

# A Note on IMPES and Some IMPES-Based Simulation Models

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## Summary

The generalized IMPES method applies to simulation models involving any number of conservation equations. The IMPES pressure equation is a linear combination of the linearized conservation equations. This article shows the generality, simplicity, uniqueness, and derivational brevity of that equation. The associated IMPES reduction vector leads directly to the value of total compressibility in a multiphase gridblock. That compressibility in turn gives several error checks on black oil pressure/volume/temperature (PVT) data.

Three IMPES-type compositional models are compared and found to be very similar, with moderate differences in efficiencies and generality. An example problem serves two comparative purposes related to IMPES model efficiency.

## IMPES Method

The acronym IMPES was used in 1968<sup>1</sup> in a description of a numerical model for simulating black oil reservoir behavior. The IMPES method was generalized in 1980<sup>2</sup> to apply to simulation models involving any number  $n$  of conservation equations, e.g., thermal, chemical flood, and compositional models. The basic principle of the method is elimination of differences in nonpressure variables from the model's set of  $n$  conservation equations to obtain a single pressure equation. This principle was attributed to Stone<sup>3</sup> and Sheldon *et al.*<sup>4</sup> Martin<sup>5</sup> used the same principle in deriving the total compressibility of multiphase black oil systems. Perhaps the first black oil IMPES model was published by Fagin and Stewart in 1966.<sup>6</sup>

Later articles<sup>7-13</sup> presented and compared derivations of the IMPES pressure equation for  $n$ -equation compositional models. The length of some of those presentations tends to obscure the fact that the IMPES pressure equation is unique, independent of the manner of derivation, choice and ordering of variables, and ordering of equations.

This article demonstrates the simplicity and uniqueness of the IMPES pressure equation, and the brevity of its derivation for the general  $n$ -equation model. A simple relationship is shown relating total compressibility of multiphase systems to the IMPES reduction vector.<sup>2</sup> This compressibility yields error checks on black oil PVT data. Several IMPES compositional models are compared, with emphasis on their similarity. Their relative efficiencies are estimated. An example problem serves some comparative purposes.

## General Model Equations

The numerical model consists of  $n+N$  equations written for each gridblock. The first  $n$  (primary) equations express conservation of  $n$  species,

$$M_i^{n+1} - M_i^n = Q_i \Delta t, \quad i = 1, 2, \dots, n, \quad (1)$$

where  $n$  denotes the timestep level and  $Q_i$  represents interblock flow and well terms. One of the  $M_i$ 's is energy in the thermal case.  $Q_i$  is  $\sum_k T_{ik}(p_k - p) - q_i$  where the summation is over all neighbor blocks  $k$ . Capillary pressure and gravity terms in the

interblock flow terms play no conceptual role in the discussions here and are neglected. Rewriting Eq. 1 in the form for Newton iteration gives

$$\delta M_i + r_i = \delta Q_i \Delta t, \quad i = 1, 2, \dots, n, \quad (2)$$

where the residual  $r_i$  is  $M_i^l - M_i^n - Q_i^l \Delta t$ ,  $\delta M_i$  is  $M_i^{l+1} - M_i^l$ ,  $M_i^{l+1}$  is the new iterate approximating  $M_i^{n+1}$ , and  $M_i^l = M_i^n$  when  $l=0$ .

A set of  $n+N$  variables  $\{P_j\}$  can always be found or chosen such that each  $M_i$  is a unique function of one or more of the  $P_j$ . With no loss of generality, the first  $n$   $P_j$ 's are called primary variables, the remaining  $N$  variables are called secondary or constraint variables, and  $P_n$  is pressure. Additional  $N$  constraint equations express phase equilibrium constraints, the saturation or volume constraint, and any other constraints required in the model. Linearizing these and Eq. 2 gives, for a Newton iteration, the  $n+N$  model equations in the  $n+N$  unknowns in the form

$$\sum_{j=1}^{n+N} g_{ij} \delta P_j + r_i = \delta Q_i \Delta t, \quad i = 1, 2, \dots, n, \quad (3a)$$

$$\sum_{j=1}^{n+N} g_{ij} \delta P_j + r_i = 0, \quad i = n+1, n+2, \dots, n+N, \quad (3b)$$

where the  $g_{ij}$  are partial derivatives arising in the linearizations.

