*Int. J. Multiphase Flow*, Vol. 1, pp. 817–844. Pergamon/Elsevier, 1975. Printed in Great Britain.

# TREATMENT OF NONLINEAR TERMS IN THE NUMERICAL SOLUTION OF PARTIAL DIFFERENTIAL EQUATIONS FOR MULTIPHASE FLOW IN POROUS MEDIA

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(*Received* 9 *November* 1973)

**Abstract**—Simultaneous flow of two or three immiscible fluids in porous media is modelled by a system of coupled, nonlinear partial differential equations. These equations are reduced to a system of nonlinear algebraic equations through the use of finite-difference approximations for derivatives. Several types of nonlinearities requiring careful analysis exist in this model. Here, we present a systematic study of all available, and some new, methods for the treatment of nonlinearities in this model. It is believed that the solution techniques presented here may also prove useful for other strongly nonlinear partial differential equations.

## INTRODUCTION

The solution of the equations for fluid flow in porous media is of great practical importance. In particular, the theory of multiphase flow is the basis of petroleum reservoir engineering (Muskat 1937; Collins 1961). During the past decade, the numerical solution of problems of multiphase flow in reservoirs has evolved into a new discipline called "reservoir simulation" which provides the engineer with the means of simulating the behaviour of a reservoir on a digital computer.

The equations describing multiphase flow of immiscible fluids in porous media are a set of strongly nonlinear, coupled partial differential equations. As such, they cannot be usually solved satisfactorily using standard numerical techniques. Consequently, a number of special, almost exclusively finite-difference, techniques have been suggested for the treatment of numerical problems of stability and truncation errors associated with various nonlinearities (Todd *et al.* 1972; Welge & Weber 1964; Blair & Weinang 1969; MacDonald & Coats 1970; Letkeman & Ridings 1970; Sonier *et al.* 1971; Nolen & Berry 1972; Robinson 1971; Coats 1968; McCreary 1971). Proper treatment of nonlinearities is extremely important since practical applications often require the use of finite-difference grids with a large number of grid points. The use of a method with limited stability would necessitate selection of small time steps, resulting in prohibitively large computer time. Also, the use of a method which gives large truncation errors requires a large number of grid points requiring large computer time in order to attain a given accuracy.

Although significant developments in the handling of these problems have been reported by earlier investigators, a direct comparison of their results is often impossible because

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various investigators have tested their methods on different problems. The objective of this work is to investigate and compare systematically all available methods, as well as some new methods, for the treatment of all essential nonlinearities in the finite-difference model of multiphase flow. In particular, Newton's method is treated in detail. The analysis presented in this paper is restricted to one-dimensional, two-phase flow. The results of this study were successfully applied to the solution of two- and three-phase problems in two dimensions; in particular, to the solution of single-well (coning) problems which are among the most difficult multiphase flow problems (Settari & Aziz 1973). The results of the two-dimensional studies have been reported (Settari & Aziz 1973; Aziz *et al.* 1973; Settari 1973).

While the topic dealt with in this work has received attention mostly in the petroleum literature, it is believed that the solution techniques presented here may prove useful for a wide variety of strongly nonlinear time-dependent equations encountered in other fields of engineering, including chemical engineering.

## 1. FORMULATION OF THE PROBLEM AND THE FINITE-DIFFERENCE EQUATIONS

Many actual situations of multiphase flow in porous media can be approximated by a mathematical model of the flow of two immiscible fluids with capillary forces and interphase mass transfer. Typically, only the solubility of the non-wetting phase in the wetting phase is significant for the mass transfer, and under the assumption of thermodynamic equilibrium it can be described by the solution ratio $R_s$ as a function of the pressure of the wetting phase. This model is known as the $\beta$-model (Douglas *et al.* 1959) and the equations are obtained by the combination of Darcy's law for every phase with the mass conservation equation for the two components. The result is (see, for example, Douglas *et al.* 1959; Craft & Hawkins 1959; for the derivation):

$$\frac{\partial}{\partial x}\left[\lambda_w\left(\frac{\partial p_w}{\partial x} - \gamma_w \frac{\mathrm{d}z}{\mathrm{d}x}\right)\right] = \phi \frac{\partial}{\partial t}\left(\frac{S_w}{B_w}\right) + q_w \qquad [1a]$$

$$\lambda_w\left(\frac{\partial p_w}{\partial x} - \gamma_w \frac{\mathrm{d}z}{\mathrm{d}x}\right)\frac{\partial R_s}{\partial x} + \frac{\partial}{\partial x}\left[\lambda_n\left(\frac{\partial p_n}{\partial x} - \gamma_n \frac{\mathrm{d}z}{\mathrm{d}x}\right)\right] = \phi\left[\frac{S_w}{B_w}\frac{\partial R_s}{\partial t} - \frac{\partial}{\partial t}\left(\frac{1 - S_w}{B_n}\right)\right] + q_n \qquad [1b]$$

where

$$\lambda_l = \frac{k k_{rl}}{\mu_l B_l} \qquad l = w, n. \qquad [2]$$

In the above equations, $x$ is the space coordinate and $z$ is another coordinate, vertical and positive downwards. Therefore $\mathrm{d}z/\mathrm{d}x = 0$ for horizontal $x$ and $\dfrac{\mathrm{d}z}{\mathrm{d}x} = -1$ for vertical $x$ oriented upwards. The pressures of wetting and non-wetting phases are denoted by $p_w$ and $p_n$ and they are related by capillary pressure, which is a function of the wetting phase saturations $S_w$:

$$P_c = p_n - p_w = f(S_w) \qquad [3]$$

$B_l$ are the formation volume factors (sometimes referred to as $\beta$-factors) accounting for

the compressibility of fluids, $\gamma_l = g\rho_l$, where $\rho_l$ is the density of phase $l$, and $\mu_l$ is the viscosity of phase $l$. All these quantities are functions of pressure; densities are related to the formation volume factors and $R_s$ by:

$$\rho_w = \frac{1}{B_w}(\rho_{wSTC} + R_s\rho_{nSTC}) \qquad [4a]$$

$$\rho_n = \frac{1}{B_n}\rho_{nSTC} \qquad [4b]$$

where the subscript $STC$ denotes standard conditions at which we assume $B_w = B_n = 1$ and $R_s = 0$. Equations [4] can serve as a definition of $B_l$; an alternative, more direct, definition is given in the nomenclature. Finally, $k$ and $\phi$ are the absolute permeability and porosity of the medium and $k_{rw}$ and $k_{rn}$ are the relative permeabilities of wetting and non-wetting phases respectively. The relative permeabilities are empirical functions of $S_w$.

If the function $P_c$ has an inverse, [3] may be used to eliminate $S_w$ from [1] and we obtain two coupled equations in two variables $p_w$, $p_n$.

The two typical examples of petroleum reservoirs that can be described by the model of [1] are gas–oil reservoirs and oil–water reservoirs. In the gas–oil reservoir, gas is the non-wetting, and oil the wetting, phase. Gas is soluble in oil; the solubility is constant if the pressure is above the bubble point and decreases with pressure below this point. Therefore, decrease in pressure causes liberation of solution gas. This gas migrates (percolates) to the top of the reservoir due to density differences between oil and gas and this phenomenon is called "gas percolation". Although the capillary pressures in a gas–oil system are usually small and may be neglected, the density changes due to compressibility and solubility are significant and cannot be neglected. In an oil–water reservoir, usually water is the wetting, and oil the non-wetting, phase. Solubility can be neglected in this case, i.e. $R_s = 0$ and compressibilities of fluids are usually small. On the other hand, capillary pressures may have significant values in many cases. In a special case of incompressible flow ($B_w = B_n = 1$) of fluids of constant viscosities in a homogeneous horizontal reservoir ($k$ = constant, $\phi$ = constant) and with zero capillary pressures, the problem has an analytical solution (Buckley–Leverett problem, see, for example, Collins 1961; Craft & Hawkins 1959). Even in the case of non-zero capillary pressure this problem may be referred to as the Buckley–Leverett problem and its description is obtained by the following simplification of [1]

$$\frac{k}{\mu_w}\frac{\partial}{\partial x}\left(k_{rw}\frac{\partial p_w}{\partial x}\right) = \phi\frac{\partial S_w}{\partial t} + q_w \qquad [5a]$$

$$\frac{k}{\mu_n}\frac{\partial}{\partial x}\left(k_{rn}\frac{\partial p_n}{\partial x}\right) = -\phi\frac{\partial S_w}{\partial t} + q_n. \qquad [5b]$$

The principal difficulty in solving [1] or [5] rests in the coefficients $k_{rl}$ on the left-hand side, which are strong functions of saturation, which, in turn, is a function of the difference of pressures. This difference is usually orders of magnitude lower than the pressures themselves. Additional difficulties arise from the non-linearity of the capillary pressure

function [2] and, in the case of oil–gas flow, from the gas percolation which is due to density differences. The viscosity of the gas phase is usually small compared to the liquid phase viscosity and this causes additional problems.

We will now discuss a finite-difference approximation of [1]. For the sake of clarity, we will assume a regular grid system; for the treatment of an irregular grid, see Settari & Aziz (1972). If the solution is sought for $x \in (0, L)$ and the total number of grid points is $N$ ($x_1 = 0, \ldots, x_N = L$), then $\Delta x = x_{i+1} - x_i = L/(N-1)$. The diffusion type terms on the left-hand side will be approximated at $x_i$ by the standard three-point formula while the first-order terms on the left-hand side of [1b] will be approximated by an average of approximations at $i + \frac{1}{2}$ and $i - \frac{1}{2}$. The right-hand side is approximated by a backward difference operator which satisfies the conservation of mass over a time step. (Detailed discussion of reasons for this choice of the finite-difference operators is given in Settari (1973).) We denote $\Delta z_{i+1/2} = z(x_{i+1}) - z(x_i)$ and define

$$\nabla\Phi_{l_{i+1/2}} = p_{l_{i+1}} - p_{l_i} - \gamma_{l_{i-1/2}}\Delta z. \tag{6}$$

The discretization of [1] can be written as

$$[T^w_{i+1/2}\nabla\Phi_{w_{i+1/2}} - T^w_{i-1/2}\nabla\Phi_{w_{i-1/2}}]^{n+1} = \phi_i\frac{\Delta x}{\Delta t}\left[\left(\frac{S_w}{B_w}\right)^{n+1} - \left(\frac{S_w}{B_w}\right)^n\right]_i + q_{w_i} \tag{7a}$$

$$\begin{aligned}&\tfrac{1}{2}[(R_{s_{i+1}} - R_{s_i})T^w_{i+1/2}\nabla\Phi_{w_{i+1/2}} + (R_{s_i} - R_{s_{i-1}})T^w_{i-1/2}\nabla\Phi_{w_{i-1/2}}]^{n+1}\\ &\quad + [T^n_{i+1/2}\nabla\Phi_{n_{i+1/2}} - T^n_{i-1/2}\nabla\Phi_{n_{i-1/2}}]^{n+1}\\ &= \phi_i\frac{\Delta x}{\Delta t}\left[\left(\frac{S_w}{B_w}\right)^n(R_s^{n+1} - R_s^n) + \left(\frac{S_n}{B_n}\right)^{n+1} - \left(\frac{S_n}{B_n}\right)^n\right]_i + q_{n_i}\end{aligned} \tag{7b}$$

where

$$S_n = 1 - S_w$$

and

$$T^l_{i+1/2} = \frac{1}{\Delta x}\left(\frac{kk_{rl}}{\mu_l B_l}\right)_{i+1/2} = \frac{\lambda_{l_{i+1/2}}}{\Delta x}, \qquad l = w, n \tag{8}$$

are the discrete transmissibilities.

