19/2 & 41 \\ 0 & 0 & 0 & -41/2 & -82 \end{Bmatrix}$$

This entire set of operations has consisted of nothing more than multiplying some equation throughout by some number, multiplying another by another number

and subtracting the second equation from the first. Such operations do not change the solution $\{x_1, x_2, ----, x_n\}$ to the system of equations.

The modified, augmented matrix B_8 gives the equations

$$\begin{aligned} x_1 - 2x_2 + x_3 - 3\ x_4 &= -12 \\ x_2 + 7/2\ x_4 &= 16 \\ x_3 + 19/2\ x_4 &= 41 \\ - 41/2\ x_4 &= -82 \end{aligned}$$

The last equation directly gives

$$x_4 = 4$$

Substituting this x_4 value into the third equation gives

$$x_3 = 41 - \frac{19}{2}\ (4) = 3$$

The second equation gives

$$x_2 = 16 - \frac{7}{2}\ (4) = 2$$

and finally the first equation gives

$$x_1 = -12 + 2\ (2) - 3 + 3\ (4) = 1$$

This simple "back-solution" for x_4, x_3, x_2 and x_1 illustrates the purpose in reducing the original equations (2.9) to an upper triangular form.

Computer solution of eqs. (2.8) gives values $\{x_i\}$ which contain round-off error. This error is due to the finite number of digits carried by the computer in its arithmetic operations. The magnitude of round-off error generally increases with the number of equations solved (n). But, in addition, this error is strongly dependent upon the degree of diagonal dominance of the matrix A. A matrix $\{a_{i,j}\}$ is termed diagonally dominant if in each row the diagonal element $a_{i,i}$ is greater in absolute value than the sum of absolute values of the off-diagonal elements,

$$|a_{i,i}| > \sum_{\substack{j=1 \\ j\neq i}}^{n} |a_{i,j}| \qquad i = 1, 2, \text{----}, n$$

The greater this degree of diagonal dominance, the less the round-off error incurred in Gaussian elimination. In some cases the equations in the set (2.8) can be rearranged prior to solution, for example by interchanging the seventh and fourth equations, in order to obtain a greater degree of diagonal dominance.

The inverse of an n x n matrix A is denoted by A^{-1} and is defined by

$$A^{-1} A = A A^{-1} = I \tag{2.10}$$

where I is the identity matrix $\{\delta_{i,j}\}$, $\delta_{i,j} = 0$ if $i \neq j$, $= 1$ if $i = j$. The inverse matrix exists only if A is nonsingular, i.e. the determinant $|A| \neq 0$.

Gaussian elimination can be employed to calculate the inverse matrix. Let the matrix $A = \{a_{i,j}\}$ be given. Temporarily denote the unknown entries in the first column of A^{-1} by $\underline{x} = (x_1, x_2, \text{----}, x_n)^T$ and denote the columns of I by $\underline{\delta}_j$ (i.e. $\underline{\delta}_2 = (0, 1, 0, \text{----}, 0)^T$. By the rule of matrix multiplication, eq. (2.10) gives

$$A\underline{x} = \underline{\delta}_1 \tag{2.11}$$

which is a set of n simultaneous equations in the n unknowns x_1, x_2, ----, x_n. To solve eqs. (2.11) by Gaussian elimination, we augment the A matrix by the column vector $\underline{\delta}_1$ and render the matrix in upper triangular form, as described in Example 2.1 above. We can then continue this Gaussian elimination process to obtain the diagonal form of the augmented matrix,

$$\begin{Bmatrix} 1 & 0 & 0 & \cdot & \cdot & \cdot & \cdot & 0 & \delta'_{1,1} \\ 0 & 1 & 0 & \cdot & \cdot & \cdot & \cdot & 0 & \delta'_{2,1} \\ \cdot & & \cdot & & & & & & \cdot \\ \cdot & & & \cdot & & & & & \cdot \\ \cdot & & & & \cdot & & & & \cdot \\ \cdot & & & & & \cdot & & & \cdot \\ \cdot & & & & & & \cdot & & \cdot \\ 0 & \cdot & \cdot & \cdot & \cdot & \cdot & 0 & 1 & \delta'_{n,1} \end{Bmatrix} \tag{2.12}$$

The solution of (2.11) is then simply $x_i = \delta'_{i,1}$, i = 1, 2, ----, n.

Now let $\underline{y} = (y_1, y_2, \text{----}, y_n)^T$ denote the unknown entries of the second column of A^{-1}. Eq. (2.10) gives

$$A\underline{y} = \underline{\delta}_2 \tag{2.13}$$

Again, application of Gaussian elimination to the A matrix augmented by $\underline{\delta}_2$ gives a result identical to (2.12) except that the last column is different, $(\delta'_{1,2}, \delta'_{2,2}, \text{----}, \delta'_{n,2})$. The second column of A^{-1} is $\underline{y}$ where $y_i = \delta'_{i,2}$.

This Gaussian elimination procedure can be repeated to determine each column of the inverse matrix as the solution of a set of n equations in n unknowns. However, we will be repeating the same operations on the elements of the A matrix

each time. Thus, a more efficient procedure would be to augment the A matrix by all columns of the I matrix and perform the Gaussian elimination one time, resulting in a modified augmented matrix of form

$$\left\{\begin{array}{ccccc|ccccc} 1 & 0 & \cdot & \cdot & 0 & \delta'_{1,1} & \delta'_{1,2} & \cdot & \cdot & \delta'_{1,n} \\ 0 & 1 & 0 & \cdot & 0 & \delta'_{2,1} & \delta'_{2,2} & & & \delta'_{2,n} \\ \cdot & & & & & \cdot & & & & \\ \cdot & & & & & \cdot & & & & \\ 0 & \cdot & \cdot & 0 & 1 & \delta'_{n,1} & \delta'_{n,2} & \cdot & \cdot & \delta'_{n,n} \end{array}\right\}$$

The inverse A^{-1} is then simply the right-hand half of this matrix, i.e. $A^{-1} = \{\delta'_{ij}\}$.

EXAMPLE 2.2

Calculate by Gaussian elimination the inverse of the matrix

$$A = \left\{\begin{array}{ccc} 1 & 2 & 4 \\ 2 & 2 & 4 \\ 4 & 8 & 8 \end{array}\right\}$$

Solution:

The augmented matrix is

$$\left\{\begin{array}{ccc|ccc} 1 & 2 & 4 & 1 & 0 & 0 \\ 2 & 2 & 4 & 0 & 1 & 0 \\ 4 & 8 & 8 & 0 & 0 & 1 \end{array}\right\}$$

We first zero out the first column below the pivot element $a_{1,1}$. Multiplying the

first row by 2, the second by 1 and subtracting the second from the first gives

$$\left\{\begin{array}{ccc|ccc} 1 & 2 & 4 & 1 & 0 & 0 \\ 0 & 2 & 4 & 2 & -1 & 0 \\ 4 & 8 & 8 & 0 & 0 & 1 \end{array}\right\}$$

Proceeding in this fashion (see EXAMPLE 2.1) we obtain the upper triangular form

$$\left\{\begin{array}{ccc|ccc} 1 & 2 & 4 & 1 & 0 & 0 \\ 0 & 1 & 2 & 1 & -\frac{1}{2} & 0 \\ 0 & 0 & \textcircled{1} & \frac{1}{2} & 0 & -\frac{1}{8} \end{array}\right\}$$

We continue the Gaussian elimination to obtain zeroes in the positions indicated by the dotted triangle. First, using the encircled $a'_{3,3}$ as pivot element, zero out the entries in the third column. Multiply the third row by 2, the second row by 1 and subtract the third from the second to obtain

$$\left\{\begin{array}{ccc|ccc} 1 & 2 & 4 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & -\frac{1}{2} & \frac{1}{4} \\ 0 & 0 & 1 & \frac{1}{2} & 0 & -\frac{1}{8} \end{array}\right\}$$

We proceed in this fashion to obtain the diagonal form,

$$\left\{\begin{array}{ccc|ccc} 1 & 0 & 0 & -1 & 1 & 0 \\ 0 & 1 & 0 & 0 & -\frac{1}{2} & \frac{1}{4} \\ 0 & 0 & 1 & \frac{1}{2} & 0 & -\frac{1}{8} \end{array}\right\}$$

The inverse is then

$$A^{-1} = \begin{Bmatrix} -1 & 1 & 0 \\ 0 & -\frac{1}{2} & \frac{1}{4} \\ \frac{1}{2} & 0 & -\frac{1}{8} \end{Bmatrix}$$

The computational efforts required by alternative methods for solving a set of equations are often compared on the basis of multiplications only. The reason for this is that the computer time required for a multiplication is typically 3 to 4 times that required for an addition or subtraction. Division requires somewhat more time than a multiplication but can generally be avoided in favor of multiplication. For example, the division of $\{a_{7,j}\}$, $j = 8, 9, ----, n$ by $a_{7,7}$ in Gaussian elimination can be performed by calculating $1/a_{7,7}$ (one division) and multiplying the result into each of the set $\{a_{7,j}\}$.

The number of multiplications required in solution of eq. (2.8) by Gaussian elimination is about $n^3/3$. An equal number of additions and subtractions is required. The number of multiplications required to obtain the inverse of a full n x n matrix by Gaussian elimination is about n^3. See Problems 2.7 and 2.9 for more precise computational efforts.

PROBLEMS

2.1. For the same block size, Δx, Δy, compare the numbers of computing (grid) points necessary in the two grids of Figures 2.1b and 2.2. If grid 2.1b has I x J grid points, how many has grid 2.2?

2.2. A closed boundary, say i = I, j = 1,J on grid of Fig. 2.1b, can be represented by either of the conditions

$$A_{I+\frac{1}{2},j} = 0$$

$$p_{I,j} = p_{I+1,j}$$

Show that the term $\Delta(A\Delta p)$ assumes exactly the same form in these blocks (I,j) regardless of which of the two conditions is used.

2.3. Show that the sum

$$\sum_{i=1}^{I} \sum_{j=1}^{J} \Delta(T\Delta p)_{i,j} \equiv 0$$

for <u>any</u> values $p_{i,j}$ for the grid of Fig. 2.1b if the exterior boundary is closed. Is it also zero for the grid of Figure 2.4?

2.4. Show that

a) $$\nabla^2 p = \nabla \cdot (\nabla p) = \frac{\partial^2 p}{\partial x^2} + \frac{\partial^2 p}{\partial y^2} + \frac{\partial^2 p}{\partial z^2}$$

b) $$\nabla \cdot (k\nabla p) = k\nabla^2 p + (\nabla k) \cdot (\nabla p)$$

2.5. The inverse A^{-1} of a matrix A is defined by

$$A\,A^{-1} = A^{-1}\,A = I$$

where I is the identity matrix. Derive the inverse of the 2 x 2 matrix $A = \{a_{ij}\}$ as

$$A^{-1} = \frac{1}{a_{11}\,a_{22} - a_{12}\,a_{21}} \begin{Bmatrix} a_{22} & -a_{12} \\ -a_{21} & a_{11} \end{Bmatrix}$$

(Hint: Denote the inverse A^{-1} by $\begin{Bmatrix} x_1 & x_2 \\ x_3 & x_4 \end{Bmatrix}$. Then use the requirement that $A^{-1}\,A = I$ or $\begin{Bmatrix} x_1 & x_2 \\ x_3 & x_4 \end{Bmatrix} \begin{Bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{Bmatrix} = \begin{Bmatrix} 1 & 0 \\ 0 & 1 \end{Bmatrix}$ to define four equations in the four unknowns x_1, x_2, x_3 and x_4.)

2.6. A is an m x n matrix. In order that $\underline{c}A$ be defined, must $\underline{c}$ be a row or column vector? What must be the length of the vector $\underline{c}$?

2.7. Show that the number of multiplications required in solution of the system $A\underline{x} = \underline{b}$ by Gaussian elimination is about

$$\frac{(n+1)\;n\;(n-1)}{3} + (n+1)\;n$$

where A is a full, n x n matrix. Hint: $\sum_{i=1}^{n} i^2 = \frac{(n+1)\;n\;(n-1)}{3} + \frac{n\;(n+1)}{2}$

2.8. Use Gaussian elimination to obtain the inverse of the matrix

$$A = \begin{Bmatrix} 1 & 2 & -1 \\ 2 & 5 & 1 \\ 3 & 1 & 6 \end{Bmatrix}$$

Show that

$$A^{-1} = \frac{1}{24} \begin{Bmatrix} 29 & -13 & 7 \\ -9 & 9 & -3 \\ -13 & 5 & 1 \end{Bmatrix}$$

2.9. Show that about $n^3 + n^2$ multiplications are required to invert a full n x n matrix by Gaussian elimination.

3. FLUID & ROCK PROPERTIES

Reservoir fluid quantities are commonly expressed in units of stock tank barrels (STB) of oil and thousands of standard cubic feet (Mcf) of gas. One STB is simply a barrel of liquid at some average stock tank temperature and pressure - generally 60°F and 14.7 psia. This volume unit may be also thought of as a fixed mass since one STB is simply 5.6146 ρ_{oST} lbs_m of oil where ρ_{oST} is oil density at stock tank conditions and 5.6146 is cubic feet per barrel. Similarly one Mcf is a thousand cubic feet of gas at standard conditions of 60°F and 14.7 psia and is a fixed mass of ρ_{gST} lbs_m of gas where ρ_{gST} is gas density at standard conditions in units of lbs_m/thousand cubic feet.

Formation volume factors B_o and B_g are defined as the volumes which one STB of oil and one Mcf of gas, respectively, occupy in the reservoir at reservoir pressure p and temperature T. The gas law pV = znRT relates volume of a fixed amount of gas at p and T to volume at standard conditions as

$$B_g = \frac{1000}{5.6146} \frac{z\, p_s\, T}{p\, T_s} \frac{RB}{Mcf} \qquad (3.1)$$

where z is gas compressibility factor, a function of pressure and reservoir temperature T. The oil formation volume factor B_o is expressed in units of reservoir barrels per stock tank barrel (RB/STB). The term b is simply the inverse of B, i.e. b_o is STB/RB and b_g is Mcf/RB.

The term R_s denotes the gas dissolved in the oil, in units of Mcf/STB. Figure 3.1 illustrates typical variations of R_s and the formation volume factors with pressure. The bubble point p_b noted on the figure is also referred to as saturation pressure; R_s is constant above p_b since gas evolution does not begin until pressure falls to p_b.

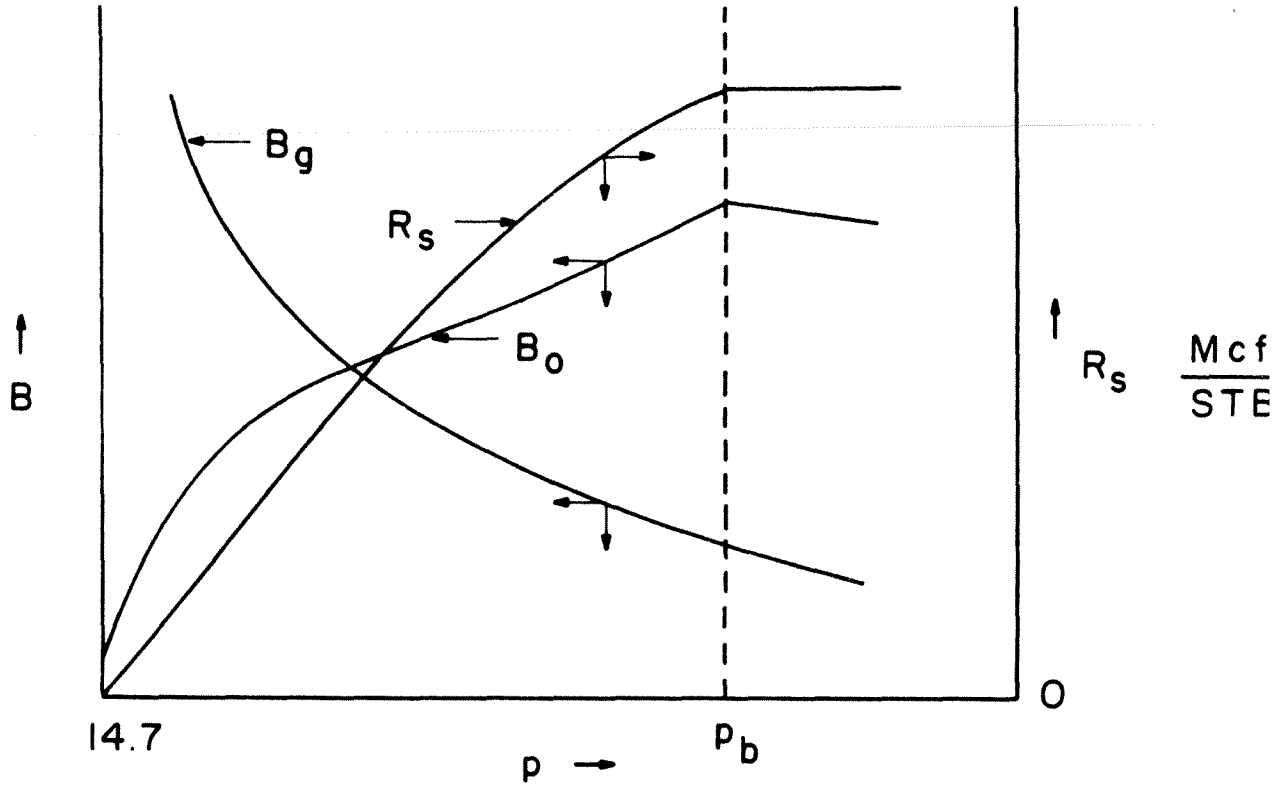


Fig. 3.1 FORMATION VOLUME FACTORS AND SOLUTION GAS VS PRESSURE

The densities of oil and gas in lbs_m/cu ft are related to R_s and the formation volume factors as

$$\rho_o = (\rho_{oST} + R_s \rho_{gST}/5.6146)\, b_o \tag{3.2}$$

$$\rho_g = \frac{\rho_{gST}}{5.6146}\, b_g \tag{3.3}$$

where ρ_{oST} is density of stock tank oil, lbs_m/cu ft, and ρ_{gST} is gas density at standard conditions, lbs_m/Mcf (see Problem 3.1).

The compressibility c of fluid is defined by

$$c \equiv -\frac{1}{V}\frac{dV}{dp} \tag{3.4}$$

where V is the volume of any fixed amount of the fluid such as one lb_m or one STB. Eq. (3.4) is thus equivalent to the relation

$$\frac{d\rho}{dp} = c\rho \tag{3.5}$$

Use of eqs. 3.5 and 3.2 and 3.3 then gives for oil at pressures above bubble point

$$c_{oil} = \frac{1}{\rho_o}\frac{d\rho_o}{dp} = \frac{1}{b_o}\frac{db_o}{dp} \tag{3.6}$$

and for gas

$$c_{gas} = \frac{1}{\rho_g}\frac{d\rho_g}{dp} = \frac{1}{b_g}\frac{db_g}{dp} \tag{3.7}$$

Compressibility is about 3×10^{-6} for water and the order of 10^{-5} psi^{-1} for oil. See Problem 3.2 for further development of gas compressibility. For slightly compressible liquids (e.g. water and most oils above their bubble points) c may often be taken as constant over the pressure range of interest and eq. (3.5) integrates to the familiar relation

$$\rho = \rho^* e^{c(p-p^*)} \tag{3.8}$$

where ρ^* is density at pressure p^*. If c is small (e.g. order of 10^{-5}) then the right hand side of eq. (3.8) is very nearly $\rho^* [1 + c (p - p^*)]$ since e^x is $1 + x + x^2/2! + x^3/3! + ----$ and for small x this is approximately $1 + x$.

Porous rock is slightly compressible and porosity is related to pressure through the following definition of rock compressibility c_f:

$$\frac{d\phi}{dp} = c_f \phi \tag{3.9}$$

The term c_f is generally of the order of 10^{-6} psi^{-1}.

Relative permeability is an experimentally determined rock property which is used in the Darcy eq. (4.2) below to relate volumetric velocity to pressure gradient when more than one phase is flowing. This relative permeability k_r is in general a nonlinear function of saturation as indicated in Figure 3.2.

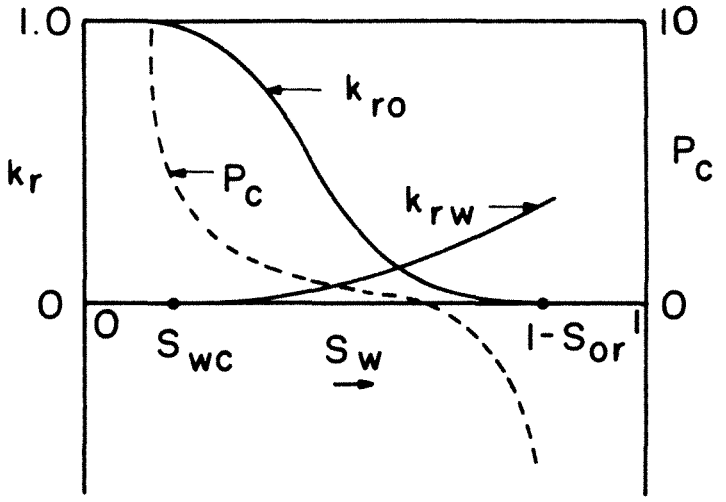


Fig. 3.2 RELATIVE PERMEABILITY AND CAPILLARY PRESSURE CURVES IN OIL-WATER SYSTEM

k_{rw} is zero at irreducible (connate) water saturation, k_{ro} is zero at residual oil saturation and relative permeability to any phase is unity when saturation of that phase is unity. Extensive laboratory experiments in multiphase fluid flow have indicated insignificant sensitivity of the k_r vs S relations to viscosities of the flowing phases.

Capillary pressure P_c is defined as the difference between non-wetting and wetting phase pressures; this pressure difference arises from the interfacial tension between the immiscible phases and the small radii of curvature of the fluid interfaces in the pore structure. In general, water and oil are the wetting phases in water-oil and gas-oil systems, respectively. Thus,

$$P_{cwo} = p_o - p_w \quad \text{and} \quad P_{cgo} = p_g - p_o \tag{3.10}$$

where one or both relations apply at a point in the reservoir depending upon the number of phases present. In a two-phase system P_c is generally represented as a single-valued function of saturation as indicated in Fig. (3.2).

The relative permeability and capillary pressure curves are dependent upon the direction of change in wetting phase saturation. A fluid displacement where wetting phase saturation is increasing (e.g. oil displacement by water) is referred to as imbibition while a displacement involving a decreasing wetting phase saturation (e.g. oil displacement by gas) is referred to as drainage. Relative permeability and capillary pressure curves experimentally determined in these two situations are referred to as imbibition and drainage curves, respectively. Fig. 3.3 indicates the difference between imbibition and drainage curves.

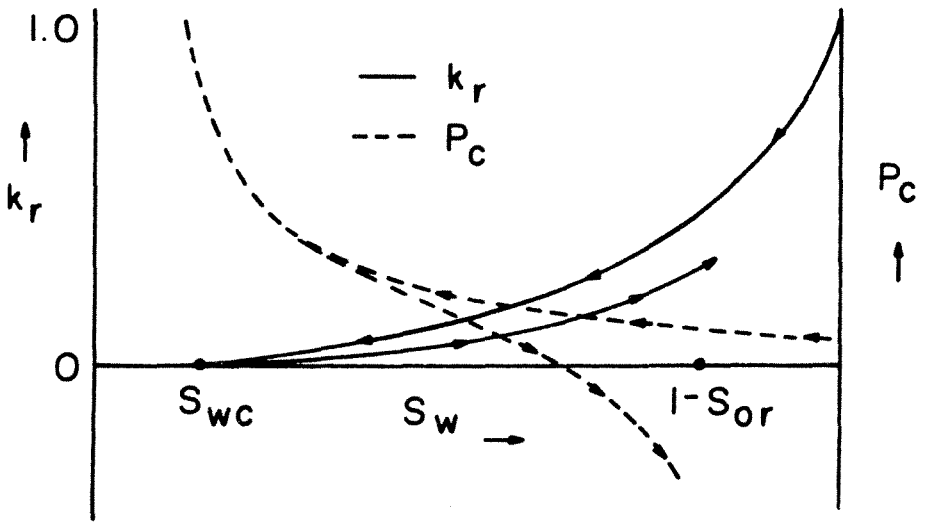


Fig. 3.3 IMBIBITION AND DRAINAGE CURVES IN WATER-OIL SYSTEM

Fortunately, many practical problems do not involve this hysteresis effect since the oil recovery process is generally one of imbibition (water-flooding or water drive) or drainage (gas injection or dissolved gas drive).

Various articles in the literature discuss functional dependence of relative permeability and capillary pressure upon saturations in three-phase systems [2, 3 In this text, water-oil capillary pressure and relative permeability to water are represented as single-valued functions of water saturation,

$$P_{cwo} = P_{cwo} \ (S_w) \qquad k_{rw} = k_{rw} \ (S_w)$$

The relative permeability to oil is a function of water and oil saturations,

$$k_{ro} = k_{ro} \ (S_w, \ S_o)$$

Relative permeability to gas and gas-oil capillary pressure are represented as single-valued functions of gas saturation.

$$k_{rg} = k_{rg} \ (S_g) \qquad P_{cgo} = P_{cgo} \ (S_g)$$

PROBLEMS

3.1. Derive eqs. (3.2) and (3.3). Hint: if B_o reservoir barrels of oil at reservoir pressure p are flashed to stock tank conditions then 1 STB of oil and R_s (evaluated at p) Mcf of gas are obtained. Equate the mass of the B_o barrels at p to the mass of 1 STB and R_s Mcf of gas.

3.2. Use eq. (3.4) and the gas law $pV = znRT$ to show that the compressibility of a gas is

$$c = \frac{1}{p}\left(1 - \frac{p}{z}\frac{dz}{dp}\right)$$

3.3. Show that at equilibrium the water saturation varies with depth in an oil-water sand as

$$S_w = .2 + \frac{1}{(P_c^* - \Delta\gamma_s\, Z)^{1/3}}$$

where: Z is depth measured positively downward, Z = 0 at free water surface ($S_w = 1$)

the capillary pressure curve is $P_c = 1/(S_w - .2)^3$

$P_c^* = P_c$ at $S_w = 1.0$

$\Delta\gamma = \gamma_w - \gamma_o$ where γ is specific weight, psi/ft

4. DARCY'S LAW

A variety of rate processes occur within a petroleum reservoir during the production of oil or gas. The relative importance of these processes in any specific case depends upon the particular exploitation scheme under which the reservoir is being produced. The rate process of fluid flow is of course dominant in all cases. For single-phase flow in a porous medium, Darcy's law relates the volumetric velocity to the pressure gradient and gravity force as

$$u_x = -\frac{k_x}{\mu}\left(\frac{\partial p}{\partial x} - \gamma\frac{\partial Z}{\partial x}\right) \tag{4.1}$$

where

u_x = volumetric velocity, cu ft/(sq ft of area normal to flow - day)

k_x = rock permeability, md x 0.00633

μ = fluid viscosity, cp

p = fluid pressure, psi

x = distance, feet

γ = specific weight, psi/ft $\left(\rho\ \frac{\text{lbs}_m}{\text{cu ft}}\ \frac{g}{g_c}\ \frac{1\text{ sq ft}}{144\text{ sq in}}\right)$

Z = elevation (vertical position) measured positively downward, ft

Similar equations apply for flow in the y and z directions. This volumetric velocity u is also referred to as superficial or Darcy velocity. Note that it is simply volumetric flow rate per unit cross-sectional area normal to flow; u is related to average pore velocity u_p by $u = \phi\ u_p$ where ϕ is rock porosity.

For multiphase fluid flow the velocity of each fluid is given by eq. (4.1) modified by relative permeability. The simultaneous flow of oil and gas is described by

$$u_{ox} = - \frac{k_x \, k_{ro}}{\mu_o} \left(\frac{\partial p_o}{\partial x} - \gamma_o \frac{\partial Z}{\partial x} \right) \tag{4.2a}$$

$$u_{gx} = - \frac{k_x \, k_{rg}}{\mu_g} \left(\frac{\partial p_g}{\partial x} - \gamma_g \frac{\partial Z}{\partial x} \right. \tag{4.2b}$$

where subscripts o and g denote oil and gas respectively. The relative permeabilities k_{ro} and k_{rg} are functions of saturation as discussed in Chapter 3.

5. A GENERALIZED CONSERVATION EQUATION

A mathematical model is simply a set of equations which describe certain physical processes occurring in the reservoir. In nearly all cases of interest these equations express conservation of some quantity which is flowing or being transported through the reservoir. Examples are conservation of mass of a flowing fluid and conservation of thermal energy in cases involving injection of hot fluids to enhance oil recovery. In general, the quantity one wishes to conserve is indicated by the verbal statement of the problem.

A generalized continuity equation can be derived for conservation of any flowing quantity. This equation is simply a material (or energy) balance about a small element of the reservoir. We choose a system consisting of a small element of space $\Delta x\ \Delta y\ \Delta z$ in the reservoir as illustrated in Fig. 5.1;

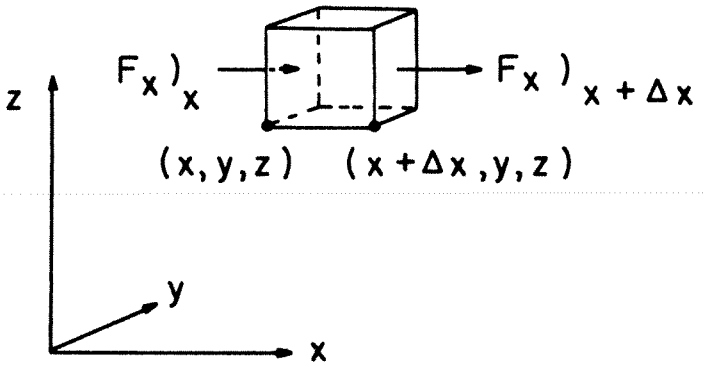


Fig. 5.1 SYSTEM FOR MASS OF HEAT BALANCE

this element contains rock and whatever fluids occupy the pore space. A general flux F is defined as the rate of flow of the quantity being conserved, per unit

cross-sectional area normal to the direction of flow. For example, F is lbs_m of fluid per sq ft per day if mass of flowing fluid were being conserved or Btu per sq ft per day if thermal energy were being conserved. Note that the flux F is a flow rate and determination of an expression for F in any particular case requires accounting for all mechanisms by which the conserved quantity flows or is transported through the reservoir. Since F is a flow rate it will in general depend upon direction as well as position (x, y, z) in the reservoir. Thus F_x will denote the flux in x direction, F_y the flux in the y direction, and F_z that in the z direction. Finally, F_x will by convention be considered as the flow rate in the positive x direction and similarly for F_y and F_z.

A general concentration C is defined as the amount of the conserved quantity per unit volume of the system. For example, C might be lbs_m per cu ft or Btu per cu ft. Note that the denominator of C, i.e. the system volume, is the entire volume $\Delta x\ \Delta y\ \Delta z$, not just the pore space therein. Finally, a sink term q_v is defined as the production rate of the conserved quantity, expressed as amount of the quantity produced per unit volume of the reservoir per unit time. Note that q_v is in general a function of position x, y, z and time t.

A balance about the system, expressing conservation of the flowing quantity over a small time increment Δt, can be simply expressed as

$$\text{IN} - \text{OUT} = \text{GAIN} \tag{5.1}$$

where IN is the amount (of the conserved quantity) flowing into the system during time Δt. OUT is the amount flowing out plus the amount produced over Δt and GAIN is the amount in the system at time $t + \Delta t$ less the original amount present at time t. Reference to Fig. 5.1 shows that flow into the system (element) occurs at the three faces of areas $\Delta y\ \Delta z$ at position x, $\Delta x\ \Delta z$ at position y and $\Delta x\ \Delta y$ at position

z. Multiplication of the fluxes at these faces by the respective cross sectional areas normal to flow and by the time increment Δt gives

$$IN = [(F_x)_x \Delta y \Delta z + (F_y)_y \Delta x \Delta z + (F_z)_z \Delta x \Delta y] \Delta t \qquad (5.2)$$

Note that the units of this term are simply those of the conserved quantity (e.g. lbs_m or Btu). Similarly, flow out of the system occurs at the three faces of areas $\Delta y \Delta z$ at position $x + \Delta x$, $\Delta x \Delta z$ at position $y + \Delta y$ and $\Delta x \Delta y$ at position $z + \Delta z$. Thus

$$OUT = q_v \Delta x \Delta y \Delta z \Delta t + [(F_x)_{x+\Delta x} \Delta y \Delta z + (F_y)_{y+\Delta y} \Delta x \Delta z + (F_z)_{z+\Delta z} \Delta x \Delta y] \Delta t \qquad (5.3)$$

Finally, the gain over the time Δt is

$$GAIN = [(C)_{t+\Delta t} - (C)_t] \Delta x \Delta y \Delta z \qquad (5.4)$$

Substitution from eqs. (5.2) - (5.4) into eq. (5.1) and division of each term in the resulting equation by $\Delta x \Delta y \Delta z \Delta t$ gives

$$-\frac{(F_x)_{x+\Delta x} - (F_x)_x}{\Delta x} - \frac{(F_y)_{y+\Delta y} - (F_y)_y}{\Delta y} - \frac{(F_z)_{z+\Delta z} - (F_z)_z}{\Delta z} - q_v = \frac{(C)_{t+\Delta t} - (C)_t}{\Delta t} \qquad (5.5)$$

In the limit as Δx, Δy, Δz and Δt approach zero, this equation becomes

$$-\frac{\partial F_x}{\partial x} - \frac{\partial F_y}{\partial y} - \frac{\partial F_z}{\partial z} - q_v = \frac{\partial C}{\partial t} \tag{5.6}$$

This result follows from the definition of the partial derivative of any function f(u, v, ...) with respect to any variable, say u, as

$$\frac{\partial f}{\partial u} = \lim_{\Delta u \to o} \frac{f(u+\Delta u, v, \ldots) - f(u, v, \ldots)}{\Delta u} \tag{5.7}$$

Equation (5.6) is a generalized continuity or material (heat) balance equation expressing conservation of a quantity flowing in a reservoir.

For the case of two-dimensional (x-y) flow in a reservoir of variable thickness h, a derivation similar to that given above yields

$$-\frac{\partial(h\, F_x)}{\partial x} - \frac{\partial(h\, F_y)}{\partial y} - h\, q_v = h\, \frac{\partial C}{\partial t} \tag{5.8}$$

6. FORMULATION OF THE MATHEMATICAL MODEL

The term multiphase flow denotes the simultaneous movement of two or more immiscible phases through a porous medium. Obvious examples are gas-oil or gas-oil-water flow. The equations describing this flow are simply the conservation eq. (5.6) written for each phase. In writing these equations we must select the quantities to be conserved. Customary quantities (or units) are stock tank barrels (STB) of water, STB of oil and Mcf of gas. As discussed above, each of these units is convertible to mass through densities at stock tank or standard conditions.

Mcf of gas exist in the reservoir both as free gas and as gas in solution in the oil, while STB of oil exists only in the "oil" (liquid hydrocarbon) phase. A volume V at pressure p in the reservoir contains $V\phi S_o b_o$ STB of oil and $V\phi (S_o b_o R_s + S_g b_g)$ Mcf of gas. Note that the STB is a quantity which undergoes no vaporization into the gas phase since it is defined as the part or component of the "oil" phase which remains in liquid form upon flashing to stock tank pressure.