## Reduced Model Equations

Writing Eq. 3 in matrix form gives an  $(n+N) \times (n+N)$  matrix  $G$ , partitioned as shown in Fig. 1. The elements  $Q_i$  of the  $\mathbf{Q}$  vector are 0 for  $i > n$ . The  $N$  constraint equations are used to eliminate the coefficients of the  $C$  matrix, giving

$$A \delta \mathbf{P} = \delta \mathbf{Q} \Delta t - \mathbf{R} \equiv \mathbf{b}, \quad (4)$$

where  $\delta \mathbf{P}$ ,  $\mathbf{R}$ ,  $\delta \mathbf{Q}$ , and  $\mathbf{b}$  are column vectors of length  $n$ . The  $n \times n$  matrix  $A$  and vector  $\mathbf{R}$  are

$$A = B - C(E^{-1}D), \quad \mathbf{R} = \mathbf{f} - C(E^{-1}\mathbf{h}), \quad (5)$$

where  $\mathbf{f}$  and  $\mathbf{h}$  denote the vectors of the first  $n$   $r_i$  and the last  $N$   $r_i$ , respectively. The reduced model Eq. 4 constitutes a set of  $n$  equations in the  $n$  primary unknowns  $P_1, P_2, \dots, P_n$ . They are the basis for both fully implicit and IMPES formulations.

## IMPES Pressure Equation<sup>2</sup>

The IMPES pressure equation is obtained by multiplying the  $i$ th equation of Eq. 4 by  $X_i$  and summing the resulting  $n$  equations. The  $X_i$ 's are determined by requiring that the resulting left-hand side coefficients on the  $\delta P_j$  are 0 for nonpressure variables ( $j < n$ ). This requirement gives  $n-1$  linear equations for the  $n$   $X_i$ . The degree of freedom translates into a vector  $\mathbf{X}$  which is unique subject to an arbitrary multiplicative constant. The IMPES reduction vector  $\mathbf{X}$  is calculated as  $(A^T)^{-1}\mathbf{e}$  from

$$A^T \mathbf{X} = \mathbf{e}, \quad (6)$$

where the elements of the vector  $\mathbf{e}$  are  $e_i = c \delta_{in}$  and  $c$  is an arbitrary constant. Setting  $X_n = 1$  and solving for  $X_1 - X_{n-1}$  from the first  $n-1$  equations of Eq. 6 gives slightly greater efficiency.

The IMPES pressure equation results from premultiplication of each term in Eq. 4 by  $\mathbf{X}^T$ . Since  $\mathbf{X}^T$  is  $\mathbf{e}^T A^{-1}$ ,  $\mathbf{X}^T A \delta \mathbf{P}$  is  $c \delta p$  and the IMPES pressure equation is

$$c \delta p = \mathbf{X} \cdot \mathbf{b}. \quad (7)$$

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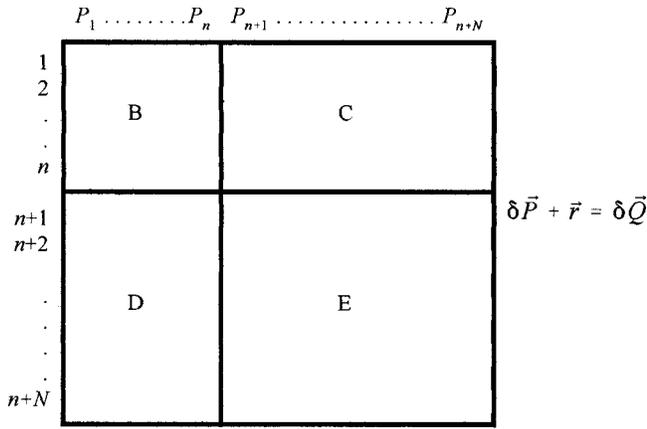


Fig. 1—Partitioning of the general model matrix.

From the last of Eq. 6,  $c$  is  $\mathbf{X} \cdot \mathbf{a}_n = \mathbf{X} \cdot \partial \mathbf{M} / \partial p$  where  $\mathbf{a}_n$  is the vector  $\{a_{in}\}$  and  $a_{in} = \partial M_i / \partial p$ . Writing out Eq. 7 to show the pressure equation transmissibilities,

$$\mathbf{X} \frac{\partial \mathbf{M}}{\partial p} \delta p = \Delta t \sum_k \mathbf{X} \cdot \mathbf{T}_k (\delta p_k - \delta p) - \mathbf{X} \cdot \mathbf{R} - \Delta t \mathbf{X} \cdot \delta \mathbf{q}. \quad (7a)$$

The transmissibility connecting the block to its neighbor  $k$  is simply  $\mathbf{X} \cdot \mathbf{T}_k$  where  $\mathbf{T}_k$  is the vector of elements  $T_{ik}$ . If the well terms  $q_i$  are implicit in pressure only, then  $\delta \mathbf{q} = \mathbf{q}' \delta p$ . Transposing all right-hand side coefficients on  $\delta p$  to the left-hand side then gives

$$\left[ \mathbf{X} \cdot \left( \frac{\partial \mathbf{M}}{\partial p} + \mathbf{q}' \Delta t \right) + \Delta t \sum_k \mathbf{X} \cdot \mathbf{T}_k \right] \delta p = \Delta t \sum_k \mathbf{X} \cdot \mathbf{T}_k \delta p_k - \mathbf{X} \cdot \mathbf{R}. \quad (7b)$$