The right-hand side of [7] must be expressed in terms of pressures. Using relation [3], we can define a "derivative" of saturation

$$S'_w = \frac{S_w^{n+1} - S_w^n}{P_c(S_w^{n+1}) - P_c(S_w^n)}. \tag{9}$$

Similarly, we can define "derivatives" of $1/B_l$ and $R_s$ by

$$\left(\frac{1}{B_l}\right)' = \left[\frac{1}{B_l(P_l^{n+1})} - \frac{1}{B_l(P^n)}\right] \Big/ [p_l^{n+1} - p_l^n], \quad l = w, n \tag{10}$$

and

$$R'_s = [R_s(p_w^{n+1}) - R_s(p_w^n)]/[p_w^{n+1} - p_w^n]. \tag{11}$$

Then the right-hand side terms may be expressed as

$$\left(\frac{S_w}{B_w}\right)^{n+1} - \left(\frac{S_w}{B_w}\right)^{n} = \left[S_w^n\left(\frac{1}{B_w}\right)'(p_w^{n+1} - p_w^n)\right] + \left[\frac{1}{B_w^{n+1}}S_w'(p_c^{n+1} - p_c^n)\right] \quad [12a]$$

$$\left(\frac{S_n}{B_n}\right)^{n+1} - \left(\frac{S_n}{B_n}\right)^{n} = \left[(1 - S_w^n)\left(\frac{1}{B_n}\right)'(p_n^{n+1} - p_n^n)\right] - \left[\frac{1}{B_n^{n+1}}S_w'(p_c^{n+1} - p_c^n)\right] \quad [12b]$$

$$\left(\frac{S_n}{B_n}\right)^{n}(R_s^{n+1} - R_s^n) = \left(\frac{S_n}{B_n}\right)^{n} R_s'(p_w^{n+1} - p_w^n). \quad [12c]$$

Substitution of [12] into [7] gives the final discretization used in this work. It may be noted that the equality in [12] is only valid if the quantities $S_w'$ etc. are defined as chords by [9]–[11]. Consequently, these quantities represent implicit coefficients.

The above set of finite difference equations can be expressed in a convenient matrix form by means of a suitable ordering of unknowns. Let us define the vector $\mathbf{P}$ as

$$\mathbf{P} = (p_{w_1}, p_{n_1}, \ldots, p_{w_i}, p_{n_i}, \ldots, p_{w_N}, p_{n_N})^T \quad [13]$$

Then the set of all difference equations can be written as:

$$T^{n+1}\mathbf{P}^{n+1} - D^{n+1}(\mathbf{P}^{n+1} - \mathbf{P}^n) + \mathbf{G}^{n+1} = \mathbf{Q} \quad [14]$$

where $T$ is the flow coefficient (transmissibility) matrix composed of coefficients [8], $D$ is the accumulation matrix composed of coefficients of expansions [12], $\mathbf{G}$ is the vector of gravity terms (containing all $T^l\gamma_l\Delta z$ terms) and $\mathbf{Q}$ is the source vector which also accounts for the flow across boundaries at $x = 0$ and $x = L$ (specified production or injection rate). According to the ordering [13], all matrices and vectors have block structure with $2 \times 2$ and $2 \times 1$ blocks, respectively; the elements within a block have the same row and column subscripts. It is easy to see that the matrix $T$ is block-tridiagonal and matrix $D$ block-diagonal.

Equation [14] can be written in a more convenient residual form. We define a residual $\mathbf{R}_m^k$ corresponding to a vector $\mathbf{P}^k$ by

$$\mathbf{R}_m^k = T^m\mathbf{P}^k - D^m(\mathbf{P}^k - \mathbf{P}^n) + \mathbf{G}^m. \quad [15]$$

The subscript $m$ in the previous definition denotes that the elements of matrices $T$, $D$ and vector $\mathbf{G}$ are evaluated as functions of a vector $\mathbf{P}^m$ which may be generally different from $\mathbf{P}^k$. Using the previous definition, we can rewrite [14] in the final form

$$(T^{n+1} - D^{n+1})(\mathbf{P}^{n+1} - \mathbf{P}^n) = -\mathbf{R}_{n+1}^n + \mathbf{Q}. \quad [16]$$

Equation [16] represents a set of $2N$ nonlinear algebraic equations. The solution of this set is the main concern of this study.

## 2. CLASSIFICATION OF NONLINEARITIES AND TEST PROBLEMS

The nonlinearities in [16] appear in matrices $T$ and $D$ and implicitly also in the vector $\mathbf{R}$. A typical element of matrix $T$[8] will be denoted for further discussion as:

$$T^l = T^l[f_1(p_l), f_2(S_w)] = GCf_1f_2 \quad [17]$$

where $GC$ is the constant part of the transmissibility, $f_1 = 1/\mu B$, and $f_2 = k_{rl}$. Functions $f_1$ and $f_2$ may be approximated on different time levels and in different ways between grid points, generally as:

$$T_{i+1/2}^{l^{n+1}} \approx T^l[f_{1i_1}^{k_1}, f_{2i_2}^{k_2}]$$

where

$$i \leq i_1, i_2 \leq i+1, \qquad n \leq k_1, k_2 \leq n+1.$$

The problem of approximating the $i + 1/2$ level in the space coordinate is referred to as the "weighting" problem. The problem of approximation of the $n + 1$ level in time is the problem of solution or linearization of the set of nonlinear equations.

A similar situation exists in approximating the matrix $D$.

All nonlinearities in [16] may be divided into two groups:

*(1) Weak nonlinearities*

All variables that are functions of the pressure of one phase only can be considered weak nonlinearities. These include $B_l^{n+1}$, $(1/B_l)'$, $R_s'$, $\gamma_l^{n+1}$ and $\mu_l^{n+1}$. An example of actual pressure dependent functions is presented by figure 1(a) and (1b) (these data are from McCreary (1971)). The effect of weak nonlinearities depends on the degree of pressure changes and disappears in problems in which pressure remains constant. It is generally satisfactory even in the case of varying pressure to evaluate pressure dependent functions one step behind, i.e. as a function of $p_l^n$ instead of $p_l^{n+1}$. Also, the approximation of the $i + 1/2$ level is not critical; in this work, we have used

$$f_{1i+1/2} \approx \tfrac{1}{2}(f_{1i} + f_{1i+1}).$$

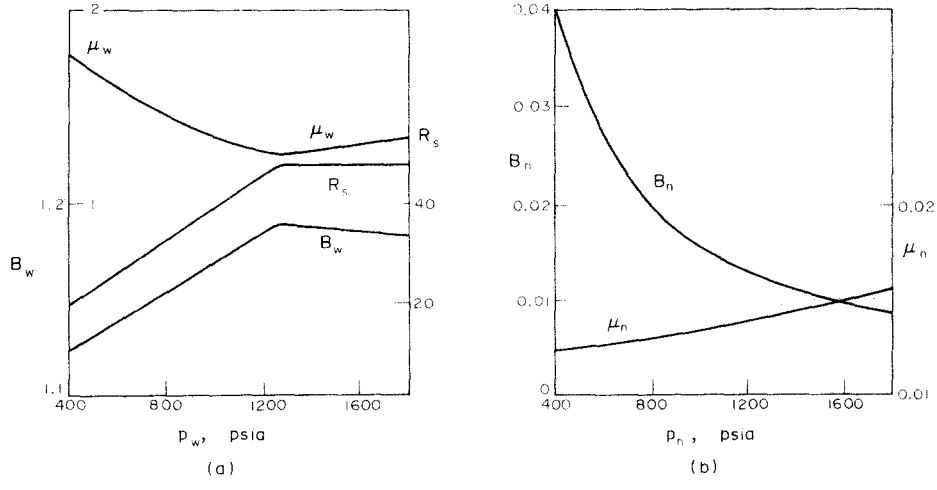


Figure 1. Typical pressure dependent functions.

*(2) Strong nonlinearities*

The coefficients dependent on saturation or capillary pressure, i.e. $k_{rl}$ and $S'_w$, are the strong nonlinearities. The nonlinearity due to gas percolation has a special character and will be discussed separately. An example of functions $k_{rw}$, $k_{rn}$ and $P_c$ is given on figure 2, which shows the data from McCreary (1971), typical of a gas–oil system. Typical data for an

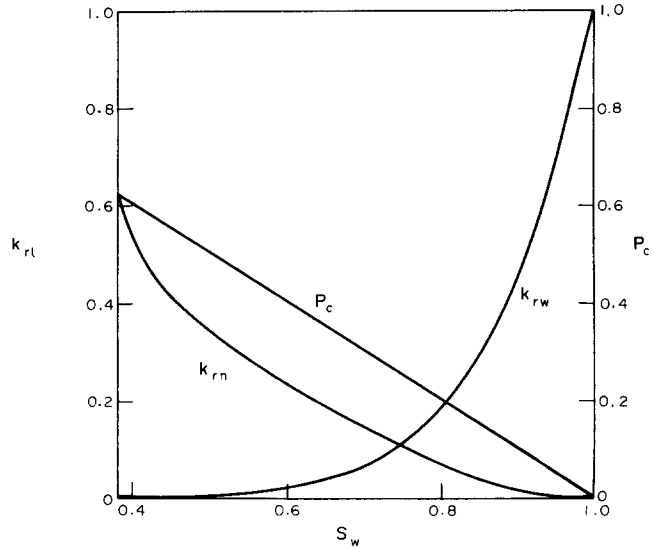


Figure 2. Typical saturation dependent functions for gas–oil systems (oil is the wetting phase).

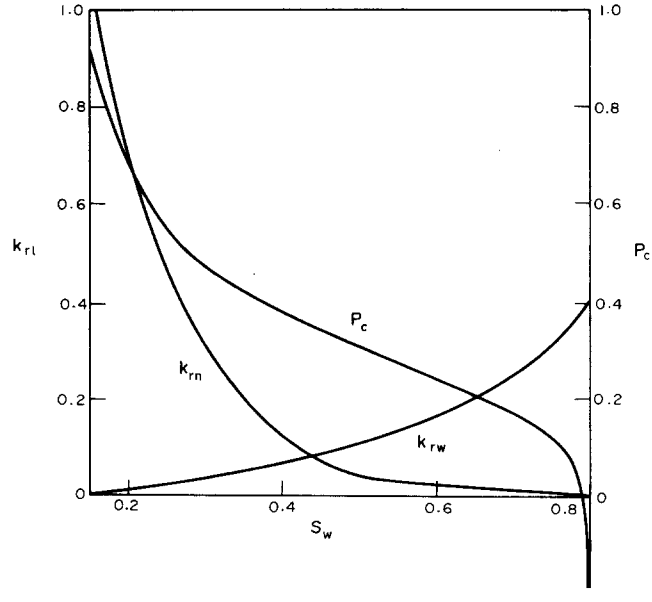


Figure 3. Typical saturation dependent functions for water–oil systems (water is the wetting phase).

oil–water system are shown on figure 3 ($k_r$ curves are from Todd *et al.* 1972, $P_c$ curve from Blair & Weinang 1969). It follows from eqn. [9] that the nonlinearity due to $S'_w$ disappears if $P_c$ is a linear function of saturation, but this is not true of $k_r$. Therefore, $k_r$ introduces the principal nonlinearity in [16].