The fluxes F_x for the three phases are

$$\left.\begin{aligned} F_{xw} &= b_w u_{xw} \\ F_{xo} &= b_o u_{xo} \end{aligned}\right\} \frac{\text{STB}}{\text{sq ft. - day}}$$

$$F_{xg} = b_g u_{xg} + b_o R_s u_{xo} \text{ Mcf/sq. ft. - day} \qquad (6.1)$$

where formation volume factor units here are STB/cu ft and Mcf/cu ft. R_s has units of Mcf of gas in solution per STB of oil. The production term q_v will be expressed in units of STB/cu ft - day or Mcf/cu ft - day and denoted by q_{vw}, q_{vo}, q_{vg}. The concentrations of the phases in units of STB/cu ft or Mcf/cu ft are

$$C_w = \phi b_w S_w \qquad C_o = \phi b_o S_o \qquad C_g = \phi (b_o R_s S_o + b_g S_g) \qquad (6.2)$$

For one-dimensional flow, the conservation eq. (5.6) can then be written for each phase as

$$-\frac{\partial(b_w u_{xw})}{\partial x} - q_{vw} = \frac{\partial(\phi b_w S_w)}{\partial t} \tag{6.3a}$$

$$-\frac{\partial(b_o u_{xo})}{\partial x} - q_{vo} = \frac{\partial(\phi b_o S_o)}{\partial t} \tag{6.3b}$$

$$-\frac{\partial(b_o R_s u_{xo} + b_g u_{xg})}{\partial x} - q_{vg} = \frac{\partial[\phi (b_o R_s S_o + b_g S_g)]}{\partial t} \tag{6.3c}$$

Substitution of Darcy's law, eq. (4.2), into these equations finally gives

$$\frac{\partial}{\partial x}\left[\frac{k_x k_{rw} b_w}{\mu_w}\left(\frac{\partial p_w}{\partial x} - \gamma_w \frac{\partial Z}{\partial x}\right)\right] - q_{vw} = \frac{\partial(\phi b_w S_w)}{\partial t} \tag{6.4a}$$

$$\frac{\partial}{\partial x}\left[\frac{k_x k_{ro} b_o}{\mu_o}\left(\frac{\partial p_o}{\partial x} - \gamma_o \frac{\partial Z}{\partial x}\right)\right] - q_{vo} = \frac{\partial(\phi b_o S_o)}{\partial t} \tag{6.4b}$$

$$\frac{\partial}{\partial x}\left\{k\left[\frac{k_{ro} b_o R_s}{\mu_o}\left(\frac{\partial p_o}{\partial x} - \gamma_o \frac{\partial Z}{\partial x}\right) + \frac{k_{rg} b_g}{\mu_g}\left(\frac{\partial p_g}{\partial x} - \gamma_g \frac{\partial Z}{\partial x}\right)\right]\right\} - q_{vg} = \frac{\partial[\phi (b_o R_s S_o + b_g S_g)]}{\partial t} \tag{6.4c}$$

These are three equations in the five unknowns p_w, p_o, p_g, S_w, S_o. Note that S_g is simply $1-S_w - S_o$. However, two additional equations are available in the capillary pressure definitions which give $p_o - p_w$ and $p_g - p_o$ as functions of saturations S_w and S_g. Thus, we have effectively three equations in three unknowns. For two or three dimensional flow, y- and z-direction flow terms, of form identical to the given x-direction flow terms, are added to the left hand

sides of eqs. (6.4).

As pointed out by Hubbert [4], a dependent variable P_w may be defined by

$$\frac{\partial p_w}{\partial x} - \gamma_w \frac{\partial Z}{\partial x} = \gamma_w \frac{\partial P_w}{\partial x} \tag{6.5}$$

or

$$P_w = \int_{p_b}^{p_w} \frac{dp}{\gamma_w(p)} - Z$$

where p_b is an arbitrary base pressure (see Problem 4.1). This transformation is valid only if specific weight γ_w is a single-valued function of p_w. Similar relations can be written defining oil and gas "potentials" P_o and P_g. Thus, an alternative, somewhat condensed form of eqs. (6.4) is

$$\frac{\partial}{\partial x}\left(\frac{k_x\, k_{rw}\, b_w\, \gamma_w}{\mu_w} \frac{\partial P_w}{\partial x}\right) - q_{vw} = \frac{\partial(\phi\, b_w\, S_w)}{\partial t} \tag{6.6a}$$

$$\frac{\partial}{\partial x}\left(\frac{k_x\, k_{ro}\, b_o\, \gamma_o}{\mu_o} \frac{\partial P_o}{\partial x}\right) - q_{vo} = \frac{\partial(\phi\, b_o\, S_o)}{\partial t} \tag{6.6b}$$

$$\frac{\partial}{\partial x}\left(\frac{k_x\, k_{ro}\, b_o\, \gamma_o\, R_s}{\mu_o} \frac{\partial P_o}{\partial x}\right) + \frac{\partial}{\partial x}\left(\frac{k_x\, k_{rg}\, b_g\, \gamma_g}{\mu_g} \frac{\partial P_g}{\partial x}\right) - q_{vg}$$

$$= \frac{\partial}{\partial t}\left[\phi\,(b_o\, R_s\, S_o + b_g\, S_g)\right] \tag{6.6c}$$

Fluid compressibility effects are generally negligible in producing operations under pressure maintenance by water and/or gas injection. Although gas compressibility may be appreciable, the maintenance of pressure results in negligible time variation of gas density. In addition, the spatial variation of gas density is usually small in relation to the gas density itself. Producing

schemes of pattern or flank waterflood and/or crestal gas injection may therefore be simulated with equations which presume fluid incompressibility.

If the fluids and rock are considered incompressible and gas evolution is assumed negligible then R_s, formation volume factors, specific weights and porosity are constants and eqs. (6.4) become

$$\frac{\partial}{\partial x}\left(\frac{k_x\, k_{rw}}{\mu_w}\frac{\partial \Phi_w}{\partial x}\right) - B_w\, q_{vw} = \phi\,\frac{\partial S_w}{\partial t} \tag{6.7a}$$

$$\frac{\partial}{\partial x}\left(\frac{k_x\, k_{ro}}{\mu_g}\frac{\partial \Phi_o}{\partial x}\right) - B_o\, q_{vo} = \phi\,\frac{\partial S_o}{\partial t} \tag{6.7b}$$

$$\frac{\partial}{\partial x}\left(\frac{k_x\, k_{rg}}{\mu_g}\frac{\partial \Phi_g}{\partial x}\right) - B_g\, q_{vg} = \phi\,\frac{\partial S_g}{\partial t} \tag{6.7c}$$

Here

$$\Phi_w = p_w - \gamma_w Z \qquad \Phi_o = p_o - \gamma_o Z \qquad \Phi_g = p_g - \gamma_g Z \tag{6.8}$$

and B is 1/b. In eqs. (6.4c) and (6.6c) q_{vg} is total gas production rate including free gas entering the wellbore and gas dissolved in the oil entering the wellbore. In eq. (6.7c) q_{vg} is free gas production only.

PROBLEMS

6.1. A vertical sand column is saturated with water and oil with an initial non-equilibrium saturation distribution. The column is closed at both ends and the fluids may be considered incompressible. Derive the partial differential equations expressing conservation of mass of oil and water. From these equations, prove that the total volumetric velocity u is zero at all z and t. Combine these equations using Darcy's to give the single equation in water saturation S,

$$\frac{\partial}{\partial z}\,\Psi\,\frac{\partial S}{\partial z} - k\;\;\Delta\rho\,\frac{df}{dS}\,\frac{\partial S}{\partial z} = \phi\,\frac{\partial S}{\partial t}$$

where $S = S_w$, z is distance measured positively downward and

$$\Psi = -\frac{\dfrac{k\,k_{rw}}{\mu_w}\,\dfrac{k_{ro}}{\mu_o}}{\dfrac{k_{rw}}{\mu_w} + \dfrac{k_{ro}}{\mu_o}}\;\;\frac{d\,P_c}{d\,S_w} \qquad f = \frac{k_{rw}/\mu_w}{\dfrac{k_{rw}}{\mu_w} + \dfrac{k_{ro}}{\mu_o}}$$

Show that the two conservation equations may be combined to give the equivalent equation

$$\frac{\partial}{\partial z}\,\Psi_1\,\frac{\partial P}{\partial z} = \phi\;S'\,\frac{\partial P}{\partial t}$$

where

$$S' = d\,S_w/d\,P_c \qquad \Psi_1 = -\frac{\dfrac{k\,k_{rw}}{\mu_w}\,\dfrac{k_{ro}}{\mu_o}}{\dfrac{k_{rw}}{\mu_w} + \dfrac{k_{ro}}{\mu_o}} \qquad P = P_c + \Delta\,\rho\,z$$

6.2. Derive the equation describing pressure as a function of x and time for one-dimensional flow of a slightly compressible fluid in a fractured matrix reservoir. The fractures are closely spaced and effective fracture permeability is 2 to 3 orders of magnitude larger than matrix permeability. Denote fracture porosity by ϕ_f and matrix porosity by ϕ_m. The transfer of fluid between fracture and matrix may be represented by

$$q \frac{\text{lbs}_m}{\text{sq ft. - day}} = K (p_f - p_m)$$

where K is a rate constant and subscripts f and m denote fracture and matrix. The 'sq ft' here denotes area of fracture face. The given specific surface σ has units of sq ft of fracture facial area per cubic foot of pore space.

6.3. Derive the equations describing two-phase (e.g. water-oil) flow in a sand under the following conditions:

1) the flow is one-dimensional
2) capillary forces may be neglected
3) the fluids may be assumed incompressible
4) dissolved gas effects may be ignored

6.4. Combine the two equations derived in 6.3 into a single equation in saturation:

$$\alpha(S) \frac{\partial S}{\partial x} = \frac{\partial S}{\partial t}$$

6.5. Starting with eqs. (6.4), derive eqs. (6.7) for the incompressible case. Show that the terms in eq. (6.4c) involving R_s disappear, as indicated by

eq. (6.7c) (Hint: use eq. (6.7b) in the gas equation). Note that q_{vg} in eq. (6.4c) is total gas production and may be expressed as $q_{vo} R_s + (q_{vg})_{free}$. The q_{vg} in eq. (6.7c) is only this free gas production rate.

7. FINITE DIFFERENCE APPROXIMATIONS TO DIFFERENTIAL EQUATIONS

7.1. Finite Difference Forms

Numerical solution of a partial differential equation refers to the process of solving a finite difference representation of the differential equation. This representation is obtained by replacing all derivatives by finite difference forms. These forms can easily be developed from a Taylor's series expansion of the dependent variable. If a function $y(x)$ and all its derivatives exist at a point x_o, then $y(x)$ can be expanded in a Taylor's series as

$$y(x) = y(x_0) + (x-x_0)\, y'(x_0) + \frac{(x-x_0)^2}{2!} y''(x_0) + \frac{(x-x_0)^3}{3!} y'''(x_0) + \ldots \tag{7.1}$$

with the notation $y_i = y(x_0 + i\Delta x)$, equation (7.1) can be written

$$y_1 = y_0 + \Delta x y_0' + \frac{\Delta x^2}{2!} y_0'' + \frac{\Delta x^3}{3!} y''' + \frac{\Delta x^4}{4!} y_0^{IV} + \ldots \tag{7.2}$$

$$y_{-1} = y_0 - \Delta x y_0' + \frac{\Delta x^2}{2'} y_0'' - \frac{\Delta x^3}{3!} y''' + \frac{\Delta x^4}{4!} y_0^{IV} + \ldots \tag{7.3}$$

If Δx is small, terms of order 3 and higher in Δx can be ignored and (7.2) can be rearranged to give

$$y_0' = \frac{y_1 - y_0}{\Delta x} + \mathcal{O}(\Delta x) \tag{7.4}$$

which is a finite difference form of the first derivative $\frac{dy}{dx}$ at the point x_0. Subtraction of (7.3) from (7.2) yields

$$y_0' = \frac{y_1 - y_{-1}}{2\Delta x} + \mathcal{O}(\Delta x^2) \tag{7.5}$$

an alternate difference form for the first derivative. Comparison of (7.4) and (7.5) shows that the truncation error (the error incurred by ignoring higher order terms in the series expansion) is of the order of Δx in (7.4) and of the order of Δx^2 in (7.5). Thus, the latter is a more accurate representation of the first derivative.

Addition of (7.2) and (7.3) yields a finite difference form of the second derivative,

$$y_0'' = \frac{y_1 - 2y_0 + y_{-1}}{\Delta x^2} + \mathcal{O}(\Delta x^2) \tag{7.6}$$

A higher order representation can be obtained by writing

$$y_2 = y_0 + 2\Delta x y_0' + \frac{4\Delta x^2}{2!} y_0'' + \frac{8\Delta x^3}{3!} y_0''' + \frac{16\Delta x^4}{4!} y_0^{IV} + \ldots \tag{7.7}$$

$$y_{-2} = y_0 - 2\Delta x y_0' + \frac{4\Delta x^2}{2!} y_0' - \frac{8\Delta x^3}{3!} y_0''' + \frac{16\Delta x^4}{4!} y_0^{IV} + \ldots \tag{7.8}$$

and manipulating (7.2), (7.3), (7.7), (7.8) to obtain

$$y_0'' = \frac{-y_2 + 16y_1 - 30y_0 + 16y_{-1} - y_{-2}}{12\Delta x^2} + \mathcal{O}(\Delta x^4) \tag{7.9}$$

The representation (7.9) is seldom used because of the increased computational labor which results.

In summary, then, the usual finite difference forms for the first and second derivatives, at any point $x = i\Delta x$, are

$$\frac{dy}{dx} \cong \frac{y_{i+1} - y_i}{\Delta x} \cong \frac{y_i - y_{i-1}}{\Delta x} \cong \frac{y_{i+1} - y_{i-1}}{2\Delta x} \tag{7.10}$$

$$\frac{d^2y}{dx^2} \cong \frac{y_{i+1} - 2y_i + y_{i-1}}{\Delta x^2} \tag{7.11}$$

where $y_i = y(i\Delta x)$.

An alternate approximation to the first derivative results from writing equation (7.1) twice, first with $x = x_0 + \frac{1}{2}\Delta x$ and again with $x = x_0 - \frac{1}{2}\Delta x$. Subtracting the two results gives

$$\left(\frac{dy}{dx}\right)_{x=i\Delta x} \cong \frac{y_{i+\frac{1}{2}} - y_{i-\frac{1}{2}}}{\Delta x} \tag{7.12}$$

This form is useful in expressing in difference form the term $\frac{\partial}{\partial x}K(x)\frac{\partial p}{\partial x}$ which appears in the equations of reservoir simulation. Using equation (7.12) we first write

$$\frac{\partial}{\partial x} K(x) \frac{\partial p}{\partial x} = \frac{\left(K \frac{\partial p}{\partial x}\right)_{i+\frac{1}{2}} - \left(K \frac{\partial p}{\partial x}\right)_{i-\frac{1}{2}}}{\Delta x} \tag{7.13}$$

Using equation (7.12) again,

$$\left(K \frac{\partial p}{\partial x}\right)_{i+\frac{1}{2}} = K_{i+\frac{1}{2}} \frac{p_{i+1} - p_i}{\Delta x} \tag{7.14a}$$

$$\left(K \frac{\partial p}{\partial x}\right)_{i-\frac{1}{2}} = K_{i-\frac{1}{2}} \frac{p_i - p_{i-1}}{\Delta x} \tag{7.14b}$$

Substituting equations (7.14) into (7.13) gives finally

$$\frac{\partial}{\partial x} K \frac{\partial p}{\partial x} = \frac{K_{i+\frac{1}{2}} p_{i+1} - (K_{i+\frac{1}{2}} + K_{i-\frac{1}{2}}) p_i + K_{i-\frac{1}{2}} p_{i-1}}{\Delta x^2} \tag{7.15}$$

7.2. Explicit and Implicit Difference Approximations

In discussions of numerical solution of partial differential equations the terms "explicit" and "implicit" appear frequently. These terms are explained by

Richtmyer [5] with reference to the parabolic partial differential equation

$$\frac{\partial^2 p}{\partial x^2} = \frac{\partial p}{\partial t} \tag{7.16}$$

Equation (7.16) is presumed to hold in some region

$$0 < x < X$$

$$0 < t$$

and this region will be represented by grid

$$x = i\Delta x,\ 0 < i < I,\ \text{where } I\Delta x = X$$

$$t = n\Delta t$$

where Δx and Δt are selected spatial and time increments. The term $p_{i,n}$ represents the value $p\ (i\Delta x, n\Delta t)$. A finite difference representation of (7.16) at the point (i,n) is, then,

$$\frac{p_{i+1,n} - 2p_{i,n} + p_{i-1,n}}{\Delta x^2} = \frac{p_{i,n+1} - p_{i,n}}{\Delta t} \tag{7.17}$$

The form $\frac{p_{i,n+1} - p_{i,n-1}}{2\Delta t}$ is not used for $\frac{\partial p}{\partial t}$ because of stability considerations which will be discussed later. Equation (7.17) is termed an <u>explicit</u> difference representation of (7.16) because at each time step only <u>one</u> unknown appears ($p_{i,n+1}$) and this unknown can therefore be solved for explicitly. Thus, rearrangement of (7.17) yields

$$p_{i,n+1} = a\, p_{i+1,n} - (2a-1)\, p_{i,n} + a\, p_{i-1,n} \tag{7.18}$$

where $a = \Delta t/\Delta x^2$. At zero time (n = 0) all $p_{i,n}$ for $0 < i < I$ are known from the initial condition and $p_{i,1}$ can be calculated explicitly <u>for all i</u> from (7.18). Knowledge of $p_{i,1}$ then allows calculation of $p_{i,2}$ and so on.

An implicit representation of (7.16) at the point (i,n) is

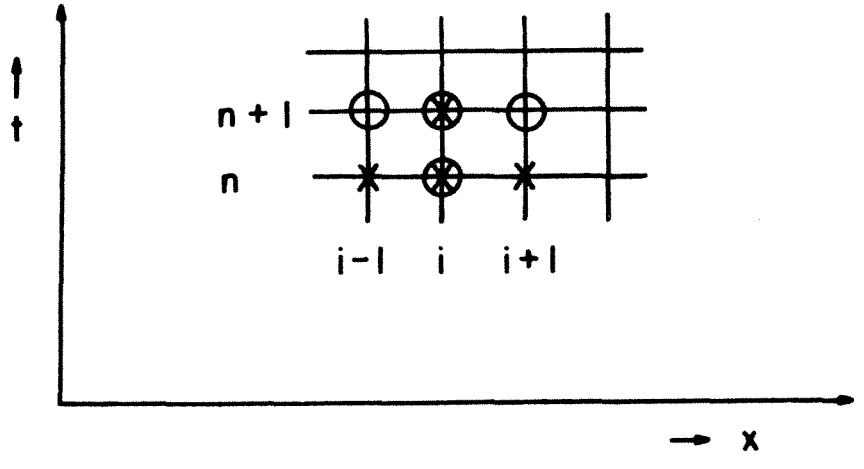
$$\frac{p_{i+1,n+1} - 2p_{i,n+1} + p_{i-1,n+1}}{\Delta x^2} = \frac{p_{i,n+1} - p_{i,n}}{\Delta t} \qquad (7.19)$$

Here the spatial derivative $\frac{\partial^2 p}{\partial x^2}$ is replaced by a difference form evaluated at $(n+1)\Delta t$ rather than $n\Delta t$ and at each time step the result contains three unknown values of the dependent variable p. Rearrangement of (7.19) yields

$$p_{i+1,n+1} - (2 + \beta)\, p_{i,n+1} + p_{i-1,n+1} = -\beta\, p_{i,n} \qquad (7.20)$$

where $\beta = \Delta x^2/\Delta t$. Thus at each time step a set of simultaneous equations which forms a tridiagonal matrix is obtained. The term "implicit" refers to the fact that the unknowns are implicitly related to one another through the set of simultaneous equations. The implicit form (7.20) seems to demand considerably more computational labor than does the explicit form (7.18). As discussed below, however, in practical applications the former is used almost exclusively in preference to the latter.

The difference between the explicit and implicit forms can be seen on the sketch below.



The explicit form utilizes p values at points marked by the x's while the implicit uses values at points marked by the circles. The explicit form (7.17) and implicit form (7.19) are often referred to as forward and backward difference approximations, respectively. This terminology refers to the time difference extending forward or backward from the time index of the spatial difference.

The Crank-Nicolson [6] implicit form of (7.16) is

$$\tfrac{1}{2}\left[\frac{p_{i+1,n+1} - 2p_{i,n+1} + p_{i-1,n+1}}{\Delta x^2} + \frac{p_{i+1,n} - 2p_{i,n} + p_{i-1,n}}{\Delta x^2}\right] = \frac{p_{i,n+1} - p_{i,n}}{\Delta t} \qquad (7.21)$$

where the spatial derivative $\frac{\partial^2 p}{\partial x^2}$ is replaced by an average of its values at $n\Delta t$ and $(n+1)\Delta t$.

7.3. Truncation Error

Truncation error is that error incurred by replacing a differential equation by a difference equation. The exact solution (i.e. no round-off error) of a difference equation differs from the solution of the corresponding differential equation due to this error.

The truncation error in a finite difference approximation is defined by

$$T = L_D p - (Lp)_{i\Delta x, n\Delta t} \qquad (7.22)$$

where

T = truncation error

$L_D p$ = difference form

Lp = differential form

EXAMPLE 7.1

Determine the truncation error of the explicit difference approximation, equation (7.17).

Solution:

$$L_D p = \frac{p_{i+1,n} - 2p_{i,n} + p_{i-1,n}}{\Delta x^2} - \frac{p_{i,n+1} - p_{i,n}}{\Delta t} \tag{7.23}$$

$$Lp = \frac{\partial^2 p}{\partial x^2} - \frac{\partial p}{\partial t} \tag{7.24}$$

From equations (7.2) and (7.3),

$$\frac{p_{i+1,n} - 2p_{i,n} + p_{i-1,n}}{\Delta x^2} = \left(\frac{\partial^2 p}{\partial x^2}\right)_{i,n} + \frac{\Delta x^2}{12}\frac{\partial^4 p}{\partial x^4} + \ldots \tag{7.25}$$

$$\frac{p_{i,n+1} - p_{i,n}}{\Delta t} = \left(\frac{\partial p}{\partial t}\right)_{i,n} + \frac{\Delta t}{2}\frac{\partial^2 p}{\partial t^2} + \ldots \tag{7.26}$$

Substituting (7.25) and (7.26) into equation (7.23) and then subtracting equation (7.24), we obtain

$$T = \frac{\Delta x^2}{12}\frac{\partial^4 p}{\partial x^4} - \frac{\Delta t}{2}\frac{\partial^2 p}{\partial t^2} \tag{7.27}$$

which would ordinarily be written

$$T = \mathcal{O}(\Delta x^2) + \mathcal{O}(\Delta t) \tag{7.28}$$

EXAMPLE 7.2

Determine the truncation error of the DuFort-Frankel approximation [7] of equation (7.16),

$$\frac{p_{i+1,n} - (p_{i,n+1} + p_{i,n-1}) + p_{i-1,n}}{\Delta x^2} = \frac{p_{i,n+1} - p_{i,n-1}}{2\Delta t}$$

Solution:

The truncation error is, from equation (7.22),

$$T = \frac{p_{i+1,n} - (p_{i,n+1} + p_{i,n-1}) + p_{i-1,n}}{\Delta x^2} - \frac{p_{i,n+1} - p_{i,n-1}}{2\Delta t}$$

$$- \left(\frac{\partial^2 p}{\partial x^2} - \frac{\partial p}{\partial t}\right)_{i,n} \qquad (7.29)$$

Taylor's series, (7.1) gives

$$p_{i,n+1} = p_{i,n} + \Delta t\, p_t + \frac{\Delta t^2}{2} p_{tt} + \frac{\Delta t^3}{6} p_{ttt} + \cdots$$

$$p_{i,n-1} = p_{i,n} - \Delta t\, p_t + \frac{\Delta t^2}{2} p_{tt} - \frac{\Delta t^3}{6} p_{ttt} + \cdots$$

$$p_{i+1,n} = p_{i,n} + \Delta x\, p_x + \frac{\Delta x^2}{2} p_{xx} + \frac{\Delta x^3}{6} p_{xxx} + \frac{\Delta x^4}{24} p_{xxxx} + \cdots$$

$$p_{i-1,n} = p_{i,n} - \Delta x\, p_x + \frac{\Delta x^2}{2} p_{xx} - \frac{\Delta x^3}{6} p_{xxx} + \frac{\Delta x^4}{24} p_{xxxx} + \cdots$$

Substituting these values for $p_{i,n+1}$, etc., into equation (7.29) gives

$$T = \frac{\Delta x^2}{12} p_{xxxx} - \left(\frac{\Delta t}{\Delta x}\right) p_{tt} - \frac{\Delta t^2}{6} p_{ttt}$$

From equation (7.16), $p_{tt} = p_{xxxx}$, so that

$$T = \left[\frac{\Delta x^2}{12} - \left(\frac{\Delta t}{\Delta x}\right)^2\right] p_{tt} - \frac{\Delta t^2}{6} p_{ttt}$$

which would ordinarily be written

$$T = \mathcal{O}\left(\frac{\Delta t^2}{\Delta x^2}\right) + \mathcal{O}(\Delta x^2) + \mathcal{O}(\Delta t^2)$$

7.4. Truncation Error in Boundary Conditions

Consider the mixed boundary condition

$$\alpha \frac{\partial p}{\partial x} + \beta p = \gamma \qquad (7.30)$$

applying along the boundary $x = 0$ of a rectangular reservoir. As discussed in Chapter 2, if α is zero then half-blocks are employed along this boundary, as shown in Fig. 2.2. The reason for this is that this grid places points on the boundary and the condition (7.30) specifies values of pressure at points on the boundary. If β were zero then full blocks along the boundary would be used as indicated in Fig. 2.1b. Note that in this case of zero β, the grid of Fig. 2.2 could be used with $\partial p/\partial x$ expressed as

$$\left.\frac{\partial p}{\partial x}\right)_{x=0} \cong \frac{p_{2,j} - p_{0,j}}{2\Delta x} \qquad (7.31)$$

This difference form is an approximation of order $(\Delta x)^2$ to $\partial p/\partial x$ at $x = 0$. We would not use

$$\left.\frac{\partial p}{\partial x}\right)_{x=0} \cong \frac{p_{2,j} - p_{1,j}}{\Delta x} \qquad (7.32)$$

since this has truncation error of order Δx. The difference in (7.32) is an approximation of order $(\Delta x)^2$ to $\partial p/\partial x$ at $x = \Delta x/2$, not at $x = 0$.

Thus, if β were zero we could use either of the grids of Figs. 2.1b or 2.2 and obtain a difference representation of $\partial p/\partial x$ with truncation error of order $(\Delta x)^2$. In the latter grid, eq. (7.31) would be used and in the former grid,

$$\left(\frac{\partial p}{\partial x}\right)_{x=0} = (p_{1,j} - p_{0,j})/\Delta x \tag{7.33}$$

would be used. If β were zero along the entire boundary $x = 0$ then the grid of Fig. 2.1b and eq. (7.33) are preferable because the truncation error in eq. (7.33) is less than that in (7.31) even though the order (Δx^2) of the errors are the same.

If β is nonzero along any part of the boundary $x = 0$ then the grid of Fig. 2.2 is required in order to handle the specification of pressure values on the boundary. The mixed boundary condition (7.30) with α and β both nonzero cannot be adequately handled by a grid of type shown in Fig. 2.1b.

PROBLEMS

7.1. Determine the truncation error for

a) the implicit difference approximation equation (7.19)

b) the Crank-Nicolson approximation equation (7.21)

7.2. Modified explicit approximations are

$$\frac{p_{i+1,n} - 2p_{i,n+1} + p_{i-1,n+1}}{\Delta x^2} = \frac{p_{i,n+1} - p_{i,n}}{\Delta t}$$

$$\frac{p_{i+1,n} - p_{i,n} - p_{i,n+1} + p_{i-1,n+1}}{\Delta x^2} = \frac{p_{i,n+1} - p_{i,n}}{\Delta t}$$

What is the truncation error for each form?

7.3. Consider numerical solution of the one-dimensional problem

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

with boundary conditions

$$\frac{\partial p}{\partial x} = \beta p - \alpha \text{ at } x = 0,\ t \geqslant 0$$

$$\frac{\partial p}{\partial x} = 0 \text{ at } x = L,\ t \geqslant 0$$

where α and β are given constants. Show a type of grid which will result in truncation error in the difference form of the boundary conditions of the order of Δx^2 (as opposed to $\mathcal{O}(\Delta x)$). Give the difference representations of the boundary conditions for this grid.

7.4. Show that the truncation error of eq. (7.31) applied to the grid of Fig. 2.2 is greater than that of eq. (7.33) applied to the grid of Fig. 2.1b.

8. METHODS FOR NUMERICAL SOLUTION OF THE DIFFUSIVITY EQUATION

Practical problems in a wide variety of fields give rise to linear systems of equations which can be characterized by

$$\left.\begin{aligned} a_{1,1}\,x_1 + a_{1,2}\,x_2 + \cdots\cdots + a_{1,n}\,x_n &= b_1 \\ a_{2,1}\,x_1 + a_{2,2}\,x_2 + \cdots\cdots + a_{2,n}\,x_n &= b_2 \\ \vdots \\ a_{n,1}\,x_1 + a_{n,2}\,x_2 + \cdots\cdots + a_{n,n}\,x_n &= b_n \end{aligned}\right\} \qquad (8.1)$$

This system is concisely represented by matrix form as

$$A\,\underline{x} = \underline{b}$$

where $\underline{x}$ is the unknown column vector $(x_1, x_2, \text{----}, x_N)^T$, $\underline{b}$ is the known column vector $(b_1, b_2, \text{----}, b_N)^T$ and A is the matrix of coefficients $\{a_{ij}\}$.

The problems of single- or multi-phase flow in reservoirs give rise to the linear system (8.2) with the matrix A assuming a special form depending upon the dimensionality of the flow. We will develop these matrix forms by considering the difference representation of the diffusivity equation

$$\frac{\partial}{\partial x}\left(\frac{k}{\mu}\frac{\partial p}{\partial x}\right) + \frac{\partial}{\partial y}\left(\frac{k}{\mu}\frac{\partial p}{\partial y}\right) + \frac{\partial}{\partial z}\left(\frac{k}{\mu}\frac{\partial p}{\partial z}\right) - q = \phi c\frac{\partial p}{\partial t} \qquad (8.3)$$

Mathematical models of reservoir processes usually include at least one equation similar in form to this diffusivity equation.

For purposes of clarity we will take k and μ as constants, and q as zero in the difference form of eq. (8.3). This in no way detracts from the generality of the numerical solution techniques which will be described. That is, the techniques apply equally well to the heterogeneous case with nonzero q. For uniform k, μ and zero q, eq. (8.3) is

$$\nabla^2 p = \frac{\partial^2 p}{\partial x^2} + \frac{\partial^2 p}{\partial y^2} + \frac{\partial^2 p}{\partial z^2} = \frac{\partial p}{\partial t} \tag{8.3a}$$

where t in this equation is actually $k/\mu\,\phi c$ times the t in eq. (8.3).

Replacing the second-order derivatives by the standard second-order differences yields

$$\Delta^2 p_{n+1} = \Delta_x^2 p + \Delta_y^2 p + \Delta_z^2 p = \frac{\Delta_t p}{\Delta t} = \frac{p_{n+1} - p_n}{\Delta t} \tag{8.4}$$

Pressure values in the terms $\Delta^2 p$ are understood to apply at the new time n+1; the subscript n+1 is suppressed for clarity. Eq. (8.4) is thus the implicit or backward-difference approximation to eq. (8.3a).

8.1. The One-Dimensional Problem - Gaussian Elimination

In the case of one-dimensional flow, eq. (8.4) becomes

$$p_{i+1} - (2+\alpha)p_i + p_{i-1} = b_i \tag{8.5}$$

where

$$b_i = -\alpha p_{i,n} \text{ and } \alpha = \Delta x^2/\Delta t$$

Consider the Dirichlet problem (i.e. boundary conditions specify values of p on the boundaries) of eq. (8.5) subject to boundary conditions

$$p_{0,n} = c_1$$

$$p_{N+1,n} = c_2 \qquad (8.6)$$

The linear system is divided into (N+1) equal increments and $x_i = i\Delta x$, $i = 0, 1, ----, N+1$. Writing eq. (8.5) at $i = 1, 2, ----, N$ yields

$$\begin{aligned}
-(2+\alpha)\, p_1 + p_2 &= b_1 - c_1 \\
p_1 - (2+\alpha)\, p_2 + p_3 &= b_2 \\
p_2 - (2+\alpha)\, p_3 + p_4 &= b_3 \\
&\vdots \\
p_{N-1} - (2+\alpha)\, p_N &= b_N - c_2
\end{aligned} \qquad (8.7)$$

This system of equations may be written as

$$\underline{A}\underline{p} = \underline{c} \qquad (8.8)$$

$$\underline{p} = \begin{Bmatrix} p_1 \\ p_2 \\ \vdots \\ p_N \end{Bmatrix} \qquad \underline{c} = \begin{Bmatrix} b_1 - c_1 \\ b_2 \\ \vdots \\ b_{N-1} \\ b_N - c_2 \end{Bmatrix}$$

and A is the tridiagonal matrix

$$A = \begin{Bmatrix} -(2+\alpha) & 1 & & & & \\ 1 & -(2+\alpha) & 1 & & 0 & \\ & 1 & -(2+\alpha) & 1 & & \\ & & \cdot & \cdot & \cdot & \\ & 0 & & \cdot & \cdot & \\ & & & & 1 & -(2+\alpha) \end{Bmatrix} \qquad (8.10)$$

Eqs. (8.7) are easily solved by Gaussian elimination. Richtmyer gives a simple algebraic representation or algorithm for this Gaussian elimination. We will derive his algorithm here through an inductive process. The derivation will proceed as follows. We <u>assume</u> a property P_i which is actually a relationship between p_{i-1} and p_i. We then show that if P_i is "true" then, using equation (8.5), P_{i+1} is also "true". Therefore, if we can show P_2 true then by induction, P_3, P_4, P_5, ----, P_{N+1}, are all true. The relationship <u>assumed</u> is

$$p_{i-1} = C_i\, p_i + D_i \qquad (8.11)$$

where C_i and D_i are given (known) coefficients. Inserting equation (8.11) into equation (8.5) we obtain

$$p_{i+1} - (2 + \alpha - C_i)\, p_i + D_i = b_i$$

or, upon rearrangement,

$$p_i = \frac{1}{2 + \alpha - C_i}\, p_i + \frac{D_i - b_i}{2 + \alpha - C_i} \qquad (8.12)$$

But equation (8.12) is of identical form to equation (8.11) and, identifying coefficients, we have

$$C_{i+1} = \frac{1}{2 + \alpha - C_i} \tag{8.13a}$$

$$D_{i+1} = \frac{D_i - b_i}{2 + \alpha - C_i} \tag{8.13b}$$

Thus, we have shown that if equation (8.11) holds at i then it also holds at i + 1 with the recursion relationships (8.13) giving C_{i+1}, D_{i+1} in terms of C_i and D_i.

Starting values C_2 and D_2 are readily available from equation (8.5) written at i = 1:

$$p_2 - (2 + \alpha)\, p_1 + c_1 = b_1$$

and rearranging,

$$p_1 = \frac{1}{2 + \alpha}\, p_2 + \frac{c_1 - b_1}{2 + \alpha} \tag{8.14}$$

Identifying coefficients in (8.14) with those of equation (8.11) gives

$$C_2 = \frac{1}{2 + \alpha} \tag{8.15a}$$

$$D_2 = \frac{c_1 - b_1}{2 + \alpha} \tag{8.15b}$$

Equations (8.15) and (8.13) allow calculation of C_i, D_i for i = 2, 3, ----, N+1. The upper boundary condition at i = N+1 is

$$p_{N+1} = c_2$$

so that, from equation (8.11)

$$p_N = C_{n+1}\, c_2 + D_{N+1}$$

and p_{N-1}, p_{N-2}, ----, p_1 can be calculated in order from equation (8.11).

8.2. The Two-Dimensional Case - Gaussian Elimination

For the case of two-dimensional flow, eq. (8.4) is

$$\Delta_x^2\, p + \Delta_y^2\, p = \frac{\Delta_t\, p}{\Delta t} = \frac{p_{n+1} - p_n}{\Delta t} \tag{8.16}$$

where, again, absence of a time subscript on p implies the new time n+1.

In expanded form, eq. (8.16) appears as

$$p_{i+1,j} + p_{i-1,j} + p_{i,j+1} + p_{i,j-1} - (4 + \alpha)\, p_{i,j} = b_{i,j} \tag{8.17}$$

where $\alpha = \Delta x^2/\Delta t$ and $b_{i,j} = -\alpha\, p_{i,j,n}$ and we have taken $\Delta y = \Delta x$.

Eq. (8.17) written at i = 1, 2, ----, I; j = 1, 2, ----, J constitutes I x J equations in the I x J unknowns $p_{i,j}$. In matrix form these equations can be written

$$A\underline{p} = \underline{b} \tag{8.18}$$

where $\underline{p}$ and $\underline{b}$ are column vectors (I x J 'long') and A is a pentadiagonal matrix. We recall the one-dimensional equation (8.5) gave rise to a tridiagonal matrix.

The correspondence of the eqs. (8.17) to a pentadiagonal matrix can be understood in reference to a modified numbering or indexing of the system indicated in Fig. 8.1 below.

