The Numerical Solution of Large Systems of Linear Differential Equations

E. J. DAVISON

University of California, Berkeley, California

In chemical engineering and process control, the numerical solution of large systems of linear, time-invariant, differential equations must often be considered. Standard numerical techniques such as the Runge-Kutta method usually require excessive computational time. Since often the time solution of only a few variables is desired in such large systems, a method has been developed to take advantage of this and allows the solution of large systems of differential equations to be obtained in an extremely fast and efficient manner. The basis of the method is to solve for the poles and zeros of the system and then to find the time solution in terms of these poles and zeros.

The numerical solution of differential equations of the type

$$\dot{\mathbf{x}} = \mathbf{A} \ \mathbf{x} + \mathbf{B} \ u(t)$$

by finite-difference methods such as the Runge-Kutta technique is generally satisfactory. Sometimes, however, the time interval h of

$$\mathbf{x} \doteq \frac{\mathbf{x}(t+h) - \mathbf{x}(t)}{h}$$

must be chosen very small to ensure stability in the computation (8), and this may mean excessive computation time to find the solution. This usually happens when there is a wide distribution of eigenvalues in the matrix A. This problem has been recently studied by Henrici (6) in a review article in which he investigated a number of classical numerical techniques as well as some recent modified techniques with respect to stability. Other studies of sta-

METHOD OF SOLUTION

Consider the linear system

$$\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{B} \ u(t) \tag{1}$$

where x and B are n dimensional vectors and A is a constant $n \times n$ matrix. Suppose it is desired to find the solution for $x_r(t)$. Initial conditions are given as x(0).

Taking the Laplace transform of (1), we get

$$(s\mathbf{I} - \mathbf{A}) \chi(s) = \mathbf{B}\mathcal{L}[u(t)] + \mathbf{x}(0) \tag{2}$$

where $\chi(s)$ is the Laplace transform of x(t). This is a set of simultaneous algebraic equations in $\chi(s)$ and so Cramer's rule may be applied to solve for the variable $\chi_r(s)$:

$$\chi_r(s) = -\frac{\det(\mathbf{A_1}^*)}{\det(s\mathbf{I} - \mathbf{A})} \mathcal{L}[u(t)] - \frac{\det(\mathbf{A_2}^*)}{\det(s\mathbf{I} - \mathbf{A})}$$
(3)

wher

$$\mathbf{A_{1}}^{\bullet} = \begin{pmatrix} -s + a_{1,1} & a_{1,2} & \dots & a_{1,\,r-1} & b_{1} & a_{1,\,r+1} & \dots & a_{1,n} \\ a_{2,1} & -s + a_{2,2} & \dots & a_{2,\,r-1} & b_{2} & a_{2,\,r+1} & \dots & a_{2,n} \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ & -s + a_{r-1,\,r-1} & b_{r} & \ddots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ a_{n,1} & a_{n,2} & \dots & a_{n,\,r-1} & b_{n} & a_{n,\,r+1} & \dots & -s + a_{n,n} \end{pmatrix}$$

$$(4)$$

bility have been carried out by Dahlquist (3), Wilf (10), Certaine (1), Chase (2), Fox (4), and more recently by Rosenbrock and Storey (9).

In the solution of large systems of differential equations which arise from such systems as chemical plants, boiler systems, nuclear reactors, etc., the system's eigenvalues are usually quite widely spread and so numerical solution is often difficult to achieve. Many times in the solution of such large systems the solution of only a very few variables of the system is actually desired, the other variables being used merely in the mathematical formulation of the problem. For example in the solution of the equations of a boiler system one is really only interested in the pressure and water-level response. The purpose of this paper is to consider the solution of such large sets of differential equations when only a few variables of the system are wanted. The basis of the method is to find the solution in terms of poles and zeros of the system.