Three test problems were selected for numerical experiments:

*Test Problem No. 1.* The first test problem is the incompressible Buckley–Leverett problem with negligible capillary pressure in which $k_r$ is the only nonlinearity. The $k_r$ functions are given by figure 3 and the other data are (see Todd *et al.*): $L = 1000$ ft, $B_w = B_n = 1$, $\mu_w = \mu_n = 1$ cp, k = 300 md, $\phi = 0.2$. Non-wetting phase is produced at $x = L$ at a rate of 426.5 ft$^3$/day and the wetting phase is injected at $x = 0$ at the same rate. The reservoir is horizontal with a cross-sectional area of 10,000 ft$^2$ and constant initial saturation $S_w = 0.16$. This problem will be used for some tests in Sections 3 and 4.

*Test Problem No. 2.* The second problem is obtained by adding the capillary pressure curve according to figure 3 to the first problem and will be used for testing in Section 5.

*Test Problem No. 3.* The third problem is the compressible oil–gas problem including gas percolation, with the nonlinear functions given in figures 1 and 2. The other data are (see McCreary 1971): $L = 135$ ft, $k = 20$ md, $\phi = 0.04$. The densities at standard conditions are $\rho_{wSTC} = 60$ lb./ft$^3$ and $\rho_{nSTC} = 0.0005$ lb./ft$^3$. Non-wetting phase is produced at $x = L$ at the rate of 2810 ft$^3$/day at standard conditions. The reservoir is a vertical column with a cross-sectional area of 5,414,929 ft$^2$, constant initial saturation $S_w = 0.19$. Initial pressure is given by gravity equilibrium with $p_w = 1750$ psia at the top of the column.

## 3. WEIGHTING OF TRANSMISSIBILITIES

### (a) *Weighting formulas*

According to our assumptions, we consider only the nonlinearity due to $k_{rl}$. The value of $k_{rl_{i+1/2}}$ must be related to $S_{w_i}$ and $S_{w_{i+1}}$. The following approximation, which seems to be most appropriate from the standpoint of numerical analysis,

$$k_{rl_{i+1/2}} = \tfrac{1}{2}[k_{rl}(S_{w_i}) + k_{rl}(S_{w_{i+1}})] \qquad [18]$$

may be called "midpoint weighting" and it is of second order. An alternative formula (apparently not discussed previously in the literature for reservoir simulation) may be defined as

$$k_{rl_{i+1/2}} = k_{rl}[\tfrac{1}{2}(S_{w_i} + S_{w_{i+1}})]. \qquad [19]$$

Although both approximations are of second-order, as shown in the Appendix, it is well known that [18] gives erroneous results. This is attributed to the hyperbolic character of the equations.

The commonly used scheme, called "upstream weighting" is given by

$$k_{rl_{i+1/2}} = \begin{cases} k_{rl}(S_{wi}) \text{ if flow is from } i \text{ to } i+1 \\ k_{rl}(S_{w_{i+1}}) \text{ if flow is from } i+1 \text{ to } i \end{cases} \qquad [20]$$

This formula gives only a first-order approximation.

Todd *et al.* (1973) proposed an asymmetric second-order approximation that uses two upstream points

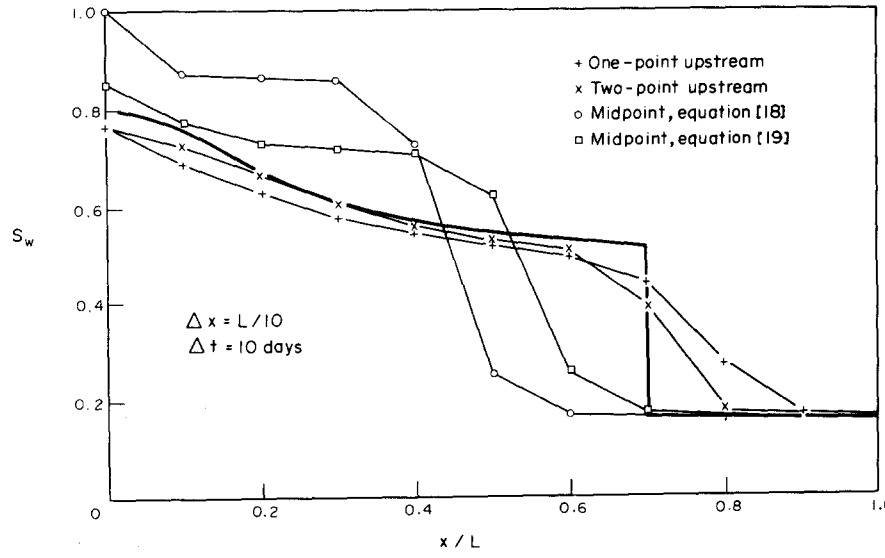


Figure 4. Comparison of weighting formulae for Test Problem No. 1 with $\Delta x = L/10$, $\Delta t = 10$ days at $t = 1500$ days.

$$k_{rl_{i+1/2}} = \begin{cases} \frac{1}{2}[3k_{rl}(S_{w_i}) - k_{rl}(S_{w_{i-1}})] \text{ for flow from } i \text{ to } i+1 \\ \frac{1}{2}[3k_{rl}(S_{w_{i+1}}) - k_{rl}(S_{w_{i-2}})] \text{ for flow from } i+1 \text{ to } i \end{cases} \quad [21]$$

The direction of flow is given by the sign of $\nabla\Phi_{l_{i+1/2}}$ given by [6]. Flow is from $i$ to $i+1$ if $\nabla\Phi < 0$ and vice versa.

Truncation errors for all methods are summarized in the Appendix. For numerical testing, the transmissibilities were approximated explicitly in time (i.e. $f_2 \approx f_2^n$) and small

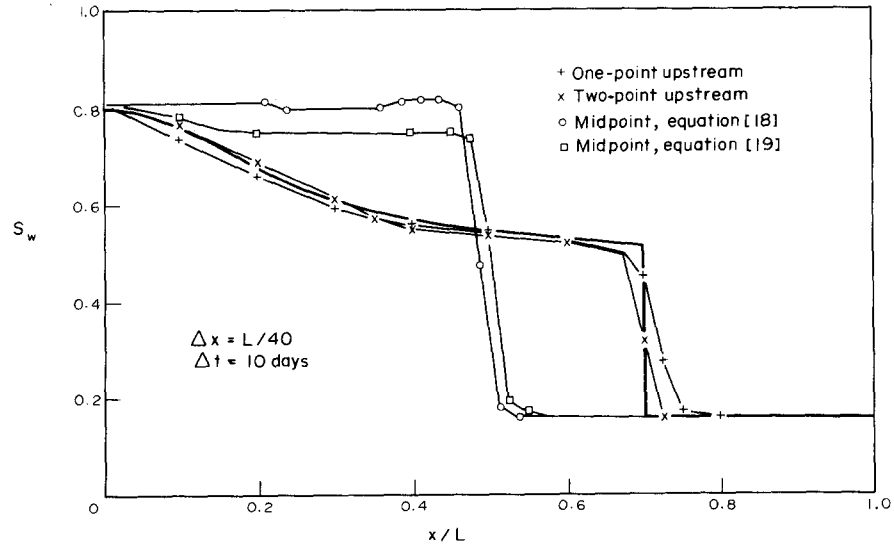


Figure 5. Comparison of weighting formulas for Test Problem No. 1 with $\Delta x = L/40$, $\Delta t = 10$ days at $t = 1500$ days.

time steps were used. Comparison of numerical results calculated by all methods with the exact solution is shown in figure 4. It shows saturation profiles at $t = 1500$ days. Both midpoint formulas give erroneous answers although [19] seems to perform better than [18]. However, results with a finer grid ($\Delta x = L/40$) given in figure 5 rendered [19] almost as unsuitable as [18]. The second-order upstream formula gives a sharper displacement front than the single-point formula. The fact that upstream weighting is superior to higher order midpoint weighting has also been observed in solving Navier–Stokes equations (Runchal & Wolfstein 1969).

One might propose that the bad performance of the second-order approximation is a consequence of inadequate space approximation of $\partial S/\partial t$ on the right-hand side of [1], which was obtained by discretization of $(\partial S_w/\partial t)_i$. If it is assumed that $\partial S_w/\partial t$ is linear between grid points, the mean value of $\partial S_w/\partial t$ between $i - \frac{1}{2}$ and $i + \frac{1}{2}$ is given by

$$\left.\frac{\overline{\partial S_w}}{\partial t}\right|_i = \frac{1}{6}\left[\frac{\partial S_{w_{i-1}}}{\partial t} + 4\frac{\partial S_{w_i}}{\partial t} + \frac{\partial S_{w_{i+1}}}{\partial t}\right]$$

Then the right-hand side of the difference equations may be obtained by discretizing $\overline{\partial S_w}/\partial t$. Approximations of this type are discussed in Collatz (1966). Unfortunately, use of such approximations gives equations of highly oscillatory character. It is likely that non-oscillatory approximation would result from the upstream type of formulas, but this idea was not pursued, since it does not have any advantage over asymmetric approximation of $k_{rl}$.

The weighting problem is an example of a problem in which the truncation error analysis such as the one carried out in the Appendix can be completely misleading. The truncation errors of the midpoint and two-point upstream formulas differ only in the coefficient of the $\Delta x^2$ term, but their performance is quite different. For the solution of practical problems, the choice is between single-point and two-point weighting. The single-point weighting scheme has a larger truncation error (additional first-order $\Delta x$ term and the mixed term $\Delta x \Delta t$) and has been found more sensitive to grid orientation in multi-dimensional problems (Todd *et al.* 1972). On the other hand, implementation of the two-point scheme requires more programming and computational effort, especially in connection with implicit approximations, which will be discussed next.

## 4. APPROXIMATION TO TRANSMISSIBILITIES IN TIME

The approximation of the time level appears to be crucial for stability of the finite-difference equations. The explicit approximation, i.e. $T^{n+1} \approx T(f_2^n)$ is only conditionally stable and therefore imposes a limitation on the size of time step. Stability problems become severe especially in the simulation of multi-dimensional flow around a single well, where high flow velocities are attained due to convergence of flow towards the sink. It was this application (coning simulation) in which the stability problem was first identified (Welge & Weber 1964). Later, it was demonstrated that the problem is a result of explicit transmissibilities (Blair & Weinaug 1969), and subsequently several methods were suggested, involving linearized (MacDonald & Coats 1970; Letkeman & Ridings 1970; Sonier *et al.*

1971), as well as nonlinear (Nolen & Berry 1972; Robinson 1971), approximations to the fully implicit transmissibilities. Although most of these methods are closely related to Newton's method (Ostrowski 1973; Ortega & Rheinboldt 1970) of solution of nonlinear equations, the use of the classical (or full) Newton's method has apparently not been discussed in the literature since the initial attempt in Blair & Weinaug (1969). It is compared with the other methods here for the first time.