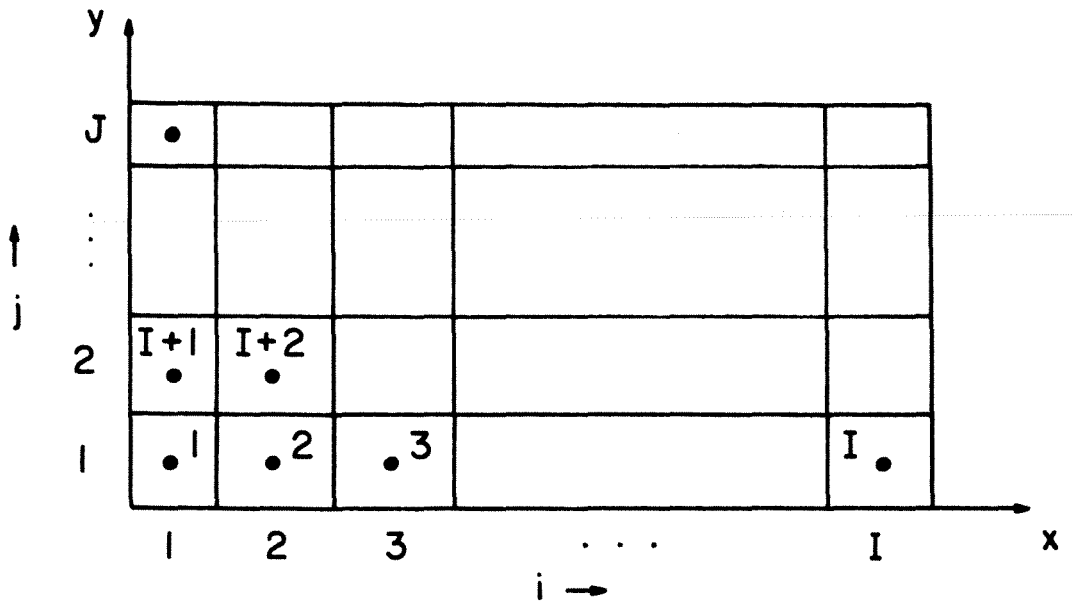


Fig. 8.1 LINEAR INDEXING OF GRID BLOCKS

The relation

$$k = (j-1) \times I + i \tag{8.19}$$

assigns a unique linear subscript k to each grid point (i,j). For example, if the number of blocks is the x direction, I, is 10 then $p_{3,4}$ in the original indexing mode becomes p_{33} in the linear subscript mode. Eqs. (8.17) become, in this linear subscript

$$p_{k+1} + p_{k-1} + p_{k+I} + p_{k-I} - (4 + \alpha)\, p_k = b_k \tag{8.20}$$

Eqs. (8.20) are identical to eq. (8.18) with the definitions

$$A = \begin{Bmatrix}
-(4+\alpha) & 1 & 0 & \cdots & 0 & 1 & 0 & \cdots & & \\
1 & -(4+\alpha) & 1 & 0 & \cdots & 0 & 1 & 0 & \cdots & \\
0 & 1 & -(4+\alpha) & 1 & \cdots & 0 & 1 & 0 & \cdots & \\
 & & & & & & & & & \\
0 & \cdots & 0 & 1 & 0 & \cdots & 1 & -(4+\alpha) & 1 & 0 & \cdots & 0 & 1 & 0 \\
0 & \cdots & 0 & 1 & 0 & \cdots & 1 & -(4+\alpha) & 1 & 0 & \cdots & 0 & 1 & \\
 & & & & & & & & & & & & & \\
0 & \cdots & & & & & 0 & 1 & 0 & \cdots & 1 & -(4+\alpha) &
\end{Bmatrix}$$

(8.20a)

$$\underline{p} = \begin{Bmatrix} p_1 \\ p_2 \\ \cdot \\ \cdot \\ \cdot \\ p_{IxJ} \end{Bmatrix} \qquad \underline{b} = \begin{Bmatrix} b_1 \\ b_2 \\ \cdot \\ \cdot \\ \cdot \\ b_{IxJ} \end{Bmatrix} \qquad (8.20b)$$

The reason for calling A a pentadiagonal matrix is obvious.

The application of Gaussian elimination to the matrix A requires a total of abou $2I^3J$ arithmetic operations. More specifically, about I^3J multiplications and I^3J additions are required to render the matrix in upper triangular form (all zeroes below the main diagonal); about I^2J multiplications and I J additions are then necessary to solve for the p values - a total of $I^2J(I+1)$ multiplications and $I^2J(I+1$ additions. Note that for a square grid (I=J=N) this is N^4 multiplications compared to $N^6/3$ multiplications ((number of unknowns)^3 / 3) required to solve a <u>full</u> matrix problem with N^2 unknowns.

In direct solution (i.e. Gaussian elimination) of eq. (8.20) we number the

grid as shown in Fig. 8.1 only if I is less than J. If J were less than I then we would number vertically along the columns, i. e.,

$$k = Jx(i-1) + j \tag{8.21}$$

The reason for this is that for the numbering scheme of Fig. 8.1 and eq. (8.19) the computational work of direct solution is $2I^3J$ while for the numbering of eq. (8.21) the work is $2J^3I$. The cubic power is attached to the number of blocks in the direction in which we number.

The implicit difference equations (8.16) can be written out in the form

$$p_{i+1,j} - 2p_{i,j} + p_{i-1,j} + p_{i,j+1} - 2p_{i,j} + p_{i,j-1} - \alpha p_{i,j} = - \alpha p_{i,j,n} \tag{8.22}$$

where absence of time index implies t_{n+1}. This form leads to an alternative (but entirely equivalent) formulation of the direct solution procedure. For definiteness and brevity we employ Von Neumann type boundary conditions

$$\left.\begin{aligned} p_{0,j} &= p_{1,j} \\ p_{I,j} &= p_{I+1,j} \end{aligned}\right\} \quad j = 1, 2, \text{----}, J$$

$$\left.\begin{aligned} p_{i,0} &= p_{i,1} \\ p_{i,J} &= p_{i,J+1} \end{aligned}\right\} \quad i = 1, 2, \text{----}, I \tag{8.23}$$

and select J = 5. If the column vector $\underline{P}_i$ is defined as

$$\underline{P}_i = \begin{Bmatrix} p_{i,1} \\ p_{i,2} \\ \cdot \\ \cdot \\ \cdot \\ p_{i,J} \end{Bmatrix} \tag{8.24}$$

then eqs. (8.22) may be written in matrix form as

$$D\,\underline{P}_{i+1} - T\,\underline{P}_i + D\,\underline{P}_{i-1} = -\,B\,\underline{P}_{i,n} \tag{8.25}$$

where (for J = 5)

$$D = \begin{Bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{Bmatrix} \tag{8.26}$$

$$T = \begin{Bmatrix} 3+\alpha & -1 & 0 & 0 & 0 \\ -1 & 4+\alpha & -1 & 0 & 0 \\ 0 & -1 & 4+\alpha & -1 & 0 \\ 0 & 0 & -1 & 4+\alpha & -1 \\ 0 & 0 & 0 & -1 & 3+\alpha \end{Bmatrix} \tag{8.27}$$

$$B = \begin{Bmatrix} \alpha & 0 & 0 & 0 & 0 \\ 0 & \alpha & 0 & 0 & 0 \\ 0 & 0 & \alpha & 0 & 0 \\ 0 & 0 & 0 & \alpha & 0 \\ 0 & 0 & 0 & 0 & \alpha \end{Bmatrix} \tag{8.28}$$

B and D are diagonal (actually scalar) matrices and T is tridiagonal.

In form, eq. (8.25) is identical to the one-dimensional difference eq. (8.5). The only difference is that, there scalars were involved while eq. (8.25) involves column vectors and matrices. Since eq. (8.25) is identical in form to eq. (8.5) we proceed with a method of solution analogous to that applied to the latter. We assume a recursion relationship of the form

$$\underline{P}_{i-1} = C_i \, \underline{P}_i + \underline{D}_i \tag{8.29}$$

where C_i is a square, J x J, matrix and $\underline{D}_i$ is a column vector. Insertion of eq. (8.29) into eq. (8.25) gives

$$D \, \underline{P}_{i+1} - (T - D \, C_i) \, \underline{P}_i + D \, \underline{D}_i = - B \, \underline{P}_{i,n}$$

or

$$\underline{P}_i = (T - D \, C_i)^{-1} \, D \, \underline{P}_{i+1} + (T - D \, C_i)^{-1} \, (D \, \underline{D}_i + B \, \underline{P}_{i,n}) \tag{8.30}$$

where superscript (-1) denotes the inverse of the matrix. Comparison of eq. (8.30) to (8.29) gives

$$C_{i+1} = (T - D \, C_i)^{-1} \, D$$

$$\underline{D}_{i+1} = (T - D \, C_i)^{-1} \, (D \, \underline{D}_i + B \, \underline{P}_{i,n}) \tag{8.31}$$

The recursion relationships (8.31) are analogous to eqs. (8.13) except that matrix

multiplication and inversion replace scalar multiplication and division.

'Starting' values of C_i and $\underline{D}_i$ are obtained by writing eq. (8.25) at i = 1 and employing the Von Neuman boundary condition $\underline{P}_0 = \underline{P}_1$:

$$D\,\underline{P}_2 - (T - D)\,\underline{P}_1 = -B\,\underline{P}_{1,n}$$

Rearrangement and comparison with eq. (8.29) gives

$$C_2 = (T - D)^{-1} D$$

$$\underline{D}_2 = (T - D)^{-1} B\,\underline{P}_{1,n} \qquad (8.32)$$

One might suspect from the sparse (diagonal, tridiagonal) form of the original matrices D, B, T that the matrices C_i and $T - D\,C_i$ would be also sparse and the work of inverting $T - D\,C_i$ would be less than the $2J^3$ operations required for a full matrix. This is not true. The matrices C_i or $T - D\,C_i$ rapidly (with increasing i) 'fill up' to become full matrices and the work of solving eq. (8.25) can be closely estimated by simply assuming C_i and $T - D\,C_i$ to be full J x J matrices.

8.3. Alternating Direction Implicit Techniques

The alternating-direction implicit procedure (ADIP) [8] is a technique for numerical solution of parabolic and elliptic partial difference equations in two space variables. Douglas and Rachford [9] developed a modified implicit method for numerical solution of parabolic and elliptic equations in two or three space variables. Brian [10] proposed a third difference method of higher-order accuracy for solution of the parabolic (heat) equation in three space variables.

Chapter presents a single, general alternating-direction formulation which

includes the above mentioned three methods. That chapter also presents truncation error and stability analyses for the various alternating-direction implicit techniques. Here we simply present ADIP (the Peaceman-Rachford, two-dimensional method) and the Douglas-Rachford three-dimensional method.

8.3.1 ADIP

The alternating-direction implicit procedure approximates the two-dimensional difference equation (8.16) by the step-wise difference equations

$$\Delta_x^2 p^* + \Delta_y^2 p_n = \frac{2}{\Delta t} (p^* - p_n) \tag{8.33a}$$

$$\Delta_x^2 p^* + \Delta_y^2 p_{n+1} = \frac{2}{\Delta t} (p_{n+1} - p^*) \tag{8.33b}$$

The term p^* may be viewed as $p_{n+\frac{1}{2}}$. Each of equations (8.33) involves solution of a "one-dimensional" (tridiagonal matrix) problem as opposed to the two-dimensional (pentadiagonal matrix) problem corresponding to the total implicit form (8.16).

8.3.2 Douglas-Rachford Implicit Procedure

The obvious extension of equation (8.33) to three dimensions,

$$\Delta_x^2 p^* + \Delta_y^2 p_n + \Delta_z^2 p_n = \frac{3}{\Delta t} (p^* - p_n)$$

$$\Delta_x^2 p^* + \Delta_y^2 p^{**} + \Delta_z^2 p_n = \frac{3}{\Delta t} (p^{**} - p^*)$$

$$\Delta_x^2 p^* + \Delta_y^2 p^{**} + \Delta_z^2 p_{n+1} = \frac{3}{\Delta t} (p_{n+1} - p^{**}) \tag{8.34}$$

is unstable. Douglas and Rachford [9] proposed the stable form

$$\Delta_x^2 p^* + \Delta_y^2 p_n + \Delta_z^2 p_n = \frac{1}{\Delta t}(p^* - p_n)$$

$$\Delta_x^2 p^* + \Delta_y^2 p^{**} + \Delta_z^2 p_n = \frac{1}{\Delta t}(p^{**} - p_n)$$

$$\Delta_x^2 p^* + \Delta_y^2 p^{**} + \Delta_z^2 p_{n+1} = \frac{1}{\Delta t}(p_{n+1} - p_n) \qquad (8.35)$$

This form is also stable in two dimensions but involves more truncation error than ADIP, equation (8.33), as will be shown below. The terms p^* and p^{**} may be viewed at first and second approximations to p_{n+1}.

8.3.3 Computational Work

As remarked above, direct solution of the matrix problem associated with

$$\Delta^2 p_{n+1} = \frac{p_{n+1} - p_n}{\Delta t}$$

requires roughly $2IJ^3$ arithmetic operations in two dimensions and $2IJ^3K^3$ operations in three dimensions per time step*. These operations are equally split between multiplications and additions.

In solving eqs. (8.35) we can solve for the changes over the time step,

$$PX = p^* - p_n$$

$$PY = P^{**} - p_n$$

$$PZ = p_{n+1} - p_n \qquad (8.36)$$

* The assumption is made here that in the two-dimensional case, J < I and in three dimensions, J < I and K < I.

from

$$\Delta_x^2 \, PX = \frac{1}{\Delta t} PX - \Delta^2 p_n$$

$$\Delta_y^2 \, PY = \frac{1}{\Delta t} PY - \frac{1}{\Delta t} PX$$

$$\Delta_z^2 \, PZ = \frac{1}{\Delta t} PZ - \frac{1}{\Delta t} PY \qquad (8.37)$$

Having obtained PX from eq. (8.37c) we form $p_{n+1} = p_n + PZ$ and proceed to the next time step.

About 46IJK operations, again equally split between additions and multiplications, are required to solve eqs. (8.37) by three successive tridiagonal calculations (in the variable coefficient case). Thus, the alternating direction procedure requires $46IJK/2IJ^3K^3$ or about $23/J^2K^2$ as much work per time step as direct solution of the full implicit form (8.4). As an example, for the cube I = J = K = 10, this is a ratio of 0.0023. The ratio becomes less favorable however as J and K decrease. For the case I = 20, J = K = 4 the ratio is only $23/16^2$ or about 0.1.

8.4. Alternating-Direction Explicit Procedure (ADEP)

The alternating-direction explicit procedure [11] is a method for solution of 1, 2 or 3-dimensional flow problems. As in the case of ADIP, the utility of the technique derives from reduced computational labor relative to direct solution of the fully implicit equation (8.16). ADEP involves replacement of eq. (8.16) at odd time steps by $t_{n+\frac{1}{2}}$ by

$$\frac{\Delta_x p_{i,j,n} - \Delta_x p_{i-1,j,n}}{\Delta x^2} + \frac{\Delta_y p_{i,j,n} - \Delta_y p_{i,j-1,n+\frac{1}{2}}}{\Delta y^2}$$

$$= \frac{p_{i,j,n+\frac{1}{2}} - p_{i,j,n}}{\Delta t/2} \qquad (8.38a)$$

and at full time steps t_n by

$$\frac{\Delta_x p_{i,j,n+1} - \Delta_x p_{i-1,j,n+\frac{1}{2}}}{\Delta x^2} + \frac{\Delta_y p_{i,j,n+1} - \Delta_y p_{i,j-1,n+\frac{1}{2}}}{\Delta y^2}$$

$$= \frac{p_{i,j,n+1} - p_{i,j,n+\frac{1}{2}}}{\Delta t/2} \qquad (8.38b)$$

Sweeping a two-dimensional grid from Southwest to Northeast using eq. (8.38a) and from Northeast to Southwest using eq. (8.38b) allows explicit calculation of $p_{i,j,n+1}$ at the new time step at each grid point.

While ADEP is an explicit procedure, it has the unconditional stability typical of implicit methods. Chapter presents a comparative analysis of truncation error and stability for ADIP and ADEP. While ADEP requires less computational effort per time step than ADIP the truncation error is larger. Thus, for the same level of truncation error, a smaller time step must be used with ADEP than with ADIP. ADEP may be extended in an obvious fashion to three dimensions. As in the case of ADIP, the intermediate solution $p_{i,j,n+\frac{1}{2}}$ is not utilized - i.e. the "numerical solutic consists of $p_{i,j,n}$ for integral n.

PROBLEMS

8.1. Consider the following linear system:

$$p_{i+1} - ap_i + p_{i-1} = b_i$$

where a is constant and b_i is a known function of i. The range on i is $o \leqslant i \leqslant N$ and the boundary conditions are

$$p_0 = 0$$

$$p_N = 1$$

Set up equations which allow explicit calculation of each p_i, $1 \leqslant i \leqslant N-1$.

8.2. Carry out numerical calculation of p_i in problem 8.1 for the case a = 2.1, $b_i = 0$ (all i) and N = 5.

8.3. Repeat problem 8.1 and 8.2 for the flux type boundary conditions

$$T_1 - T_0 = 1$$

$$T_{N+1} - T_N = 0$$

That is, set up recursion relationships similar to equations (8.13) and derive starting values C_2, D_2 and a relationship giving p_N. Solve for p_i, i = 1, ----, 5.

8.4. Derive the matrix A and column vector $\underline{b}$ (eq. (8.18)) for solution by Gaussian elimination of the two-dimensional, variable coefficient equation

$$\Delta(T\ \Delta\ p)_{ij} + Q_{ij} = s_{ij}\ \Delta_t p \tag{8.39}$$

where s_{ij} is a storage coefficient, $T_{i+\frac{1}{2},j}$, $T_{i,j+\frac{1}{2}}$, etc. are transmissibilities and Q_{ij} is injection for the block.

8.5. Verify that about I^3J multiplications are necessary to solve the matrix problem of eq. (8.18) or of problem 8.4 using Gaussian elimination.

8.6. Expand the j^{th} row eq. (8.25) to show that the result is eq. (8.22).

8.7. Show that the work of solving eq. (8.25) is about $2J^3I$ arithmetic operations.

8.8. Derive (verify) eqs. (8.37).

8.9. Write the ADIP equations for the two-dimensional variable coefficient eq. (8.39). Express the x-sweep and y-sweep equations in a residual form similar to eqs. (8.37). Do this for the definitions

$$PX = p^* - p_n$$

$$PY = p_{n+1} - p^*$$

and again for the definitions

$$PX = p^{*} - p_n$$

$$PY = p_{n+1} - p_n$$

Which resulting residual equation form do you prefer? Why? For the Neumann problem (closed boundaries), derive the recursion relationships required for solution of the two separate one-dimensional problems (x-sweep and y-sweep).

8.10. Repeat Problem 8.9 for the three-dimensional case, using the Douglas-Rachford procedure and the residual definitions of eqs. (8.36).

8.11. Verify the computational work of 46IJK operations required to solve the equations developed in Problem 8.10.

8.12. Write the ADEP equations for solution of eq. (8.39) in three dimensions.

9. ANALYSIS OF STABILITY

A finite-difference approximation to the equation

$$\frac{\partial^2 p}{\partial x^2} = \frac{\partial p}{\partial t} \tag{9.1}$$

is stable if an error introduced in p at some grid point and at some time level decays with increasing time. If the error in p due to this introduced error grows with time then the difference equation is unstable. Let $p^*_{i,n}$ be the exact solution (infinite digit computing machine) of some difference representation of eq (9.1) corresponding to given boundary and initial conditions. Let $p_{i,n}$ be the actual machine solution of the same difference equation. The error $\varepsilon_{i,n}$ in the solution obtained is defined by $p_{i,n} = p^*_{i,n} + \varepsilon_{i,n}$. This error arises due to round-off error and/or to error in initial or boundary conditions. The difference equation is called stable if

$$\left| \frac{\varepsilon_{i,n+1}}{\varepsilon_{i,n}} \right| \leq 1 \tag{9.2}$$

and unstable otherwise. Eq (9.2) holds for all i and n.

Stability analyses may be performed in several different ways. The method of analysis given here is generally referred to as the Von Neumann method. The error $\varepsilon_{i,n}$ is represented by

$$\varepsilon_{i,n} = \lambda^n e^{\hat{\imath}\beta i} \tag{9.3}$$

where $\hat{\imath}$ denotes $\sqrt{-1}$. The stability condition (9.2) is then

$$| \lambda | < 1 \tag{9.4}$$

9.1 Stability of Forward- and Backward-Difference Equations

We will first consider the explicit (forward-) difference approximation to eq (9.1)

$$p_{i+1,n} - 2p_{i,n} + p_{i-1,n} = \alpha \, (p_{i,n+1} - p_{i,n}) \tag{9.5}$$

where $\alpha = \Delta x^2/\Delta t$. Let $p^*_{i,n}$ denote the exact solution of the difference eq (9.5), $p_{i,n}$ the machine solution (erroneous due to round-off error) and $\varepsilon_{i,n}$ the difference between them. Then by these definitions, p^* satisfies eq (9.5)

$$p^*_{i+1,n} - 2p^*_{i,n} + p^*_{i-1,n} = \alpha \, (p^*_{i,n+1} - p^*_{i,n}) \tag{9.6}$$

and so does p,

$$p^*_{i+1,n} + \varepsilon_{i+1,n} - 2(p^*_{i,n} + \varepsilon_{i,n}) + p^*_{i-1,n} + \varepsilon_{i-1,n}$$

$$= \alpha \, (p^*_{i,n+1} + \varepsilon_{i,n+1} - p^*_{i,n} - \varepsilon_{i,n}) \tag{9.7}$$

Subtracting eq (9.6) from (9.7) yields

$$\varepsilon_{i+1,n} - 2\varepsilon_{i,n} + \varepsilon_{i-1,n} = \alpha \, (\varepsilon_{i,n+1} - \varepsilon_{i,n}) \tag{9.8}$$

Thus the error ε satisfies the same difference equation as the pressure p.

Substitution of (9.3) into (9.8) and multiplication of each term by $\lambda^{-n} \, e^{-\hat{i}\beta i}$ gives

$$e^{\hat{i}\beta} - 2 + e^{-\hat{i}\beta} = \alpha\ (\lambda-1) \tag{9.9}$$

Use of this eq and definition $\cos x = (e^{\hat{i}x} + e^{-\hat{i}x})/2$ gives

$$\lambda = 1 - \frac{2(1-\cos\ \beta)}{\alpha}$$

The stability condition (9.4) is then

$$-1 < 1 - \frac{2(1-\cos\ \beta)}{\alpha} < 1 \tag{9.10}$$

The right hand inequality is obviously satisfied for any positive α but the left hand inequality gives

$$-2 < \frac{2(1-\cos\ \beta)}{\alpha}$$

or rearranging and replacing α by $\Delta x^2/\Delta t$.

$$\Delta t < \frac{1}{1-\cos\ \beta}\ \Delta x^2 \tag{9.11}$$

This inequality must hold for all values of β and the restriction is most severe when $\cos\ \beta = -1$ or

$$\Delta t < \frac{\Delta x^2}{2}$$

Thus the explicit difference scheme (9.5) is stable provided the time step does not exceed $\frac{1}{2}\Delta x^2$.

The implicit difference approximation to eq (9.1) is

$$p_{i+1,n+1} - 2p_{i,n+1} + p_{i-1,n+1} = \alpha\,(p_{i,n+1} - p_{i,n}) \qquad (9.12)$$

and is stable for any positive Δt. Again, the error ε satisfies the same equation as the pressure,

$$\varepsilon_{i+1,n+1} - 2\varepsilon_{i,n+1} + \varepsilon_{i-1,n+1} = \alpha\,(\varepsilon_{i,n+1} - \varepsilon_{i,n}) \qquad (9.13)$$

Substitution of ε from eq (9.3) into this equation and multiplication by $\lambda^{-n}\, e^{-\hat{i}\beta i}$ gives

$$-2\,(1-\cos\beta)\,\lambda = \alpha(\lambda-1)$$

or

$$\lambda = \frac{1}{1+\frac{2}{\alpha}\,(1-\cos\beta)}$$

This ratio is positive and less than 1 for any positive value of α and hence there is no restriction on Δt to ensure stability. That is, the backward difference eq (9.12) is unconditionally stable.

9.2 Stability of ADIP

Eqs (8.33) define the Alternating-Direction Implicit Procedure for solving the diffusivity equation (8.3a). Proceeding in the manner described in eqs (9.6) and (9.7), we find that the propagated error $\varepsilon_{i,j,n}$ satisfies the same equation

$$\begin{aligned} \Delta_x^2\,\varepsilon^* + \Delta_y^2\,\varepsilon_n &= \frac{2}{\Delta t}\,(\varepsilon^* - \varepsilon_n) \\ \Delta_x^2\,\varepsilon^* + \Delta_y^2\,\varepsilon_{n+1} &= \frac{2}{\Delta t}\,(\varepsilon_{n+1} - \varepsilon^*) \end{aligned} \qquad (9.14)$$

Let

$$\varepsilon_{i,j,n} = \lambda_n \, e^{\hat{i}\beta i} \, e^{\hat{i}\gamma j}$$
$$\varepsilon^*_{i,j} = \lambda_* \, e^{i\beta\hat{i}} \, e^{\hat{i}\gamma j} \qquad (9.15)$$

and define

$$\lambda \equiv \frac{\varepsilon_{i,j,n+1}}{\varepsilon_{i,j,n}} = \frac{\lambda_{n+1}}{\lambda_n} = \frac{\lambda_*}{\lambda_n} \frac{\lambda_{n+1}}{\lambda_*}$$

as the error amplification factor for the complete time step. The stability condition is again eq (9.4).

Substituting from eqs (9.15) into eqs (9.14) and division of eqs (9.14) by $e^{\hat{i}\beta i} \, e^{\hat{i}\gamma j}$ gives

$$-\lambda_* \frac{(2 - 2\cos\beta)}{\Delta x^2} - \lambda_n \frac{(2 - 2\cos\gamma)}{\Delta y^2} = \frac{2}{\Delta t}(\lambda_* - \lambda_n) \qquad (9.16a)$$

$$-\lambda_* \frac{(2 - 2\cos\beta)}{\Delta x^2} - \lambda_{n+1} \frac{(2 - 2\cos\gamma)}{\Delta y^2} = \frac{2}{\Delta t}(\lambda_{n+1} - \lambda_*) \qquad (9.16b)$$

Use of the identity $2 - 2\cos x = 4 \sin^2(x/2)$ and solution of eq (9.16a) for λ_*/λ_n, eq (9.16b) for λ_{n+1}/λ_* gives

$$\lambda = \frac{\lambda_*}{\lambda_n} \frac{\lambda_{n+1}}{\lambda_*} = \frac{\left[\frac{2}{\Delta t} - \frac{4 \sin^2(\gamma/2)}{\Delta y^2}\right]\left[\frac{2}{\Delta t} - \frac{4 \sin^2(\beta/2)}{\Delta x^2}\right]}{\left[\frac{2}{\Delta t} + \frac{4 \sin^2(\gamma/2)}{\Delta y^2}\right]\left[\frac{2}{\Delta t} + \frac{4 \sin^2(\beta/2)}{\Delta x^2}\right]} \qquad (9.17)$$

This equation shows that the stability condition (9.4) is satisfied, i.e. $|\lambda| < 1$, for all β, γ, for any positive time increment Δt. Thus ADIP is unconditionally stable

9.3. Stability of a Waterflood Equation

Chapter describes application of the equation

$$-\frac{\partial f}{\partial x} = \frac{\partial S}{\partial t} \tag{9.18}$$

in two-dimensional simulation of a normal or thickened waterflood in a 5-spot pattern. Fractional flow of water, f, is presumed to be single-valued function of water saturation S. A reason for interest in numerical solution of this equation is the coupling between it and a concentration equation in simulation of thickened waterflooding.

Following are some difference representations of eq (9.18):

$$-\frac{f_{i+1,n} - f_{i-1,n}}{2\Delta x} = \frac{S_{i,n+1} - S_{i,n-1}}{2\Delta t} \tag{9.19}$$

$$-\frac{f_{i+1,n} - f_{i-1,n}}{2\Delta x} = \frac{S_{i,n+1} - S_{i,n}}{\Delta t} \tag{9.20}$$

$$-\frac{f_{i,n} - f_{i-1,n}}{\Delta x} = \frac{S_{i,n+1} - S_{i,n-1}}{2\Delta t} \tag{9.21}$$

$$-\frac{f_{i,n} - f_{i-1,n}}{\Delta x} = \frac{S_{i,n+1} - S_{i,n}}{\Delta t} \tag{9.22}$$

$$-\frac{f_{i+1,n+1} - f_{i-1,n+1}}{2\Delta x} = \frac{S_{i,n+1} - S_{i,n-1}}{2\Delta t} \tag{9.23}$$

$$-\frac{f_{i+1,n+1} - f_{i-1,n+1}}{2\Delta x} = \frac{S_{i,n+1} - S_{i,n}}{\Delta t} \tag{9.24}$$

$$-\frac{f_{i,n+1} - f_{i-1,n+1}}{\Delta x} = \frac{S_{i,n+1} - S_{i,n}}{\Delta t} \tag{9.25}$$

The stability of these equations can be analyzed in a manner similar to that described above. $S^*_{i,n}$ is defined as the exact solution and $f^*_{i,n}$ is $f(S^*_{i,n})$ (recall that f is a single-valued function of S). $S_{i,n}$ is the actual machine solution which contains an error $\varepsilon_{i,n}$ defined by $S_{i,n} = S^*_{i,n} + \varepsilon_{i,n}$. Since S^* and S both satisfy the difference equation, we have, using eq (9.19) as an example,

$$- (f_{i+1,n} - f_{i-1,n}) \frac{\Delta t}{\Delta x} = S_{i,n+1} - S_{i,n-1} \tag{9.26}$$

and

$$- (f^*_{i+1,n} - f^*_{i-1,n}) \frac{\Delta t}{\Delta x} = S^*_{i,n+1} - S^*_{i,n-1} \tag{9.27}$$

Subtracting the second from the first yields

$$- [(f_{i+1,n} - f^*_{i+1,n}) - (f_{i-1,n} - f^*_{i-1,n})] \frac{\Delta t}{\Delta x} = \varepsilon_{i,n+1} - \varepsilon_{i,n-1} \tag{9.28}$$

From Taylor's series, for small ε,

$$f(S) = f(S^*) + (S-S^*) f'(\bar{S})$$

where $\bar{S}$ is some saturation between S and S^*.

Thus

$$f_{i+1,n} = f^*_{i+1,n} + \varepsilon_{i+1,n} f'$$

and eq (9.28) is

$$-(\varepsilon_{i+1,n} - \varepsilon_{i-1,n})\, c = \varepsilon_{i,n+1} - \varepsilon_{i,n-1} \qquad (9.29)$$

where c is $f'\Delta t/\Delta x$. This same procedure yields a difference equation in ε corresponding to each of the eqs (9.19) - (9.25).

The following examples demonstrate application of the Von Neumann method in determination of stability of the eqs (9.19) - (9.25).

EXAMPLE 9.1

Determine the stability of eq (9.19).

Solution:

Replacing ε in eq (9.29) in accordance with $\varepsilon_{i,n} = \lambda^n e^{\hat{i}\beta i}$ and subsequent division by $\lambda^n e^{\hat{i}\beta i}$ gives

$$-(e^{\hat{i}\beta} - e^{-\hat{i}\beta})\, c = \lambda - 1/\lambda$$

or

$$\lambda^2 + (2\hat{i}c \sin \beta)\, \lambda - 1 = 0$$

The roots of this equation are

$$\lambda = -\hat{i}c \sin \beta \pm \sqrt{1 - c^2 \sin^2 \beta}$$

If $c \sin \beta > 1$ then one of these roots exceeds unity in absolute value; if $c \sin \beta \leq 1$ then both roots satisfy $|\lambda| = 1$. Thus the stability condition is $c \sin \beta \leq 1$ or

$$c \leq 1$$

which gives

$$\Delta t \leq \Delta x/f' \tag{9.30}$$

We have treated f' as a constant here although it is actually a function of S. Thus this analysis is only approximate. In practice, we often take such variable coefficients as constants for the purpose of stability analysis. Then in the final result (9.30), a conservative upper limit on the time step is obtained by inserting extremal values for all variable coefficients which were taken as constants. Thus if f' in this case ranges from .2 to 2 we would insert f' = 2 in eq (9.30) and obtain

$$\Delta t \leq \Delta x/2$$

In practice we would not expect to attain stability with a time step much larger than this.

EXAMPLE 9.2

Determine the stability of eq (9.21).

Solution:

The corresponding error equation is

$$-2c\,(\varepsilon_{i,n} - \varepsilon_{i-1,n}) = \varepsilon_{i,n+1} - \varepsilon_{i,n-1}$$

Substitution of $\lambda^n e^{\hat{i}\beta i}$ for $\varepsilon_{i,n}$ gives

$$-2c\,(1 - e^{-\hat{i}\beta}) = \lambda - 1/\lambda$$

or

$$\lambda^2 + 2c(1 - \cos\beta + \hat{i}\sin\beta)\lambda - 1 = 0$$

Further analysis is simplified in this case if we take $\sin\beta = 0$, $\cos\beta = -1$ at this point so that

$$\lambda^2 + 4c\lambda - 1 = 0$$

The roots are

$$\lambda = -2c \pm \sqrt{1 + 4c^2}$$

One of these roots exceeds unity in absolute value for any positive c, however, small. Thus the difference equation (9.21) is unconditionally unstable.

Results of similar stability analyses of the remaining equations of (9.19) - (9.25) are tabulated in Table 9.1 Truncation errors of the various equations are also tabulated. Truncation error is defined as

$$T = L_D S - LS = L_D S - \left(-\frac{\partial f}{\partial x} - \frac{\partial S}{\partial t}\right)_{i\Delta x,\, n\Delta t}$$

where $L_D S$ is the difference equation.

TABLE 9.1

STABILITY AND TRUNCATION ERROR OF EQS (9.19) - (9.25)

EQ.	STABILITY CONDITION	TRUNCATION ERROR
(9.19)	$c \leq 1$	$\frac{1}{6}(S_{xxt}\,\Delta x^2 - S_{ttt}\,\Delta t^2)$
(9.20)	Uncond. Unstable	
(9.21)	Uncond. Unstable	
(9.22)	$c \leq 1$	
(9.23)	Uncond. Stable	
(9.24)	Uncond. Stable	
(9.25)	Uncond. Stable	

A nonlinear difference equation may be stable but, at the same time, non-convergent under a certain iterative scheme of solution. Stability is concerned with the growth of error amplitude from time step to time step. Convergence is concerned with the growth or damping of error from iteration to iteration at a fixed time step. The unconditionally stable eq (9.24) provides a good example of the distinction between stability and convergence. Since f is a nonlinear function of S, let $S_{i,n+1}$ be determined from eq (9.24) by the following iterative process:

$$- (f^k_{i+1,n+1} - f^k_{i-1,n+1})\frac{\Delta t}{2\Delta x} = S^{k+1}_{i,n+1} - S_{i,n} \tag{9.31}$$

where

$$f^k = f(S^k) \tag{9.32}$$

and k is iteration index. We will denote the solution of eq (9.31) by $S_{i,n+1}$, $f_{i,n+1}$ and the question of convergence is then whether

$$\lim_{k\to\infty} S^k_{i,n+1} = S_{i,n+1}$$

is true.

The solution $S_{i,n+1}$ satisfies eq (9.24) by definition so that

$$-(f_{i+1,n+1} - f_{i-1,n+1})\frac{\Delta t}{2\Delta x} = S_{i,n+1} - S_{i,n} \qquad (9.33)$$

We define ε^k_i as the difference between the true solution and the k th iterate, i.e.

$$S^k_{i,n+1} = S_{i,n+1} + \varepsilon^k_i$$

Subtraction of eq (9.33) from (9.31) then gives

$$-[(f^k_{i+1,n+1} - f_{i+1,n+1}) - (f^k_{i-1,n+1} - f_{i-1,n+1})]\frac{\Delta t}{2\Delta x} = \varepsilon^{k+1}_i$$

Use of a Taylor's series expansion of $f(S^k)$ in terms of $f(S)$ gives

$$-[\varepsilon^k_{i+1} - \varepsilon^k_{i-1}]\frac{c}{2} = \varepsilon^{k+1}_i$$

where, again, c is $f'\Delta t/\Delta x$. Substitution of $\lambda^k e^{\hat{i}\beta i}$ for ε^k_i gives

$$-[e^{\hat{i}\beta} - e^{-\hat{i}\beta}]\frac{c}{2} = \lambda$$

or

$$\lambda = - \hat{i}\, c \sin \beta \tag{9.34}$$

Note that, as in the stability analyses above, λ is the error amplification factor,

$$\lambda = \frac{\varepsilon_i^{k+1}}{\varepsilon_i^{k}}$$

The condition for convergence of the iterative process is $|\lambda| < 1$. From eq (9.34) convergence is obtained only if

$$c \leq 1$$

Thus while the difference eq (9.24) is <u>unconditionally stable</u>, the particular iterative process eq (9.31) for obtaining $S_{i,n+1}$ is <u>conditionally convergent</u>.