 A_2 * is the same as matrix A_1 * except that the column

$$\begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix} \quad \text{is replaced by the column } \mathbf{x}(0) = \begin{pmatrix} x_1(0) \\ x_2(0) \\ \vdots \\ x_n(0) \end{pmatrix}$$

The right-hand side terms of Equation (3) can now be factored by using numerical methods into the following (see Appendix 1):

$$\chi_{r}(s) = \frac{K(s - \alpha_{1})(s - \alpha_{2}) \dots (s - \alpha_{m})}{(s - \beta_{1})(s - \beta_{2}) \dots (s - \beta_{k})^{1}(s - \beta_{k+1}) \dots (s - \beta_{n})} \mathcal{L}[u(t)] + \frac{x_{r}(0)(s - \delta_{1})(s - \delta_{2}) \dots (s - \delta_{n-1})}{(s - \beta_{1})(s - \beta_{2}) \dots (s - \beta_{k})^{1}(s - \beta_{k+1}) \dots (s - \beta_{n})}$$
(5)

where $0 \le m \le (n-1)$. (If m=0 the numerator of the first term becomes K.)

K is known as the gain of the system. The β_i are known as the poles of the system and α_i, δ_i are known as the zeros of the system. The poles and zeros may be either real or complex; when they are complex, a conjugate pole or zero will also occur. It is assumed (for simplicity only) that one pole of the system β_k is repeated l times; in the general case there may be other poles occurring which are also repeated. It is straightforward to include these other repeated poles in the analysis which follows. It makes no difference in the analysis if the zeros are repeated. If it happens that some particular pole or zero are equal to each other, then they may be cancelled out of the expression. This is unlikely to happen however since this implies that the system of Equations (1) represents an unobservable system (7).

The input u(t) is assumed to be such that its Laplace transform $\mathcal{L}[u(t)]$ may be expressed as a rational function in s:

$$\mathcal{L}[u(t)] = \frac{P(s)}{Q(s)}$$

where P(s) is a polynomial of order p and Q(s) is a polynomial of order q and

$$0 \le p \le q$$

Most time functions which are of physical interest such as step inputs, ramp inputs, sinusoidal inputs, etc., have Laplace transforms of this type or at least can be approximated by Laplace transforms of this type.

Assume now that

$$\frac{P(s)}{Q(s)} = K_0 \frac{(s - \alpha_{m+1})(s - \alpha_{m+2}) \dots (s - \alpha_{m+p})}{(s - \beta_{n+1})(s - \beta_{n+2}) \dots (s - \beta_{n+q})}$$
(6)

Then Equation (5) may be written as

TABLE 1. TIME REQUIRED TO FIND EIGENVALUES OF MATRIX ON THE IBM 7094II DIGITAL COMPUTER

Order of matrix	Sec.
n = 10	0.5
n = 30	14
n = 50	60
n = 70	160

Table 2. Time Required to Solve $\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{B}\;u(t)$ on the IBM 7094II Digital Computer

Order of Matrix A	Solution by pole-zero method, min.	Solution by Runge- Kutta, min.
n = 10	0.02	40
n = 30	0.5	360*
n = 50	2	900*
n = 70	5	1,800*

^{*} These times are estimated.

TABLE 3. POLES AND ZEROS OF SYSTEM

Poles of System	Zeros of System
n = 10	n = 10
$\beta_2 = -0.4950069 \times 10^{-1}$	$\alpha_1 = -0.1598099$
$\beta_3 = -0.1499985$	$\alpha_2 = -0.4496683$
$\beta_4 = -0.4499994$	$\alpha_3 = -0.1350000 \times 10^1$
$\beta_5 = -0.1349998 \times 10^1$	$\alpha_4 = -0.4050000 \times 10^1$
$\beta_6 = -0.4049995 \times 10^{1}$	$\alpha_5 = -0.1214999 \times 10^2$
$\beta_7 = -0.1214999 \times 10^2$	$\alpha_6 = -0.3644997 \times 10^2$
$\beta_8 = -0.3644997 \times 10^2$	$\alpha_7 = -0.1093500 \times 10^3$
$\beta_9 = -0.1093499 \times 10^3$	$\alpha_8 = -0.3280503 \times 10^3$
$\beta_{10} = -0.3280498 \times 10^3$	
$\beta_{11} = -0.9841502 \times 10^3$	

$$\chi_{r}(s) = \frac{KK_{0}(s-\alpha_{1})(s-\alpha_{2})\dots(s-\alpha_{m})(s-\alpha_{m+1})\dots(s-\alpha_{m+p})}{(s-\beta_{1})(s-\beta_{2})\dots(s-\beta_{k})^{1}(s-\beta_{k+1})\dots(s-\beta_{n})(s-\beta_{n+1})\dots(s-\beta_{n+q})} + \frac{x_{r}(0)(s-\delta_{1})(s-\delta_{2})\dots(s-\delta_{n-1})}{(s-\beta_{1})(s-\beta_{2})\dots(s-\beta_{k})^{1}(s-\beta_{k+1})\dots(s-\beta_{n})}$$
(7)

where the β_i terms have been combined so that they are all different from one another.