In the rest of this paper, we assume single-point, upstream weighting (equation [20]) for the approximation in space.

(a) *Explicit transmissibilities*

As mentioned above, the approximation:

$$T^{n+1} \approx T(f_2^n) \qquad [22]$$

is only conditionally stable. This is demonstrated in figure 6 where the solutions obtained with different time steps are shown in comparison with the exact solution. Instead of using $\mathbf{P}^n$ one might extrapolate pressure from two previous time steps, i.e.

$$\mathbf{P}^k = \mathbf{P}^n + \frac{\Delta t^{n+1}}{\Delta t^n}(\mathbf{P}^n - \mathbf{P}^{n-1})$$

and use $T(f_2^k)$. This gives only a slight improvement in stability.

(b) *Simple iteration on matrix T*

Such a method for solving [16] with $T^{n+1}$ may be written as:

$$[\mathbf{T}^{(v)} - D]\,[\mathbf{P}^{(v+1)} - \mathbf{P}^{(v)}] = -R_{(v)}^{(v)} + \mathbf{Q}$$
$$v = 0, 1, \ldots; \qquad \mathbf{P}^{(0)} = \mathbf{P}^{(n)} \qquad [23]$$

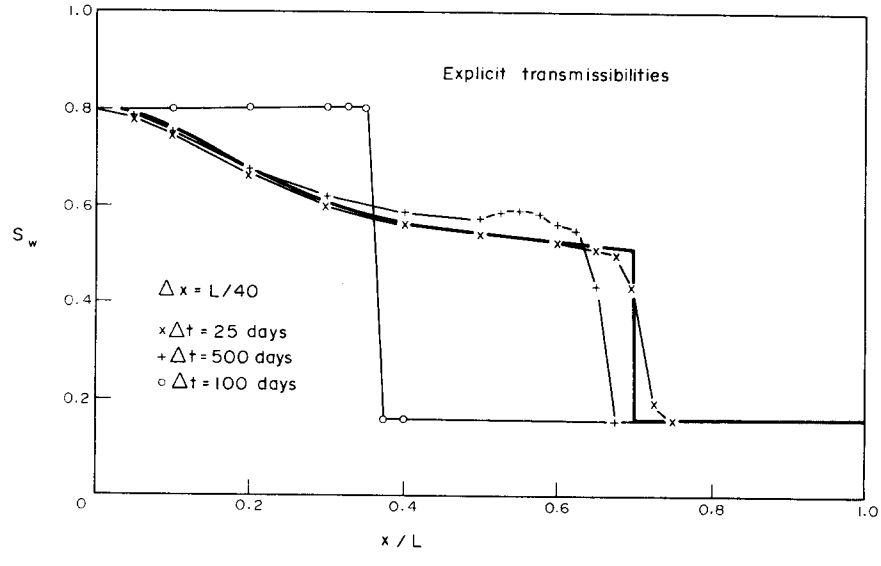


Figure 6. Stability of the explicit method [22] for Test Problem No. 1 at $t$ = 1500 days.

where $T^{(\nu)} = T(f_2^{(\nu)})$. It has been found through numerical experiments that [23] converges for $\Delta t < \Delta t_{cr}$, where $\Delta t_{cr}$ is the stability limit for the explicit approximation of [22]. In the iterative process, the saturations oscillate with decreasing amplitude if $\Delta t < \Delta t_{cr}$, and increasing amplitude if $\Delta t > \Delta t_{cr}$. In the latter case, the oscillations can be "damped out", if only a part of the saturation change in the current iteration is carried over for re-evaluation of $T$. This may be achieved by defining $T^{(\nu)}$ by a weighted average:

$$T^{(\nu)} = T^{(\nu-1)} + d\frac{\Delta t_{cr}}{\Delta t^{n+1}}[T(f_2^{(\nu)}) - T^{(\nu-1)}] \qquad [24]$$

where $d$ is a damping factor, $0 < d < 1$. This damping scheme has been found convergent for time steps of an order of magnitude larger than $\Delta t_{cr}$, when tested on a two-dimensional problem. However, it has several features that make it impractical to use; in particular, the necessity of estimating $\Delta t_{cr}$ and the choice of a suitable damping strategy.

(c) *Linearized implicit transmissibilities*

The method in its original formulation (MacDonald & Coats 1970; Letkeman & Ridings 1970) consists of extrapolating $T^l$ by the first-order approximation to $f_2^{n+1}$ as follows:

$$T^{ln+1} \approx T^l(f_2^n) + \frac{\partial T^l}{\partial P_c}(P_c^{n+1} - P_c^n) \qquad [25]$$

where

$$\frac{\partial T^l}{\partial P_c} = GC(f_1)\left(\frac{df_2}{dS_w}\right)\left(\frac{dS_w}{dP_c}\right)$$

is the derivative with respect to the upstream point. These extrapolated transmissibilities are introduced into $T\mathbf{P}$ and the nonlinear terms are linearized. For example, the nonlinear part of a typical term of $T\mathbf{P}$, $T^{ln+1}_{i+1/2}(P_{li+1} - P_{li})^{n+1}$, is linearized by the following assumption

$$(p_{li+1} - p_{li})^{n+1}\frac{\partial T^l}{\partial P_c}(p_c^{n+1} - p_c^n) \approx (p_{li+1} - p_{li})^n\frac{\partial T^l}{\partial P_c}(p_c^{n+1} - p_c^n). \qquad [26]$$

We will now show that this method of linearization can be interpreted as the first iteration of Newton's method. The equation to be solved, [16], can be written as (combining [14] and [15]):

$$\mathbf{R}_{n+1}^{n+1} = T^{n+1}\mathbf{P}^{n+1} - D^{n+1}(\mathbf{P}^{n+1} - \mathbf{P}^n) + \mathbf{G}^{n+1} = \mathbf{Q} \qquad [27]$$

and the classical Newton's method for [27] is an iterative process defined by

$$DR^{(\nu)}[\mathbf{P}^{(\nu+1)} - \mathbf{P}^{(\nu)}] = -\mathbf{R}_{(\nu)}^{(\nu)} + \mathbf{Q},$$
$$\nu = 0, 1, \ldots; \qquad \mathbf{P}^{(0)} = \mathbf{P}^{(n)}. \qquad [28]$$

Let us now assume that $D$ and $\gamma_l$ are constant and examine the Jacobi matrix $DR$. By definition, elements of $DR$ are partial derivatives of vector $\mathbf{R}$. In the notation introduced

earlier, the block element of $DR$ in the $i$th row and $j$th column will consist of derivatives $\partial R_{l_i}/\partial P_{k_j}$, where $l, k = w, n$:

$$\begin{vmatrix} \dfrac{\partial R_{w_i}}{\partial p_{w_j}} & \dfrac{\partial R_{w_i}}{\partial p_{n_j}} \\ \dfrac{\partial R_{n_i}}{\partial p_{w_j}} & \dfrac{\partial R_{n_i}}{\partial p_{n_j}} \end{vmatrix}.$$

It can be readily seen that the matrix $DR$ can only have non-zero elements in the locations of the three block-diagonals of matrix $T$ (note that this is not true if two-point upstream weighting, [21], is used). Under the above assumptions, derivatives of $\gamma_l$ are zero and derivations of $D\mathbf{P}$ give again matrix $D$. A typical element of $T\mathbf{P} + \mathbf{G}$ is:

$$T^l_{i+1/2}(p_{l_{i+1}} - p_{l_i} - \gamma_l \Delta z) = T^l_x \qquad [29]$$

and it has, at most, four non-zero derivatives if the single-point upstream weighting is used. Let us denote:

$$T^{l'}_{i+1/2} = \nabla\Phi_{l_{i+1/2}} \frac{\partial T^l_{i+1/2}}{\partial P_c} \qquad [30]$$

where the derivative without a subscript is understood with respect to the upstream point. Then the derivatives of the term [29] are:

$$\frac{\partial T^l_x}{\partial p_{k_i}} = -\delta_{kl} T^l_{i+1/2} + T^{l'}_{i+1/2} \cdot \frac{\partial P_c}{\partial p_{k_i}}$$

$$\frac{\partial T^l_x}{\partial p_{k_{i+1}}} = \delta_{kl} T^l_{i+1/2} + T^{l'}_{i+1/2} \cdot \frac{\partial P_c}{\partial p_{k_{i+1}}} \qquad k, l = w, n$$

where $\delta_{kl}$ is the Kronecker delta and $P_c$ is the upstream value (i.e. $P_c = (p_n - p_w)_i$ or $(p_n - p_w)_{i+1}$). After collecting all terms it is easy to see that the matrix $DR$ may be written as:

$$DR = T + T' - D \qquad [31]$$

where $T'$ is a matrix composed of $T^{l'}$. The form of $T'$ is generally dependent on the direction of flow. In a special case, when the flow is in the direction of increasing $i$ for all grid points and for both phases, $T'$ will be a lower block-triangular matrix with non-zero entries in only the main diagonal and the subdiagonal. If the diagonal block-element of matrix $T'$ for the row $i$ is denoted by $TC_i$ and the subdiagonal element by $TX_i$, then for the general case with solubility terms:

$$TX_i = \begin{vmatrix} -T^{w'} & T^{w'} \\ -T^{n'} + RT' & T^{n'} - RT' \end{vmatrix}_{i-1/2}$$

where:

$$RT'_{i+1/2} = \frac{1}{2}(R_{s_{i+1}} - R_{s_i}) \nabla\Phi_{w_{i+1/2}} \frac{\partial T^w_{i+1/2}}{\partial P_c} \qquad [32]$$

and:

$$TC_i = TX_{i+1} + 2\begin{vmatrix} 0 & 0 \\ -RT' & RT' \end{vmatrix}_{i+1/2}.$$

The derivatives $\partial T^l/\partial P_c$ and the $\nabla\Phi$ terms in [30] and [32] may be evaluated at different time levels $m$ and $k$ and the matrix $T'$ will then be denoted $T'^k_m$ in analogy with the definition of **R** [15].

For the classical Newton's method with tangents, both $k$ and $m$ are at the level of the previous iteration, i.e. $T' = T'^{(v)}_{(v)}$ and $\partial T^l/\partial P_c$ are tangents at $\mathbf{P}^{(v)}$. If it is now assumed that only one Newton's iteration, [28], will be performed per time step, $\mathbf{P}^{(1)} = \mathbf{P}^{n+1}$ and one obtains, with respect to [31], the equation:

$$(T^n + T'^n_n - D)(\mathbf{P}^{n+1} - \mathbf{P}^n) = -R^n_n + \mathbf{Q} \qquad [33]$$

which is the matrix formulation of the linearized method, [26]. Therefore, we have the result: *Linearized method* [26] *is the first iteration of Newton's method*, [28].

Numerical results for the method of [33] are on figure 7. The method is about twice as stable as the explicit method [22]. It should be noted again, that the one-dimensional problem we study here is not the most severe from the point of view of stability. Instability of explicit equations occurs, when the time step approaches a value at which the saturation front advances one grid point per time step. In multi-dimensional (especially single-well) problems, instability of explicit equations occurs for much smaller time steps and the improvement by using the linearized method of [33] is much larger than indicated by the results shown on figure 7.