A superior iterative method of solving eq (9.24) which avoids this conditional convergence is replacement of f_{n+1} on the left hand side by

$$f_{n+1} = f_n + (S_{n+1} - S_n)f' \tag{9.35}$$

where

$$f' \equiv \frac{f_{n+1} - f_n}{S_{n+1} - S_n} \tag{9.36}$$

Note that the definition (9.36) causes (9.35) to be an identity, not an approximate relation. Substitution from (9.35) into (9.24) gives

$$- [f_{i+1,n} + (S_{i+1,n+1} - S_{i+1,n})f'_{i+1} - (f_{i-1,n} + (S_{i-1,n+1} - S_{i-1,n})f'_{i-1})]\frac{\Delta t}{2\Delta x} = S_{i,n+1} - S_{i,n} \qquad (9.37)$$

Now this equation cannot be solved for $S_{i,n+1}$ unless f'_i is known, but f'_i cannot be determined (see eq (9.36)) unless $S_{i,n+1}$ is known.

Hence we define the iterative process

$$- [f_{i+1,n} + (S^{k+1}_{i+1,n+1} - S_{i+1,n})f'^{k}_{i+1} - (f_{i-1,n} + (S^{k}_{i-1,n+1} - S_{i-1,n})f'^{k}_{i-1})]\frac{\Delta t}{2\Delta x} = S^{k+1}_{i,n+1} - S_{i,n} \qquad (9.38)$$

where

$$f'^{k}_{i} = w\, f'^{k-1}_{i} + (1-w)\frac{f^{k}_{i} - f_{i,n}}{S^{k}_{i,n+1} - S_{i,n}} \qquad (9.39)$$

and f^{k}_{i} is simply $f(S^{k}_{i,n+1})$. The term w is a weight factor, say 0.5. Eqs (9.38) for i = 1,2,3,--- give a tridiagonal matrix in the unknows and hence are solved by application of the Richtmyer algorithm (see page). The reader should verify that if f'^{k}_{i} is treated as a constant, eq (9.38) is unconditionally convergent.

PROBLEMS

9.1. Show that the following difference approximation to eq (9.1) is unconditionally unstable:

$$p_{i+1,n} - 2p_{i,n} + p_{i-1,n} = \frac{\alpha}{2}\,(p_{i,n+1} - p_{i,n-1})$$

Show that the amplification factor obeys the quadratic equation

$$\lambda^2 + (\frac{8}{\alpha}\sin^2\frac{\beta}{2})\lambda - 1 = 0,$$

solve for λ and show that $|\lambda| > 1$ for some β for any Δt, however small.

9.2. Show that the DuFort-Frankel scheme

$$p_{i+1,n} - (p_{i,n+1} + p_{i,n-1}) + p_{i-1,n} = \frac{\alpha}{2}\,(p_{i,n+1} - p_{i,n-1})$$

is unconditionally stable ($\alpha = \Delta x^2/\Delta t$).

Hint: Show that $\lambda = \dfrac{\cos\beta \pm \sqrt{\frac{\alpha^2}{4} - \sin\beta}}{1 + \frac{\alpha}{2}}$ and treat the two cases $\frac{\alpha^2}{4} \geq \sin^2\beta$ and $\frac{\alpha^2}{4} < \sin^2\beta$. Use the relation $|a \pm \hat{i}\, b| = \sqrt{a^2 + b^2}$ in the second case.

9.3. Analyse the stability of the forward (explicit) and backward (implicit) difference approximations to eq (9.1) in two and three dimensions. Show that the explicit difference equation in three dimensions is conditionally stable and that

$$\Delta t < \tfrac{1}{2} \frac{1}{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}}$$

must be satisfied for stability.

9.4. Consider the two-dimensional equation

$$\frac{\partial^2 p}{\partial x^2} + \frac{\partial^2 p}{\partial z^2} = \frac{\partial p}{\partial t}$$

in a rectangle of dimensions L_x, L_z where $L_x >> L_z$. Such regions arise in calculation of flow in two-dimensional cross-sections or vertical slices of reservoirs. As determined in problem 9.3, the explicit difference approximation to this equation is stable for

$$\Delta t \leq \frac{1}{2} \frac{1}{\frac{1}{\Delta x^2} + \frac{1}{\Delta z^2}}$$

which is approximately

$$\Delta t \leq \frac{\Delta x^2}{2}$$

since $\Delta z << \Delta x$. This is a severe limitation since Δz is small. Suppose then we approximate the differential equation implicitly only in the z-direction and explicitly in the x-direction, i.e.

$$\Delta_x^2 p_n + \Delta_z^2 p_{n+1} = \frac{1}{\Delta t} (p_{n+1} - p_n)$$

Do we now obtain the less severe time step limitation of $\Delta t \leq \Delta x^2/2$? Determine the stability of this difference equation. (NOTE: There is no "alternating direction" here. We proceed every time step implicitly in the z-direction only.)

9.5. Determine the stability of the Douglas-Rachford three-dimensional alternating-direction technique, eqs (8.35).

9.6. Determine the stability of the following approximation (similar to ADEP) to eq (9.1).

$$\frac{\Delta_x p_{i,n} - \Delta_x p_{i-1,n+1}}{\Delta x^2} = \frac{1}{\Delta t}\left(p_{i,n+1} - p_{i,n}\right)$$

9.7. The DuFort-Frankel approximation to eq (9.1) in two dimensions is

$$\frac{p_{i+1,n} - (p_{n+1} + p_{n-1}) + p_{i-1,n}}{\Delta x^2} + \frac{p_{j+1,n} - (p_{n+1} + p_{n-1}) + p_{j-1,n}}{\Delta y^2}$$

$$= \frac{1}{2\,\Delta t}\left(p_{n+1} - p_{n-1}\right)$$

Determine the stability of this equation.

9.8. Determine the truncation error and stability of the following difference approximation to eq (9.18)

$$-\frac{f_{i,n} - f_{i-1,n+1}}{\Delta x} = \frac{S_{i,n+1} - S_{i,n}}{\Delta t}$$

9.9. Verify the truncation errors and stability conditions tabulated in Table 9.1.

10. SOLUTION OF ELLIPTIC EQUATIONS BY ALTERNATING DIRECTION PROCEDURES

In Chapter 8 we discussed solution of the parabolic equation (8.3a) by alternating-direction methods. We now consider solution of the elliptic equation

$$\nabla^2 p = 0 \tag{10.1}$$

in the rectangle with either p specified on the boundary (Dirichlet problem) or with $\partial p/\partial n$ (n is normal to boundary) specified there (Neumann problem). The difference equation

$$\Delta^2 p = 0 \tag{10.2}$$

can be solved directly by Gaussian elimination. However, the work involved is $2IJ^3K^3$ in three dimensions, as discussed above.

The alternating-direction procedure may be used to solve equation (10.2) in the following manner [8, 9]. The solution p(x, y, z) to equation (10.1) may be viewed as the steady-state or large-time solution to the parabolic or transient problem

$$\nabla^2 p = \frac{\partial p}{\partial t} \tag{10.3}$$

That is, we could arrive at the desired solution p to equation (10.1) by solving (10.3) for a sequence of time steps until we reached steady state. In that case we would solve

$$\Delta^2 p = \frac{1}{\Delta t}\left(p_{n+1} - p_n\right) \tag{10.4}$$

by the alternating direction procedure. Since, however, we are not interested in the transient solution, we inquire whether "judicious" time step values might be chosen so that the steady state solution is reached in as few steps as possible. These Δt values may introduce considerable truncation error in the transient solution but,

to repeat, we are not interested in the transient solution. Thus there is no need to retain the terminology time, n, Δt, and we re-write equation (10.4) as

$$\Delta^2 p^{k+1} = H_k \, (p^{k+1} - p^k) \tag{10.5}$$

where H_k is the iteration parameter and k is iteration index; from the above discussion, H_k may be viewed as the inverse of a pseudo time step and k as the total number of time steps.

10.1 The Douglas-Rachford Alternating-Direction Iterative Technique

To avoid the labor of direct solution we employ the Douglas-Rachford alternating-direction procedure, equation (8.35), and solve equation (10.5) in three dimensions by

$$\Delta_x^2 p^* + \Delta_y^2 p^k + \Delta_z^2 p^k = H_k \, (p^* - p^k) \tag{10.6a}$$

$$\Delta_x^2 p^* + \Delta_y^2 p^{**} + \Delta_z^2 p^k = H_k \, (p^{**} - p^k) \tag{10.6b}$$

$$\Delta_x^2 p^* + \Delta_y^2 p^{**} + \Delta_z^2 p^{k+1} = H_k \, (p^{k+1} - p^k) \tag{10.6c}$$

To insure convergence, the same value of H_k is used in each of the three steps. However, H_k is varied from one iteration to the next.

Solution for p^* from equation (10.6a), p^{**} from (10.6b) and p^{k+1} from (10.6c) constitutes one *iteration*. K iterations constitute one *cycle*. Thus one cycle involves solution of equation (10.6) for k = 1, 2, ---, K, using parameters H_1, H_2, ---, H_K. Cycles are repeated until convergence is obtained. Douglas, Rachford and Peaceman discuss selection of iteration parameters in several papers [8, 9, 12]; we will consider that problem below.

The alternating-direction iterative procedure is equally applicable to the parabolic equation. Consider the parabolic case with a source term,

$$\nabla^2 p + q(x,y,z) = \alpha \frac{\partial p}{\partial t} \tag{10.7}$$

In implicit difference form this equation becomes

$$\Delta^2 p_{n+1} + Q = \frac{\alpha}{\Delta t} (p_{n+1} - p_n)$$

or

$$\Delta^2 p_{n+1} - \frac{\alpha}{\Delta t} p_{n+1} = - \frac{\alpha}{\Delta t} p_n - Q = - B_{ijk} \quad (10.8)$$

where ijk denotes spatial grid point (x_i, y_j, z_k). We obtain p_{n+1} by iteration as

$$\Delta_x^2 p^* + \Delta_y^2 p^k + \Delta_z^2 p^k - \frac{\alpha}{\Delta t} p^* = H_k (p^* - p^k) - B \quad (10.9a)$$

$$\Delta_x^2 p^* + \Delta_y^2 p^{**} + \Delta_z p^k - \frac{\alpha}{\Delta t} p^{**} = H_k (p^{**} - p^k) - B \quad (10.9b)$$

$$\Delta_x^2 p^* + \Delta_y^2 p^{**} + \Delta_z^2 p^{k+1} - \frac{\alpha}{\Delta t} p^{k+1} = H_k (p^{k+1} - p^k) - B \quad (10.9c)$$

where p^k, p^*, p^{**}, and p^{k+1}, etc., are successive approximations to the new time step values p_{n+1}.

The Douglas-Rachford procedure applies in two dimensions to eq (10.8) as

$$\Delta_x^2 p^* + \Delta_y^2 p^k - \frac{\alpha}{\Delta t} p^* = H_k (p^* - p^k) - B \quad (10.10a)$$

$$\Delta_x^2 p^* + \Delta_y^2 p^{k+1} - \frac{\alpha}{\Delta t} p^{k+1} = H_k (p^{k+1} - p^k) - B \quad (10.10b)$$

Iterative solution of equation (10.8) for p_{n+1} has the advantage that any time step, however large, may be accommodated. If equation (10.8) is solved by the noniterative application of the alternating-direction procedure, equation (8.35) as described in Chapter 8, then a limited time step (smaller as compressibility α becomes smaller) must be employed to insure smoothness and accuracy in the solution.

10.2 The Peaceman-Rachford Iterative Technique

The two-dimensional Peaceman-Rachford procedure applies to eq (10.8) as

$$\Delta_x^2 p^* + \Delta_y^2 p^k - \frac{\alpha}{\Delta t} p^* = H_k (p^* - p^k) - B \tag{10.11a}$$

$$\Delta_x^2 p^* + \Delta_y^2 p^{k+1} - \frac{\alpha}{\Delta t} p^{k+1} = H_k (p^{k+1} - p^*) - B \tag{10.11b}$$

Note that the only difference between this method and the Douglas-Rachford technique in two dimensions is the use of p^* as opposed to p^k on the right-hand side of the second (y-sweep) equation.

10.3 Iteration Parameters for the Two-Dimensional Problem

The convergence analysis which yields formulae for selection of iteration parameters is discussed in the literature [8, 13, 14] and is presented in detail in Chapter below. Here we will simply give guidelines based on this analysis which are often satisfactory. Consider a two-dimensional elliptic difference equation,

$$\Delta(T \Delta p) = - C_{ij} \tag{10.12}$$

where C_{ij} is a known term at each grid point $x = i\Delta x$, $y = j\Delta y$ and $\Delta T \Delta p$ is defined in eq (2.3). Application of the Peaceman-Rachford alternating-direction iterative method to this equation gives

$$\Delta_x T \Delta_x p^* + \Delta_y T \Delta_y p^k = H_k (p^* - p^k) - C_{ij} \tag{10.13a}$$

$$\Delta_x T \Delta_x p^* + \Delta_y T \Delta_y p^{k+1} = H_k (p^{k+1} - p^*) - C_{ij} \tag{10.13b}$$

In practice the iteration parameters are normalized as defined by

$$H_k = h_k (\Sigma T)_{ij} \tag{10.14}$$

where $\Sigma T_{ij} = T_{i+\frac{1}{2},j} + T_{i-\frac{1}{2},j} + T_{i,j+\frac{1}{2}} + T_{i,j-\frac{1}{2}}$. If N_x and N_y denote the numbers of grid points in the x and y directions, respectively, then the minimum iteration parameter is

$$h_{min} = \text{Min.} \left\{ \frac{\pi^2}{2N_x^2} \frac{1}{1 + \frac{T_y}{T_x}}, \frac{\pi^2}{2N_y^2} \frac{1}{1 + \frac{T_x}{T_y}} \right\} \tag{10.15}$$

while the maximum parameter is 1 if $T_x = T_y$ and 2 if $T_x >> T_y$ or $T_y >> T_x$. Strictly speaking, this formula applies only to the Peaceman-Rachford (two dimensional) alternating-direction procedure. However, the formula has been used with success in selecting parameters for three-dimensional problems using the Douglas-Rachford iterative technique.

As pointed out in Chapter 12 below, except for relative permeabilities

$$T_x = k_x \frac{\Delta y}{\Delta x} \qquad T_y = k_y \frac{\Delta x}{\Delta y}$$

Insertion of these definitions into equation (10.15) gives

$$h_{min} = \text{Min.} \left\{ \frac{\pi^2}{2N_x^2} \frac{1}{1 + \frac{k_y}{k_x} \frac{\Delta x^2}{\Delta y^2}}, \frac{\pi^2}{2N_y^2} \frac{1}{1 + \frac{k_x}{k_y} \frac{\Delta y^2}{\Delta x^2}} \right\} \tag{10.16}$$

For an areal (two-dimensional) problem, generally $\Delta x \cong \Delta y$ and if $k_x = k_y$, then the two terms in equation (10.10) are equal. For cross-sectional problems, however, generally

$$N_x >> N_y \qquad \Delta x >> \Delta y$$

and the first term in equation (10.16) is the smaller.

Iteration parameters should be spaced as a geometric sequence [8, 12] i.e.

$$\frac{h_{k+1}}{h_k} = \alpha, \text{ a constant} \tag{10.17}$$

If a total of K parameters are chosen per cycle, then

$$\frac{h_K}{h_1} = \alpha^{K-1} \tag{10.18}$$

If h_1, h_K (minimum and maximum parameters) and the number of parameters per cycle, K, are known then α may be calculated from equation (10.18) as

$$\ell n\ \alpha = \frac{\ell n\ (h_K/h_1)}{K-1} \tag{10.19}$$

The number of parameters K is generally chosen as 4 or 5 for a small range on the h_k (e.g., .01-2) and as 6 to 8 for a large range (e.g., .0001-2). The writer has generally used the h_k in order of increasing magnitude--i.e., the smallest h_k first, etc.

Equation (10.16) provides only an estimate of the minimum parameter. Some problems exhibit considerable sensitivity to this h_{min} with respect to ease of convergence. In such cases only the minimum parameter is important in gaining a rapidly convergent calculation. That is, whether a maximum h_k of .5, 1, or 2 is used is generally immaterial. A difference from .0001 to .005 in h_1, however, may be critical. In cases where sensitivity to h_{min} exists, three or four trial runs over the first few time steps with different sets of h_k are usually sufficient to determine an h_k set which will be satisfactory for the entire time prediction.

A satisfactory rate of convergence is, in the writer's experience, convergence within two cycles--i.e. 6 to 12 iterations per time step.

Example 10.1. Estimate an iteration parameter set for a cross-sectional two-dimensional problem with the following data:

$N_x = 30$

$N_y = 8$

$k_x = 100$ md

$k_y = 20$ md

$L_x = 6000$ ft

$L_y = 160$ ft

where L_x and L_y are reservoir length in the x and y directions, respectively.

Solution: The grid size is $\Delta x = 6000/30 = 200$, $\Delta y = 160/8 = 20$. Equation (10.16) gives

$$h_{min} = \text{Min} \left\{ \frac{\pi^2}{2(30)^2} \frac{1}{1 + \frac{20}{100}\left(\frac{200}{20}\right)^2}, \frac{\pi^2}{2(8)^2} \frac{1}{1 + \frac{100}{20}\left(\frac{20}{200}\right)^2} \right\}$$

The first of these two numbers is smaller and therefore

$$h_{min} = h_1 = \frac{5}{900} \frac{1}{1 + .2(100)} = \frac{5}{900} \frac{1}{21} = .0003$$

Since $T_y >> T_x$, $h_K = 2$ and using K = 7 parameters per cycle, equation (10.19) gives

$$\ln \alpha = \frac{\ln (2/.0003)}{6} = 1.47$$

$$\alpha = 4.35$$

Thus the set is

$$\begin{aligned} h_1 &= .0003 \\ h_2 &= 4.35\ (.0003) = .0013 \\ h_3 &= 4.35\ (.0013) = .00566 \\ h_4 &= 4.35\ (.00566) = .0246 \\ h_5 &= 4.35\ (.0246) = .107 \\ h_6 &= 4.35\ (.107) = .466 \\ h_7 &= 4.35\ (.466) = 2 \end{aligned}$$

11. DIFFERENCE APPROXIMATIONS TO THE RESERVOIR SIMULATION EQUATIONS

The reservoir simulation equations (6.11) contain second-order spatial derivatives of type $\frac{\partial}{\partial x}\left(K \frac{\partial p}{\partial x}\right)$ and first-order derivatives in time. In three dimensions, the oil flow eq. (6.13b) is

$$\frac{\partial}{\partial x}\left(\frac{k\, k_{ro}\, b_o\, \gamma_o}{\mu_o} \frac{\partial P_o}{\partial x}\right) + \frac{\partial}{\partial y}\left(\frac{k\, k_{ro}\, b_o\, \gamma_o}{\mu_o} \frac{\partial P_o}{\partial y}\right) + \frac{\partial}{\partial z}\left(\frac{k\, k_{ro}\, b_o\, \gamma_o}{\mu_o} \frac{\partial P_o}{\partial z}\right)$$

$$- q_{vo} = \frac{\partial}{\partial t}\left(\phi\, b_o\, S_o\right) \qquad (11.1)$$

We will develop difference approximations to eq. (11.1) for the uses of regular and variable grid spacing.

11.1. Regular Grid Spacing

The standard central-difference approximation is employed for the spatial derivatives, i.e.

$$\frac{\partial}{\partial x}\left(K_o \frac{\partial P_o}{\partial x}\right) \cong \frac{K_{oi+\frac{1}{2}}\left(P_{oi+1} - P_{oi}\right) - K_{oi-\frac{1}{2}}\left(P_{oi} - P_{oi-1}\right)}{\Delta x^2}$$

where $K_o = k\, k_{ro}\, b_o\, \gamma_o/\mu_o$. The P values in these spatial differences are understood to apply at the new time level t_{n+1}. The backward time difference is employed,

$$\frac{\partial}{\partial t}\left(\phi\, b_o\, S_o\right) \cong \frac{\left(\phi\, b_o\, S_o\right)_{n+1} - \left(\phi\, b_o\, S_o\right)_n}{\Delta t}$$

Using these difference approximations in eq. (11.1) and multiplying each term in the equation by $\Delta x\ \Delta y\ \Delta z$ gives

$$\Delta(T_o \Delta P_o)_{ijk} - q_{oijk} = \frac{V_{ijk}}{\Delta t} \Delta_t (\phi b_o S_o)_{ijk} \qquad (11.2)$$

where

$$\Delta(T_o \Delta P_o) = \Delta_x (T_o \Delta_x P_o) + \Delta_y (T_o \Delta_y P_o) + \Delta_z (T_o \Delta_z P_o)$$

$$\Delta_x (T_o \Delta_x P_o) = T_{oi+\frac{1}{2}} (P_{oi+1} - P_{oi}) - T_{oi-\frac{1}{2}} (P_{oi} - P_{oi-1})$$

$$T_{oi+\frac{1}{2}} = \left(\frac{k\, k_{ro}\, b_o\, \gamma_o\, \Delta y\, \Delta z}{\Delta x}\right)_{i+\frac{1}{2}}$$

q_{oijk} = STB/day oil production rate from block (i,j,k)

$$\Delta_t (\phi b_o S_o) = (\phi b_o S_o)_{i,j,k,n+1} - (\phi b_o S_o)_{i,j,k,n}$$

V_{ijk} = block volume, $\Delta x\, \Delta y\, \Delta z$

The term $T_{oi+\frac{1}{2}}$ is oil-phase transmissibility for x-direction oil flow between blocks (i,j,k) and (i+1,j,k). In fact, $T_{oi+\frac{1}{2}} (P_{oi+1,j,k} - P_{oi,j,k})$ is simply the rate of oil flow, STB/day, in the x direction from block (i+1,j,k) to block (i,j,k). Transmissibility for y-direction flow is $T_{oj+\frac{1}{2}} = (k\, k_{ro}\, b_o\, \gamma_o\, \Delta x\, \Delta z/\Delta y)_{i,j+\frac{1}{2},k}$.

EXAMPLE 11.1

Express in difference form the equations (6.14) describing incompressible, two-phase (water-oil) flow in three dimensions.

Solution:

In three dimensions, eq. (6.14a) (6.14b) are

$$\frac{\partial}{\partial x}\left(\frac{k_x k_{rw}}{\mu_w}\frac{\partial \Phi_w}{\partial x}\right) + \frac{\partial}{\partial y}\left(\frac{k_y k_{rw}}{\mu_w}\frac{\partial \Phi_w}{\partial y}\right) + \frac{\partial}{\partial z}\left(\frac{k_z k_{rw}}{\mu_w}\frac{\partial \Phi_w}{\partial z}\right) - B_w q_{vw} = \phi \frac{\partial S}{\partial t}$$

$$\frac{\partial}{\partial x}\left(\frac{k_x k_{ro}}{\mu_o}\frac{\partial \Phi_o}{\partial x}\right) + \frac{\partial}{\partial y}\left(\frac{k_y k_{ro}}{\mu_o}\frac{\partial \Phi_o}{\partial y}\right) + \frac{\partial}{\partial z}\left(\frac{k_z k_{ro}}{\mu_o}\frac{\partial \Phi_o}{\partial z}\right) - B_o q_{vo} = -\phi \frac{\partial S}{\partial t}$$

Replacing the spatial derivatives by the second-order differences and multiplication by $\Delta x\, \Delta y\, \Delta z$ gives

$$\Delta(T_w \Delta \Phi_w)_{ijk} - B_w q_{wijk} = \frac{V_{pijk}}{\Delta t} \Delta_t S$$

$$\Delta(T_o \Delta \Phi_o)_{ijk} - B_o q_{oijk} = -\frac{V_{pijk}}{\Delta t} \Delta_t S$$

where

$$\Delta(T_w \Delta \Phi_w)_{ijk} = \Delta_x (T_w \Delta_x \Phi_w)_{ijk} + \Delta_y (T_w \Delta_y \Phi_w)_{ijk} + \Delta_z (T_w \Delta_z \Phi_w)_{ij}$$

$$\Delta_x (T_w \Delta_x \Phi_w)_{ijk} = T_{wi+\frac{1}{2},j,k} (\Phi_{wi+1,j,k} - \Phi_{wijk}) - T_{wi-\frac{1}{2},j,k} (\Phi_{wijk} - \Phi_{wi-1,j,k})$$

$$T_{wi+\frac{1}{2},j,k} = \left(\frac{k_x k_{rw}}{\mu_w}\frac{\Delta y\, \Delta z}{\Delta x}\right)_{i+\frac{1}{2},j,k}$$

$$V_{pijk} = (\phi\, \Delta x\, \Delta y\, \Delta z)_{ijk} = \text{block pore volume}$$

Transmissibility for flow in the y- and z-directions are defined similarly. The term q_{wijk} is production rate for the block (i,j,k), STB/day.

11.2. Variable Grid Spacing

This procedure for obtaining the difference equation applies equally well to the case of a variable grid. Consider numerical solution of eq. (11.1)

$$\frac{\partial}{\partial x}\left(K_o \frac{\partial P_o}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_o \frac{\partial P_o}{\partial y}\right) - q_{vo} = \frac{\partial}{\partial t}\left(\phi\, b_o\, S_o\right) \qquad (11.3)$$

in two dimensions using the grid of Fig. 11.1. The term K_o here is

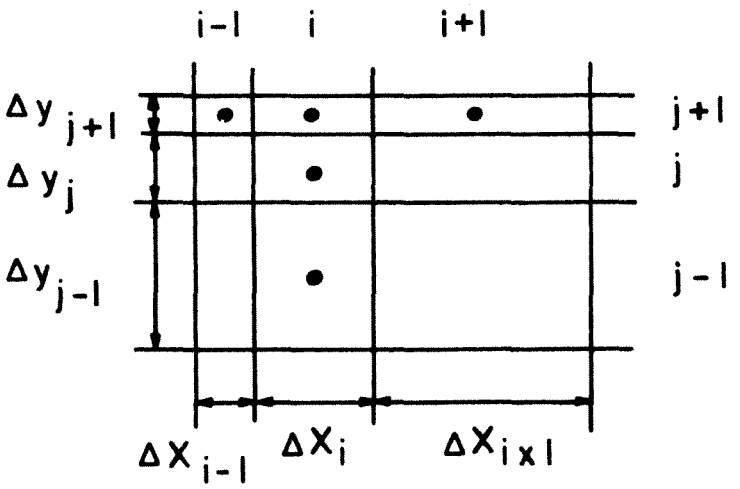


Fig. 11.1 VARIABLE GRID

$k\, k_{ro}\, b_o\, \gamma_o/\mu_o$. We will denote distance between points (block centers) by ℓ, that is

$$\ell_{i+\frac{1}{2}} = .5\ (\Delta x_i + \Delta x_{i+1})$$

$$\ell_{j-\frac{1}{2}} = .5\ (\Delta y_j + \Delta y_{j-1})$$

A difference approximation to $\frac{\partial}{\partial x}\left(K_o \frac{\partial P_o}{\partial x}\right)$ at the point x_i, y_i is

$$\frac{\partial}{\partial x}\left(K_o \frac{\partial P_o}{\partial x}\right) \cong \left[\left(K_o \frac{\partial P_o}{\partial x}\right)_{i+\frac{1}{2},j} - \left(K_o \frac{\partial P_o}{\partial x}\right)_{i-\frac{1}{2},j}\right]/\Delta x_i$$

where $i+\frac{1}{2}$ denotes the position $x_i + \Delta x_i/2$. Further differencing gives

$$\frac{\partial}{\partial x}\left(K_o \frac{\partial P_o}{\partial x}\right) \cong K_{oi+\frac{1}{2},j} \frac{P_{oi+1,j} - P_{oi,j}}{\Delta x_i \, \ell_{i+\frac{1}{2}}} - K_{oi-\frac{1}{2},j} \frac{P_{oi,j} - P_{oi-1,j}}{\Delta x_i \, \ell_{i-\frac{1}{2}}}$$

A similar differencing of the term $\frac{\partial}{\partial y}\left(K_o \frac{\partial P_o}{\partial y}\right)$ in eq. (11.3) and multiplication by $h \, \Delta x_i \, \Delta y_j$ (where h is reservoir thickness) gives

$$\Delta(T_o \, \Delta \, P_o)_{ij} - q_{oij} = \frac{V_{ij}}{\Delta t} \Delta_t \, (\phi \, b_o \, S_o)_{ij} \qquad (11.4)$$

where

$$T_{oi+\frac{1}{2},j} = \left(\frac{K_o \, \Delta y_i \, h}{\ell}\right)_{i+\frac{1}{2},j}$$

$$T_{oi,j+\frac{1}{2}} = \left(\frac{K_o \, h \, \Delta x_i}{\ell}\right)_{i,j+\frac{1}{2}}$$

V_{ij} = block volume, $h \ \Delta x_i \, \Delta y_j$

q_{oij} = oil production rate for block i,j, STB/day

11.3. Difference Approximation to the Time Derivative

Expansion of the difference $\Delta_t \, (\phi \, b_o \, S_o)$ must be carefully performed so that the expanded form reduces identically to $(\phi \, b_o \, S_o)_{n+1} - (\phi \, b_o \, S_o)_n$. For example

$$\Delta_t \, (\phi \, b_o \, S_o) = \phi_n \, b_{on} \, \Delta_t \, S_o + \phi_n \, S_{on} \, \Delta_t \, b_o + b_{on} \, S_{on} \, \Delta_t \, \phi \qquad (11.5)$$

is clearly incorrect since, as the reader should verify, the right-hand side does

not reduce to $(\phi\, b_o\, S_o)_{n+1} - (\phi\, b_o\, S_o)_n$. One of several correct expansions is

$$\Delta_t\,(\phi\, b_o\, S_o) = \phi_{n+1}\, b_{on+1}\, \Delta_t\, S_o + \phi_{n+1}\, S_{on}\, \Delta_t\, b_o + b_{on}\, S_{on}\, \Delta_t\, \phi \tag{11.6}$$

Further expansion of the right hand side of eq. (11.2) is given in Chapter 15 in conjunction with the description of methods for solving the equations describing multiphase, multidimensional flow.

11.4. Calculation of Interblock Transmissibilities

The transmissibilities $T_{oi+\frac{1}{2},j}$ etc., in eq. (11.2) contain pressure-dependent terms (b_o, γ_o, μ_o) and saturation-depandent terms (k_{ro}). These variables are generally evaluated at the old time step (t_n) regardless of whether P_o on the left hand side of eq. (11.2) is taken implicitly (at t_{n+1}) or explicitly (at t_n). The truncation error incurred by taking these b_o, k_{ro}, etc., at the old time step is generally negligible in practical problems. As pointed out by Blair [13], however, problems which involve "converging" flow, such as coning problems, may be solved in some cases with larger time steps if the transmissibilities are taken at $t_{n+\frac{1}{2}}$ or t_{n+1}. In any event, the truncation error associated with use of explicit (time level n) transmissibilities can be estimated by repeating portions of a calculation using smaller time steps. If the calculated answers are largely insensitive to the change at Δt then this truncation error is not significant. Use of smaller time steps in an explicit transmissibility model allows estimation of the effect of using implicit transmissibilities simply because the transmissibilities are more frequently updated when a smaller time step is used.

In calculating the interblock transmissibility

$$T_{o+\frac{1}{2},j,k} = \left(\frac{k\, k_{ro}\, b_o\, \gamma_o\, \Delta y_j\, \Delta z_k}{\mu_o\, \ell}\right)_{i+\frac{1}{2},j,k}$$

values of k_{ro}, b_o, etc., are required at the position $i+\frac{1}{2}$ (or $x_i + \Delta x_i/2$) between points (i,j,k) and (i+1,j,k). However, pressures and saturations are known only at the points. The pressure-dependent quantities b_o, γ_o, and μ_o are generally arithmetically averaged or taken at the upstream point. The upstream point is (i+1,j,k) if flow is from (i+1,j,k) to (i,j,k) and is (i,j,k) if flow is in the opposite direction. In most practical cases, the calculated answers are insensitive to the choice of upstream weighting as opposed to averaging of pressure-dependent quantities in the transmissibilities.

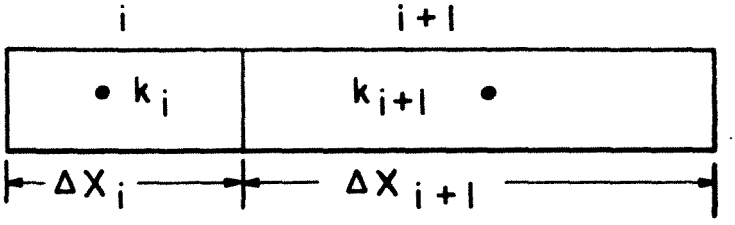
An interblock relative permeability value between points i and i+1 can be obtained as a) the weighted average

$$k_{ri+\frac{1}{2}} = \omega(k_r)_{\text{upstream}} + (1-\omega)\,(k_r)_{\text{downstream}} \qquad (11.7)$$

b) the value of k_r at a weighted saturation $\omega S_i + (1-\omega)\, S_{i+1}$, or c) the harmonic or "series resistance" value $2k_{ri}\, k_{ri+1}/(k_{ri} + k_{ri+1})$. This writer strongly recommends use of the upstream weighting, i.e. eq. (11.7) with ω=1. This handling of interblock relative permeability is intuitively correct if we consider the extreme case of oil draining from a block (1) of low oil saturation to an adjacent block (2) of high oil saturation. If k_{ro1} were (say) .05 and k_{ro2} were .8 and simple arithmetic averaging were used to obtain $k_{ro1+\frac{1}{2}}$, a relative permeability of .425 would be used and oil would drain out of block 1 at a rapid, highly erroneou rate. However, an upstream weighting would give an interblock transmissibility corresponding to a relative permeability of .05 which would result in a more realistic, retarded rate of gravity drainage. More pertinent to this weighting problem, however, is a comparison between a Buckley-Leverett saturation profile and several numerical, one-dimensional calculations using various values of ω in eq. (11.7). Use of ω = 1 or nearly 1 yields much better agreement than use of

$\omega = .5$ as shown in Example 11.2 below. The harmonic mean gives highly erroneous results in the vicinity of relatively sharp saturation fronts (areas where saturation varies sharply with distance). As an extreme example, consider the flow of water from block i having $k_{r\omega i} = .7$ to block i+1 having $k_{r\omega i+1} = 0$. The harmonic mean is 0 and would not allow water to enter the block i+1.

The remaining term k/ℓ in the interblock transmissibility should be taken as the harmonic value. Consider the geometry shown in the sketch consisting of adjacent blocks of different lengths and permeabilities



For steady-state flow between points i and i+1, Darcy's law correctly relates pressu drop to flow rate as

$$q = \left(\frac{k}{\ell}\right)_m \frac{A}{\mu} (p_i - p_{i+1})$$

where A is cross-sectional area and

$$\left(\frac{k}{\ell}\right)_m = \frac{1}{\frac{\Delta x_i/2}{k_i} + \frac{\Delta x_{i+1}/2}{k_{i+1}}} = \frac{2k_i\ k_{i+1}}{k_i\ \Delta x_{i+1} + k_{i+1}\ \Delta x_i}$$

If $\Delta x_i = \Delta x_{i+1}$ then this is

$$\left(\frac{k}{\ell}\right)_m = \frac{1}{\Delta x} \frac{2k_i\ k_{i+1}}{k_i + k_{i+1}}$$

If the arithmetic average of k/ℓ for the two blocks is used in the transmissibility then the calculations will give an erroneous pressure gradient if and when the flow regime approaches a steady-state.

In summary, the transmissibility in eq. (11.2) is calculated for use in the new time step's calculation (t_{n+1}) as

$$T_{oi+\frac{1}{2},j,k} = \frac{2k_i\, k_{i+1}}{k_i\, \Delta x_{i+1} + k_{i+1}\, \Delta x_i} (\Delta y_j\, \Delta z_k)\, (k_{ro})_{\text{upstream}} \left(\frac{b_o\, \gamma_o}{\mu_o}\right)_{\text{upstrea}}$$
$$\text{or aver}$$

All pressure- and saturation-dependent components are evaluated from the old time level's (t_n) pressure and saturation distributions.