 $\chi_r(s)$ may now be broken up into partial fractions in the usual way. Consider the first term of Equation (7) initially:

$$\chi_{r}(s) = \frac{A_{1}}{s - \beta_{1}} + \frac{A_{2}}{s - \beta_{2}} + \dots + \frac{A_{k-1}}{s - \beta_{k-1}} + \frac{A_{k}}{(s - \beta_{k})^{l}} + \frac{A_{k+1}}{(s - \beta_{k})^{l-1}} + \dots + \frac{A_{k+l-1}}{(s - \beta_{k})} + \frac{A_{k+l}}{(s - \beta_{k+l})} + \dots + \frac{A_{n+q}}{(s - \beta_{n+q})} + \frac{x_{r}(0)(s - \delta_{1})\dots(s - \delta_{n-1})}{(s - \beta_{1})(s - \beta_{2})\dots(s - \beta_{n})} \tag{8}$$

Table 4. Coefficients of Solution of System when n=10

where the coefficients
$$A_1, A_2, \dots A_{n+q}$$
 are evaluated as
$$A_1 = \frac{KK_0(s - \alpha_1) \dots (s - \alpha_{m+p})}{(s - \beta_2) \dots (s - \beta_{n+q})} \Big|_{s = \beta_1}$$

$$A_2 = \frac{KK_0(s - \alpha_1) \dots (s - \alpha_{m+p})}{(s - \beta_1)(s - \beta_3) \dots (s - \beta_{n+q})} \Big|_{s = \beta_2}$$

$$\vdots$$

$$\vdots$$

$$A_k = \frac{KK_0(s - \alpha_1) \dots (s - \alpha_{m+p})}{(s - \beta_1) \dots (s - \beta_{k-1})(s - \beta_{k+1}) \dots (s - \beta_n)}$$

$$A_{k+1} = \frac{d}{ds} \frac{KK_0(s - \alpha_1) \dots (s - \alpha_{m+p})}{(s - \beta_1) \dots (s - \beta_{k-1})(s - \beta_{k+1}) \dots (s - \alpha_{m+p})}$$

$$A_{k} = \frac{KK_{0}(s - \alpha_{1}) \dots (s - \alpha_{m+p})}{(s - \beta_{1}) \dots (s - \beta_{k-1}) (s - \beta_{k+1}) \dots (s - \beta_{n+q})} \Big|_{s = \beta_{k}}$$

$$A_{k+1} = \frac{d}{ds} \frac{KK_{0}(s - \alpha_{1}) \dots (s - \alpha_{m+p})}{(s - \beta_{1}) \dots (s - \beta_{k-1}) (s - \beta_{k+1}) \dots (s - \beta_{n+q})} \Big|_{s = \beta_{k}}$$

$$\vdots$$

$$\vdots$$

$$\vdots$$

$$\vdots$$

$$\vdots$$

$$\vdots$$

$$A_{k+l-1} = \frac{d^{(l-1)}}{ds^{(l-1)}} \frac{KK_{0}(s - \alpha_{1}) \dots (s - \alpha_{m+p})}{(s - \beta_{1}) \dots (s - \beta_{k-1}) (s - \beta_{k+1}) \dots (s - \beta_{n+q})} \Big|_{s = \beta_{k}}$$

$$A_{k+1} = \frac{KK_{0}(s - \alpha_{1}) \dots (s - \beta_{k}) (s - \beta_{k+l+1}) \dots (s - \beta_{n+q})}{(s - \beta_{1}) \dots (s - \beta_{k}) (s - \beta_{k+l+1}) \dots (s - \beta_{n+q})} \Big|_{s = \beta_{k}}$$

$$A_{n+q} = \frac{KK_0(s-\alpha_1)\dots(s-\alpha_{m+p})}{(s-\beta_1)\dots(s-\beta_{n+q-1})} \bigg|_{s=\beta_{n+q}}$$
(9)

Numerical differentiation must be used in evaluating $A_{k+1}, A_{k+2}, \ldots A_{k+l-1}$ and this usually is not a desirable operation. However, it was rarely found necessary to evaluate more than the first derivative in all systems considered to date. It was very unusual in fact to find any poles of the system repeated at all.