(d) *Semi-implicit method of Nolen & Berry* (1972)

These authors retain the nonlinearity in [26]. If we assume that the derivatives in $T'$

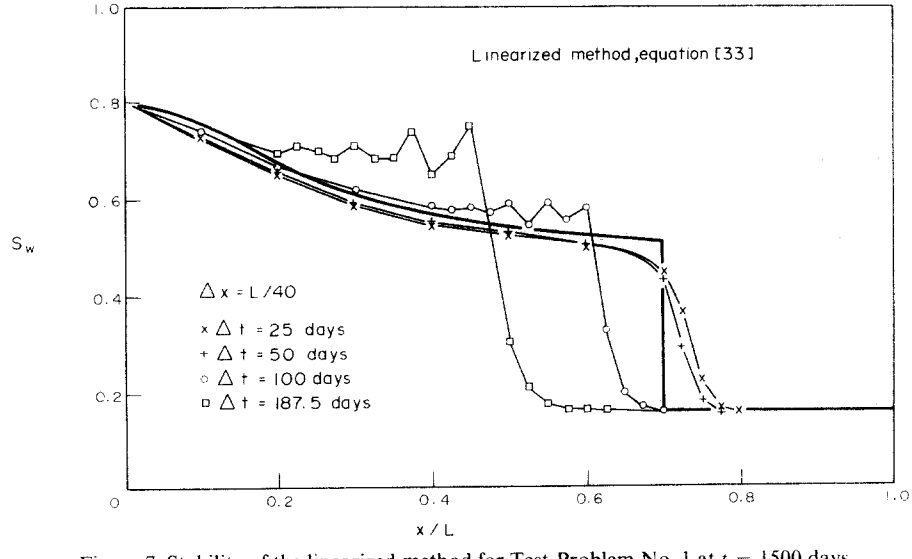


Figure 7. Stability of the linearized method for Test Problem No. 1 at $t$ = 1500 days.

are still evaluated at the level $n$, the matrix formulation of the method is:

$$(T^n + T_n'^{n+1} - D)(\mathbf{P}^{n+1} - \mathbf{P}^n) = -\mathbf{R}_n^n + \mathbf{Q} \qquad [34]$$

which represents a system of nonlinear equations. The nonlinearity $T_n'^{n+1}(\mathbf{P}^{n+1} - \mathbf{P}^n)$ was solved by Newton's iteration. This is equivalent to iteration on the left-hand side of [26] as follows

$$\begin{aligned}
&(p_{l_{i+1}} - p_{l_i})^{(v+1)} \frac{\partial T^l}{\partial P_c}(P_c^{(v+1)} - P_c^n) \\
&\quad = (p_{l_{i+1}} - p_{l_i})^{(v)} \frac{\partial T^l}{\partial P_c}(P_c^{(v+1)} - P_c^{(v)}) \\
&\qquad + [(p_{l_{i+1}} - p_{l_i})^{(v+1)} - (p_{l_{i+1}} - p_{l_i})^{(v)}] \frac{\partial T^l}{\partial P_c}(P_c^{(v)} - P_c^n) \\
&\qquad + (p_{l_{i+1}} - p_{l_i})^{(v)} \frac{\partial T^l}{\partial P_c}(P_c^{(v)} - P_c^n), \qquad v = 1, 2, \ldots
\end{aligned} \qquad [35]$$

We observe immediately the following properties of the above method:

(1) *If* $\mathbf{P}^{(v)} = \mathbf{P}^{(n)}$ *and only one iteration* [35] *is performed, the method of Nolen & Berry becomes the linearized method* [33].

(2) *If the functions* $k_{rl}(S_w)$ *are linear, the method of Nolen & Berry gives the solution of the implicit equations* [16].

Note that statement (2) above is not true for the case of the linearized method [33].

Numerical results for this method are presented in figure 8. For Test Problem 1, the iterative method [35] started to diverge for a time step of 100 days, although only three iterations were necessary for convergence for smaller time steps. The convergence was

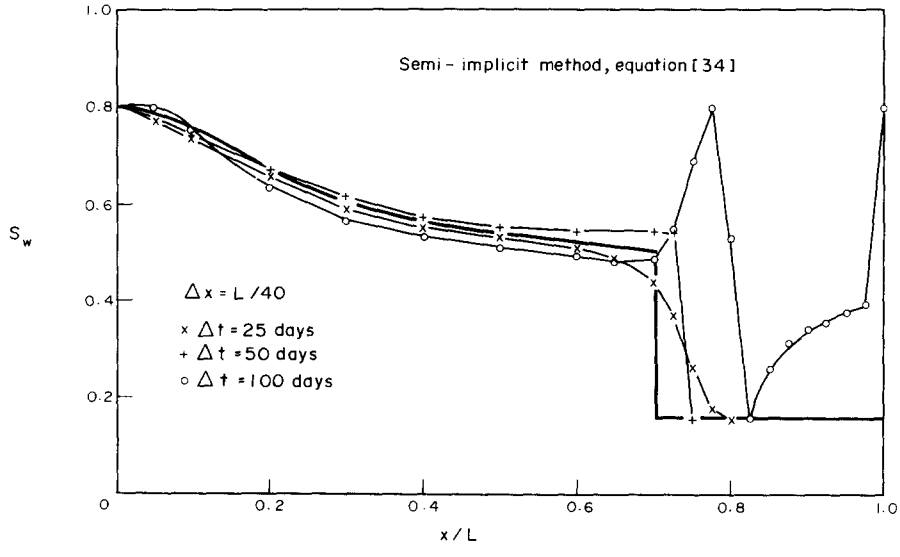


Figure 8. Stability of the semi-implicit tangent method for Test Problem No. 1 at $t$ = 1500 days.

measured by the $l_\infty$ norm of saturation change, i.e. by $\delta S_w = \max_i |S_{w_i}^{(\nu+1)} - S_{w_i}^{(\nu)}|$ with the closure $\delta S_w = 0.001$. The relatively bad performance of [35] is only seemingly in contradiction with the original work of Nolen & Berry (1972), where the authors concluded that this method is superior to the linearized method. The reason is that, in the original work, the semi-implicit method was used with chords instead of tangents in the matrix $T'$. We will discuss the performance of secant methods in (g).

(e) *Linearized second-order method*

Instead of the approximation [25], the implicit transmissibility may be approximated by a second-order expression

$$T^{ln+1} \approx T^{ln} + \frac{\partial T^l}{\partial P_c}(P_c^{n+1} - P_c^n) + \frac{1}{2}\frac{\partial^2 T^l}{\partial P_c^2}(P_c^{n+1} - P_c^n)^2. \qquad [36]$$

The expression [36] is itself nonlinear. In order to use it in a linearized method, we will first linearize it by assuming:

$$(P_c^{n+1} - P_c^n)^2 = (P_c^{n+1} - P_c^n)(P_c^n - P_c^{n-1}) \qquad [37]$$

in the second-order term. After linearization of $T\mathbf{P}$ similar to [26], the method may be written in matrix form as:

$$(T^n + T_n'^n + \tfrac{1}{2}T_n''^n - D)(\mathbf{P}^{n+1} - \mathbf{P}^n) = -R_n^n + \mathbf{Q} \qquad [38]$$

where $T''$ is a matrix of second derivatives, similar in structure to matrix $T'$. Numerical results for the method [38] are shown in figure 9. Although the method seems to have less truncation error than the first-order linearization for smaller time steps, it behaves erratically for large time steps, when the approximation [37] is not adequate.

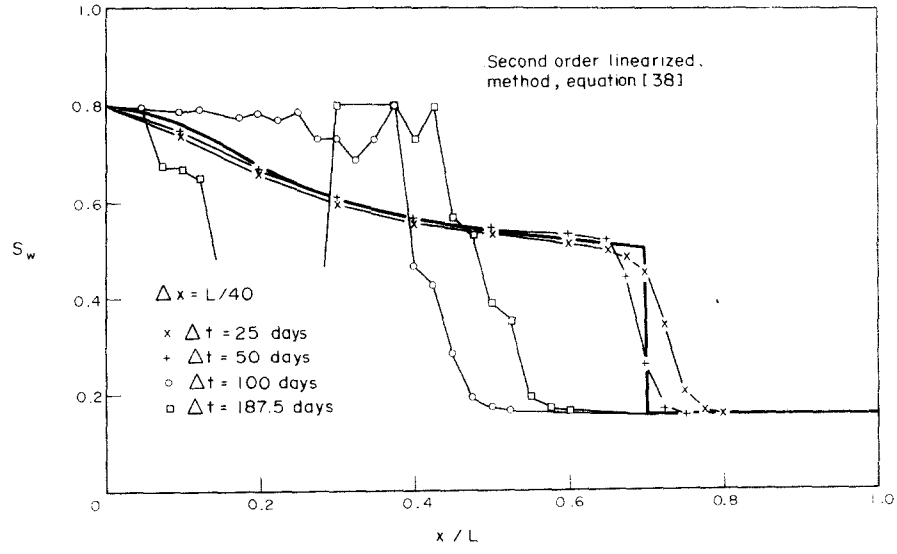


Figure 9. Stability of the second-order linearized method for Test Problem No. 1 at $t = 1500$ days.

(f) *Solution of implicit equations by Newton's method*

All methods discussed so far have incorporated only some approximation to the implicit scheme [16]. Equations [16] may also be solved by Newton's method, derived already in (c). Using the notation already introduced, the tangent method may be written as

$$[T^{(\nu)} + T'^{(\nu)}_{(\nu)} - D][\mathbf{P}^{(\nu+1)} - \mathbf{P}^{(\nu)}] = -\mathbf{R}^{(\nu)}_{(\nu)} + \mathbf{Q}$$
$$\nu = 0, 1, 2, \ldots; \qquad \mathbf{P}^{(0)} = \mathbf{P}^n. \qquad [39]$$

Theoretical treatment of Newton's method becomes quite complicated for systems of equations (see, for example, Ortega & Rheinboldt 1970) and the conditions for convergence, existence, and uniqueness of solution are not easily established for practical problems. The essential conditions are that the functions $R_i^{n+1}$ have continuous second derivatives and the Jacobi matrix $DR$ has an inverse, and they are usually met for practical problems.

Rate of convergence is crucial for the feasibility of the method [39] as well as for the semi-implicit method [34], because one iteration needs approximately the same amount of work as does the solution of one time step for any linearized method. This relation is based on the assumption that each iteration by Newton's method is solved to the same degree of accuracy as the solution of linearized equations. While this is always true when a direct method is used for the solution of the linearized matrix, the work ratio may be more favourable for Newton's method when an iterative method is used, since the equations for every Newton's iteration may be solved only approximately in the latter case.