EXAMPLE 11.2

Numerically solve the equations for one-dimensional displacement of oil by water and examine error in the solution as a function of the weighting employed on relative permeabilities in the transmissibilities. Fluids may be treated as incompressible. Relative permeability curves are given in Fig. 11.2 and other data are:

k = 300 md $\quad \mu_o = \mu_w$ = 1 cp $\quad \phi$ = .2

L_x = reservoir length = 1000' $\quad L_y$ = width = 100' $\quad h$ = 100'

Injection rate = 76 BPD

The reservoir is horizontal and initial water saturation is .16.

Solution:

For the case of incompressible, one-dimensional flow of oil and water, eqs. (6.14) are

$$\frac{\partial}{\partial x}\left(\frac{k\, k_{rw}}{\mu_w}\frac{\partial \Phi_w}{\partial x}\right) - q_{vw} = \phi \frac{\partial S_w}{\partial t}$$

$$\frac{\partial}{\partial x}\left(\frac{k\, k_{ro}}{\mu_o}\frac{\partial \Phi_o}{\partial x}\right) - q_{vo} = -\phi \frac{\partial S_w}{\partial t}$$

where $\Phi = p - \gamma Z$ and S is water saturation. In finite-difference form these equation are

$$\Delta_x \left(T_w \Delta_x \Phi_w\right)_i - q_{wi} = \frac{V_{pi}}{\Delta t} \Delta_t S$$

$$\Delta_x \left(T_o \Delta_x \Phi_o\right)_i - q_{oi} = -\frac{V_{pi}}{\Delta t} \Delta_t S \qquad (11.8)$$

where

$$T_{wi+\frac{1}{2}} = \left(\frac{k\, k_{rw}\, L_y\, h}{\Delta x}\right)_{i+\frac{1}{2}}$$

$$\Delta_x \left(T_w \Delta_x \Phi_w\right) \equiv T_{wi+\frac{1}{2}} \left(\Phi_{wi+1} - \Phi_{wi}\right) - T_{wi-\frac{1}{2}} \left(\Phi_{wi} - \Phi_{wi-1}\right)$$

and similarly for the oil phase. V_{pi} is simply the block pore volume $\phi h\, L_y\, \Delta x$.

The results discussed here were obtained by simultaneous solution of eqs. (11.8 as described in Chapter 15. Forty spatial increments ($\Delta x = 1000/40 = 25'$) and a time step of 10 days were employed.

Figure 11.3 shows water saturation vs distance after injection of .32 pore volumes. The solid curve is the analytical (Buckley-Leverett) solution. The open circles are numerical results using upstream weighting on both water and oil relative permeabilities in the transmissibilities. The solid circles are numerical results using mid-point weighting ($\omega = .5$ in eq. (11.7)) on the relative permeabilit The considerably superior accuracy obtained by upstream weighting is apparent.

Figure 11.4 compares saturation profiles calculated using a) upstream weighting on both water and oil relative permeabilities and b) upstream weighting on the oil (displaced phase) and midpoint weighting on the water (displacing phase). The good agreement between these profiles and poor agreement between the profiles on Fig. 11.3 shows that the only important weighting factor is that on the displaced phase. That is, it is generally immaterial whether midpoint or upstream weighting is used on the displacing phase. However, upstream weighting on the displaced phase is highly preferable to midpoint weighting.

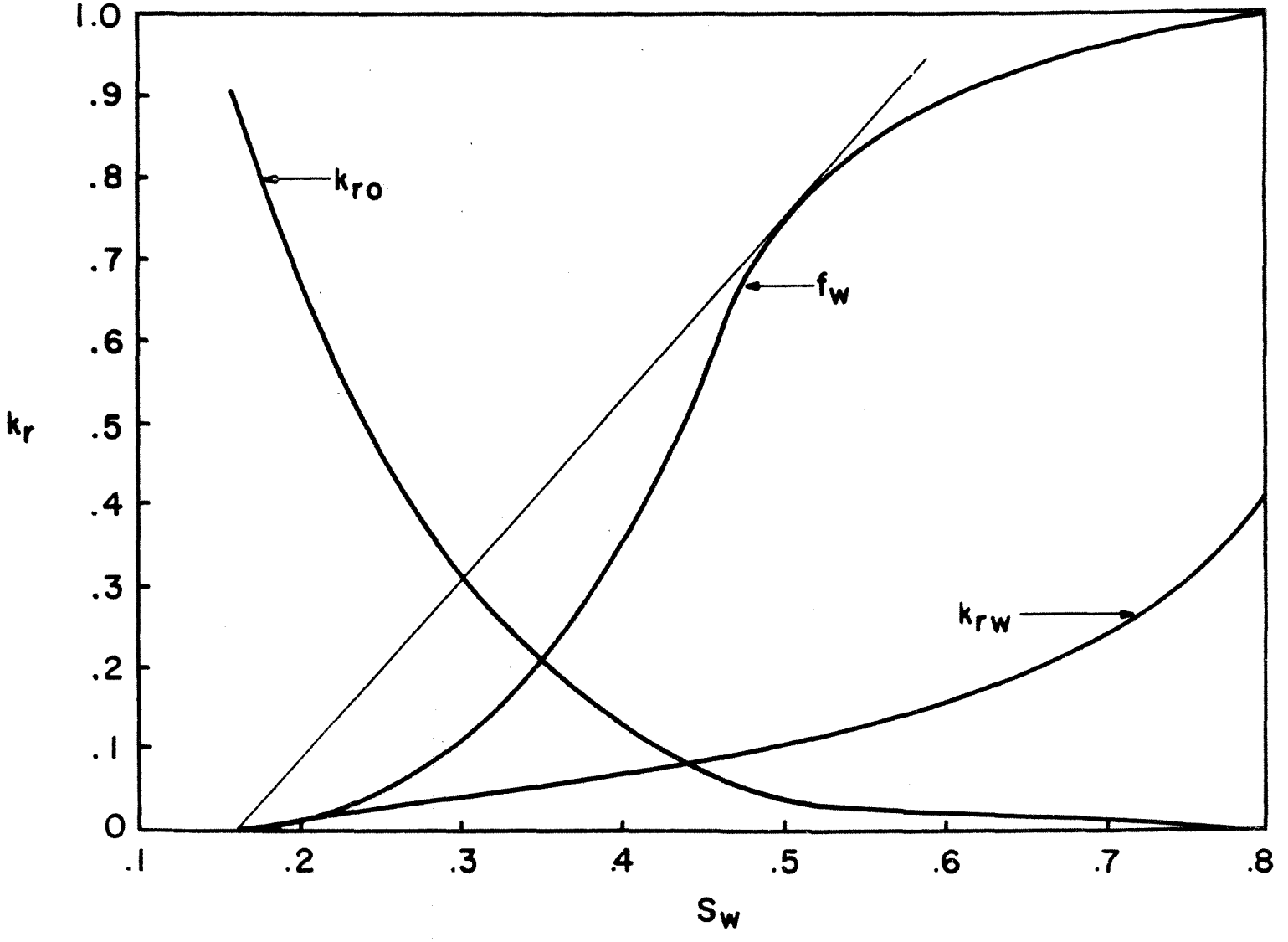


FIG. 11.2 WATER-OIL RELATIVE PERMEABILITY CURVES

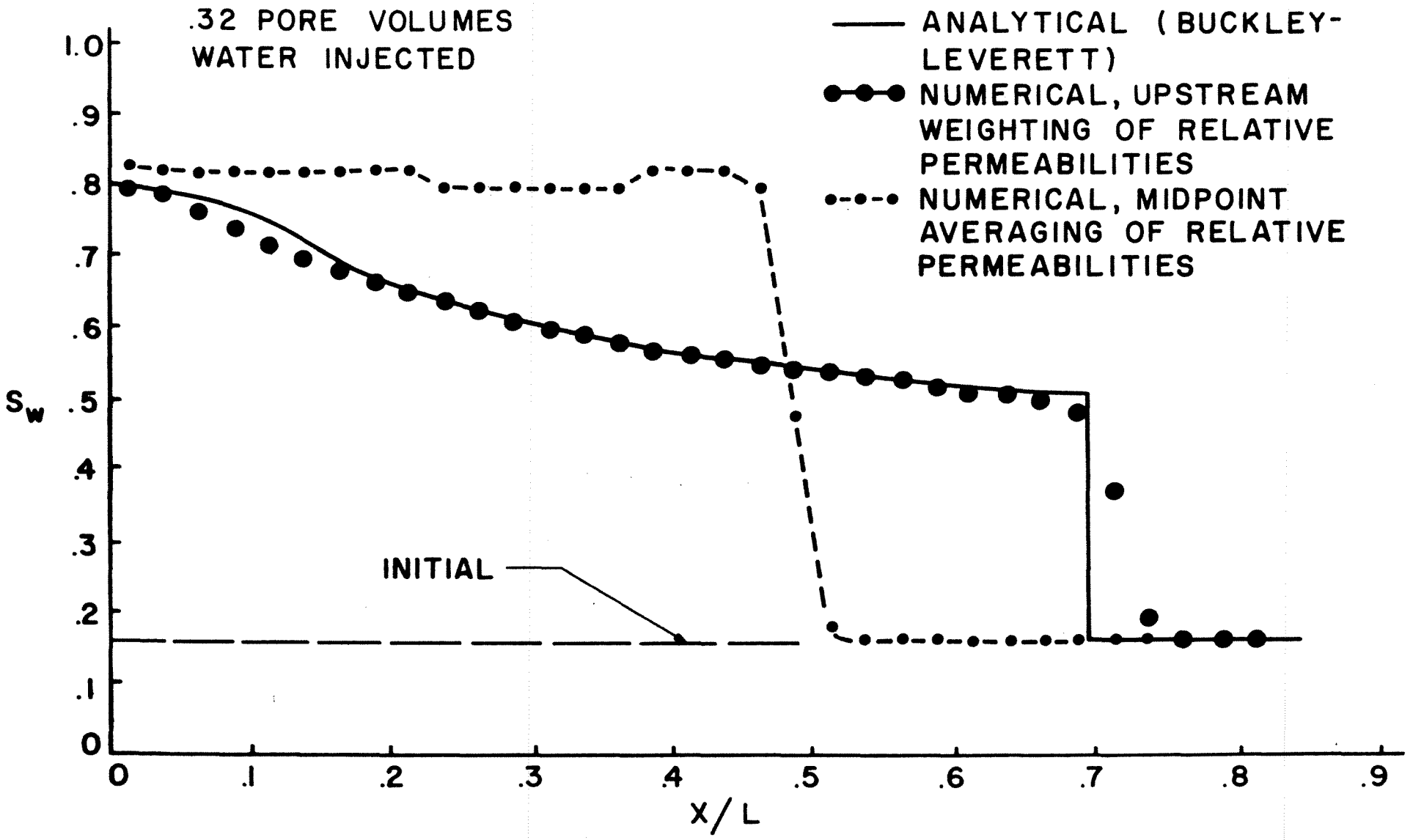


FIG. II.3 ONE-DIMENSIONAL WATER-OIL DISPLACEMENT

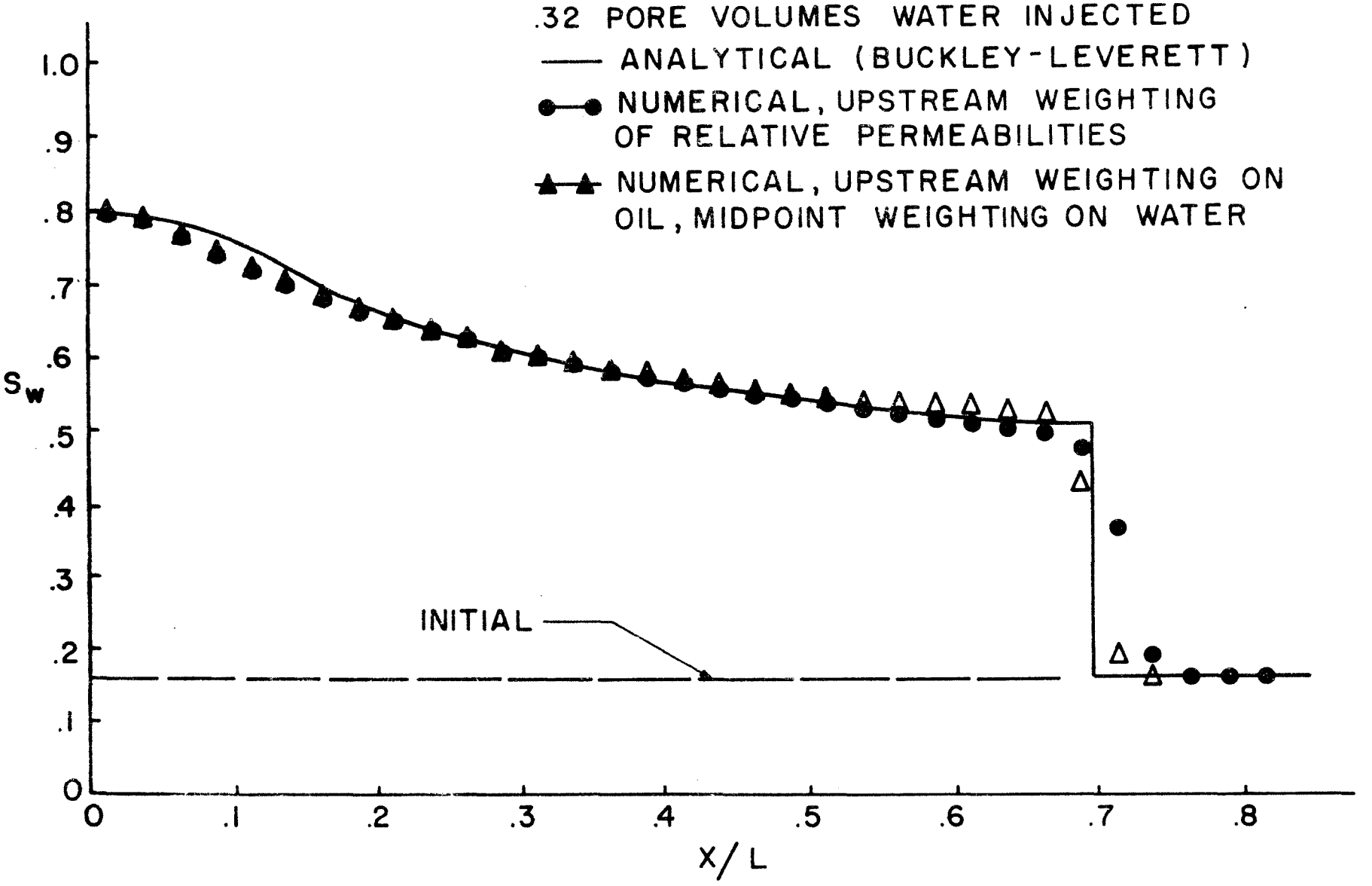


FIG. II.4 ONE-DIMENSIONAL WATER-OIL DISPLACEMENT

12. METHODS OF HANDLING INDIVIDUAL WELLS

The finite-difference equations describing the flow in a reservoir contain a production term q_{ijk}. This term is the entire production rate for the block (i,j,k). If more than one well is located in the block then q is the sum of the rates for all wells. Sections below discuss calculation of q_{ijk} for the two cases of specified well rates and specified flowing well pressure.

12.1. Case of Specified Well Rates

In two-dimensional areal calculations the term $q_{i,j}$ is given directly for injection wells by the specified injection rate. That is, if a well located at i = 11, j = 7 is injecting 250 STB/day of water then $q_{wll,7}$ is (-250) STB/d.

In two-dimensional areal calculations, individual phase production rates can be calculated from specified oil or total production rates. If the well's oil production rate is specified then gas and water production rates are calculated for the block as

$$q_w = \left(M_{wo} \frac{b_w}{b_o}\right)_n q_o \qquad (12.1a)$$

$$q_g = \left(M_{go} \frac{b_g}{b_o}\right)_n q_o \qquad (12.1b)$$

where q_o is the specified oil production rate in STB/d and

$$M_{wo} = \frac{k_{rw}/\mu_w}{k_{ro}/\mu_o} \qquad M_{go} = \frac{k_{rg}/\mu_g}{k_{ro}/\mu_o} \qquad (12.2)$$

Subscripts i,j on all quantities are suppressed. Formation volume factors are STB/RB for liquids and Mcf/RB for gas. These calculated production rates are for

use in the coming or new time step n+1.

Eqs. (12.1) represent an explicit production routine since the mobility ratios M are evaluated using the oil time level (n) relative permeabilities. In most two-dimensional areal calculations, this explicit routine is adequate. However, if the producing block is "small" or if the total reservoir flow rate converges upon the producing block, as in the case of an areal 5-spot calculation, then use of this explicit routine can give rise to saturation oscillations. These oscillations can be reduced or eliminated by use of the implicit production routine:

$$q_w = \left(\frac{b_w}{b_o}\right)_n (M_{wo})_{n+\frac{1}{2}} q_o \tag{12.3a}$$

$$q_g = \left(\frac{b_g}{b_o}\right)_n (M_{go})_{n+\frac{1}{2}} q_o + (R_s)_n q_o \tag{12.3b}$$

These time-centered mobility ratios can be calculated as

$$(M_{wo})_{n+\frac{1}{2}} = (M_{wo})_n + .5\, M'_{wo}\, \Delta_t\, S_w \tag{12.4a}$$

$$(M_{go})_{n+\frac{1}{2}} = (M_{go})_n + .5\, M'_{go}\, \Delta_t\, S_g \tag{12.4b}$$

Eqs. (12.4) assume that water-oil and gas-oil mobility ratios are single-valued functions of water and gas saturations, respectively. The "derivatives" are actually chord slopes, defined as

$$M'_{wo} = \frac{(M_{wo})_{n+1} - (M_{wo})_n}{S_{wn+1} - S_{wn}}$$

$$M'_{go} = \frac{(M_{go})_{n+1} - (M_{go})_n}{S_{gn+1} - S_{gn}} \tag{12.5}$$

These chord slopes can generally be estimated from the relative permeability tables

at the beginning of the time step and retained without updating for the time step's calculation. Results are generally insensitive to updating of the pressure dependent formation volume factor ratios. Substitution of eqs. (12.4) into (12.3) gives equations for q_w and q_g of type

$$q = C_1 + C_2 \Delta_t S \tag{12.6}$$

The term $C_2 \Delta_t S$ combines with the term $\Delta_t S$ already present on the right hand side of the difference equation. For an example, see the right-hand side of expansion given in eq. (15.9). Thus, use of an implicit as opposed to explicit production routine requires very little additional computational labor.

If total producing rate, as opposed to oil rate, is specified in a two-dimensional areal problem, then that total must be split into individual phase producing rates. Assuming the total rate q is specified as (RB of total fluid)/day, we have

$$q_w = M_w b_w q \quad \text{STB water/day} \tag{12.7a}$$

$$q_o = M_o b_o q \quad \text{STB oil/day} \tag{12.7b}$$

$$q_g = M_g b_g q + R_s q_o \quad \text{Mcf/day} \tag{12.7c}$$

where M is the ratio of mobility of phase ℓ to total mobility. For example, M_o is $(k_{ro}/\mu_o)/(k_{ro}/\mu_o + k_{rg}/\mu_g + k_{rw}/\mu_w)$. Again, the mobility ratios can be expressed at time level n or at $n+\frac{1}{2}$ depending upon whether an explicit or implicit production routine is desired. In the implicit case, the assumption that M_ℓ is a function only of S_ℓ (where $\ell = \omega, o, g$) gives

$$q_w = q\, b_{wn} [M_{wn} + .5\, M'_w \Delta_t S_w] \tag{12.8a}$$

$$q_o = q\, b_{on}\, [M_{on} + .5\, M'_o\, \Delta_t\, S_o] \tag{12.8b}$$

$$q_g = q\, b_{gn}\, [M_{gn} + .5\, M'_g\, \Delta_t\, S_g] + R_{sn}\, q_o \tag{12.8c}$$

where M'_ω, etc., are defined in eq. (12.5).

In two-dimensional cross-sectional or three-dimensional calculation, a specified well production rate must be allocated among the grid layers as well as split into individual phase rates. Let a well at areal position i,j be completed (perforated) in layers k_1, k_1+1, k_1+2, ----, k_L. As above, we will suppress the subscripts i,j on all quantities. We denote the mobility of phase ℓ in the k^{th} layer by*

$$\lambda_{\ell k} = \left(\frac{k\, \Delta z\, k_{r\ell}}{\mu_\ell}\right)_k , \tag{12.9}$$

total mobility of the k^{th} layer as

$$\lambda_k = \lambda_{wk} + \lambda_{ok} + \lambda_{gk} \tag{12.10}$$

and the total mobility of all layers as

$$\lambda = \sum_{k=k_1}^{k_L} \lambda_k \tag{12.11}$$

If q RB/d is the specified total fluid producing rate then

$$q_k = \frac{\lambda_k}{\lambda}\, q \tag{12.12}$$

is the RB/d produced from layer k and individual phase producing rates from layer

*Note that layer index k is used only as a subscript. That is, k inside the parentheses is absolute permeability, md.

k are

$$q_{\ell k} = b_{\ell k} \frac{\lambda_{\ell k}}{\lambda k} q_k = b_{\ell k} \frac{\lambda_{\ell k}}{\lambda} q \frac{STB}{day} \tag{12.13a}$$

for $\ell = \omega$ and o, and

$$q_{gk} = b_{gk} \frac{\lambda_{gk}}{\lambda} q + R_{sk} q_{ok} \frac{Mcf}{day} \tag{12.13b}$$

This calculation of individual phase production rates for each block assumes that the difference between reservoir pressure and sandface flowing pressure is about the same for all layers. This is a good assumption if sufficiently good vertical communication exists in the sand over the perforated interval. That is, flow potential should vary little with depth (z) compared with the radial variation out from the well. The assumption is clearly a poor one in stratified reservoirs where a number of non-communicating sands are connected vertically only by the wells. In simulation of a reservoir where vertical fluid communication exists between the grid layers in which the well is completed, the assumption of small vertical gradients in flow potentials can be checked by simply printing them out.

Considerable programming difficulty is avoided in relation to eqs. (12.13) if in the implicit case the total mobility λ in the denominator is evaluated at the old time level n. The "implicit" mobility ratio for any phase ℓ is then calculated as

$$M_{\ell k, n+\frac{1}{2}} = \frac{(\lambda_{\ell k})_{n+\frac{1}{2}}}{\lambda_n} = M_{\ell k, n} + .5\, M'_{\ell k}\, \Delta_t\, S_\ell \tag{12.14}$$

where M'_k is defined in eq. (14.5) and the assumption is made that mobility to phase ℓ is a single-valued function of S_ℓ.

For a water injection well in a two-dimensional cross-sectional or three-dimensional calculation, the water is generally allocated on a total mobility

basis. That is, the water injection rate into the k^{th} layer is calculated as

$$q_{wk} = \frac{(b_w \lambda)_k}{\sum_{k=k_1}^{k_L} (b_w \lambda)_k} q_w \quad \frac{STB}{day} \tag{12.15}$$

where $(-q_w)$ is the specified injection rate in STB/d and λ is the sum of water, oil and gas mobilities. Eq. (12.9) defines the individual phase mobilities.

For a gas injection well in a cross-sectional or three-dimensional calculation, the recommended procedure is allocation of gas on a gas mobility basis. The gas injection rate into the k^{th} layer is calculated as

$$q_{gk} = \frac{(b_g \lambda_g)_k}{\sum_{k=k_1}^{k_L} (b_g \lambda_g)_k} q_g \quad \frac{Mcf}{day} \tag{12.16}$$

where $(-q_g)$ is specified gas injection rate in Mcf/d.

The allocation of gas on a basis of gas as opposed to total mobility is recommende because of the ease with which gas flows vertically in a reservoir. Consider the case of a gas injection well perforated through four vertically communicating, 15-feet thick layers in an oil leg. Until gas saturation builds up sufficiently in the upper layers, any gas injected into the bottom layers will flow very rapidly upwards. This high flow rate will lead to computational instability or will require a very small time step with resultant large computer time. We can put gas where we like but we cannot keep it there against strong prevailing gravity and viscous forces. A remedy to this problem is injection of gas only into the top block, or, equivalently, inject it into the layers in accordance with gas mobility of the layers. The gas injected into the top block will move downward into lower blocks of its own accord when gravity

and viscous forces dictate that downward movement. The movement of gas away from the well and out into the reservoir is almost completely insensitive to whether the gas is injected into all four layers or only the top layer. In short, the gas will go where it pleases regardless of where or how we inject it. Calculations performed with gas injection only into the top layer have been compared in several cases with (very difficult and expensive) calculations involving injection into all layers. Computed results for all blocks once or twice removed from the injection well were virtually identical in the two calculations in all cases.

This injection of gas into the top layer or in accordance with gas mobility is not recommended for reservoirs having zero or negligible vertical communication. Injection of gas into a well completed in several noncommunicating layers will in general result in gas flow into all the sands. The relative amounts of gas entering the various layers must be calculated taking into account the differences between injection pressure and pressure at the well in each of the sands. This is discussed below.

15. MULTIDIMENSIONAL, MULTIPHASE FLOW

Eqs. (6.11) describe the three-dimensional flow of water, oil, and gas in a porous medium:

$$\nabla \cdot [K_w (\nabla p_w - \gamma_w \nabla Z] - q_{vw} = \frac{\partial(\phi b_w S_w)}{\partial t} \qquad (15.1a)$$

$$\nabla \cdot [K_o (\nabla p_o - \gamma_o \nabla Z) - q_{vo} = \frac{\partial(\phi b_o S_o)}{\partial t} \qquad (15.1b)$$

$$\nabla \cdot [K_o R_s (\nabla p_o - \gamma_o \nabla Z)] + \nabla \cdot [K_g (\nabla p_g - \gamma_g \nabla Z)]$$

$$- q_{vg} = \frac{\partial}{\partial t} (\phi b_o R_s S_o + \phi b_g S_g) \qquad (15.1c)$$

where

$$K_w = \frac{k k_{rw} b_w}{\mu_w} \qquad K_o = \frac{k k_{ro} b_o}{\mu_o} \qquad K_g = \frac{k k_{rg} b_g}{\mu_g}$$

We will outline two methods for solving eqs. (15.1): a) an implicit pressure - explicit saturation method (IMPES) which is an extension of methods proposed in 1960 by Sheldon et al [14] and Stone [15], and b) a method of simultaneous solution which is an extension of a method proposed in 1959 by Douglas, Peaceman and Rachford [16] for solution of two-dimensional, two-phase incompressible flow problems.

In presentation of these methods, the boundary conditions are assumed to be no-flow. Any flow across a boundary is accounted for by the production terms in the boundary blocks. An aquifer may be handled by extending the areal grid to encompass the aquifer using increasingly larger blocks at increasing distance from the reservoir. Alternatively, an aquifer can be handled by restricting the grid to

the reservoir proper and accounting for water influx in the edge blocks in the manner described in Section . The no-flow boundary conditions are imposed by simply setting to zero all transmissibilities for flow across the reservoir boundaries.

As discussed in Chapter 11, the difference approximations to eqs. (15.1) are

$$\Delta[T_w (\Delta p_w - \gamma_w \Delta Z)] - q_w = \frac{V}{\Delta t} \Delta_t (\phi b_w S_w)$$

$$\Delta[T_o (\Delta p_o - \gamma_o \Delta Z)] - q_o = \frac{V}{\Delta t} \Delta_t (\phi b_o S_o)$$

$$\Delta[T_o R_s (\Delta p_o - \gamma_o \Delta Z)] + \Delta[T_g (\Delta p_g - \gamma_g \Delta Z)] - q_g$$

$$= \frac{V}{\Delta t} \Delta_t (\phi b_o R_s S_o + \phi b_g S_g) \qquad (15.3)$$

where for x-direction flow

$$T_{wi+\frac{1}{2},j,k} = \left[\frac{k\, k_{rw}\, b_w}{\mu_w} \frac{\Delta y\, \Delta z}{\Delta x}\right]_{i+\frac{1}{2},j,k}$$

and similar definitioss hold for the oil and gas transmissibilities. The term V is block volume, $\Delta x\, \Delta y\, \Delta z$. The spatial and time difference notation is defined on in Chapter 2. Eqs. (15.3) apply at each grid point i,j,k in the reservoir.

Eqs. (15.3) are three equations in the six unknowns p_w, p_o, p_g, S_w, S_o, and S_g. Three additional equations are

$$S_w + S_o + S_g = 1 \qquad (15.4)$$

$$P_{cgo} = p_g - p_o = P_{cgo}(S_g) \qquad (15.5)$$

$$P_{cwo} = p_o - p_w = P_{cwo}\ (S_w) \tag{15.6}$$

15.1. The Implicit Pressure - Explicit Saturation Method

The name of this method implies the implicit solution for pressure and explicit solution for saturation. The basis of the method is the reduction of eqs. (15.3) to a single equation in oil pressure with no terms on the right hand side of type Δ_t S. That is, the pressure equation is obtained from eqs. (15.3) by eliminating $\Delta_t\ S_w$, $\Delta_t\ S_o$, and $\Delta_t\ S_g$.

A very important, but often overlooked, matter is consistency in expansion of the right hand side terms in eqs. (15.3). These terms of type Δ_t (abc) are material balance terms and their proper expansion is critical in obtaining a calculation which preserves a good material balance. For example, $V\ \Delta_t\ (\phi\ b_o\ S_o)$ is quite simply the gain in STB of oil in the grid block over the time step. Any expansion of a term Δ_t (abc) must preserve the definition of the difference operator, namely

$$\Delta_t\ (abc) = (abc)_{n+1} - (abc)_n$$

Consistency of an expansion simply denotes satisfaction of the definition of $\Delta_t\ X = X_{n+1} - X_n$. Thus

$$\Delta_t\ (ab) = a_{n+1}\ \Delta_t\ b + b_n\ \Delta_t\ a \tag{15.7}$$

is consistent while

$$\Delta_t\ (ab) = a_n\ \Delta_t\ b + b_n\ \Delta_t\ a$$

is not. Using eq. (15.7) we can perform the consistent expansion

$$\Delta_t (\phi b_o S_o) = (\phi b_o)_{n+1} \Delta_t S_o + S_{on} \Delta_t (\phi b_o) = (\phi b_o)_{n+1} \Delta_t S_o$$

$$+ S_{on} \phi_{n+1} \Delta_t b_o + S_{on} b_{on} \Delta_t \phi \qquad (15.8)$$

Using the definition of rock compressibility

$$c_f = \frac{1}{\phi} \frac{d\phi}{dp}$$

we have

$$\phi \cong \phi_b [1 + c_f (p - p_b)]$$

where ϕ_b is base porosity at arbitrary base pressure p_b. Thus

$$\Delta_t \phi \cong \phi_b c_f \Delta_t p$$

Also, by definition of

$$b'_o = \frac{b_{on+1} - b_{on}}{p_{on+1} - p_{on}}$$

we have

$$\Delta_t b_o = b'_o \Delta_t p_o$$

Thus, eq. (15.8) becomes

$$\Delta_t (\phi b_o S_o) = S_{on} [\phi_{n+1} b'_o + b_{on} \phi_b c_f] \Delta_t p + (\phi b_o)_{n+1} \Delta_t S_o$$

(15.9)

where p is oil pressure.

Similarly consistent expansions of the time differences on the right hand sides of the water and gas equations (15.3a and c) gives

$$\frac{V}{\Delta t}\Delta_t\,(\phi\, b_w\, S_w) = C_{10}\,\Delta_t\, p + \sum_{\ell=1}^{3} C_{1\ell}\Delta_t\, S_\ell$$

$$\frac{V}{\Delta t}\Delta_t\,(\phi\, b_o\, S_o) = C_{20}\,\Delta_t\, p + \sum_{\ell=1}^{3} C_{2\ell}\,\Delta_t\, S_\ell$$

$$\frac{V}{\Delta t}\Delta_t\,(\phi\, b_o\, R_s\, S_o + \phi\, b_g\, S_g) = C_{30}\,\Delta_t\, p + \sum_{\ell=1}^{3} C_{3\ell}\,\Delta_t\, S_\ell \qquad (15.10)$$

where subscripts of 1, 2, 3 on S denote water, oil, and gas, respectively. The coefficients C_{ij} are

$$C_{10} = \frac{V}{\Delta t}\; S_{wn}\,[\phi_{n+1}\, b_{wb}\, c_w + b_{wn}\,\phi_b\, c_f]$$

$$C_{11} = \frac{V}{\Delta t}\;(\phi\, b_w)_{n+1}$$

$$C_{12} = C_{13} = 0$$

$$C_{20} = \frac{V}{\Delta t}\; S_{on}\,[\phi_{n+1}\, b_o' + b_{on}\,\phi_b\, c_f]$$

$$C_{21} = 0$$

$$C_{22} = \frac{V}{\Delta t}\,(\phi\, b_o)_{n+1}$$

$$C_{23} = 0$$

$$C_{30} = \frac{V}{\Delta t} \{S_{gn} [\phi_{n+1} b'_g + b_{gn} \phi_b c_f] + S_{on} [\phi_{n+1} (b_o R_s)' + (b_o R_s)_n \phi_b c_f]\}$$

$$C_{31} = 0$$

$$C_{32} = \frac{V}{\Delta t} (\phi b_o R_s)_{n+1}$$

$$C_{33} = \frac{V}{\Delta t} (\phi b_g)_{n+1}$$

Definitions of terms newly introduced are

$$b'_g = \frac{b_{gn+1} - b_{gn}}{p_{gn+1} - p_{gn}}$$

$$(b_o R_s)' = \frac{(b_o R_s)_{n+1} - (b_o R_s)_n}{p_{on+1} - p_{on}}$$

$$b_w = b_{wb} [1 + c_w (p_w - p_{wb})]$$

We have used the identity $\Delta_t p_w = \Delta_t p_g = \Delta_t p$, where p is oil pressure, in accordance with the assumption of "explicit saturation" in this technique. That is, in obtaining the pressure equation we ignore change of capillary pressure over the time step.

To repeat, the equations here of type (15.9) are rigorous expansions in accordance with the definition $\Delta_t X = X_{n+1} - X_n$. That is, the dating of certain terms at time n and others at n+1 on the right hand side of eq. (15.9) and other expansions is not arbitrary and introduces no assumptions or approximations. The appearance of saturation at time level n in the coefficients C_{ij} in no way reflects

any "explicit" dating or specification of saturation. We could have performed the expansion in (15.8) equally consistently as

$$\Delta_t (\phi b_o S_o) = S_{on+1} \Delta_t (\phi b) + (\phi b)_n \Delta_t S_o$$

However, this type of expansion would result in unknown saturations at time n+1 in the coefficients C_{ij}. We would then have to follow a calculational procedure at each time step of: a) solve the pressure equation, b) solve saturation equations for new saturations, c) update (reevaluate) C_{ij}'s, d) resolve the pressure equation, etc. Using the expansions of type (15.8) we have C_{ij}'s which are dependent only upon new time level values of pressure. We can, thus, solve the pressure equation independently of and prior to the calculation of new time level saturations.