When β_j is complex a conjugate pole $\widetilde{\beta}_j$ occurs with it and only one coefficient A_j need be computed, the co-

efficient occurring with B_i being A_i . Complex arithmetic must be used to evaluate such a coefficient:

$$A_{j} = \frac{KK_{0}(s-\alpha_{1})\ldots(s-\alpha_{m+p})}{(s-\beta_{1})\ldots(s-\beta_{j-1})(s-\beta_{j+1})\ldots(s-\beta_{n+q})}$$
$$= Re(A_{j}) + i Im(A_{j})$$

It is obvious that evaluation of the coefficients A_i , i =1,2, . . . (n+q) will become inaccurate whenever a pole β_k of the system approaches β_i . In this case the best procedure to follow is to set the two poles equal $\beta_k = \beta_i$ and evaluate the coefficients as though the system had a repeated pole at β_i .

The second term of Equation (7) can similarly be broken up into partial fractions.

The time solution $x_r(t)$ of Equation (1) can now be immediately written as

$$x_r(t) = A_1 e^{\beta_1 t} + A_2 e^{\beta_2 t} + \dots + A_{k-1} e^{\beta_{k-1} t}$$

$$+ \left(A_{k} \frac{t^{l-1}}{|l-1|} + A_{k+1} \frac{t^{l-2}}{|l-2|} + \ldots + A_{k+l-2} \frac{t}{|1|} + A_{k+l-1} \right) e^{\beta_{k}t}$$

$$+ \ldots + 2\{Re(A_{j}) \cos [Im(\beta_{j})t]\} + Im(A_{j}) \sin [I_{m}(\beta_{j})t]\} e^{Re(\beta_{j})t} + \ldots$$

$$\ldots + A_{n+q}e^{\beta_{n+q}t} + \widetilde{A}_1e^{\beta_1t} + \widetilde{A}_2e^{\beta_2t} + \ldots + \widetilde{A}_ne^{\beta_nt} \quad (10)$$

where \widetilde{A}_1 , \widetilde{A}_2 ,..., \widetilde{A}_n are the coefficients of the partial fraction expansion of the second term of Equation (7).

NUMERICAL EXAMPLE OF A DIFFUSION PROCESS

The main part of the computation is spent in calculating the poles and zeros of the system and therefore the time needed to solve the system of equations given by Equation (1) is approximately three times the time needed to find eigenvalues of the matrix A (if initial conditions are zero, the factor is two). The time required to solve for each variable after this is one-third of this value. It is important therefore that a fast efficient method be used for finding eigenvalues.

Typical times needed to find eigenvalues of full matrices of various order on the IBM 7094II are given in Table 1. The QR transformation (5) was used for this calculation. Computation time necessary to solve Equation (1) can then be immediately estimated from this table.

The following set of equations was solved for variable x₁ with the above procedure and compared with the fourth-order Runge-Kutta method. They are typical of the types of equations occurring in process control and chemical engineering and represent a process which has some type of diffusion or mass transfer occurring.

 $s = Re(\beta_j) + i Im(\beta_j)$

$$\mathbf{x} = \mathbf{A}\mathbf{x} + \mathbf{B}\,\mathbf{u}(t), \quad \mathbf{x}(o) = \mathbf{O}$$

where u(t) is an unit step function and A and B are given below:

$$\begin{array}{lll} \mathbf{A} = (a_{i,j}) \text{ where} \\ a_{i,i} = -0.05 \ k^{i-1} &, \ i = 1, 2, \dots, n \\ a_{i+1,i} = 0.005 \ k^{i-1} &, \ i = 1, 2, \dots, (n-1) \\ a_{i,i+1} = 0.01 &, \ i = 1, 2, \dots, (n-1) \\ a_{n,i} = 0.02 &, \ i = 1, 2, \dots, (n-2) \\ a_{i,n} = 0.002 &, \ i = 1, 2, \dots, (n-2) \end{array}$$

and k = 1.17 when n = 70, k = 1.25 when n = 50, k = 1.45 when n = 30, and k = 3.00 when n = 10.