Numerical results for the method [39] are on figure 10. The closure for convergence was $\delta S_w = 0.001$ and the average number of iterations to meet it was 3 for $\Delta t = 25$ and 50 days, 4 for $\Delta t = 100$ days, and 5 for $\Delta t = 187.5$ days. With closure relaxed to $\delta S_w = 0.01$, almost all cases could be solved in just two iterations, which shows that the convergence is very

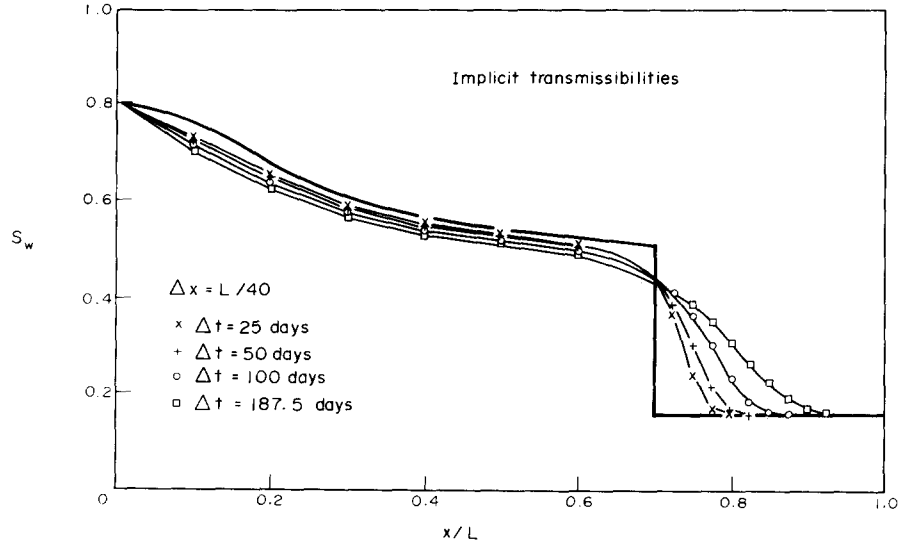


Figure 10. Stability of the implicit method for Test Problem No. 1 at $t = 1500$ days.

rapid. The results also demonstrate clearly the superiority of the fully implicit transmissibilities to all previously considered methods. The same conclusions have been reached for multi-dimensional, two- and three-phase problems (Settari 1973).

(g) *Secant methods*

The methods discussed in previous paragraphs may be called tangent methods, since the derivatives $\partial T^l/\partial P_c$ were evaluated as tangents at the level $n$ (or, generally, at the previous iteration level). A better rate of convergence may be expected if the derivative is approximated by a secant (chord) between $\mathbf{P}^n$ and a reasonable estimate of $\mathbf{P}^{n+1}$, denoted $\mathbf{P}^k$

$$\frac{\partial T^l}{\partial P_c} \approx \frac{T^l(S_w^k) - T^l(S_w^n)}{S_w^k - S_w^n} \frac{\mathrm{d}S_w}{\mathrm{d}P_c}. \qquad [40]$$

The matrix $T'$ may then be denoted as $T'_{n+1/2}$ and secant methods are obtained through the replacement of $T'_n$ by $T'_{n+1/2}$. If the chord is chosen reasonably, the secant method has a better rate of convergence than the corresponding tangent method (Ortega & Rheinboldt 1970). Since the prediction of $\Delta S_w = S_w^k - S_w^n$ is difficult for every grid point, a constant chord, $\Delta S_w$, is usually used, which is calculated from the maximum anticipated change of saturation, i.e. $\Delta S_w \approx \delta S_w$.

Such chord methods were compared during this investigation with tangent methods for the linearized method [33], the semi-implicit method [34], and Newton's method [39]. The improvement for the linearized method was marginal. For the other two methods, the only effect is in the rate of convergence, which changed very little for the Newton's method. However, the rate of convergence for the semi-implicit method improved dramatically and

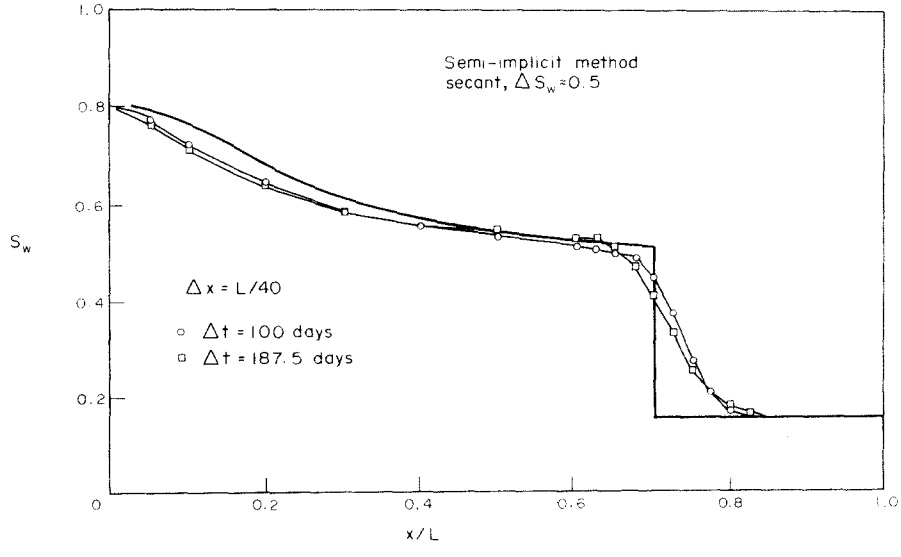


Figure 11. Stability of the semi-implicit secant method for Test Problem No. 1 at $t$ = 1500 days.

convergence in 4 iterations was obtained for $\Delta t = 100$ and 187.5 days. These results are shown in figure 11 and have considerably less truncation error than the fully implicit solution on figure 10.

(h) *Comparison of methods*

We have shown the effect of various treatments of the time level in the handling of transmissibilities. As we progress from fully explicit to fully implicit treatment, the numerical stability of the equations increases. However, this improvement is gained at the expense of larger truncation errors. This can be seen by comparison of figure 6 with figures 7–10 for $\Delta t = 25$ days. The behaviour is also confirmed by the truncation error analysis included in the Appendix. Since $C_w > 0$, the first-order error term for the implicit method is always larger than the corresponding term for the explicit method, as pointed out first in MacDonald & Coats (1970). Comparison of the implicit and linearized method shows that the $\Delta t$ and $\Delta x$ components of the first-order term have the same sign for the implicit method (equation [A12]), while they have opposite signs for the linearized method (equation [A10]). This is also confirmed by numerical results. The errors for implicit solution on figure 10 are of one sign and increase with $\Delta t$. The errors for linearized method (figure 7) change sign with $\Delta t$, which opens an interesting possibility of minimizing the discretization errors by an appropriate choice of $\Delta t$.

The semi-implicit method does not lend itself easily to similar analysis, but the results suggest that the behaviour is not monotonic and the secant method has a relatively small truncation error.

All three methods are efficient for solving the stability problem. The linearized method is embedded in both the semi-implicit and the implicit method. The advantage of Newton's method is in its relative insensitivity to the choice of chords; the advantage of the semi-implicit method is in lower truncation errors.

## 5. HANDLING OF THE NONLINEARITY DUE TO $P_c$ FUNCTION

When the function $S_w = f(P_c)$ is not linear, the elements of matrix $D$ become implicit: $D = D^{n+1}$. We will consider, for clarity, again the incompressible flow given by equations [5]; in this case the $i$th block of matrix $D$ simplifies to

$$D_i^{n+1} = \phi_i \frac{\Delta x}{\Delta t} (S'_w)_i^{n+1} \begin{vmatrix} -1 & 1 \\ 1 & -1 \end{vmatrix}. \qquad [41]$$

The nonlinearity due to $S'_w$ enters also in the matrix $T'$, its effect on this term is, however, small and will not be considered separately. In order for $S'_w$ to satisfy equation [9], some iterative method must be used to obtain the solution. In the case that an iterative method is used to solve for implicit transmissibilities, the iterations on $D$ will generally be sub-iterations of such an iterative method. In order to simplify the discussion, we will consider methods for solving [16] with implicit matrix $D^{n+1}$ in connection with the linearized method only.

(a) *Simple iteration*

Based on the last iteration $\mathbf{P}^{(\nu)}$, the derivative of $S_w$ is updated as

$$S_w'^{(\nu)} = \frac{S_w(P_c^{(\nu)}) - S_w(P_c^n)}{P_c^{(\nu)} - P_c^n}. \tag{42}$$

If the corresponding matrix $D$ is denoted as $D^{(\nu)}$, the iterative scheme for the linearized method [33] may be written as

$$(T^n + T_n'^n - D^{(\nu)})(\mathbf{P}^{(\nu+1)} - \mathbf{P}^n) = -\mathbf{R}_n^n + \mathbf{Q}^{n+1},$$
$$\nu = 0, 1, 2, \ldots; \qquad \mathbf{P}^{(\nu)} = \mathbf{P}^{(n)}. \tag{43}$$

The method [43] was found to converge for small time steps, but its stability limit was about 1/4 of the stability of the linearized method and, in fact, even lower than the stability limit of the equations with explicit transmissibilities. Also, the derivative $S_w'$ must be continuous in order that the method converges at all. Numerically it means that the method requires at least second-order interpolation if the function $P_c$ is given in the form of a table. In order to take full advantage of the stability of the treatment of matrix $T$, we must search for a better method.

(b) *Newton's iteration*

We can define a vector **DS** by

$$\mathbf{DS}^{n,n+1} = D^{n+1}(\mathbf{P}^{n+1} - \mathbf{P}^n). \tag{44}$$

In terms of $S_w$, the element of **DS** will be

$$DS_i^{n,n+1} = \begin{vmatrix} S_w^{n+1} - S_w^n \\ -(S_w^{n+1} - S_w^n) \end{vmatrix}.$$

Let us substitute [44] into [33] and apply Newton's method, considering **DS** to be the only nonlinearity. From [44] it is easy to see that the derivative of **DS** is just $D$, therefore the method can be written as

$$(T^n + T_n'^n - D^{(\nu)})(\mathbf{P}^{(\nu+1)} - \mathbf{P}^{(\nu)}) = -\mathbf{R}_n^n - (T^n + T_n'^n)(\mathbf{P}^{(\nu)} - \mathbf{P}^n) + \mathbf{DS}^{n,(\nu)} + \mathbf{Q},$$
$$\nu = 0, 1, \ldots; \qquad \mathbf{P}^{(0)} = \mathbf{P}^n. \tag{45}$$

In terms of $S_w$, this is equivalent to iteration of the form:

$$S_w^{(\nu+1)} = S_w^{(\nu)} + S_w'^{(\nu)}(P_c^{(\nu+1)} - P_c^{(\nu)}) \tag{46}$$

where now $S_w'^{(\nu)}$ is a tangent at $P_c^{(\nu)}$.

The method [45] when applied to the $P_c$ curve of figure 3, failed to converge for any reasonable value of time step. The reason for this becomes clear if we realize that, except for $S_w^{n+1}$, all other terms in [45] depend only weakly on $P_c^{n+1}$. Therefore, the equation at a grid point $i$ can be approximately replaced by the following problem:

$$F(P_{c_i}^{n+1}) = S_w(P_{c_i}^{n+1}) - S_{w_i}^n + C = 0 \tag{47}$$

where $C$ is a certain constant. For the particular $P_c$ function, the function $F$ is depicted on

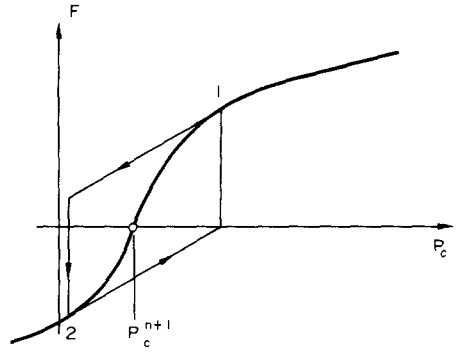


Figure 12. Divergence of Newton's method for Test Problem No. 2.

figure 12. Because the function $F$ has small derivatives at the ends of the interval in which solution is sought, Newton's method may converge or diverge depending on the initial guess (cf. Ostrowski 1973).