Substituting eqs. (15.10) into eq. (15.3) gives

$$\Delta(T_w (\Delta p_w - \gamma_w \Delta Z)) - q_w = C_{10} \Delta_t p + C_{11} \Delta_t S_w$$

$$\Delta(T_o (\Delta p_o - \gamma_o \Delta Z)) - q_o = C_{20} \Delta_t p + C_{22} \Delta_t S_o$$

$$\Delta(T_o R_s (\Delta p_o - \gamma_o \Delta Z)) + \Delta(T_g (\Delta p_g - \gamma_g \Delta Z)) - q_g$$

$$= C_{30} \Delta_t p + C_{32} \Delta_t S_o + C_{33} \Delta_t S_g \quad (15.11)$$

To eliminate all terms of type $\Delta_t S$ from these equations we multiply the first by a_1, the second by a_2, and the third by a_3 and add to obtain

$$a_1 \Delta(T_w (\Delta p_w - \gamma_w \Delta Z)) + a_2 \Delta(T_o (\Delta p_o - \gamma_o \Delta Z))$$

$$+ a_3 \Delta(T_o R_s (\Delta p_o - \gamma_o \Delta Z)) + a_3 \Delta(T_g (\Delta p_g - \gamma_g \Delta Z)$$

$$-q = C \Delta_t p + a_1 C_{11} \Delta_t S_w + (a_2 C_{22} + a_3 C_{32})$$

$$\Delta_t S_o + a_3 C_{33} \Delta_t S_g \qquad (15.12)$$

where

$$q = a_1 q_w + a_2 q_o + a_3 q_g$$

$$C = a_1 C_{10} + a_2 C_{20} + a_3 C_{30} \qquad (15.13)$$

We now seek values of a_1, a_2, a_3 such that

$$a_1 C_{11} \Delta_t S_w + (a_2 C_{22} + a_3 C_{32}) \Delta_t S_o + a_3 C_{33} \Delta_t S_g = 0$$

Since $\Delta_t S_g = - \Delta_t S_w - \Delta_t S_o$ this requirement is

$$(a_1 C_{11} - a_3 C_{33}) \Delta_t S_w + (a_2 C_{22} + a_3 (C_{32} - C_{33})) \Delta_t S_o = 0$$

This equation is satisfied if

$$a_1 C_{11} - a_3 C_{33} = 0$$

$$a_2 C_{22} + a_3 (C_{32} - C_{33}) = 0$$

These two equations in the three unknowns a_1, a_2, a_3 give one degree of freedom which we use by specifying $a_2 = 1$. Then

$$a_3 = \frac{C_{22}}{C_{33} - C_{32}}$$

$$a_1 = a_3 \frac{C_{33}}{C_{11}}$$

$$a_2 = 1 \qquad (15.14)$$

These values of a_i reduce the right hand side of eq. (15.12) to simply $C \Delta_t p$. However, the left hand side still contains the three unknowns p_w, p_o and p_g. We use eqs. (15.5) and (15.6) to eliminate p_w and p_g in terms of oil pressure p to obtain from (15.12),

$$\{a_1 \Delta(T_w \Delta p_{n+1}) + a_2 \Delta(T_o \Delta p_{n+1}) + a_3 \Delta(T_o R_s \Delta p_{n+1}) + a_3 \Delta(T_g \Delta p_{n+1}$$

$$- \{a_1 \Delta(T_w \Delta P_{cwo}) - a_3 \Delta(T_g \Delta P_{cgo})\}_n$$

$$- \{a_1 \Delta(T_w \gamma_w \Delta Z) + a_2 \Delta(T_o \gamma_o \Delta Z)$$

$$+ a_3 \Delta(T_o R_s \gamma_o \Delta Z) + a_3 \Delta(T_g \gamma_g \Delta Z)\} - q$$

$$= C \Delta_t p \qquad (15.15)$$

Oil pressure is taken implicitly at time n+1 while capillary pressures are taken explicitly ("explicit saturation") at time n. The capillary pressure and gravitational spatial differences and production term in eqs. (15.15) are known from the time level n pressure and saturation distributions so that eq. (15.15) is of type

$$\Delta(T \Delta p)_{ijk} - B_{ijk} = C_{ijk} \Delta_t p_{ijk} \qquad (15.16)$$

This pressure equation is easily solved by iterative alternating direction as discussed in Chapter 10. At the end of each iteration, the new pressure iterate is used to update the C_{ij}'s and recalculate the coefficients a_1 and a_3 from eqs. (15.14).

After solution of (15.16) for $p_{i,j,k,n+1}$ the new water and oil saturations are calculated directly from eqs. (15.11a and b). All terms in these two equations are known except $\Delta_t S_w$ and $\Delta_t S_o$. The new saturations S_{wn+1} and S_{on+1} are then used to obtain the new capillary pressures P_{cwon+1} and P_{cgon+1}. This completes the time step's calculations.

15.2. The Method of Simultaneous Solution

Using the definition of the "potential"

$$P_p = \int^{P_\ell} \frac{dp}{\gamma_\ell(p)} - Z \qquad (15.17)$$

where ℓ = w, o and g, we can write eqs. (15.1) as

$$\nabla \cdot [K_w \gamma_w \nabla P_w] - q_{vw} = \frac{\partial(\phi b_w S_w)}{\partial t}$$

$$\nabla \cdot [K_o \gamma_o \nabla P_o] - q_{vo} = \frac{\partial(\phi b_o S_o)}{\partial t}$$

$$\nabla \cdot [K_o R_s \gamma_o \nabla P_o] + \nabla \cdot [K_g \gamma_g \nabla P_g] - q_{vg} = \frac{\partial}{\partial t} (\phi b_o R_s S_o + \phi b_g S_g$$

(15.18)

In implicit difference form these equations are

$$\Delta(T_w \Delta P_{wn+1}) - q_w = \frac{V}{\Delta t} \Delta_t (\phi b_w S_w)$$

$$\Delta(T_o \Delta P_{on+1}) - q_o = \frac{V}{\Delta t} \Delta_t (\phi b_o S_o)$$

$$\Delta(T_o R_s \Delta P_{on+1}) + \Delta(T_g \Delta P_{gn+1}) - q_g = \frac{V}{\Delta t} \Delta_t (\phi b_o R_s S_o + \phi b_g S_g)$$

(15.19)

where the transmissibilities here are

$$T_{wi+\frac{1}{2},j,k} = \left(\frac{k k_{rw} b_w \gamma_w}{\mu_w} \frac{\Delta y \Delta z}{\Delta x}\right)_{i+\frac{1}{2},j,k} \qquad (15.20)$$

and similarly for oil and gas. We seek expansions of the right hand sides of these equations of the form

$$\frac{V}{\Delta t} \Delta_t (\phi b_w S_w) = C_{11} \Delta_t P_w + C_{12} \Delta_t P_o + C_{13} \Delta_t P_g$$

$$\frac{V}{\Delta t} \Delta_t (\phi b_o S_o) = C_{21} \Delta_t P_w + C_{22} \Delta_t P_o + C_{33} \Delta_t P_g$$

$$\frac{V}{\Delta t} \Delta_t (\phi b_o R_s S_o + \phi b_g S_g) = C_{31} \Delta_t P_w + C_{32} \Delta_t P_o + C_{33} \Delta_t P_g$$

(15.21)

Insertion of these expansions into eqs. (15.19) then yields three equations in the three unknowns P_{wn+1}, P_{on+1}, and P_{gn+1} for which these equations can be simultaneously solved.

We will demonstrate the procedure for obtaining the coefficients C_{ij} by expanding the term $\Delta_t (\phi b_o S_o)$. As given in eq. (15.8)

$$\Delta_t (\phi b_o S_o) = (\phi b_o)_{n+1} \Delta_t S_o + S_{on} \phi_{n+1} \Delta_t b_o + S_{on} b_{on} \Delta_t \phi$$

(15.8)

Using the definitions of capillary pressures, eqs. (15.5) and (15.6)

$$\Delta_t S_o = - \Delta_t S_w - \Delta_t S_g = - S'_w \Delta_t P_{cwo} - S'_g \Delta_t P_{cgo}$$

$$= - S'_w (\Delta_t P_o - \Delta_t P_w) - S'_g (\Delta_t P_g - \Delta_t P_o) \qquad (15.22)$$

where

$$S'_w = \frac{S_{wn+1} - S_{wn}}{P_{cwon+1} - P_{cwon}} \qquad S'_g = \frac{S_{gn+1} - S_{gn}}{P_{cgon+1} - P_{cgon}} \qquad (15.23)$$

Eq. (15.17) gives $dP_\ell = \frac{1}{\gamma_\ell} dp_\ell$ at any fixed spatial point so that

$$\Delta_t p_\ell = \bar{\gamma}_\ell \Delta_t P_\ell \qquad (15.24)$$

where ℓ = w, o, or g and $\bar{\gamma}_\ell$ is an average specific weight over the pressure interval $P_{\ell,n}$ to $P_{\ell,n+1}$. Thus, eq. (15.22) is

$$\Delta_t S_o = S'_w \bar{\gamma}_w \Delta_t P_w - (S'_w - S'_g) \bar{\gamma}_o \Delta_t P_o - S'_g \bar{\gamma}_g \Delta_t P_g \qquad (15.25)$$

From eq. (15.7a)

$$\Delta_t \phi = \phi_b c_f \Delta_t p_w = \phi_b c_f \bar{\gamma}_w \Delta_t P_w \qquad (15.26)$$

Finally

$$\Delta_t b_o = b'_o \Delta_t P_o \tag{15.27}$$

where

$$b'_o = \frac{b_{on+1} - b_{on}}{P_{on+1} - P_{on}} \tag{15.28}$$

Substitution from eqs. (15.25), (15.26), and (15.27) into (15.8) gives

$$\Delta_t (\phi b_o S_o) = \bar{\gamma}_w [(\phi b_o)_{n+1} S'_w + S_{on} b_{on} \phi_b c_f] \Delta_t P_w$$

$$+ [S_{on} \phi_{n+1} b'_o - \bar{\gamma}_o (S'_w - S'_g) (\phi b_o)_{n+1}] \Delta_t P_o$$

$$- \bar{\gamma}_g S'_g (\phi b_o)_{n+1} \Delta_t P_g \tag{15.28}$$

Similar expansions of the right hand sides of eqs. (15.19a and c) gives eqs. (15.21) with the following coefficients:

$$C_{11} = \frac{V}{\Delta t} \bar{\gamma}_w [S_{wn} \phi_b c_f b_{wn} + S_{wn} \phi_{n+1} b_{wb} c_w - (\phi b_w)_{n+1} S'_w]$$

$$C_{12} = (\phi b_w)_{n+1} S'_w \bar{\gamma}_o$$

$$C_{13} = 0$$

$$C_{21} = \frac{V}{\Delta t} \bar{\gamma}_w [(\phi b_o)_{n+1} S'_w + S_{on} b_{on} \phi_b c_f]$$

$$C_{22} = \frac{V}{\Delta t} [S_{on} \phi_{n+1} b'_o - \bar{\gamma}_o (S'_w - S'_g) (\phi b_o)_{n+1}]$$

$$C_{23} = -\frac{V}{\Delta t}\,\bar{\gamma}_g\,S'_g\,(\phi\,b_o)_{n+1}$$

$$C_{31} = \frac{V}{\Delta t}\,\bar{\gamma}_w\,[(\phi\,b_o\,R_s)_{n+1}\,S'_w + (S_{on}\,b_{on} + S_{gn}\,b_{gn})\,\phi_b\,c_f]$$

$$C_{32} = \frac{V}{\Delta t}\,[S_{on}\,\phi_{n+1}\,(b_o\,R_s)' - \bar{\gamma}_o\,(S'_w - S'_g)\,(\phi\,b_o\,R_s)_{n+1} - (\phi\,b_g)_{n+1}\,S'_g\,\bar{\gamma}$$

$$C_{33} = \frac{V}{\Delta t}\,[S_{gn}\,\phi_{n+1}\,b'_g + S'_g\,\bar{\gamma}_g\,[(\phi\,b_g)_{n+1} - (\phi\,b_o\,R_s)_{n+1}]]$$

Definitions of newly introduced terms are

$$b'_g = \frac{b_{gn+1} - b_{gn}}{P_{gn+1} - P_{gn}} \qquad (b_o\,R_s)' = \frac{(b_o\,R)_{s_{n+1}} - (b_o\,R_s)_n}{P_{on+1} - P_{on}} \qquad (15.30)$$

The term b is defined on page 126.

Substitution of eqs. (15.21) into (15.19) gives the three flow equations

$$\Delta(T_w\,\Delta\,P_{wn+1}) - q_w = C_{11}\,\Delta_t\,P_w + C_{12}\,\Delta_t\,P_o + C_{13}\,\Delta_t\,P_g$$

$$\Delta(T_o\,\Delta\,P_{on+1}) - q_o = C_{21}\,\Delta_t\,P_w + C_{22}\,\Delta_t\,P_o + C_{23}\,\Delta_t\,P_g$$

$$\Delta(T_o\,R_s\,\Delta\,P_{on+1}) + \Delta(T_g\,\Delta\,P_{gn+1}) - q_g = C_{31}\,\Delta_t\,P_w + C_{32}\,\Delta_t\,P_o + C_{33}\,\Delta_t$$

(15.31)

We can write these equations as the single matrix equation

$$\Delta\,T\,\Delta\,\underline{P}_{ijk,n+1} - \underline{q}_{ijk} = C_{ijk}\,\Delta_t\,\underline{P}_{ijk} \qquad (15.32)$$

$$\underline{T} = \begin{Bmatrix} T_w & 0 & 0 \\ 0 & T_o & 0 \\ 0 & T_o R_s & T_g \end{Bmatrix} \qquad \underline{C} = \begin{Bmatrix} C_{11} & C_{12} & C_{13} \\ C_{21} & C_{22} & C_{23} \\ C_{31} & C_{32} & C_{33} \end{Bmatrix}$$

$$\underline{P} = \begin{Bmatrix} P_w \\ P_o \\ P_g \end{Bmatrix} \qquad \underline{q} = \begin{Bmatrix} q_w \\ q_o \\ q_g \end{Bmatrix} \tag{15.33}$$

Eq. (15.32) applies at each grid point in the reservoir.

Eq. (15.32) is implicit both in pressure and saturation. That is, there is no explicit dating of capillary pressure at the old time level as in the IMPES method. The changes in pressure over the time step automatically account for the changes in saturation through equations of type (15.22).

We solve eq. (15.32) by iterative, Douglas-Rachford alternating-direction. The x-sweep is

$$\Delta_x T \Delta_x \underline{P}^* + \Delta_y T \Delta_y \underline{P}^k + \Delta_z T \Delta_z \underline{P}^k - \underline{q} = C (\underline{P}^* - \underline{P}_n)$$

$$+ H_k (\underline{P}^* - \underline{P}^k) \tag{15.34a}$$

Similarly, the y- and z- direction sweeps are

$$\Delta_x T \Delta_x \underline{P}^* + \Delta_y T \Delta_y \underline{P}^{**} + \Delta_z T \Delta_z \underline{P}^k - \underline{q} = C (\underline{P}^{**} - \underline{P}^k)$$

$$+ H_k (\underline{P}^{**} - \underline{P}^k) \tag{15.34b}$$

$$\Delta_x T \Delta_x \underline{P}^* + \Delta_y T \Delta_y \underline{P}^{**} + \Delta_z T \Delta_z \underline{P}^{k+1} - \underline{q} = C (\underline{P}^{k+1} - \underline{P}_n)$$

$$+ H_k (\underline{P}^{k+1} - \underline{P}^k) \qquad (15.34c)$$

The matrix H_k is

$$H_{kijk} = \begin{Bmatrix} h_k (\Sigma T_w)_{ijk} & 0 & 0 \\ 0 & h_k (\Sigma T_o)_{ijk} & 0 \\ 0 & h_k (\Sigma T_o R_s)_{ijk} & h_k (\Sigma T_g)_{ijk} \end{Bmatrix} \qquad (15.35)$$

The term h_k is iteration parameter as given by eq. ( ). The terms of type ΣT are the sums of the six transmissibilities for flow across the six faces of the grid block.

Effects of round-off error are minimized by solving for changes over the iteration. We define

$$\underline{PX} = \underline{P}^* - \underline{P}^k \qquad \underline{PY} = \underline{P}^{**} - \underline{P}^k \qquad \underline{PZ} = \underline{P}^{k+1} - \underline{P}^k \qquad (15.36)$$

Adding and subtracting $\Delta_x T \Delta_x \underline{P}^k$ to eq. (15.34) and rearranging the result gives

$$\Delta_x T \Delta_x \underline{PX}_{ijk} - (C + H_k) \underline{PX}_{ijk} = - \underline{R}_{ijk} \qquad (15.37a)$$

where the residual R_{ijk} is simply the eq. (15.32) itself,

$$\underline{R}_{ijk} = \Delta T \Delta \underline{P}^k_{ijk} - \underline{q}_{ijk} - C (\underline{P}^k - \underline{P}_n)_{ijk} \qquad (15.38)$$

This residual approaches zero as the iterate $\underline{P}^k$ approaches the desired solution $\underline{P}_{n+1}$.

Subtraction of eq. (15.34a) from (15.34b) gives

$$\Delta_y T \Delta_y \underline{PY} - (C + H_k) \underline{PY} = - (C + H_k) \underline{PX} \qquad (15.37b)$$

and subtraction of (15.34b) from (15.34c) yields for the z-sweep

$$\Delta_z T \Delta_z \underline{PZ} - (C + H_k) \underline{PZ} = - (C + H_k) \underline{PY} \qquad (15.37c)$$

Each of eqs. (15.38) are of one-dimensional type and can be solved by application of the Richtmyer algorithm. Eq. (15.37a) is first solved for $\underline{PX}_{ijk}$ for all i,j,k. Eq. (15.37b) is then solved for $\underline{PY}_{ijk}$ at all grid points and finally eq. (15.37c) is solved for $\underline{PZ}_{ijk}$. The new iterate is then calculated as

$$\underline{P}^{k+1} = \underline{P}^k + \underline{PZ} \qquad (15.39)$$

This solution of eqs. (15.37) constitutes one iteration.

We now proceed to outline the application of the Richtmyer algorithm to each of eqs. (15.37). Each of these three equations is of the same type so that we will demonstrate the solution for only the x-sweep, eq. (15.37a). At any j,k grid line, that equation is

$$T_{i+\frac{1}{2}} \underline{PX}_{i+1} = (T_{i+\frac{1}{2}} + T_{i-\frac{1}{2}} + C_i + H_{ki}) \underline{PX}_i + T_{i-\frac{1}{2}} \underline{PX}_{i-1} = - \underline{R}_i \qquad (15.40)$$

where we suppress the fixed j,k on all terms. Extending the Richtmyer algorithm

to this matrix equation, we write

$$\underline{PX}_{i-1} = E_i \, \underline{PX}_i + \underline{F}_i \tag{15.41}$$

Where E_i is the matrix and $\underline{F}_i$ the column vector

$$E_i = \begin{Bmatrix} e_{11i} & e_{12i} & e_{13i} \\ e_{21i} & e_{22i} & e_{23i} \\ e_{31i} & e_{32i} & e_{33i} \end{Bmatrix} \qquad \underline{F}_i = \begin{Bmatrix} f_{1i} \\ f_{2i} \\ f_{3i} \end{Bmatrix} \tag{15.42}$$

Substitution of $\underline{PX}_{i-1}$ from (15.41) into (15.40) gives

$$T_{i+\frac{1}{2}} \, \underline{PX}_{i+1} - (T_{i+\frac{1}{2}} + T_{i-\frac{1}{2}} \, (I - E_i) + C_i + H_{ki}) \, \underline{PX}_i$$

$$+ T_{i-\frac{1}{2}} \, \underline{F}_i = - \underline{R}_i$$

and solution for $\underline{PX}_i$ gives

$$\underline{PX}_i = A_i^{-1} \, T_{i+\frac{1}{2}} \, \underline{PX}_{i+1} + A_i^{-1} \, [T_{i-\frac{1}{2}} \, \underline{F}_i + \underline{R}_i] \tag{15.43}$$

where the matrix A_i^{-1} is the inverse of

$$A_i = T_{i+\frac{1}{2}} + T_{i-\frac{1}{2}} \, (I - E_i) + C_i + H_{ki} \tag{15.44}$$

Comparison of eqs. (15.43) and (15.41) gives

$$E_{i+1} = A_i^{-1} \, T_{i+\frac{1}{2}}$$

$$\underline{F}_{i+1} = A_i^{-1} [T_{i-\frac{1}{2}} \underline{E}_i + \underline{R}_i] \qquad (15.45)$$

These recursion relationships allow calculation of E_2, $\underline{F}_2$, $\underline{E}_3$, $\underline{F}_3$, ---- $\underline{F}_{N_x+1}$ where N_x is the number of grid blocks in the x direction. Note that E_2 can be calculated from (15.45) without knowing E_1 because $T_{\frac{1}{2}}$ is zero by the noflow boundary conditions. Similarly E_{N_x+1} is zero because $T_{N_x+\frac{1}{2}}$ is zero.

After calculating all E_i and $\underline{F}_i$ from (15.45), the value of $\underline{PX}_{N_x}$ is obtained from (15.41) as

$$\underline{PX}_{N_x} = \underline{F}_{N_x+1}$$

and values of $\underline{PX}_{N_x-1}$, $\underline{PX}_{N_x-2}$, ----- $\underline{PX}_1$ are obtained by successive use of eq. (15.41). This solution for $\underline{PX}_i$ along the x-direction line at j,k is performed for all x-direction lines in the reservoir.

After obtaining $\underline{P}^{k+1}$ from eq. (15.39), the components P_w^{k+1}, P_o^{k+1}, P_g^{k+1} are used to update time level n+1 terms in the coefficients C_{ij}. That is, R_{sn+1}, b_{wn+1}, b_{on+1}, b_{gn+1} and the various chord slopes in eqs. (15.23), (15.28), (15.30) are recalculated.

The residual $\underline{R}_{ijk}$ of eq. (15.38) provides a simple closure tolerance for this iterative solution. This residual vector is

$$\underline{R}_i = \begin{Bmatrix} R_w \\ R_o \\ R_g \end{Bmatrix}$$

where the oil equation residual R_o is

$$R_{oijk} = \Delta T_o \Delta P_o^k - q_o - C_{21} \Delta_t P_w^k - C_{22} \Delta_t P_o^k - C_{23} \Delta_t P_g^k$$

This residual has the same units as q_o, namely STB/day. Thus, any nonzero value of R_o is interpretable as an erroneous production rate from the block. The sum $(\sum_{ijk} R_{oijk})\ \Delta t$ is simply the total STB of oil created or destroyed during the time step due to error in the computed solution. A simple tolerance is then

$$\varepsilon_1 = \frac{\sum_{ijk} R_{oijk}}{\sum_{ijk} q_{oijk}} \tag{15.46}$$

That is, we iterate until the total amount of oil "destroyed" is a specified small fraction ε_1 of the total amount of oil produced during the time step. This tolerance can be misleading since cancellation of errors due to sign can occur in $\sum_{ijk} R_{oijk}$. A more severe tolerance is

$$\varepsilon_2 = \sum_{ijk} | R_{oijk} | / \sum_{ijk} q_{oijk} \tag{15.47}$$

A generally satisfactory procedure is to use ε_1 = (say) .002 as a closure tolerance on the iterations but to monitor, that is print out, the value of ε_2.

15.3. The Role of Capillary Pressure in the IMPES and Simultaneous Solution Methods

The method of simultaneous solution (SS method) is dependent upon a nonzero level of capillary forces. The reason for this dependence is that the terms of type $\Delta_t S$ are replaced by terms of type $S' \Delta_t P_c$ in the manner of eq. (15.22). If capillary pressure curves corresponding to P_c = constant are used then S' is ∞ and the SS method is invalid.

Since a dP_c/dS of zero cannot be used in the calculations, the question arises as to what minimal level of capillary forces, i.e. minimal values of dP_c/dS, are necessary for the calculations to converge. Extensive experience with this SS method has shown that this minimal level of P_c' is considerably less than the value at which

the capillary forces cease to affect the computed results. This situation is indicated graphically in Fig. 15.1.

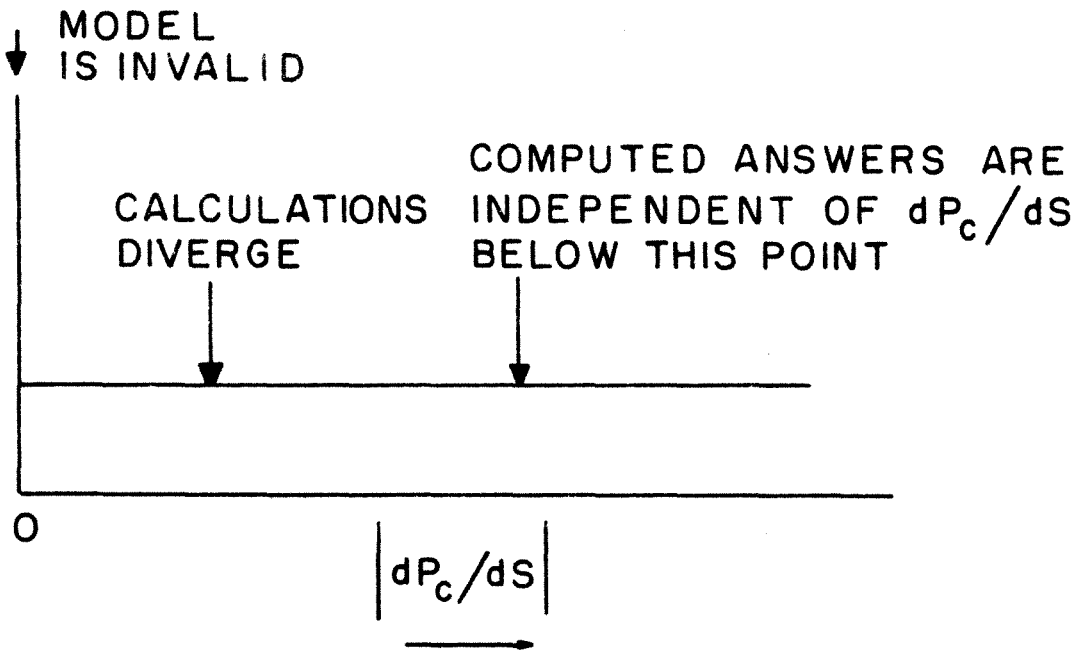


Fig. 15.1 DEPENDENCE OF SS METHOD ANSWERS UPON VALUES OF dP_c/dS

Because of this independence of answers upon P_c' below some minimal P_c' value, the SS model can be run to simulate systems where capillary forces are effectively absent. The IMPES method can be run with or without a nonzero level of capillary forces. Numerous comparisons have shown excellent agreement between IMPES and SS method results where zero capillary pressure was used in the former and small values of P_c' were used in the latter.

EXAMPLE 15.1

A computer program utilizing the SS method was run to simulate a waterflood of the linear oil sand described in Example 11.2. Forty spatial increments were used along with a time step of 10 days. Two runs were performed, with linear capillary

pressure curve slopes dP_{cwo}/dS_w Of 0.5 and 0.1 psi, respectively. The calculated saturations are listed vs x in Table 15.1. This table is presented in preference to a figure because of the virtual identity of the results in the two cases.

TABLE 15.1

Calculated Water Saturation vs x after 1500 Days of Injection at 76 BPD

Linear Reservoir of Example 11.2

	S_w	
$(x=(i - \frac{1}{2})\ \Delta x)$	dP_c/dS = .5 psi	dP_c/dS = .1 psi
1	.7975	.7976
3	.7661	.7672
5	.7181	.7189
7	.6797	.6802
9	.6483	.6487
11	.6215	.6218
13	.5995	.5997
15	.5807	.5809
17	.5641	.5643
19	.5510	.5511
21	.5392	.5394
23	.5253	.5256
25	.5115	.5119
27	.4994	.4999
29	.3704	.3652
30	.1911	.1854
31	.1609	.1606
32	.1600	.1600
33	.1600	.1600
40	.1600	.1600

15.4. Stability of IMPES and SS Methods

The eqs. (15.1) describing multiphase flow contain two sources of instability. First a conditional stability, i.e. a time step restriction, can arise by explicit treatment of certain variables. For example, if a nonzero level of capillary pressure

is used in the IMPES method, then a conditional stability results. The stability condition is unimportant in areal (x-y) calculations where grid block dimensions are roughly equal. The time step restriction may be severe, however, in two-dimensional cross-sectional or three-dimensional calculation where Δz is much less than Δx or Δy. This conditional stability due to explicit handling of P_c of course disappears if capillary pressure of zero is used in the calculations.

Since the SS method handles both pressure and saturation (capillary pressure) implicitly, it is unconditionally stable - insofar as instabilities caused by explicit handling of the primary variables is concerned.

A second source of instability exists in both the IMPES and SS methods. This is the explicit handling of the saturation-dependent transmissibilities. If these transmissibilities were taken at time level $n+\frac{1}{2}$ or $n+1$ as described by Blair and Weinaug [13], this source of instability would not exist. However, except in coning problems, the time step restriction associated with the conditional stability due to explicit transmissibilities is generally not severe.

Analysis of stability with respect to primary variables and with respect to transmissibilities of the set of three flow equations is somewhat complicated. We, therefore, summarize the results here and follow with the detailed analyses.

The conditional stability of IMPES caused by the explicit treatment of capillary pressure is

$$\Delta t \leq \frac{\phi \, \Delta x \, \Delta y \, \Delta z \, \left(\frac{\mu_o}{k_{ro}} + \frac{\mu_g}{k_{rg\ min}}\right)}{2 \, P'_{cwo} \left[k_x \frac{\Delta y \, \Delta z}{\Delta x} + k_y \frac{\Delta x \, \Delta z}{\Delta y} + k_z \frac{\Delta x \, \Delta y}{\Delta z}\right]} \qquad (15.80a)$$

for reservoir regions where primarily only gas and oil are flowing. For regions where oil and water only are flowing,

$$\Delta t \leq \frac{\phi\, \Delta x\, \Delta y\, \Delta z\, \left(\frac{\mu_w}{k_{rw}} + \frac{\mu_o}{k_{ro}}\right)_{min}}{2\, P'_{cwo}\, \left[k_x \frac{\Delta y\, \Delta z}{\Delta x} + k_y \frac{\Delta x\, \Delta z}{\Delta y} + k_z \frac{\Delta x\, \Delta y}{\Delta z}\right]} \qquad (15.80b)$$

The terms P'_c are $P'_{cgo} = d\, P_{cgo}/d\, S_g$ and $P'_{cwo} = -d\, P_{cwo}/d\, S_w$, both positive quantities. These time step restrictions do not reflect any time step restriction caused by explicit handling of transmissibilities. These stability conditions also do not reflect the mitigating effect of fluid compressibility. The effect on stability of compressibility is to slightly relax the restrictions given here.

In three-dimensional or two-dimensional cross-sectional problems where $k_z\, \Delta x\, \Delta y/\Delta z$ is much greater than $k_x\, \Delta y\, \Delta z/\Delta x$ and $k_y\, \Delta x\, \Delta z/\Delta y$, these stability conditions simplify to

$$\Delta t \leq \frac{\phi\, \Delta z^2\, \left(\frac{\mu_o}{k_{ro}} + \frac{\mu_g}{k_{rg}}\right)_{min}}{2\, k_z\, P'_{cwo}} \qquad (15.81a)$$

in the gas-oil flow regions and

$$\Delta t \leq \frac{\phi\, \Delta z^2\, \left(\frac{\mu_o}{k_{ro}} + \frac{\mu_w}{k_{rw}}\right)_{min}}{2\, k_z\, P'_{cwo}} \qquad (15.81b)$$

in the regions of water-oil flow. For two-dimensional areal calculations, k_z is zero in eqs. (15.80a and b) and for $\Delta x \cong \Delta y$ we have

$$\Delta t \leq \text{Min}\left\{\frac{\phi\, \Delta x\, \Delta y\, \left(\frac{\mu_o}{k_{ro}} + \frac{\mu_g}{k_{rg}}\right)_{min}}{4\, k\, P'_{cgo}}\,,\ \frac{\phi\, \Delta x\, \Delta y\, \left(\frac{\mu_o}{k_{ro}} + \frac{\mu_w}{k_{rw}}\right)_{min}}{4\, k\, P'_{cwo}}\right\} \qquad (15.82)$$

Comparison of eqs. (15.81) and (15.82) shows that, using IMPES, the ratio of maximum time step in cross-sectional or three-dimensional studies to the maximum time step

in an areal study is about

$$\frac{\Delta t_{3\text{-}D}}{\Delta t_{areal}} \cong \frac{k}{k_z} \frac{2\ \Delta z^2}{\Delta x\ \Delta y} \tag{15.83}$$

This ratio is often the order of .01 to .001.

Ignoring the conditional stability associated with the explicit transmissibilities, we find below that the SS method is unconditionally stable.

The stability condition for both the IMPES and SS methods which is imposed by explicit transmissibilities is derived for the assumptions of zero capillary pressure and zero fluid compressibility. As above, the effect of fluid compressibility is slight relaxation of the time step restriction derived here for the incompressible case. The fractional flow of each phase is assumed to depend primarily upon the saturation of that phase. That is,

$$\frac{\lambda_m}{\lambda_w + \lambda_o + \lambda_g} = f\ (S_m) \tag{15.84}$$

for m = w, o, g where λ is mobility, relative permeability divided by viscosity. The stability condition is

$$\Delta t \lesssim \min_{m=w,o,g} \left[\frac{\phi}{f'_m} \frac{1}{\frac{u_x}{\Delta x} + \frac{u_y}{\Delta y} + \frac{u_z}{\Delta z}}\right] \tag{15.85}$$

where u_x, u_y, u_z are total superficial or Darcy velocities in the three directions. As derived below using the method of characteristics, the term $f'_m\ u_\ell\ \Delta t/\phi\Delta\ell$ is simply the ratio of (distance advanced in direction ℓ by a phase m flood front in time Δt) to the block length $\Delta\ell$ in that direction. If we denote this ratio by r_m then eq. (15.85) is

$$\max_{m=w,o,g} (r_{mx} + r_{my} + r_{mz}) < 1 \qquad (15.86)$$

EXAMPLE 15.5

A reservoir is undergoing natural depletion with natural water drive and gas cap expansion. Using IMPES with P'_{cgo} = 2 psi and P'_{cwo} = 1.5 psi, what are the time step restrictions for two-dimensional areal and three-dimensional studies? What time step restrictions are there for the SS method? Available data are

ϕ = .15 $\quad \Delta x = \Delta y = 500'$ $\quad \Delta z = 10'$ $\quad k_x = k_y$ = 200 md

k_z = 100 md $\quad \mu_w$ = 1 cp $\quad \mu_o$ = 2 cp $\quad \mu_g$ = .02 cp

the relative permeability curves give

$$\left(\frac{\mu_o}{k_{ro}} + \frac{\mu_g}{k_{rg}}\right)_{min} \cong 2.3 \qquad \left(\frac{\mu_o}{k_{ro}} + \frac{\mu_w}{k_{rw}}\right)_{min} \cong 7$$

Solution:

From eqs. (15.80) and (15.81), the time step restriction for IMPES in the two-dimensional areal calculation is (k_z = 0 here)

$$\Delta t \leq \text{Min} \left\{ \frac{\phi \, \Delta x \, \Delta y \left(\frac{\mu_o}{k_{ro}} + \frac{\mu_g}{k_{rg}}\right)_{min}}{2 \, P'_{cgo} \left(k_x \frac{\Delta y}{\Delta x} + k_y \frac{\Delta x}{\Delta y}\right)}, \frac{\phi \, \Delta x \, \Delta y \left(\frac{\mu_w}{k_{rw}} + \frac{\mu_o}{k_{ro}}\right)_{min}}{2 \, P'_{cwo} \left[k_x \frac{\Delta y}{\Delta x} + k_y \frac{\Delta x}{\Delta y}\right]} \right\}$$

Using the given data we find

$$\Delta t \leq \text{Min} \left\{ \frac{.15 \, (500)^2 \, (2.3)}{2(2) \, (200 + 200) \, (.00633)}, \frac{.15 \, (500)^2 \, (7)}{2(1.5) \, (200 + 200) \, (.00633)} \right\}$$

$$= 8500 \text{ days}$$

This "restriction" is obviously of no importance whatsoever.

In a two-dimensional cross-sectional (x-z) or three-dimensional case, eq. (15.82 and 15.83) give the time step restriction using IMPES as

$$\Delta t \leq \text{Min}\left\{\frac{\phi\,\Delta z^2\,\left(\frac{\mu_o}{k_{ro}}+\frac{\mu_g}{k_{rg\,min}}\right)}{2\,k_z\,P'_{cgo}}\,,\ \frac{\phi\,\Delta z^2\,\left(\frac{\mu_o}{k_{ro}}+\frac{\mu_w}{k_{rw\,min}}\right)}{2\,k_z\,P'_{cwo}}\right\}$$

$$\leq \text{Min}\left\{\frac{.15\ (100)\ (2.3)}{2\ (100)\ (.00633)\ (2)}\,,\ \frac{.15\ (100)\ (7)}{2\ (100)\ (.00633)\ (1.5)}\right\} = 13.6 \text{ days}$$

The time step restriction of eq. (15.8) applies to both the IMPES and SS methods. This is a difficult restriction to quantify in the two- or three-dimensional case. Experience indicates that in general it is satisfied if saturation change in each block per time step is less than 15%. Again, in general, time truncation error in the calculated results becomes significant at about 10-15% saturation change per time step so that this stability condition is often of little practical importance.