$$\mathbf{B}=(b_i)$$
 where $b_i=0$, $i=1,2,\ldots,(n-1)$ $b_i=1$, $i=n$

Table 2 gives a comparison of times required to solve this set of equations for different values of n on the IBM 7094II. In all cases the step size chosen in the Runge-Kutta was taken to be as large as possible to just maintain stability. It is seen that the pole-zero method is significantly faster than the Runge-Kutta method, being almost 2,000 times faster for the system of ten differential equations and 300 times faster for the system of seventy differential equations. Full accuracy is also preserved; the solutions of the equations obtained by the pole-zero method were found to always have at least five-figure accuracy.

The poles and zeros occurring in the system when

under Grant AF-AFOSR-139-66.

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APPENDIX 1: NUMERICAL CALCULATION OF POLES AND ZEROS OF A SYSTEM

It is desired to find the poles and zeros of the system. Consider finding the zeros α_1 , α_2 , ..., α_m only, since the zeros $\delta_1, \delta_2, \ldots, \delta_{n-1}$ can be found in exactly the same way. The poles of the system are simply the eigenvalues of A and were obtained by the QR transformation (5). The zeros are the solution of the following equation:

$$det \begin{pmatrix} a_{1,1} - s & a_{1,2} & & & & a_{1,r-1} \\ a_{2,1} & a_{2,2} - s & & & & a_{2,r-1} \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ a_{n,1} & a_{n,2} & & & & a_{n,r-1} \end{pmatrix}$$

n = 10 are listed in Table 3. The gain K of the system in this case was calculated as $K = 0.2000244_{10} - 2$.

The solution of the system when n = 10 was calculated as follows:

$$\begin{aligned} x_1 &= A_1 + A_2 e^{\beta_2 t} + A_3 e^{\beta_3 t} + A_4 e^{\beta_4 t} \\ &\quad + A_5 e^{\beta_5 t} + A_6 e^{\beta_6 t} + A_7 e^{\beta_7 t} + A_8 e^{\beta_8 t} \\ &\quad + A_9 e^{\beta_9 t} + A_{10} e^{\beta_{10} t} + A_{11} e^{\beta_{11} t} \end{aligned}$$

where the coefficients $A_1, A_2, \ldots, A_{10}, A_{11}$ are given in Table 4.

CONCLUSIONS

Solutions of different equations by finite-difference methods are generally satisfactory, but computation time may be excessively long when large systems of equations are considered because of the small time interval needed to ensure stability of the solution. A method is given which avoids this problem for large systems of linear differential equations when the solution of only a few variables is desired.

ACKNOWLEDGMENT

The work reported herein has been supported by the National Research Council of Canada and the Joint Services Electronics Program (U.S. Army, U.S. Navy, and U.S. Air Force)

$$\begin{vmatrix}
b_1 & a_{1,r+1} & \dots & a_{1,n} \\
b_2 & a_{2,r+1} & \dots & a_{2,n} \\
\vdots & \vdots & \vdots & \vdots \\
\vdots & \vdots & \vdots & \vdots \\
b_r & \vdots & \vdots & \vdots \\
\vdots & a_{r+1,r+1} - s & \vdots \\
\vdots & \vdots & \vdots & \vdots \\
b_n & a_{n,r+1} & \dots & a_{n,n} - s
\end{vmatrix} = 0$$
(1a)

This is a polynomial equation in s of order m, $0 \le m \le$ (n-1). It is possible to change this into an eigenvalue problem by modifying the matrix. Consider the following equation:

where Γ is an arbitrary constant. This has the same roots as Equation (1a).