(c) *Modified Newton's method*

We will start with the observation that, in the case that the matrix $T + T'$ was actually independent of $P_c$, we could obtain an exact solution after the first iteration [45] simply by solving [47] for $S_w^{n+1}$ at every point. This is possible because we have assumed at the beginning that the inverse function $S_w(P_c)$ is known explicitly together with $P_c(S_w)$. Then we can calculate $P_c^{n+1}(S_w^{n+1})$. This idea of "inverse iteration" can be applied also in the general case as follows:

(1) Let $\mathbf{P}^{(c)}$ be the result of the solution of [45] on the $(v+1)$th iteration. Calculate first the saturation vector $\mathbf{S}^{(v+1)}$ by

$$S_{w_i}^{(v+1)} = S_{w_i}^{(v)} + S'^{(v)}_{w_i}(P_c^{(c)} - P_c^{(v)})_i \qquad i = 1, \ldots, N. \tag{48}$$

(2) Re-calculate the pressure vector as $\mathbf{P}^{(v+1)} = f(\mathbf{S}^{(v+1)})$. For example, we may define

$$P_{n_i}^{(v+1)} = P_{n_i}^{(c)}$$
$$P_{w_i}^{(v+1)} = P_{n_i}^{(v+1)} - P_c(S_{w_i}^{(v+1)}), \qquad i = 1, \ldots, N \tag{49}$$

The vectors $P^{(v+1)}$ and $S^{(v+1)}$ are then used for the next iteration.

Since capillary pressure is usually small compared to pressure variations, we would expect this method to have a good convergence. This was confirmed by numerical experiments. Sample results for $\Delta x = L/10$ and $\Delta t = 50$ days are shown in table 1. The first column gives the results with the original $P_c$ curve. In the second column, the $P_c$ curve was amplified 10 times. The convergence is extremely rapid even in the second case, when $P_c$ is of the same order as $\nabla\Phi$. Also, the method was found to be insensitive to the manner in which the derivatives in $D^{(v)}$ are treated. Because $\delta S^{(v)}$ is always extremely small, the second iteration is really used only to terminate the process and may be omitted. Therefore, there is no need to iterate in order to obtain a solution with $D^{n+1}$ if the method [48]–[49] is used.

Table 1. Convergence of the modified Newton's method [48] and [49] for Test Problem no. 2

| Time step | Original $P_c$ curve | | Amplified $P_c$ curve | |
|---|---|---|---|---|
| | $\delta S^{(1)}$ | $\delta S^{(2)}$ | $\delta S^{(1)}$ | $\delta S^{(2)}$ |
| 1 | 0.2133 | 0.00000 | 0.21330 | 0.00000 |
| 2 | 0.1316 | 0.00018 | 0.11090 | 0.00326 |
| 3 | 0.0795 | 0.00389 | 0.07028 | 0.00172 |
| 4 | 0.0755 | 0.00176 | 0.06621 | 0.00223 |
| 5 | 0.0568 | 0.00052 | 0.04210 | 0.00147 |
| 6 | 0.0564 | 0.00070 | 0.05010 | 0.00105 |
| . | . | . | . | . |
| . | . | . | . | . |
| . | . | . | . | . |

This method has apparently not been given in the literature previously. It may be noted in this connection that some authors use a different formulation of the basic flow equations (with $S_w$ as one of the variables) in which the $P_c$ nonlinearity is much less severe in the matrix $D$.

## 6. GAS PERCOLATION

In a two-phase oil–gas flow problem with solution gas, free gas will be released from solution if the pressure decreases below the bubble point. Because of the very small viscosity of the gas, its mobility is high and gas flows upwards with relatively high velocities. Serious stability problems arise in a standard numerical solution of [1] in the case of a vertical or inclined coordinate, as soon as the gas phase becomes mobile (i.e. $k_{rn} > 0$). This instability is essentially due to the explicit treatment of transmissibilities. The two factors that contribute to instability in this particular case are the large difference in densities of oil and gas and the stronger nonlinearity of pressure-dependent functions for gas.

The first method for controlling this nonlinearity (Coats 1968) was developed before the importance of implicit treatment of coefficients was recognized. Later a similar, but simpler, method was proposed (McCreary 1971). Several investigators (MacDonald & Coats 1970; Letkeman & Ridings 1970; Nolen & Berry 1972) claimed that the use of the linearized or semi-implicit method, discussed here, also solves the stability problem associated with gas percolation. None of these works showed, however, how these methods compare with the earlier methods (Coats 1968; McCreary 1971).

We will give such a comparison here for the problem studied in McCreary (1971). We have solved the problem by the linearized method and compared the results with the results for the methods of Coats and McCreary, reported in McCreary (1971). Saturations calculated by all three methods for a selected time $t = 900$ days are shown on figure 13. The solid line represents the reference solution computed by McCreary using very small time steps and explicit transmissibilities. Obviously, the linearized method gives a much more accurate solution than the other two methods. This is especially true in the oil zone, where the

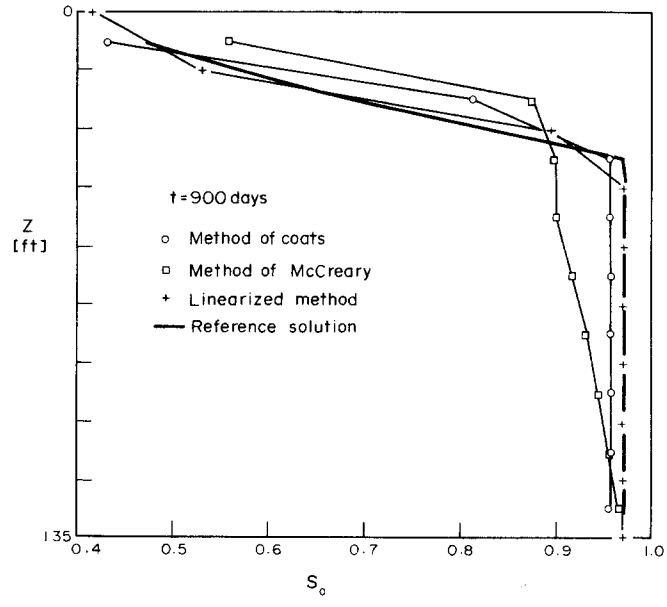


Figure 13. Comparison of three methods for the gas percolation problem of McCreary (Test Problem No. 3).

saturation of gas is only slightly higher than the critical saturation at which gas starts to flow. The common feature of the methods of Coats (1968) and McCreary (1971) is that they restrict the mobility of gas regardless of the relationship $k_{rn} = f(S_w)$, which permits development of large gas saturations in the oil zone. This is especially true of the method of McCreary.

The stability of the linearized method was, for this problem, about equal to the method of Coats, while McCreary's method permitted use of about two times larger time steps. However, in view of the poor accuracy of McCreary's method, its gain in stability is not significant.

As far as the comparison of various approximations to implicit transmissibilities is concerned, the general conclusions of Section 4(h) may be expected to hold also for gas percolation problems. Some results of comparisons, reported by Settari (1973) showed that the semi-implicit method is superior to Newton's method for a case of a reservoir with variable permeability (data described in Nolen & Berry 1972).

## CONCLUSIONS

We have studied and compared numerous methods for the handling of strong nonlinearities in the equations of two-phase flow in porous media.

It has been shown that:

(1) There are several methods that solve the problem of instability due to the treatment of transmissibilities, namely the linearized, semi-implicit, and Newton's, methods. Generally, the stability is gained at the expense of discretization error or sensitivity to the treatment of chords.

(2) The "inverse iteration" method of Section 5(c) solves the problem of handling the nonlinearity due to capillary pressure effectively without need for iteration.

(3) The methods investigated in Sections 4 and 5 can also be used to solve the stability problem due to gas percolation, and are generally superior to special earlier methods.

The conclusions made here, which are based on investigation of one-dimensional problems, were also confirmed for two-dimensional, two- and three-phase problems (Settari & Aziz 1973; Aziz *et al.* 1973; Settari 1973).

*Acknowledgements*—The financial support of the National Research Council of Canada is gratefully acknowledged.

## NOMENCLATURE

| | |
|---|---|
| $A$ | differential operator |
| $B_n$ | formation volume factor of non-wetting phase, $B_n = V_n(p)/V_{nSTC}$ where $V_n(p)$ is the volume of the non-wetting phase at pressure $p$ and $V_{nSTC}$ is the volume of the same mass of non-wetting phase at standard (stock-tank) conditions. |
| $B_w$ | formation volume factor of wetting phase. Wetting phase has two components, wetting and dissolved non-wetting. $B_w = (V_w(p) + V_{dn}(p))/V_{wSTC}$, where $V_w(p) + V_{dn}(p)$ is the total volume occupied by a certain mass of wetting component with the maximum amount of dissolved non-wetting component at pressure $p$, and $V_{wSTC}$ is the volume of the same mass of wetting component at standard conditions. This definition implies that $V_{dnSTC} = 0$, i.e. solubility is zero at $STC$. |
| $D$ | accumulation matrix. |
| **DS** | accumulation vector. |
| $DR$ | Jacobi matrix of **R**. |
| $e$ | discretization error. |
| $F$ | function, equation [47]. |
| $f_w$ | fractional flow coefficient of wetting phase. |
| **G** | vector of gravity terms. |
| $k$ | absolute permeability. |
| $k_{rl}$ | relative permeability of phase $l$. |
| $L$ | difference operator. |
| $P_c$ | capillary pressure. |
| $p_l$ | pressure of phase $l$. |
| **P** | pressure vector. |
| $q_l$ | source term for phase $l$. |
| **Q** | source vector. |
| **R** | residual vector. |
| $\mathbf{R}_m^k$ | coefficients evaluated at $m$ and pressures at $k$ level of time or iteration. |
| $R_s$ | solution ratio of non-wetting phase in wetting phase, $R_s = (V_{dnSTC}/V_{wSTC}$, where $V_{wSTC}$ is a volume of a certain mass of wetting component at $STC$, and $V_{dnSTC}$ is the $STC$ volume of the amount of non-wetting component that can, at thermodynamic equilibrium, be dissolved in that mass of wetting component at a pressure $p$. |
| $S_w$ | saturation of wetting phase. |
| $T^l_{i+1/2}$ | transmissibility coefficient. |
| $T$ | transmissibility matrix. |
| $T'$, $T''$ | "derivatives" of transmissibility matrix. |
| $T'^k_m$ | derivatives evaluated at $m$ and pressures at $k$ level of time or iteration. |
| $TX$, $TC$ | elements of matrix $T'$. |
| $t$ | time. |
| $u$ | Darcy's velocity. |
| $x$ | space coordinate. |
| $z$ | vertical coordinate, positive downwards. |

*Greek symbols*

$\gamma_l$ specific gravity, $\gamma = g\rho$.
$\delta S$ norm of saturation change.
$\Delta$ increment.
$\phi$ porosity.
$\Phi$ potential, $\Phi = p - \gamma z$.
$\lambda_l$ transmissibility or mobility of phase $l$, $\lambda = kk_{rl}/(\mu B)_l$ for compressible flow, $\lambda = kk_{rl}/\mu_l$ for incompressible flow.
$\mu$ dynamic viscosity.
$\rho$ density.