15.4.1 Derivation of IMPES Stability Condition

If fluids are considered incompressible and transmissibilities are taken constant along any given direction, then eqs.(15.3) become

$$T_w\,\Delta^2 p_w - B_w\,q_w = \frac{V_p}{\Delta t}\,\Delta_t\,S_w$$

$$T_o\,\Delta^2 p_o - B_o\,q_o = \frac{V_p}{\Delta t}\,\Delta_t\,S_o$$

$$T_g\,\Delta^2 p_g - B_g\,q_g = \frac{V_p}{\Delta t}\,\Delta_t\,S_g \qquad (15.90)$$

where

$$T\,\Delta^2 p \equiv T_x\,\Delta_x^2 p + T_y\,\Delta_y^2 p + T_z\,\Delta_z^2 p \tag{15.91}$$

and transmissibilities are

$$T_{wx} = \frac{k_x\,k_{rw}}{\mu_w}\frac{\Delta y\,\Delta z}{\Delta x} \qquad T_{wy} = \frac{k_y\,k_{rw}}{\mu_w}\frac{\Delta x\,\Delta z}{\Delta y} \qquad T_{wz} = \frac{k_z\,k_{rw}}{\mu_w}\frac{\Delta x\,\Delta y}{\Delta z}$$

Using linear capillary pressure curves gives

$$T_w\,\Delta^2 p - P'_{cwo}\,T_w\,\Delta^2 S_w - B_w\,q_w = \frac{Vp}{\Delta t}\,\Delta_t\,S_w$$

$$T_o\,\Delta^2 p - B_o\,q_o = -\frac{Vp}{\Delta t}\,\Delta_t\,S_w - \frac{Vp}{\Delta t}\,\Delta_t\,S_g$$

$$T_g\,\Delta^2 p + P'_{cgo}\,T_g\,\Delta^2 S_g - B_g\,q_g = \frac{Vp}{\Delta t}\,\Delta_t\,S_g \tag{15.93}$$

where p is oil pressure. These are three equations in the three unknowns S_w, S_g, and p. The errors ε_1, ε_2, ε_3 in these three variables satisfy the same equations

$$T_w\,\Delta^2 \varepsilon_3)_{n+1} + \overline{T}_w\,\Delta^2 \varepsilon_1)_n = \frac{Vp}{\Delta t}\,\Delta_t\,\varepsilon_1$$

$$T_o\,\Delta^2 \varepsilon_3)_{n+1} = -\frac{Vp}{t}\,\Delta_t\,\varepsilon_1 - \frac{Vp}{\Delta t}\,\Delta_t\,\varepsilon_2$$

$$T_g\,\Delta^2 \varepsilon_3)_{n+1} + \overline{T}_g\,\Delta^2 \varepsilon_2)_n = \frac{Vp}{\Delta t}\,\Delta_t\,\varepsilon_2 \tag{15.94}$$

where $\overline{T}_w = -P'_{cwo}\,T_w$, a positive number and $\overline{T}_g = P'_{cgo}\,T_g$, also positive. The time notation on left hand side terms in eq. (15.94) reflects the fact that the IMPES

method takes pressure implicitly and capillary pressure or saturation explicitly.

As discussed in Chapter 9, the replacement

$$\varepsilon_{ijkn} = f_n \, e^{\hat{\imath}\,\alpha_x\, i} \; e^{\hat{\imath}\,\alpha_y\, j} \; e^{\hat{\imath}\,\alpha_z\, k} \tag{15.95}$$

gives

$$\Delta_x^2 \, \varepsilon_{ijkn} = -\gamma_x \, \varepsilon_{ijkn} \qquad \Delta_y^2 \, \varepsilon_{ijkn} = -\gamma_y \, \varepsilon_{ijkn}$$

$$\Delta_z^2 \, \varepsilon_{ijkn} = -\gamma_z \, \varepsilon_{ijkn} \tag{15.96}$$

where $\gamma_x = 4 \sin^2 \frac{\alpha_x}{2}$, $\gamma_y = 4 \sin^2 \frac{\alpha_y}{2}$, $\gamma_z = 4 \sin^2 \frac{\alpha_z}{2}$ and f_n is a function of n. α_x, α_y, α_z range from nearly 0 to π but not more than 2 of the three values are simultaneously π. We then have

$$T_\ell \, \Delta^2 \, \varepsilon_\ell = T_{\ell x} \, \Delta_x^2 \, \varepsilon_\ell + T_{\ell y} \, \Delta_y^2 \, \varepsilon_\ell + T_{\ell z} \, \Delta_z^2 \, \varepsilon_\ell = -\lambda_\ell \, \gamma_\ell \, \varepsilon_\ell \tag{15.97}$$

where $\lambda_\ell = k_{r\ell}/\mu_\ell$

$$\gamma_\ell = \frac{4 \, k_x \, \Delta y \, \Delta z}{\Delta x} \sin^2 \frac{\alpha_x}{2} + \frac{4 \, k_y \, \Delta x \, \Delta z}{\Delta y} \sin^2 \frac{\alpha_y}{2} + \frac{4 \, k_z \, \Delta x \, \Delta y}{\Delta z} \sin^2 \frac{\alpha_z}{2} \tag{15.98}$$

Substitution from (15.97) into (15.94) gives

$$-\lambda_w \, \gamma_3 \, \varepsilon_{3n+1} - \bar{\lambda}_w \, \gamma_1 \, \varepsilon_{1n} = \alpha \, (\varepsilon_{1n+1} - \varepsilon_{1n})$$

$$- \lambda_o \gamma_3 \varepsilon_{3n+1} = - \alpha (\varepsilon_{1n+1} - \varepsilon_{1n}) - \alpha (\varepsilon_{2n+1} - \varepsilon_{2n})$$

$$- \lambda_g \gamma_3 \varepsilon_{3n+1} - \bar{\lambda}_g \gamma_2 \varepsilon_{2n} = \alpha (\varepsilon_{2n+1} - \varepsilon_{2n}) \qquad (15.99)$$

where $\bar{\lambda}_w$ is $- P'_{cwo} \lambda_w$ and $\bar{\lambda}_g$ is $P'_{cgo} \lambda_g$ and $\alpha = Vp/\Delta t$. Adding these three equations (note the right hand side adds to zero because $\sum_{\ell=1}^{3} \Delta_t S_\ell = 0$), solving the result for $\gamma_3 \varepsilon_{3n+1}$ and substituting the latter into (15.99b and c) gives the two equations

$$\alpha \varepsilon_{1n+1} = (\alpha - \frac{\bar{\lambda}_w}{\lambda} (\lambda_o + \lambda_g) \gamma_1) \varepsilon_{1n} + \frac{\lambda_w \bar{\lambda}_g}{\lambda} \gamma_2 \varepsilon_{2n}$$

$$\alpha \varepsilon_{1n+1} + \alpha \varepsilon_{2n+1} = (\alpha - \frac{\lambda_o \bar{\lambda}_w}{\lambda} \gamma_2) \varepsilon_{1n} + (\alpha - \frac{\lambda_o \bar{\lambda}_g}{\lambda} \gamma_2) \varepsilon_{2n} \qquad (15.100)$$

λ is total mobility $\lambda_w + \lambda_o + \lambda_g$. These two equations are, in matrix form,

$$a \underline{\varepsilon}_{n+1} = b \underline{\varepsilon}_n \qquad (15.101)$$

where

$$\underline{\varepsilon}_n = \begin{Bmatrix} \varepsilon_{1n} \\ \varepsilon_{2n} \end{Bmatrix} \qquad (15.102)$$

Solving for $\underline{\varepsilon}_{n+1}$ gives

$$\underline{\varepsilon}_{n+1} = a^{-1} b \underline{\varepsilon}_n = B \underline{\varepsilon}_n \qquad (15.103)$$

where a^{-1} is the inverse of the two x two matrix a.

The matrix B is

$$B = \frac{1}{\alpha} \begin{bmatrix} \alpha - \gamma_1 \bar{\lambda}_w \left(1 - \frac{\lambda}{\lambda_w}\right) & \frac{\lambda_w \bar{\lambda}_g}{\lambda} \gamma_2 \\ \frac{\bar{\lambda}_w \lambda_g \gamma_1}{\lambda} & \alpha - \frac{\bar{\lambda}_g \gamma_2}{\lambda} (\lambda_o + \lambda_w) \end{bmatrix} \quad (15.104)$$

Successive application of eq. (15.103) gives the error vector after n time steps as

$$\underline{\varepsilon}_n = B^n \underline{\varepsilon}_o$$

where $\underline{\varepsilon}_o$ is the initial error. For stability we require that

$$\lim_{n \to \alpha} B^n = 0 \text{ (null matrix)} \quad (15.105)$$

Varga [17] states that (15.105) is true - i.e. the matrix B is <u>convergent</u> - if the spectral radius (largest eigenvalue in absolute value) is less than unity. Denoting the entries in the B matrix by b_{ij} we have for the eigenvalues the equation

$$\begin{vmatrix} b_{11} - \sigma & b_{12} \\ b_{21} & b_{22} - \sigma \end{vmatrix} = 0$$

and, upon expansion of this determinant and solution of the resulting quadratic,

$$\sigma = \frac{b_{11} + b_{22} \pm \sqrt{(b_{11} + b_{22})^2 - 4 \Delta_b}}{2} \quad (15.106)$$

where

$$\Delta_b = b_{11}\, b_{22} - b_{12}\, b_{21}$$

After considerably algebraic manipulation we find that the maximum value of $|\sigma|$ given by eq. (15.106) is

$$\sigma = \frac{1}{2\alpha}\{2\alpha - \frac{\gamma_1 \bar{\lambda}_w (\lambda_o + \lambda_g)}{} - \frac{\gamma_2 \bar{\lambda}_g (\lambda_o + \lambda_w)}{} - \frac{1}{\lambda}\sqrt{[\gamma_1 \bar{\lambda}_w (\lambda_o + \lambda_g) - \gamma_2 \bar{\lambda}_g (\lambda_o + \lambda_w)]^2 + 4\lambda_w \lambda_g \bar{\lambda}_w \bar{\lambda}_g \gamma_1 \gamma_2}\}$$

This σ is always $< +1$ but the restriction $-1 < \sigma$ gives

$$\Delta t \leq \frac{4\, Vp}{\frac{\gamma_1 \bar{\lambda}_w (\lambda_o+\lambda_g)}{\lambda} + \frac{\gamma_2 \bar{\lambda}_g (\lambda_o+\lambda_w)}{\lambda} + \frac{1}{\lambda}\sqrt{\quad}} \qquad (15.108)$$

For water-oil regions of the reservoir, we set $\lambda_g = \bar{\lambda}_g = 0$ and obtain (15.80b). For gas-oil regions we set $\lambda_w = \bar{\lambda}_w = 0$ and obtain (15.80a). In obtaining these equations (15.80), we use the fact that the most severe restriction on Δt in eq. (15.108) occurs when the $\sin^2$ terms in γ_1 and γ_2 (see eq. (15.98)) have their maximum values of 1 or nearly 1.

15.4.2 Derivation of the SS Method Stability

The stability of the SS method is examined here for the case of incompressible two-phase flow. The compressible, three-phase flow case can be examined in the

same manner to obtain the same result of unconditional stability. The simpler case is treated here to minimize the algebraic complexity and preserve some clarity regarding the method of analysis. For flow of incompressible water and oil, eqs. (15.18) are

$$\nabla \cdot (K_w \nabla \Phi_w) - q_{vw} = \phi \frac{\partial S_w}{\partial t}$$

$$\nabla \cdot (K_o \nabla \Phi_o) - q_{vo} = \phi \frac{\partial S_o}{\partial t} \qquad (15.109)$$

Using the SS formulation, we have in difference form

$$T_w \Delta^2 \Phi_{wn+1} - q_w = C \Delta_t \Phi_w - C \Delta_t \Phi_o$$

$$T_o \Delta^2 \Phi_{on+1} - q_o = - C \Delta_t \Phi_w + C \Delta_t \Phi_o \qquad (15.110)$$

where C is $- Vp (d S_w/d P_{cwo})/\Delta t$, a positive number. For the purpose of analysis we take T_{wx}, T_{wy}, etc. as constants. Notation is defined in eqs. (15.91) and (15.92).

The errors in Φ_w and Φ_o will be denoted ε_1 and ε_2 respectively so that

$$T_w \Delta^2 \varepsilon_{1n+1} = C \Delta_t \varepsilon_1 - C \Delta_t \varepsilon_2$$

$$T_o \Delta^2 \varepsilon_{2n+1} = - C \Delta_t \varepsilon_1 + C \Delta_t \varepsilon_2 \qquad (15.111)$$

Following eqs. (15.95) - (15.98) we have

$$- \lambda_w \gamma_1 \varepsilon_{1n+1} = C (\varepsilon_{1n+1} - \varepsilon_{1n}) - C (\varepsilon_{2n+1} - \varepsilon_{2n})$$

$$- \lambda_o \gamma_2 \varepsilon_{2n+1} = - C (\varepsilon_{1n+1} - \varepsilon_n) + C (\varepsilon_{2n+1} - \varepsilon_{2n}) \qquad (15.112)$$

where λ_ℓ and γ_ℓ are defined in eqs. (15.98).

Eqs. (15.112) can be written

$$\underline{\varepsilon}_{n+1} = B\,\underline{\varepsilon}_n \tag{15.113}$$

where $\underline{\varepsilon}_n = \begin{bmatrix} \varepsilon_{1n} \\ \varepsilon_{2n} \end{bmatrix}$

$$B = \frac{C}{C\,(\lambda_w\,\gamma_1 + \lambda_o\,\gamma_2) + \lambda_w\,\lambda_o\,\gamma_1\,\gamma_2} \begin{bmatrix} \lambda_o\,\gamma_2 & -\lambda_o\,\gamma_2 \\ -\lambda_w\,\gamma_1 & \lambda_w\,\gamma_1 \end{bmatrix} \tag{15.114}$$

As above in analysis of IMPES, for stability we require $\lim_{n\to\infty} B^n$ = the null matrix or that the maximum eigenvalue (in absolute value) of the matrix B be less than 1. We find this maximum eigenvalue to be

$$\sigma_{max} = \frac{C\,(\lambda_o\,\gamma_2 + \lambda_w\,\gamma_1)}{C\,(\lambda_o\,\gamma_2 + \lambda_w\,\gamma_1) + \lambda_w\,\lambda_o\,\gamma_1\,\gamma_2} \tag{15.115}$$

This ratio is positive and less than 1 since γ_1 and γ_2 are positive and never zero (see below eq. (15.96)).

15.4.3 Analysis of Stability with Respect to Transmissibilities

The equations describing three-phase incompressible flow are

$$-\nabla \cdot \vec{u}_w - q_{vw} = \phi \frac{\partial S_w}{\partial t}$$

$$-\nabla \cdot \vec{u}_o - q_{vo} = \phi \frac{\partial S_o}{\partial t}$$

$$-\nabla \cdot \vec{u}_g - q_{vg} = \phi \frac{\partial S_g}{\partial t} \tag{15.120}$$

where $\vec{u}_\ell$ is the superficial (Darcy) velocity vector for phase ℓ. Adding these equations gives

$$\nabla \cdot \vec{u} = - q_v \tag{15.121}$$

where $\vec{u}$ is the total superficial velocity $\vec{u}_w + \vec{u}_o + \vec{u}_g$.

The fractional flow of water is defined by

$$u_{wx} = f_{wx}\, u_x \qquad u_{wy} = f_{wy}\, u_y \qquad u_{wz} = f_{wz}\, u_z \tag{15.122}$$

The fractional flow f_w has different values for flow in different directions because of the gravitational component due to fluid density differences. Further, fractional flow is a function of two saturations (any two since $S_w + S_o + S_g = 1$). As an approximation for the purpose of this stability analysis, we take f_ℓ for each phase as a single-valued function of the corresponding saturation S_ℓ. Thus

$$\vec{u}_\ell = f_\ell\, \vec{u} \tag{15.123}$$

Substituting from (15.123) into the water eq. (15.120a), using the fact that $\nabla \cdot f_\ell \vec{u} = f_\ell \nabla \cdot \vec{u} + \vec{u} \cdot \nabla f_\ell$ and using eq. (15.121), we obtain

$$- \vec{u} \cdot \nabla f_w + f_w q_v - q_{vw} = \phi \frac{\partial S_w}{\partial t} \tag{15.124}$$

Setting $q_{vw} = f_w q_v$ and using the assumption that f_w is a single-valued function of S_w, we obtain

$$- f_w' \vec{u} \cdot \nabla S_w = \phi \frac{\partial S_w}{\partial t} \tag{15.125}$$

where

$$f'_w = d\, f_w / d\, S_w$$

With no loss in generality we consider a point where u_x, u_y, and u_z are all positive. In accordance with the upstream weighting of explicit transmissibilities, we express (15.125) in the following difference form:

$$-\frac{f'_w\, \Delta t}{\phi}\left[u_x \frac{S_i - S_{i-1}}{\Delta x} + u_y \frac{S_j - S_{j-1}}{\Delta y} + u_z \frac{S_k - S_{k-1}}{\Delta z}\right]_n = S_{n+1} - S_n \tag{15.126}$$

where $S = S_w$ and centered values of i,j,k,n are omitted from the subscripts. Defining

$$U_x = f'_w\, u_x\, \Delta t/\phi\, \Delta x \qquad U_y = f'_w\, u_y\, \Delta t/\phi\, \Delta y \qquad U_z = f'_w\, u_z\, \Delta t/\phi\, \Delta z \tag{15.127}$$

eq. (15.126) is

$$U_x\, (S_{i-1} - S_i)_n + U_y\, (S_{j-1} - S_j)_n + U_z\, (S_{k-1} - S_k)_n = S_{n+1} - S_n \tag{15.128}$$

The error ε in water saturation S satisfies this same equation. Making the Fourier replacement,

$$\varepsilon_{ijkn} = \beta^n\, e^{\hat{\imath}\, \alpha_x\, i}\, e^{\hat{\imath}\, \alpha_y\, j}\, e^{\hat{\imath}\, \alpha_z\, k} \tag{15.129}$$

gives

$$U_x (e^{-\hat{i}\alpha_x} - 1) + U_y (e^{\hat{i}\alpha_y} - 1) + U_z (e^{\hat{i}\alpha_z} - 1) = \beta - 1$$

(15.130)

Solving for β, we obtain the complex form a + ib. The absolute value of β is $\sqrt{a^2 + b^2}$ and

$$\beta^2 = 1 - 4 \left[U_x (1 - U_x) \sin^2 \frac{\alpha_x}{2} + U_y (1 - U_y) \sin^2 \frac{\alpha_y}{2} + U_z (1 - U_z) \sin^2 \frac{\alpha_z}{2}\right]$$

$$+ 2 \{U_x U_y [4 \sin^2 \frac{\alpha_x}{2} \sin^2 \frac{\alpha_y}{2} + \sin \alpha_x \sin \alpha_y]$$

$$+ U_x U_z [4 \sin^2 \frac{\alpha_x}{2} \sin \frac{\alpha_z}{2} + \sin \alpha_x \sin \alpha_z]$$

$$+ U_y U_z [4 \sin^2 \frac{\alpha_y}{2} \sin \frac{\alpha_z}{2} + \sin \alpha_y \sin \alpha_z]\}$$

(15.131)

This result shows that for stability ($| \beta | < 1$) each of U_x, U_y, U_z must be less than 1. For example, set $\alpha_y = \alpha_z = 0$ and $\alpha_x = \pi$ to find that

$$\beta^2 = 1 - 4 U_x (1 - U_x) \qquad (15.132)$$

and β^2 exceeds 1 if $U_x > 1$. Furthermore, setting $\alpha_x = \alpha_y = \alpha_z = \pi$ gives

$$\beta^2 = 1 - 4 U (1 - U) \qquad (15.133)$$

where $U = U_x + U_y + U_z$ so that $U \leq 1$ is a necessary, more stringent, condition for stability. This analysis and results for the water equation applies also to the oil and gas equations, leading to the stability condition (15.85).

15.5 Handling of Aquifer Water Drive

A reservoir-aquifer system can be treated with the grid indicated in Fig. 15.2. Small blocks define the reservoir while increasingly larger blocks are used away from the reservoir to define the aquifer. A disadvantage of

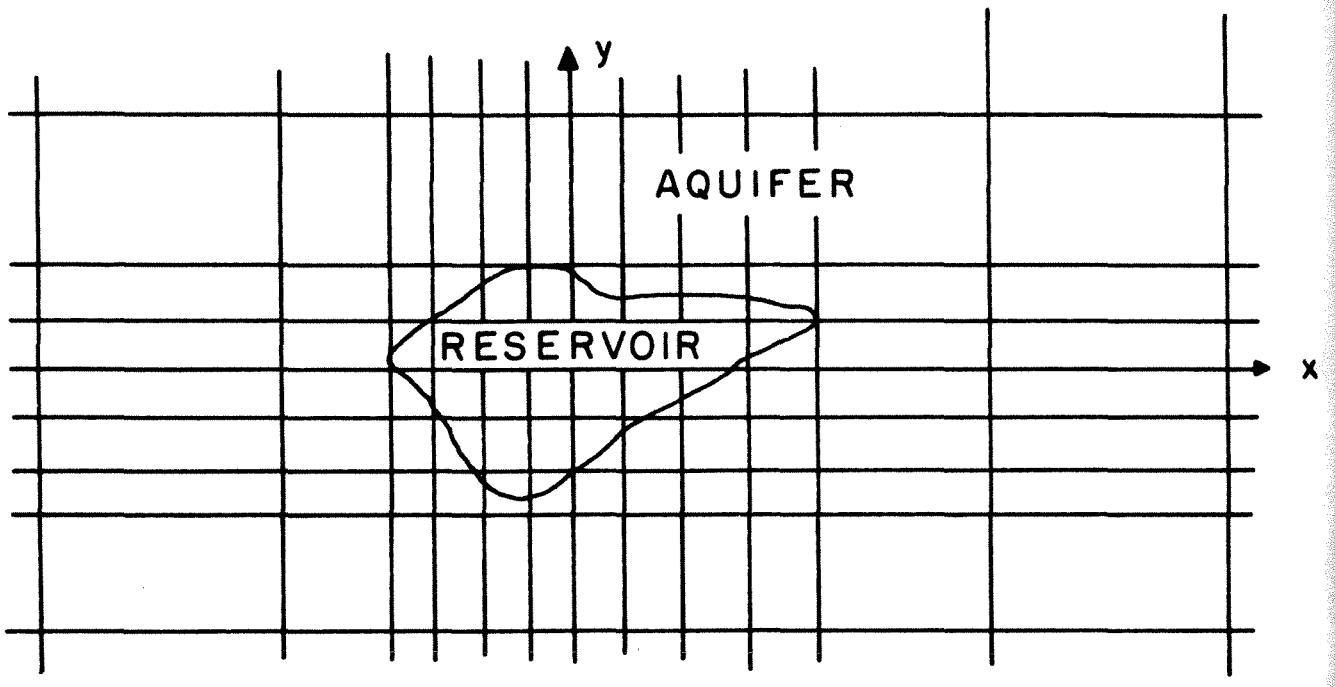


Fig. 15.2 EXTENDED GRID FOR RESERVOIR-AQUIFER SYSTEM

this handling of an aquifer is the increased computer storage and computing time required for the grid blocks in the aquifer.

An alternative method of accounting for the aquifer is to restrict the grid to the reservoir, as in Fig. 15.3, and represent the influx into the reservoir by the production term in eq. (15.3a). Actually the grid of Fig. 15.3 is generally extended somewhat so that the boundary blocks of the grid lie in the aquifer.

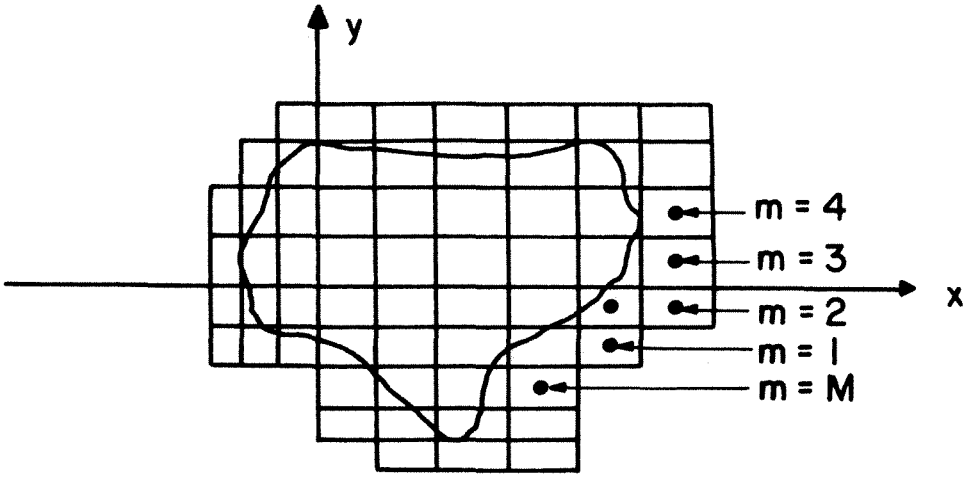


Fig. 15.3 GRID RESTRICTED TO RESERVOIR

The simplest representation of an aquifer is the "pot" aquifer. This is a relatively small aquifer with a closed exterior boundary. A semi-steady state pressure distribution is assumed to exist in the aquifer at any time so that the rate of water influx into the reservoir is

$$e_w = - c\, Vpa \frac{\partial \bar{p}_w}{\partial t} \quad RB/day \tag{15.60}$$

where

c = water + rock compressibility, 1/psi

Vpa = pore volume of aquifer, RB

$\bar{p}_w$ = average pressure at reservoir-aquifer boundary

The reservoir boundary blocks are designated by the single subscript m, as indicated on Fig. 15.3, and a fraction α_m of this total influx is associated with boundary block m as

$$q_{wm} = \alpha_m \, b_{wm} \, c \, Vpa \, \frac{\partial \, p_{wm}}{\partial t} \quad STB/day \tag{15.61}$$

The factor α_m reflects the frontage area of block m as a fraction of field perimeter and possibly the heterogeneity around the field boundary. The derivative $\partial p_{wm}/\partial t$ is expressed in difference form as $\Delta_t \, p_{wm} / \Delta t$ and combines with the identical term on the right hand side of eq. (15.3a) (see eq. (15.10) or (15.23a)). Thus, the representation of aquifer water influx by eq. (15.6) requires only a slight modification in the definition of the coefficients C_{10} in IMPES or C_{11} in the SS method. Eq. (15.61) shows that the pot aquifer concept leads to a water influx rate which is dependent only upon the rate of change and not upon the level of pressure. That is, reservoir boundary pressure could be well below initial aquifer pressure but no water influx would occur if $\partial p_w/\Delta t$ were zero.

A second representation of an aquifer is the Schilthuis steady-state [18] or Katz "pound-day" [19] model. Schilthuis calculates cumulative water influx into a reservoir as

$$W_e \, (t) = C \int_o^t (p^{(i)} - \bar{p}_w) \, dt \tag{15.62}$$

This equation is equivalent to using a linear influence function, $Q(t) = Ct$, where the influence function is defined by eq. (15.63)

$$W_e \, (t) = (p^{(i)} - \bar{p}) \, Q(t) \tag{15.63}$$

for the case of a constant pressure $\bar{p}$ at the reservoir boundary. Further, eq. (15.62)

reflects the assumption of a steady-state pressure distribution in the aquifer from $p = \bar{p}_w$ at the reservoir-aquifer boundary to $p = p_o$ at the aquifer exterior boundary.

Katz [19] proposed in the 1940's use of a similar concept in calculating water movement about gas storage reservoirs. He calculated cumulative water influx as

$$(W_e) = C \sum_{j=1}^{n} (p_o - \bar{p}_{w,j}) \Delta t_j \qquad (15.64)$$

where $\bar{p}_{w,j}$ is an average reservoir-aquifer boundary pressure during the time period from t_{j-1} to t_j. The time increment Δt_j is $t_j - t_{j-1}$. Using eq. (15.64), we have the water influx rate into the boundary block as

$$- q_{wm} = b_{wm} [(W_e)_{t_{n+1}} - (W_e)_{t_n}]/\Delta t \quad \text{STB/d}$$

or

$$- q_{wm} = \frac{\alpha_m b_{wm} C (p_o - p_{wm,n})}{\Delta t} - \frac{.5 b_{wm} \alpha_m C}{\Delta t} \Delta_t p_{wm} \qquad (15.65)$$

The first term on the right hand side is known while the second combines with a term on the right hand side of eq. (15.3a) to modify the definition of C_{10} in IMPES or C_{11} in the SS method. Eq. (15.65) relates water influx rate to the level as well as rate of change of the boundary block pressure.

A third method of representing aquifer water influx by the q_w term is use of a nonlinear aquifer influence function Q(t), defined by eq. (15.63). The storage requirements and calculational complexity of handling the resulting superposition formulas [20] can be largely eliminated by use of the Carter-Tracy approximate water influx method [21].

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ITERATIVE METHODS OF SOLVING SYSTEMS OF LINEAR EQUATIONS

H. S. Price

I. Point Iterative Methods

Consider the following system of linear simultaneous equations

$$\begin{aligned}
a_{1,1}\,x_1 + a_{1,2}\,x_2 + \cdots + a_{1,n}\,x_n &= k_1 \\
a_{2,1}\,x_1 + a_{2,2}\,x_2 + \cdots + a_{2,n}\,x_n &= k_2 \\
&\vdots \\
a_{n,1}\,x_1 + a_{n,2}\,x_2 + \cdots + a_{n,n}\,x_n &= k_n
\end{aligned}$$

which in matrix notation becomes

$$A\,\underline{x} = \underline{k} \tag{1}$$

where

$$A = \begin{bmatrix} a_{1,1} & a_{1,2} & \cdots & a_{1,n} \\ a_{2,1} & a_{2,2} & \cdots & a_{2,n} \\ \vdots & & & \vdots \\ a_{n,1} & a_{n,2} & \cdots & a_{n,n} \end{bmatrix}, \quad \underline{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}, \quad \text{and} \quad \underline{k} = \begin{bmatrix} k_1 \\ k_2 \\ \vdots \\ k_n \end{bmatrix}.$$

We will assume the matrix A is non-singular to insure the existence of a unique solution. Moreover we assume that the diagonal entries $a_{i,i}$ are all nonzero.

Let us now express the matrix A as the sum

$$A = D - B$$

where D is the diagonal matrix

$$D = \begin{bmatrix} a_{1,1} & & & \\ & a_{2,2} & & \\ & & \ddots & \\ & & & a_{n,n} \end{bmatrix} \qquad (2)$$

and the elements of B are the negatives of the off diagonal elements of A.

We can now define the following iterative scheme for solving (1)

$$D\,\underline{x}^{(m+1)} = B\,\underline{x}^{(m)} + \underline{k} \qquad (3)$$

or written out as

$$a_{ii}\,x_i^{(m+1)} = -\sum_{\substack{j=1 \\ j\neq i}}^{m} a_{i,j}\,x_j^{(m)} + k_i \qquad 1 \leq i \leq n,\ m \geq 0\ . \qquad (4)$$

Since the elements of D are nonzero (4) becomes

$$x_i^{(m+1)} = -\sum_{\substack{j=1 \\ j\neq i}}^{n} \left(\frac{a_{i,j}}{a_{i,i}}\right) x_j^{(m)} + \frac{k_i}{a_{i,i}}\ , \qquad 1 \leq i \leq n,\ m \geq 0\ .$$

or in matrix notation

$$\underline{x}^{(m+1)} = D^{-1}\,B\,\underline{x}^{(m)} + D^{-1}\underline{k} \qquad (5)$$

This method is known as the point Jacoby method and the matrix

$$D^{-1}\,B$$

is called the point Jacoby matrix.

Noticing that this method does not use updated information we now consider the iterative method

$$a_{i,i}\,x_i^{(m+1)} = -\sum_{j=1}^{i-1} a_{i,j}\,x_j^{m+1} - \sum_{j=i+1}^{n} a_{i,j}\,x_j^{(m)} + k_i \qquad 1 \leq i \leq n,\ m \geq 0\ . \qquad (6)$$

Or if we write the matrix A as the sum

$$A = D - L - U$$

where D is given by (2) and

$$L = \begin{bmatrix} 0 & & & & \\ -a_{21} & 0 & & \bigcirc & \\ -a_{31} & -a_{32} & 0 & & \\ \vdots & \vdots & \ddots & \ddots & \\ -a_{n1} & -a_{n2} & \cdots & -a_{n\,n-1} & 0 \end{bmatrix} \quad \text{and} \quad U = \begin{bmatrix} 0 & -a_{12} & -a_{13} & \cdots & -a_{1n} \\ 0 & 0 & -a_{23} & \cdots & -a_{2n} \\ & & \ddots & \ddots & \vdots \\ & \bigcirc & & \ddots & a_{n-1,n} \\ & & & & 0 \end{bmatrix}$$

Now (6) can be written in matrix form as

$$(D-L)\,\underline{x}^{(m+1)} = U\,\underline{x}^{(m)} + \underline{k} \qquad n \geq 0$$

or since D - L is non-singular if D is non-singular we have

$$\underline{x}^{(m+1)} = (D-L)^{-1}\,U\,\underline{x}^{(m)} + (D-L)^{-1}\underline{k} \tag{7}$$

and this iterative scheme is called the point Gauss Seidel method. The matrix

$$L = (D-L)^{-1}\,U$$

is called the point Gauss Seidel Matrix.

We now introduce a third basic iterative method which is very closely related to the point Gauss Seidel iterative method. Starting directly with the Gauss Seidel iterative method, we define the components of an auxilary vector $\tilde{\underline{x}}$ from

$$a_{i,i}\,\tilde{x}_i^{(m)} = -\sum_{j=1}^{i-1} a_{i,j}\,x_j^{(m+1)} - \sum_{j=i+1}^{n} a_{i,j}\,x_j^{(m)} + k_i, \quad 1 \leq i \leq n, \; m \geq 0. \tag{8}$$

Then the actual components $x_i^{(m+1)}$ of this iterative method are defined from

$$x_i^{(m+1)} = x_i^{(m)} + \omega\{\tilde{x}_i^{(m+1)} - x_i^{(m)}\} = (1-\omega)x_i^{(m)} + \omega\tilde{x}_i^{(m+1)}. \tag{9}$$

The quantity ω is a relaxation factor, and $x_i^{(m+1)}$ is seen to be a weighted mean of $x_i^{(m)}$ and $\tilde{x}_i^{(m+1)}$ with weights $(1-\omega)$ and ω. When $0 \leq \omega \leq 1$ the weights are non-negative and we shall call this underrelaxation. When $\omega > 1$ we call this overrelaxation. Combining (8) and (9) into a single equation

$$a_{i,i}\, x_i^{(m+1)} = a_{i,i}\, x_i^{(m)} + \omega\{-\sum_{j=1}^{i-1} a_{i,j}\, x_i^{(m+1)} - \sum_{j=i+1}^{m} a_{i,j}\, x_j^{(m)} + k_i - a_{i,i}\, x_i^{(m)}\}.$$

We can now rewrite this in matrix notation as

$$(D-\omega L)\underline{x}^{(m+1)} = \{(1-\omega)D + \omega U\}\underline{x}^{(m)} + \omega\underline{k},\ m \geq 0,$$

and as $(D-\omega L)$ is non-singular we have

$$\underline{x}^{(m+1)} = (D-\omega L)^{-1}\{(1-\omega)\, D + \omega U\}\, \underline{x}^{(m)} + (D-\omega L)^{-1}\, \omega\underline{k},\ m \geq 0,$$

which is the point successive overrelaxation method. The matrix

$$L_\omega = (D-\omega L)^{-1}\{(1-\omega)D + \omega U\}$$

is called the point successive overrelaxation matrix.

II. Convergence of These Methods

Each of the above schemes can be looked at as a scheme of the following form

$$\underline{x}^{(m+1)} = M\,\underline{x}^{(m)} + \underline{g} \tag{10}$$

if $\underline{x}$ is the exact solution of (1) then

$$\underline{x} = M\,\underline{x} + \underline{g} \tag{11}$$

and if the error vector after m iterations is defined by

$$\underline{\varepsilon}^{(m)} = \underline{x}^{(m)} - \underline{x} \tag{12}$$

then subtracting (11) from (10) gives

$$\underline{\varepsilon}^{(m+1)} = M\,\underline{\varepsilon}^{(m)}, \quad m \geq 0. \tag{13}$$

Since (13) holds for all $m \geq 0$ we have

$$\underline{\varepsilon}^{(m)} = M\,\underline{\varepsilon}^{(m-1)} = M^2\,\underline{\varepsilon}^{(m-2)} = \cdots = M^m\,\underline{\varepsilon}^{(0)}$$

and so it is easily seen that

$$\lim_{m\to\infty} \underline{\varepsilon}^{(m)} = 0$$

if and only if

$$\lim_{m\to\infty} M^m = 0, \tag{14}$$

and by Theorem 1.4 page 13, (Varga), (14) is true if the spectral radius $\rho(M) < 1$ where

$$\rho(M) = \max_{1\leq i\leq n} |\lambda_i|$$

where the λ_i's are eigenvalues of the matrix M.