It can now be shown that the roots of Equation (1a) are just the eigenvalues of the matrix.

$$\overline{A} = \begin{pmatrix} a_{1,1} & a_{1,2} & \dots & \Gamma b_1 & \dots & a_{1,n} \\ a_{2,1} & a_{2,2} & \dots & \Gamma b_2 & \dots & a_{2,n} \\ \vdots & \vdots & & & \vdots \\ a_{n,1} & a_{n,2} & \dots & \Gamma b_n & \dots & a_{n,n} \end{pmatrix}$$
(3a)

in the limit as $\Gamma \to \infty$. This may be verified by expanding the determinant of Equation (2a) about the Γb_i column and comparing terms obtained with the corresponding expansion of $det(\overline{\mathbf{A}} - \lambda \mathbf{I}) = 0.$

There will be associated with the eigenvalues of matrix A a number of extraneous eigenvalues which are not roots of Equation (1a); these are easily recognized, however, as they are of order $\sqrt{\Gamma}$ greater than the other eigenvalues of \overline{A} where m is the number of roots of Equation (1a). This may be established by comparing coefficients of the characteristic equation of (2a) with the corresponding expansion of det $(\overline{\mathbf{A}} - \lambda \mathbf{I}) = 0$. A typical value of Γ used to obtain zeros of the system was $\Gamma = 10^{15}$.

The gain K occurring in Equation (5) may be calculated as

follows:

Consider the system of Equation (1)

$$\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{B}\,u(t) \tag{4a}$$

when u(t) is a unit step function and $t \to \infty$. Then

$$\lim_{t \to \infty} \mathbf{x}(t) = -\mathbf{A}^{-1}\mathbf{B} \tag{5a}$$

provided Equation (1) represents a stable system (that is, eigenvalues of A are all in the left-hand part of the complex plane, this is normally the case for the types of equations considered in this paper).

From (5)

$$\lim x_r(t) = \lim s \, \chi_r(s)$$

$$= \lim_{s\to 0} s \frac{K(s-\alpha_1)(s-\alpha_2)\dots(s-\alpha_m)}{(s-\beta_1)(s-\beta_2)\dots(s-\beta_n)} \frac{1}{s}$$
 (6a)

$$=K(-)^{m-n}\frac{\alpha_1\alpha_2\ldots\alpha_m}{\beta_1\beta_2\ldots\beta_n}$$
 (7a)

Therefore the equating of (7a) and (5a) gives

$$K = (-)^{m-n-1} \frac{\beta_1 \beta_2 \dots, \beta_n}{\alpha_1 \alpha_2 \dots, \alpha_m} (\mathbf{A}^{-1} \mathbf{B})_r$$
 (8a)

where $(A^{-1}B)_r$ is the r^{th} element of the vector $(A^{-1}B)$.

Manuscript received November 16, 1966; revision received March 1, 1967; paper accepted March 2, 1967.

Multiphase Viscoelastic Flow Through Porous Media

JOHN C. SLATTERY

Mobil Oil Corporation, Dallas, Texas

Local volume averaging of the equations of continuity and of motion over each phase in a porous medium is discussed. For a Noll simple material, inertial effects may be neglected with respect to viscous effects as the product of a Reynolds number with a Weissenberg number goes to zero (in the limit of a Newtonian fluid, inertial effects may be neglected as the Reynolds number goes to zero). When inertial effects can be neglected, a resistance transformation for each phase is introduced which in part maps the local volume-averaged velocity vector into the local force per unit volume which that phase exerts on the pore walls and the moving phase interfaces. Capillary pressure is defined through a local surface average of the jump balance for momentum. The shape of the curve denoting capillary pressure as a function of saturation in a two-phase flow may vary with the contact angle. For an isotropic multiphase flow of incompressible materials, the functional dependence of the resistance coefficient for a Noll simple material and for a Newtonian fluid is discussed by means of the Buckingham-Pi theorem,

In an attempt to treat two-phase flows of Newtonian fluids in a porous medium, Darcy's law is written for each phase i (1, p. 653),

$$\nabla P^i + \frac{\mu_i}{\alpha_i \, k} \, \mathbf{V}^i = 0 \tag{1}$$

John C. Slattery is also at Northwestern University, Evanston, Ill.

Here P^i and V^i are understood to represent local averages of pressure and velocity, respectively, over phase i; α_i is termed the relative permeability, which is assumed to be a function of the local saturation of phase i alone (by saturation of phase i we mean the volume of phase i per unit volume of pores); k is the permeability of the rock to a single phase Newtonian fluid; μ_i is the viscosity of phase *i*. The local pressures P^1 and P^2 of the two phases