*Superscripts and subscripts*

$i$ grid point index.
$l$ denotes phase $l$, $l = w, n$.
$n$ non-wetting phase.
$n$ time level (superscript only).
$STC$ standard (or stock-tank) conditions.
$w$ wetting phase.

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## APPENDIX

### *Truncation errors for different approximations to transmissibilities*

The truncation error analysis for various difference approximations to [1] or [5] is difficult because of the coupling of these equations. However, in the incompressible case [5] can be formulated as a single equation in saturation (see, e.g. Fayers & Sheldon 1959; Hiatt 1968) for derivation). If we consider, for simplicity, a horizontal coordinate $x$, and fluids of equal density, this equation may be written as:

$$-u_T f'_w \frac{\partial S_w}{\partial x} = \phi \frac{\partial S_w}{\partial t} \qquad [A1]$$

where

$$u_T = u_w + u_n = -(\lambda_w + \lambda_n)\frac{\partial p}{\partial x}$$

is the total superficial (Darcy) velocity and $f'_w = \mathrm{d}f_w/\mathrm{d}S_w$, where

$$f_w = \frac{\lambda_w}{\lambda_n + \lambda_w}.$$

For a one-dimensional problem, $u_T = \text{const.} = q$ where $q$ is the flow rate per unit area imposed as a boundary condition. The formulation [A1] is more suitable for error analysis than [5]. Since there is no direct correspondence between the difference equations for the two formulations, the analogy is based on the assumption that the treatment of $k_{rl}$ in [5] is equivalent to the treatment of $S_w$ on the left-hand side of [A1]. The operator to be approximated will be denoted as

$$AS_w = \frac{\partial S_w}{\partial x} - C_w \frac{\partial S_w}{\partial t} = 0. \qquad [A2]$$

A difference operator approximating $A$ at the point $x_i$ will be denoted by $L(S_{w_i})$ and the truncation error of $L$ is defined as $e = AS_w(x_i) - L(S_{w_i})$.

## WEIGHTING OF TRANSMISSIBILITIES (EXPLICIT APPROXIMATIONS)

### A.1 *Explicit approximations*

Both midpoint weighting formulae [18] and [19] are represented by the same approximation

$$L_m(S_{w_i}^{n+1}) = -\frac{(S_{w_{i+1}} - S_{w_{i-1}})^n}{2\Delta x} - C_{w_i}\frac{(S_{w_i}^{n+1} - S_{w_i}^n)}{\Delta t}. \qquad [A3]$$

The truncation error at the $n + 1$ time level is found to be:

$$e_m = -\frac{\Delta t}{2}[2S'' + C_w S^{\cdot\cdot}] + \frac{\Delta t^2}{6}[3S'' + C_w S^{\cdot\cdot\cdot}] + \frac{\Delta x^2}{6} S''' + O(\Delta^3)$$

where $S' = \partial S_w/\partial x$ and $S^{\cdot} = \partial S_w/\partial t$.

This can be further simplified if it is assumed that $C_w$ is locally constant. Then $-C_wS^{\cdot\cdot} = S^{\prime\cdot}$, and $-C_wS^{\cdots} = S^{\prime\cdot\cdot}$, and the final expression is

$$e_m = -\frac{\Delta t}{2}S^{\prime\cdot} + \frac{\Delta t^2}{6}S^{\prime\cdot\cdot} + \frac{\Delta x^2}{6}S''' + O(\Delta^3). \qquad [A4]$$

For the upstream weighting, assume flow from $i-1$ to $i+1$, then the single-point formula [20] is represented by:

$$L_u(S_{w_i}^{n+1}) = \frac{(S_{w_i} - S_{w_{i-1}})^n}{\Delta x} - C_{w_i}\frac{(S_{w_i}^{n+1} - S_{w_i}^n)}{\Delta t} = 0 \qquad [A5]$$

and the truncation error may be simplified as above to give

$$e_u = \left(-\frac{\Delta t}{2} + C_{w_i}\frac{\Delta x}{2}\right)S^{\prime\cdot} + \frac{\Delta t^2}{3}S^{\prime\cdot\cdot} + \frac{\Delta x \Delta t}{2}S^{\prime\cdot\cdot} + \frac{\Delta x^2}{6}S''' + O(\Delta^3). \qquad [A6]$$

For the two-point upstream weighting [21] the operator is

$$L_{2u}(S_{w_i}^{n+1}) = -\frac{(3S_{w_i} - S_{w_{i-1}})^n - (3S_{w_{i-1}} - S_{w_{i-2}})^n}{2\Delta x} - C_{w_i}\frac{(S_{w_i}^{n+1} - S_{w_i}^n)}{\Delta t}$$

$$= -\frac{(3S_{w_i} - 4S_{w_{i-1}} + S_{w_{i-2}})}{2\Delta x} - C_{w_i}\frac{(S_{w_i}^{n+1} - S_{w_i}^n)}{\Delta t} = 0. \qquad [A7]$$

The discretization error of [A7] is found to be

$$e_{2u} = -\frac{\Delta t}{2}S^{\prime\cdot} + \frac{\Delta t^2}{3}S^{\prime\cdot\cdot} - \frac{\Delta x^2}{3}S''' + O(\Delta^3). \qquad [A8]$$

All three error expressions have a first-order time truncation term. While [A4] and [A8] have only second-order terms in $\Delta x$, [A6] has a first-order term as well as the mixed term $\Delta x \Delta t$.

A.2 *Implicit approximations*

Only single-point upstream weighting will be considered, with flow from $i-1$ to $i+1$.

The analog of the linearized method of Section 4a may be obtained as follows: Extrapolation of $k_{rl}$ according to [25] is equivalent to extrapolation of $S_w$ as:

$$S_w^{n+1} \approx S_w^n + \left(\frac{\partial S_w}{\partial t}\right)^n \Delta t$$

and the derivative is obtained from

$$-(S_{w_i} - S_{w_{i-1}})^n / \Delta x = C_{w_i}\left(\frac{\partial S_{w_i}}{\partial t}\right)^n.$$

After substitution of extrapolated values of $S_w$ in the first part of [A5] the operator will be

$$L_{ex}(S_{w_i}^{n+1}) = \frac{1}{\Delta x}\left[S_{w_i}^n - \frac{\Delta t}{\Delta x C_{w_i}}(S_{w_i} - S_{w_{i-1}})^n - S_{w_{i-1}}^n + \frac{\Delta t}{\Delta x C_{w_{i-1}}}(S_{w_{i-1}} - S_{w_{i-2}})^n\right]$$

$$- C_{w_i}\frac{(S_{w_i}^{n+1} - S_{w_i}^n)}{\Delta t} = 0.$$

If it is assumed that $C_{w_{i-1}} = C_{w_i}$ this can be written as

$$L_{ex}(S_{w_i}^{n+1}) = L_u(S_{w_i}^{n+1}) + \frac{\Delta t}{C_{w_i}\Delta x^2}[S_{w_i}^n - 2S_{w_{i-1}}^n + S_{w_{i-2}}^n] = 0. \quad [A9]$$

Then the error term is

$$e_{ex} = e_u + \frac{\Delta t}{C_{w_i}\Delta x}\left[\Delta x S'' - \Delta x \Delta t S''' - \frac{\Delta x^2}{6}S''''\right] + O(\Delta^3)$$

Since $S'' = -C_w S'$, $S''' = -C_w S''$, and $S'''' = -C_w S'''$, the final expression is

$$e_{ex} = \left(-\frac{3}{2}\Delta t + C_{w_i}\frac{\Delta x}{2}\right)S' + \frac{4\Delta t^2}{3}S'' + \frac{2\Delta x \Delta t}{3}S''' + \frac{\Delta x^2}{6}S'''' + O(\Delta^3). \quad [A10]$$

The fully implicit approximation with $k_{rl} = k_{rl}(S_w^{n+1})$ has a straightforward analog in:

$$\bar{L}_u = -\frac{(S_{w_i} - S_{w_i})^{n+1}}{\Delta x} - C_{w_i}\frac{(S_{w_i}^{n+1} - S_{w_i}^n)}{\Delta t} = 0 \quad [A11]$$

with discretization error

$$\bar{e}_u = \left(\frac{\Delta t}{2} + C_{w_i}\frac{\Delta x}{2}\right)S' + \frac{\Delta t^2}{6}S'' + \frac{\Delta x^2}{6}S'''' + O(\Delta^3). \quad [A12]$$

Note that the first-order $\Delta t$ terms have opposite signs in [A10] and [A12].

**Résumé**—La modélisation mathématique de l'écoulement simultané de deux ou trois fluides non miscibles dans un milieu poreux met en jeu un système d'équations aux dérivées partielles non linéaires couplées. Ces équations se réduisent à un système d'équations algébriques non linéaires par l'utilisation d'approximations aux différences finies pour les dérivées.

Ce modèle comporte plusieurs types de non-linéarités qui demandent une analyse soignée. On présente ici une étude systématique de toutes les méthodes disponsibles, et de quelques nouvelles, pour le traitement de ces non-linéarités.

Les techniques de solution présentées peuvent également s'avérer utiles dans le cas d'autres systèmes d'équations aux dérivées partielles fortement non linéaires.

**Auszug**—Die gleichzeitige Stroemung von zwei oder drei nicht mischbarer. Fluessigkeiten in einem prooesen Medium wird durch ein System gekoppelter nichtlinearer partieller Differentialgleichungen modelliert. Diese Gleichungen werden auf ein System nichtlinearer algebraischer Gleichungen zurueckgefuehrt, wobei die Ableitungen mit Hilfe endlicher Differenzen angenaehert werden. In diesem Modell gibt es verschiedene Typen von Nichlinearitaeten, die eine sorgfaeltige Analyse erfordern. Alle bekannten und einige neuen Methoden fuer die Behandlung der Nichtlinearitaeten dieses Modells werden systematisch untersucht. Es wird vermutet, dass die hier angegebenen Loesungstechniken auch fuer andere stark nichtlineare Systeme partieller Differentialgleichungen brachbar sind.

**Резюме**—Моделировоно совместное течение двух или трех несмешивающихся жидкостей в пористой среде посредством системы парных нелинейных частных дифференциальных уравнений. Эти уравнения упрощены до системы нелинейных алгебраических уравнений посредством метода конечных разностей. В данной модели существует несколько нелинейных типов, уравнений, требующих тщательного анализа. Здесь представлено систематическое исследование всех наличных и нескольких новых методов к разрешению нелинейности этой модели. Предполагается, что может быть также доказана применимость приведенной в работе техники решения к другим резко отличающимся от линейных уравнениям в частных производных.