Before presenting a simple test for convergence we need the following definitions:

Definition 1: For $n \geq 2$, an $n \times n$ matrix A is reducible if there exists a permutation† matrix P such that

$$PAP^T = \begin{bmatrix} A_{1,1} & A_{1,2} \\ 0 & A_{2,2} \end{bmatrix}$$

where $A_{1,1}$ is an $r \times r$ submatrix and $A_{2,2}$ is an $(n - r) \times (n - r)$ submatrix, where $1 \leq r < n$. If no such permutation matrix exists, then A is irreducible.

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† A permutation matrix is a square matrix which in each row and each column has some one entry unity, all others zero.

The simple matrix

$$A = \begin{bmatrix} 1 & 1 \\ 0 & 3 \end{bmatrix}$$

is obviously reducible while

$$A = \begin{bmatrix} 1 & 1 \\ 2 & 3 \end{bmatrix}$$

is irreducible.

The geometrical interpretation of irreducibility is quite useful in determining when a matrix A is irreducible. Let $A = (a_{i,j})$ be any n x n matrix, and consider n distinct points $P_1, P_2, \ldots, P_n$, in the plane, which we shall call nodes. For every nonzero entry $a_{i,j}$ of the matrix, we connect the node P_i to the node P_j by a path directed from P_i to P_j (see figure below).

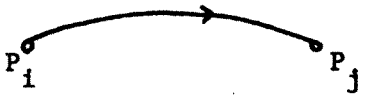


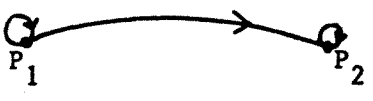
Figure 1

Once this is completed if there exists a path from every node P_i to every node P_j, then the matrix is irreducible.

The graph for

$$A = \begin{bmatrix} 1 & 1 \\ 0 & 3 \end{bmatrix}$$

is



and since there is no path from P_2 to P_1 the matrix is reducible.

Definition 2: An n x n complex matrix $A = (a_{i,j})$ is diagonally dominant if

$$|a_{i,i}| \geq \sum_{\substack{j=1 \\ j \neq i}}^{n} |a_{i,j}| \tag{15}$$

for all $1 \leq i \leq n$. An n x n matrix A is strictly diagonally dominant if strict inequality is valid in (15) for all $1 \leq i \leq n$.

We are now ready to state our convergence criteria:

The matrix M of (10) derived from A of (1) in one of the ways considered above is convegent (i.e. $\rho(M) < 1$) if the matrix A is strictly diagonally dominant or irreducible and diagonally dominant with strick inequality holding in (15) for at least one i. This last property will be called irreducibly diagonally dominant.

Exercise 1: Which of the following matrices are reducible?

a.
$$\begin{bmatrix} -1 & 0 & 3 & 1 \\ 3 & 2 & 1 & -2 \\ 2 & 0 & 0 & 4 \\ 0 & 0 & 1 & -1 \end{bmatrix}$$

b.
$$\begin{bmatrix} -1 & 0 & 3 & 1 \\ 3 & 2 & 1 & -2 \\ 0 & 2 & 0 & 4 \\ 0 & 0 & 1 & -1 \end{bmatrix}$$

c.
$$\begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & -1 \\ 2 & 1 & 0 \end{bmatrix}$$

d.
$$\begin{bmatrix} 1 & 2 & 0 \\ 1 & 1 & 1 \\ 2 & 1 & 0 \end{bmatrix}$$

e.
$$\begin{bmatrix} 2 & -1 & & & & \\ -1 & 2 & -1 & & 0 & \\ & \cdot & \cdot & \cdot & & \\ & & \cdot & \cdot & \cdot & \\ & 0 & & \cdot & 2 & -1 \\ & & & & -1 & 2 \end{bmatrix}$$

f.
$$\begin{bmatrix} 2 & -1 & & & \\ 0 & 2 & \cdot & & 0 \\ & \cdot & \cdot & \cdot & \\ & & \cdot & \cdot & \cdot \\ & 0 & & \cdot & 2 & -1 \\ & & & & 0 & 2 \end{bmatrix}$$

Exercise 2:

a. Derive the central difference equation for

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = -2, \quad (x,y) \in [0,1] \times [0,1]$$

and

$$u(x,y) = 0 \quad \text{on the boundary for} \quad \Delta x = \Delta y = \tfrac{1}{3}.$$

b. Show that this matrix is irreducible and diagonally dominant with strict inequality for at least one row.

c. Derive the point Jacoby Matrix and the point successive overrelaxation matrix.

d. Assuming that the initial error vector $\underline{\varepsilon}^{(0)}$ has all components - 1 show that

$$(D^{-1}B)^m \underline{\varepsilon}^{(0)} = \frac{-1}{2^m} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \quad \text{and} \quad (L_1)^m \underline{\varepsilon}^{(0)} = \frac{-1}{4^m} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}.$$

Exercise 3:

Let A be the 5 x 5 matrix defined by

$$A = \begin{bmatrix} 2 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & 0 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & -1 & 1 \end{bmatrix}$$

Derive its associated point Jacobi matrix, point Gauss Seidel matrix, and point successive overrelaxation matrix.

a. Show that the point Jacoby matrix is non-negative, irreducible, and convergent.

b. Show that the point Gauss Seidel matrix is non-negative, reducible, and convergent.

c. Show that for $0 < \omega < 1$ the point successive overrelaxation matrix is non-negative and convergent.

III. Block Iterative Methods

We shall begin this section by stating a very important theorem about Block Successive Overrelaxation.

Theorem: Let $A = D - E - E^T$ be an n x n Symmetric matrix where D is symmetric and positive definite (i.e. all the eigenvalues of D are positive), and $D - \omega E$ is non-singular for $0 \leq \omega \leq 2$. Then $\rho(L_\omega) < 1$ if and only if A is positive definite and $0 < \omega < 2$.

As an application of this theorem let the n x n matrix A be partitioned into the form

$$A = \begin{bmatrix} A_{1,1} & A_{1,2} & \cdots & A_{1,N} \\ A_{2,1} & A_{2,2} & \cdots & A_{2,N} \\ \vdots & & & \\ A_{N,1} & A_{N,2} & \cdots & A_{N,N} \end{bmatrix}$$

where the diagonal blocks $A_{i,i}$, $1 < i < N$ are all square and nonempty. From this partitioning of the matrix A, we define the matrices

$$D = \begin{bmatrix} A_{1,1} & & \\ & A_{2,2} & 0 \\ & 0 & \ddots \\ & & A_{N,N} \end{bmatrix},$$

$$E = -\begin{bmatrix} 0 & 0 & \cdots & 0 \\ A_{2,1} & 0 & \cdots & 0 \\ \cdot & & & \cdot \\ \cdot & & & \cdot \\ \cdot & & & \cdot \\ A_{N,1} & A_{N,2} & \cdots & 0 \end{bmatrix},$$

$$F = -\begin{bmatrix} 0 & A_{1,2} & \cdots & A_{1,N} \\ 0 & 0 & & A_{2,N} \\ \cdot & & & \cdot \\ \cdot & & & \cdot \\ \cdot & & & \cdot \\ 0 & 0 & \cdots & 0 \end{bmatrix},$$

where the matrices E and F are respectively lower and upper triangular matrices, and $A = D - E - F$. If we assume that A is symmetric, it follows that D is symmetric, and $E^T = F$. If we further assume that D is positive definite, then, from the form of the matrices D and E, it follows that $D - \omega E$ is non-singular for all values of ω. If the column vectors $\underline{x}$ and $\underline{k}$ of the system of linear equations $A\underline{x} = \underline{k}$ are partitioned relative to the partitioning of A then the system of equations can be written as

$$\begin{bmatrix} A_{1,1} & A_{1,2} & \cdots & A_{1,N} \\ A_{2,1} & A_{2,2} & \cdots & A_{2,N} \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ A_{N,1} & A_{N,2} & \cdots & A_{N,N} \end{bmatrix} \begin{bmatrix} \underline{x}_1 \\ \underline{x}_2 \\ \cdot \\ \cdot \\ \cdot \\ \underline{x}_N \end{bmatrix} = \begin{bmatrix} \underline{k}_1 \\ \underline{k}_2 \\ \cdot \\ \cdot \\ \cdot \\ \underline{k}_N \end{bmatrix}$$

or equivalently

$$A_{i,i}\,\underline{x}_i^{(m+1)} = A_{i,i}\,\underline{x}_i^{(m)} + \omega\{-\sum_{j=1}^{i-1} A_{i,j}\,\underline{x}_j^{(m+1)} - \sum_{j=i+1}^{n} A_{i,j}\,\underline{x}_j^{(m)} + k_i - A_{i,i}\,\underline{x}_i^{(m)}\},\ m > 0 \qquad (16)$$

where we have assumed that matrix equations such as $A_{i,i}\,\underline{x}_i = \underline{G}_i$ can be solved directly for $\underline{x}_i$, given $\underline{G}_i$. As is readily verified, this iterative procedure can be written as

$$(D - \omega E)\,\underline{x}^{(m+1)} = \{\omega F + (1-\omega)D\}\,\underline{x}^{(m)} + \omega k \qquad (17)$$

We shall now consider a simple example to illustrate the two most important Block SOR methods (i.e., 1 line and 2 line SOR). If we consider the problem of exercise 2 for the unit square with $\Delta x = \Delta y = 1/5$ (see Figure 2, The numbered points of this correspond to the rows of A below) the linear system of equations which must be solved are

5.
$$\left[\begin{array}{cccc|cccc|cccc|cccc}
4 & -1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-1 & 4 & -1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -1 & 4 & -1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -1 & 4 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\hline
-1 & 0 & 0 & 0 & 4 & -1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 & -1 & 4 & -1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -1 & 0 & 0 & -1 & 4 & -1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -1 & 0 & 0 & -1 & 4 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\
\hline
0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 4 & -1 & 0 & 0 & -1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & -1 & 4 & -1 & 0 & 0 & -1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & -1 & 4 & -1 & 0 & 0 & -1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & -1 & 4 & 0 & 0 & 0 & -1 \\
\hline
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 4 & -1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & -1 & 4 & -1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & -1 & 4 & -1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & -1 & 4
\end{array}\right]
\left[\begin{array}{c} x_1 \\ x_2 \\ x_3 \\ x_4 \\ \hline x_5 \\ x_6 \\ x_7 \\ x_8 \\ \hline x_9 \\ x_{10} \\ x_{11} \\ x_{12} \\ \hline x_{13} \\ x_{14} \\ x_{15} \\ x_{16} \end{array}\right]
=
\left[\begin{array}{c} 2 \\ 2 \\ 2 \\ 2 \\ \hline 2 \\ 2 \\ 2 \\ 2 \\ \hline 2 \\ 2 \\ 2 \\ 2 \\ \hline 2 \\ 2 \\ 2 \\ 2 \end{array}\right]$$

The dashed lines indicate the partitioning for one line block SOR. For this simple problem

$$A_{i,i} = 25 \begin{bmatrix} 4 & -1 & 0 & 0 \\ -1 & 4 & -1 & 0 \\ 0 & -1 & 4 & -1 \\ 0 & 0 & -1 & 4 \end{bmatrix}, \quad 1 \leq i \leq 4$$

$$A_{i,i+1} = 25 \begin{bmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}, \quad 1 \leq i \leq 3$$

$$A_{i-1,i} = 25 \begin{bmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}, \quad 2 \leq i \leq 4$$

and the remaining $A_{i,j}$'s are zero.

We can now directly apply (16) for some choice of ω noticing that we must solve the tridiagonal system of equations directly

$$A_{i,i}\, \underline{x}_i = \underline{G}_i , \quad 1 \leq i \leq 4$$

for each iteration.

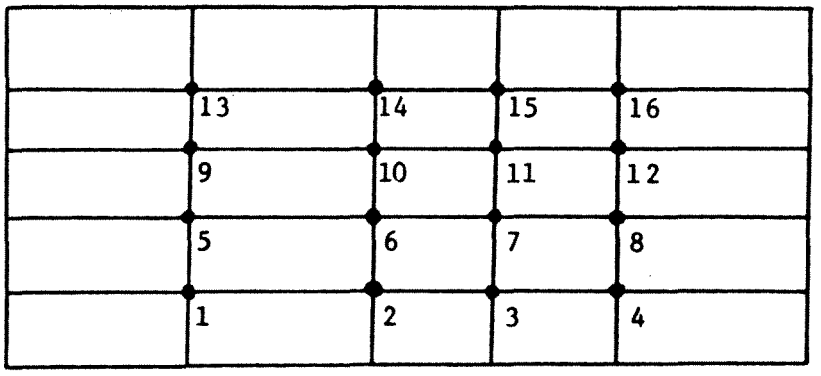


Figure 2

When one uses a 2-line method a renumbering of the points makes this computationally more efficient. See Figure 3 below for the numbering and the matrix A is given by (18) with the dashed lines again indicating the partitioning.

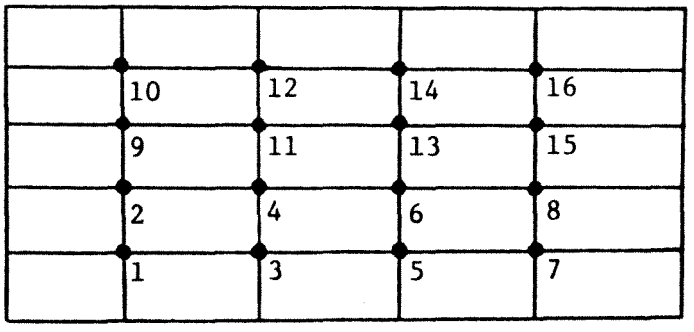


Figure 3

$$A = \left[\begin{array}{cccccccc|cccccccc}
4 & -1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-1 & 4 & 0 & -1 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-1 & 0 & 4 & -1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -1 & -1 & 4 & 0 & -1 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -1 & 0 & 4 & -1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -1 & -1 & 4 & 0 & -1 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -1 & 0 & 4 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -1 & -1 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\
\hline
0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & -1 & -1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 4 & 0 & -1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & -1 & 0 & 4 & -1 & -1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & -1 & 4 & 0 & -1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & -1 & 0 & 4 & -1 & -1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & -1 & 4 & 0 & -1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & -1 & 0 & 4 & -1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & -1 & 4
\end{array}\right]$$

Here again we just use the iterative scheme of (16) with the partitioning of A as given above. Notice that now when solving

$$A_{i,i}\,\underline{x}_i = K_i \qquad 1 \leq i \leq 2\ ,$$

one must invert a five diagonal matrix directly. We could continue in this way defining multiline methods; however, what is gained in improved rates of convergence is usually lost by increased work per iteration and the 2-line Block SOR is generally the best.

Exercise 4:

Let the 4 x 4 matrix A be given by

$$A = \begin{bmatrix} 4 & -1 & 0 & 0 \\ -1 & 4 & -1 & 0 \\ 0 & -1 & 4 & -1 \\ 0 & 0 & -1 & 4 \end{bmatrix}$$

and let $D_1 = 4I$,

$$D_2 = \begin{bmatrix} 4 & -1 & 0 & 0 \\ -1 & 4 & 0 & 0 \\ 0 & 0 & 4 & 0 \\ 0 & 0 & 0 & 4 \end{bmatrix}, \text{ and } D_3 = \begin{bmatrix} 4 & -1 & 0 & 0 \\ -1 & 4 & -1 & 0 \\ 0 & -1 & 4 & 0 \\ 0 & 0 & 0 & 4 \end{bmatrix}$$

and

$$D_4 = \begin{bmatrix} 4 & -1 & 0 & 0 \\ -1 & 4 & 0 & 0 \\ 0 & 0 & 4 & -1 \\ 0 & 0 & -1 & 4 \end{bmatrix}$$

With $A = D_i - F_i$ defining the matrices F_i, $1 \leq i \leq 4$, find $\rho(D_i^{-1} F_i)$ for $1 \leq i \leq 4$.

IV. Rates of Convergence

Let us define the average rate of convergence of a convergent matrix A to be

$$R_\infty (A) = - \ln \rho(A)$$

Now it is easily shown that it takes approximately $1/R_\infty$ iterations to reduce the length of the initial error vector by a factor of e. Therefore, if you wish to meet a convergence criteria ε and if m is chosen so that $e^{-m} < \varepsilon$ then the method will take about (m/R_∞) iterations. As an example if one wants to reduce the relative error to less than 1.0×10^{-4} then the number of iterations required is $(9.2/R_\infty)$. Therefore, if the spectral radius of the iteration matrix is .6, 18 iterations will be required to accomplish this.

A brief comparison of the various Block SOR methods will be constructive for example

$$\frac{R_\infty\ [L_\omega,\ \text{point}]}{R_\infty\ [L_\omega,\ 1\ \text{line}]} \cong \frac{1}{\sqrt{2}}$$

and

$$\frac{R_\infty\ [L_\omega,\ 1\ \text{line}]}{R_\infty\ [L_\omega,\ 2\ \text{line}]} \cong \frac{1}{\sqrt{2}}$$

so 2-line Block SOR is about twice as fast as point SOR.

V. Optimal ω

As one can see from Figure 4 below the rate of convergence of SOR depends critically on the choice of ω. Therefore, this section will

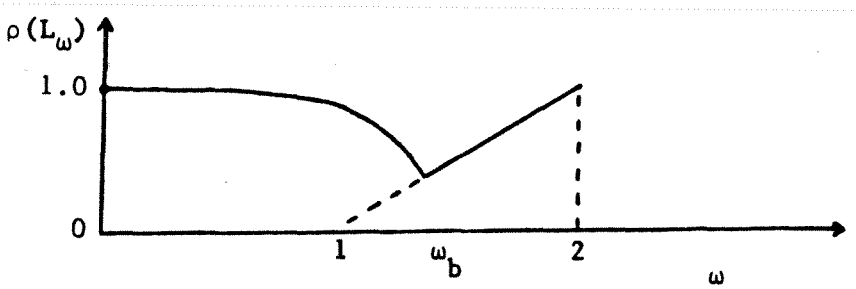


Figure 4

be devoted to selecting an optimum ω.

It is not yet known how to choose an optimum ω for all partitionings of the matrix A; however, for the ones mentioned above the theory has been worked

out. In fact if B is the block Jacoby matrix derived from A (that is if $A = D - F$ then $B = D^{-1} F$) and if there exists a permutation matrix P such that

$$PBP^T = \begin{bmatrix} 0 & B_{1,2} \\ B_{2,1} & 0 \end{bmatrix} \tag{20}$$

then B is called weakly cyclic of index 2 and an optimal ω can be found. Notice that the partitioning of equation (19) is already in the form (20) so P is just the identity matrix I. It is also easily verified that the Block Jacoby matrix derived from the matrix of equation (18) can be put in the form (20) if

$$P = \begin{bmatrix} I & 0 & 0 & 0 \\ 0 & 0 & I & 0 \\ 0 & I & 0 & 0 \\ 0 & 0 & 0 & I \end{bmatrix}$$

where the I's are 4 x 4 identity matrices.

It can also be easily verified that the point Jacoby matrix can be put in the form of (20). Therefore, these important SOR iterative techniques lend themselves to a theoretical determination of ω_b (the optimal ω).

The optimal ω, for the case when the derived block Jacoby matrix B is weakly cyclic of index 2, is given by

$$\omega_b = \frac{2}{1 + \sqrt{1 - \rho^2(B)}}$$

Therefore, all one needs to know if the spectral radius of B and one can determine ω_b. Moreover

$$\rho(\mathcal{L}_1) = \rho^2(B)$$

so a determination of $\rho(\mathcal{L}_1)$ is all that is necessary. This can be done in the following simple way. Let $\underline{x}^{(0)}$ be any vector with positive components; then

defining $\underline{x}^{(m+1)}$ through

$$(D-L)\underline{x}^{(m+1)} = U\underline{x}^{(m)} \qquad m \geq 0$$

where the matrices D, L, and U are chosen as above, that is so that $\mathcal{L}_1 = (D-L)^{-1} U$ (see sections I - III). It can now be easily shown that if the $x_i^{(m)}$'s are the components of the vector $\underline{x}^{(m)}$ then the $x_i^{(m)}$'s > 0 for all $1 \leq i \leq n$ and $m \geq 0$. Because of this, we can define the positive numbers

$$\underline{\lambda}_m \equiv \underset{1\leq i\leq n}{\text{Min}} \left(\frac{x_i^{(m+1)}}{x_i^{(m)}}\right), \quad \overline{\lambda}_m \equiv \underset{1\leq i\leq n}{\text{Max}} \left(\frac{x_i^{(m+1)}}{x_i^{(m)}}\right), \quad m \geq 0$$

and it can be shown that

$$\underline{\lambda}_m \leq \underline{\lambda}_{m+1} \leq \rho(\mathcal{L}_1) \leq \overline{\lambda}_{m+1} \leq \overline{\lambda}_m, \qquad m \geq 0$$

Therefore

$$\lim_{m\to\infty} \underline{\lambda}_m = \lim_{m\to\infty} \overline{\lambda}_m = \rho(\mathcal{L}_1).$$

Consequently if one has programmed the solution of

$$A\,\underline{x} = \underline{k}$$

using Block SOR all one must do to find $\rho(\mathcal{L}_1)$ is to choose $\omega = 1$, $\underline{k} \equiv 0$, and $\underline{x}^{(0)} \equiv \underline{e}$, where $\underline{e}$ is a vector with all ones as components in this program and calculate $\underline{\lambda}_m$ and $\underline{\lambda}^m$ from the successive iterates until a satisfactory value of $\rho(\mathcal{L}_1)$ is obtained. For other ways to calculate an optimal ω see Wachspress (pp 105).

Exercise 5

Given the matrix

$$A = \begin{bmatrix} 2 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 2 \end{bmatrix}$$

fill in the entries in the table below by using the method described above. As an initial guess choose $\underline{x}^{(0)} = \underline{e}$.

m	$\underline{\lambda}_m$	$\bar{\lambda}_m$	$\underline{\omega}_m$	$\bar{\omega}_m$
0				
1				
2				
3				

$$\underline{\omega}_m = \frac{2}{1 + \sqrt{1 - \underline{\lambda}_m}}$$

and

$$\bar{\omega}_m = \frac{2}{1 + \sqrt{1 - \bar{\lambda}_m}}$$

Exercise 6

For the partitioning of A given below repeat exercise 5.

$$A = \left[\begin{array}{cc|cc} 2 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ \hline 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 2 \end{array}\right].$$

VI. Cyclic Chebyshev Method

By means of Chebyshev polynomials one can improve the convergence rates of the iterative schemes defined above. This is quite effective if the derived block Jacoby matrix is weakly cyclic of index 2 (see (20)).

We wish to solve the matrix problem

$$A\,\underline{x} = \underline{k}$$

and we shall assume that A is symmetric and positive definite and that if

$$A = D - C$$

then D is symmetric and positive definite and that $D^{-1}C$ is of the form (20). Obviously if there exists a P such that

$$PD^{-1}CP^{T} = \begin{bmatrix} 0 & B_{1,2} \\ B_{2,1} & 0 \end{bmatrix}$$

then

$$M \equiv PD^{-\frac{1}{2}}CD^{-\frac{1}{2}}P^{T} = \begin{bmatrix} 0 & F \\ F^{T} & 0 \end{bmatrix} . \qquad (21)$$

Once we have our problem in the form (22) the cyclic Chebyshev semi-iterative method is defined for the problem

$$\begin{bmatrix} \underline{x}_1 \\ \underline{x}_2 \end{bmatrix} = \begin{bmatrix} 0 & F \\ F^{T} & 0 \end{bmatrix} \begin{bmatrix} \underline{x}_1 \\ \underline{x}_2 \end{bmatrix} + \begin{bmatrix} \underline{g}_1 \\ \underline{g}_2 \end{bmatrix}$$

by

$$\underline{x}_1^{(2m+1)} = \omega_{2m+1}\{F\,\underline{x}_2^{(2m)} + \underline{g}_1 - \underline{x}_1^{(2m-1)}\} + \underline{x}_1^{(2m-1)}, \quad m \geq 1$$

$$\underline{x}_2^{(2m+2)} = \omega_{2m+2}\{F^{T}\,\underline{x}_1^{(2m+1)} + \underline{g}_2 - \underline{x}_2^{(2m)}\} + x_2^{(2m)}, \quad m \geq 0$$

where $\underline{x}_1^{(1)} = F\underline{x}_2^{(0)} + \underline{g}_1$. The ω_i's are given by

$$\omega_1 = 1$$

$$\omega_{i+1} = \frac{1}{1 - (\frac{\rho^2(B)\omega_i}{4})}, \quad i \geq 2.$$

This is illustrated schematically by

$$\begin{bmatrix} \underline{x}_1^{(0)} \\ \underline{x}_2^{(0)} \end{bmatrix} \nearrow \begin{bmatrix} \underline{x}_1^{(1)} \\ \underline{x}_2^{(1)} \end{bmatrix} \searrow \begin{bmatrix} \underline{x}_1^{(2)} \\ \underline{x}_2^{(2)} \end{bmatrix} \nearrow \begin{bmatrix} \underline{x}_1^{(3)} \\ \underline{x}_2^{(3)} \end{bmatrix} \searrow$$

V. Variational Methods

Recently, the use of variational methods to derive difference approximations of high order accuracy has become very popular. This section illustrates how to formally use a Galerkin-type process for deriving high order approximations of a simple parabolic partial differential equation.

In the region $R \equiv \{ (x,t)/0 < x < 1,\ 0 < t < \infty \}$, we seek a solution of the equation

$$L\ [u] \equiv \frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} + \lambda \frac{\partial u}{\partial x} = 0, \quad (x,t)\varepsilon R, \qquad \text{(22)}$$

subject to the initial-boundary conditions

$$u(x,0) = 0,\ 0 < x \leq 1$$

and

$$u(0,t) = 1.0,\ \frac{\partial u}{\partial x}(1,t) = 0,\ t > 0. \qquad \text{(23)}$$

Our approach is to "discretize" first only the space variables, leaving the time variable continuous, by means of a Galerkin-type process. The resulting system of ordinary differential equations is then discretized in the time variable to obtain a discrete approximation to (22), (23) which may be solved on a digital computer. In particular, we discuss here the use of high-order polynomials and/or piecewise-polynomials in the Galerkin process for obtaining high-order semi-discretizations.

Let S denote the class of all real-valued, piecewise continuously differentiable functions, $w(x)$, on $[0,1]$ such that $w(0) = 0$, $(\frac{dw}{dx})_{x=1} = 0$. Let S_m be a m-dimensional subspace of S spanned by the m basis functions $\{w_i(x)\}_{i=1}^{m}$. We seek an approximation to the solution of (22), (23) in the form

$$u_m(x,t) = \sum_{k=1}^{m} C_{m,k}(t) w_k(x) + w_0(x)$$

. . . . . (24)

where the coefficients $C_{m,k}(t)$ are determined by the condition that $L[u_m]$ be orthogonal (in L_2) to S_m for all $t > 0$, and that u_m satisfy the boundary conditions (23), i.e.,

$$\int_0^1 \left\{ L\left[u_m\right] \right\} w_k dx = 0, k=1,2,\ldots,m, \; t > 0$$

..... (25)

and

$$\begin{cases} w_0(0) = 1.0, \; \dfrac{dw_0(1)}{dx} = 0, \\ \displaystyle\sum_{k=1}^{m} C_{m,k}(t) \left(\frac{dw_k(x)}{dx} \right)_{x=1} = 0, \\ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \end{cases} \quad (26)$$

and the coefficients $C_{m,k}(0)$ are uniquely determined such that

$$\left|\left| w_0(x) + \sum_{k=1}^{m} C_{m,k}(0) w_k(x) \right|\right|_{L^2} =$$

$$\underset{a_i}{\text{MIN}} \left|\left| w_0(x) + \sum_{k=1}^{m} a_k w_k(x) \right|\right|_{L^2}. \quad \ldots\ldots (27)$$

Equation (25) takes the form

$$\int_0^1 \sum_{j=1}^{m} \left\{ C'_{m,j}(t)w_j(x) - C_{m,j}(t)w''_j(x) + \lambda C_{m,j}(t)w'_j(x) \right\} w_k(x)dx = \int_0^1 w''_0(x)w_k(x)dx - \lambda \int_0^1 w'_0(x)w_k(x)dx$$

$k=1,2,\ldots m$ or after integrating by parts and noting that

$$w_k(0) = \frac{dw_k(1)}{dx} = 0, \quad k=1,2,\ldots,m,$$

we have

$$\sum_{j=1}^{m} C'_{m,j}(t) \int_0^1 w_j(x)w_k(x)dx + \sum_{j=1}^{m} C_{m,j}(t) \int_0^1 w'_j(x)w'_k(x)dx + \lambda \sum_{j=1}^{m} C_{m,j}(t) \int_0^1 w'_j(x)w_k(x)dx = - \int_0^1 w'_0(x)(\lambda w_k(x) + w'_k(x))dx, \quad k=1,2,\ldots m$$

..... (28)

or

$$\begin{bmatrix} \int_0^1 w_1 w_1 dx & \cdots & \int_0^1 w_m w_1 dx \\ \vdots & & \vdots \\ \int_0^1 w_1 w_m dx & \cdots & \int_0^1 w_m w_m dx \end{bmatrix} \cdot \begin{bmatrix} C'_{m,1}(t) \\ \vdots \\ C'_{m,m}(t) \end{bmatrix}$$

$$+ \begin{bmatrix} \int_0^1 (w_1' w_1' + \lambda w_1' w_1) dx & \cdots & \int_0^1 (w_m' w_1' + \lambda w_m' w_1) dx \\ \vdots & & \vdots \\ \int_0^1 (w_1' w_m' + \lambda w_1' w_m) dx & \cdots & \int_0^1 (w_m' w_m' + \lambda w_m' w_m) dx \end{bmatrix} \cdot \begin{bmatrix} C_{m,1}(t) \\ \vdots \\ C_{m,m}(t) \end{bmatrix} =$$

$$\begin{bmatrix} -\int_0^1 w_0'(x) \, (\lambda w_1(x) + w_1'(x)) dx \\ \vdots \\ -\int_0^1 w_0'(x) \, (\lambda w_m(x) + w_m'(x)) dx \end{bmatrix} \quad \ldots (29)$$

The following example using chapeau base functions should illustrate the use of equation (29) to derive a semi-discretization of (22), (23).

The unit interval is divided into m mesh blocks of length h, and the chapeau basis functions are defined to be

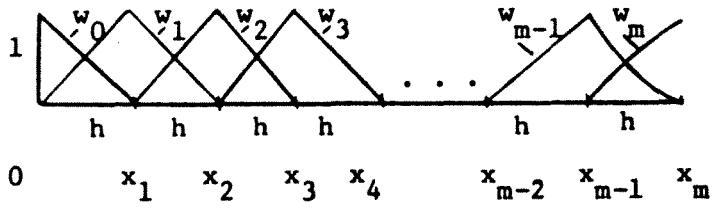
$$w_0(x)\begin{cases} = -(x-h)/h & , \ 0<x<h \\ = 0 & , \ h\leq x\leq 1 \end{cases}$$

$$w_i(x)\begin{cases} = (x-(i-1)h)/h & , \ (i-1)h\leq x\leq ih \\ = ((i+1)h-x)/h & , \ ih\leq x\leq (i+1)h \\ & \quad i = 1,2,\ldots, m-2 \\ = 0 & \quad \text{elsewhere} \end{cases}$$

$$w_{m-1}(x)\begin{cases} = (x-(m-2)h)/h & , \ (m-2)h\leq x\leq (m-1)h \\ = (mh-x)^2/h^2 & , \ (m-1)h\leq x\leq mh=1 \\ = 0 & \quad 0\leq x\leq (m-2)h \end{cases}$$

$$w_m(x)\begin{cases} = -((x-mh)^2-h^2)/h^2, & (m-1)h\leq x\leq mh=1, \\ = 0 & \quad 0\leq x\leq (m-1)h, \end{cases}$$

which is illustrated below



We see, by performing the simple integrations in (29) that this leads to the following matrix differential equation

$$B\frac{d\underline{C}_m}{dt} = -A\,\underline{C}_m + \underline{S}, \quad \ldots\ldots (30)$$

where

$$B=h\begin{bmatrix} \frac{2}{3} & \frac{1}{6} & & & & \\ \frac{1}{6} & \frac{2}{3} & \frac{1}{6} & & & \\ & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} & & \\ & & \frac{1}{6} & \frac{8}{15} & \frac{2}{15} & \\ & & & \frac{2}{15} & \frac{8}{15} & \end{bmatrix}; \qquad \ldots\ldots (31)$$

$$A=\frac{1}{h}\begin{bmatrix} 2 & -(1-\alpha) & & & & \\ -(1+\alpha) & 2 & -(1-\alpha) & & & \\ & -(1+\alpha) & 2 & -(1-\alpha) & & \\ & & -(1+\alpha) & \frac{7}{3} & -(\frac{4}{3}-\alpha) & \\ & & & -(\frac{4}{3}+\alpha) & (\frac{4}{3}+\alpha) & \end{bmatrix} \qquad \ldots\ldots (32)$$

$$\underline{S}=\frac{1}{h}\begin{bmatrix} (1+\alpha) \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \text{ and } \alpha = \frac{\lambda h}{2}. \qquad \ldots\ldots (33)$$

The other base functions used in the text are defined as follows:

Smooth Cubics

If the unit interval is divided into $\frac{m}{2}$ mesh blocks of length h, the smooth cubic base functions are given by

$$w_0(x) \begin{cases} = (2x+h)(x-h)^2/h^3, & 0 \le x \le h \\ = 0, & h \le x \le 1 \end{cases}$$

$$w_1(x) \begin{cases} = x(x-h)^2/h^2, & 0 \le x \le h \\ = 0, & h \le x \le 1 \end{cases}$$

$$w_{2i}(x) \begin{cases} = (-2x+(1+2i)h)(x-(i-1)h)^2/h^3, \\ \quad (i-1)h \le x \le ih \\ = (2x+(1-2i)h)(x-(i+1)h)^2/h^3, \\ \quad ih \le x \le (i+1)h \\ \quad i=1,2,\ldots,\frac{m}{2}-1 \\ = 0 \quad \text{elsewhere} \end{cases}$$

$$w_{2i+1}(x) \begin{cases} = (x-ih)(x-(i-1)h)^2/h^2, \\ \quad (i-1)h \le x \le ih \\ = (x-ih)(x-(i+1)h)^2/h^2, \\ \quad ih \le x \le (i+1)h \\ \quad i=1,2,\ldots,\frac{m}{2}-1 \\ = 0 \quad \text{elsewhere} \end{cases}$$

$$w_m(x) \begin{cases} = (-2x+(1+m)h)(x-(\frac{m}{2}-1)h)^2/h^3, \\ \quad (\frac{m}{2}-1)h \le x \le 1 \\ = 0 \quad \text{elsewhere} \end{cases}$$

Non-Smooth Quintics

If the unit interval is divided into m equally spaced blocks of length h, the 5m+1 basis functions will be the following

$$w_0(x)\begin{cases} = (h-x)/h & , \ 0 \le x \le h \\ = 0 & , \ h \le x \le 1 \end{cases}$$

$$\left.\begin{aligned} w_{5(i-1)+1}(x)&\begin{cases} = (x-(i-1)h)(x-ih), \\ \quad (i-1)h \le x \le ih \\ = \quad 0 \qquad \text{elsewhere} \end{cases} \\ w_{5(i-1)+2}(x)&\begin{cases} = (x-(i-1)h)(x-ih)x, \\ \quad (i-1)h \le x \le ih \\ = \quad 0 \qquad \text{elsewhere} \end{cases} \\ w_{5(i-1)+3}(x)&\begin{cases} = (x-(i-1)h)(x-ih)x^2, \\ \quad (i-1)h \le x \le ih \\ = \quad 0 \qquad \text{elsewhere} \end{cases} \\ w_{5(i-1)+4}(x)&\begin{cases} = (x-(i-1)h)(x-ih)x^3, \\ \quad (i-1)h \le x \le ih \\ = \quad 0 \qquad \text{elsewhere} \end{cases} \end{aligned}\right\} 1 \le i \le m$$

$$w_{5i}(x)\begin{cases} = (x-(i-1)h)/h, \\ \quad (i-1)h \le x \le ih \\ = ((i+1)h-x)/h, \\ \quad ih \le x \le (i+1)h \\ = \quad 0 \qquad \text{elsewhere} \end{cases} 1 \le i \le m-1$$

$$w_{5m}(x)\begin{cases} = (x-(m-1)h)/h, \\ \quad (m-1)h \le x \le 1 \\ = \quad 0 \qquad \text{elsewhere} \end{cases}$$

Exercises 7

Derive the matrices A and B and the vector S of equation (30) as in (31), (32), and (33) for the smooth cubic basis functions.

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