The IMPES pressure Eq. 7 is unique, independent of the choice and ordering of variables, and ordering of equations. The reduction vector  $\mathbf{X}/c$  is unique. No vector not a multiple of  $\mathbf{X}$  satisfies the IMPES requirement that differences of all nonpressure variables are absent from the pressure Eq. 7. The Appendix illustrates the general framework of Eqs. 3-7 for three compositional models.<sup>7-9</sup>

### Multiphase Compressibility

The IMPES reduction procedure leads directly to the value of total compressibility  $c_t$  in a multiphase gridblock. Total compressibility is  $-(1/V)dV/dp$  for a system of fixed amounts of the  $n$  conserved species,  $Vm_i$ , in an original reservoir (bulk) volume  $V$ . Differentiating at constant amount of each species,

$$d(Vm_i) = 0 = m_i dV + V dm_i = m_i dV + V \sum_{j=1}^n \frac{\partial m_i}{\partial P_j} dP_j, \quad (8)$$

$i = 1, 2, \dots, n.$

Multiplying each of these equations by  $V_b$ , and noting that the resulting terms  $\partial M_i / \partial P_j$  are the entries  $a_{ij}$  of  $A$ , we obtain Eq. 8 as

$$\mathbf{M} dV = -V A d\mathbf{P}. \quad (8a)$$

Taking the dot product of both sides with  $\mathbf{X}$  gives

$$\mathbf{X} \cdot \mathbf{M} dV = -V \mathbf{X} \cdot (A d\mathbf{P}) = -V dp, \quad (9)$$

because  $\mathbf{X} \cdot (A d\mathbf{P}) = c dp$  (see the sentence prior to Eq. 7). The compressibility is then

$$c_t = -\frac{1}{V} \frac{dV}{dp} = \frac{c}{\mathbf{X} \cdot \mathbf{M}}. \quad (10)$$

For the isothermal compositional model,  $M_i$  is  $V_b \phi (S_w \rho_w w_i + S_o \rho_o x_i + S_g \rho_g y_i)$ ,  $i = 1, n$ . For any model, Eq. 10 gives the total

(rock+fluid) compressibility value for use in analysis of multiphase well test results generated by the model. Eq. 10 does not apply in fully implicit well cells.

Eq. 10 applies for gridblocks containing any number of phases. The term  $M_i$  for a given  $i$  may be energy or a component mass or combination of individual component masses, e.g., the sum of masses of components  $1 - n_c$ . For the thermal model, this total  $c_t$  is neither an isothermal nor an adiabatic compressibility. But it is the  $c_t$  value which appears in the multiphase, thermal model pressure equation of type Eq. 11 below.

Martin<sup>5</sup> derived the equation

$$\phi c_t \frac{\partial p}{\partial t} = k \lambda_t \nabla^2 p, \quad (11)$$

used in the analysis of well pressure drawdown and buildup tests under conditions of multiphase flow. This is the well known diffusivity equation for single phase flow of a slightly compressible fluid, modified to use total mobility and compressibility. Martin derived the expression for  $c_t$ , starting from the black oil Eq. 12. He used zero  $r_s$  and constant  $\phi$ :

$$\frac{\partial [\phi (b_o S_o + b_g r_s S_g)]}{\partial t} = k (\lambda_o b_o + \lambda_g b_g r_s) \nabla^2 p, \quad (12a)$$

$$\frac{\partial [\phi (b_g S_g + b_o r_s S_o + b_w R_{sw} S_w)]}{\partial t} = k (\lambda_o b_o R_s + \lambda_g b_g + \lambda_w b_w R_{sw}) \nabla^2 p, \quad (12b)$$

$$\frac{\partial (\phi b_w S_w)}{\partial t} = k \lambda_w b_w \nabla^2 p. \quad (12c)$$

Using  $dS_w = -dS_o - dS_g$  and linearization gives the left-hand side in the form  $\sum_{j=1}^3 a_{ij} \partial P_j / \partial t$  where  $P_1 = S_o, P_2 = S_g, P_3 = p$ , and  $i = 1, 2, 3$  denotes the three equations. Using the IMPES reduction vector with  $c = 1$  to eliminate  $\partial S_o / \partial t$  and  $\partial S_g / \partial t$ , gives Eq. 11 the form

$$\frac{\partial p}{\partial t} = \frac{k \lambda_t}{\phi c_t} \nabla^2 p, \quad (11a)$$

and  $c_t$  as

$$c_t = S_w c_w + S_o c_o + S_g c_g + c_r, \quad (13)$$

where

$$c_w = \frac{b'_w}{b_w} + \frac{R'_{sw} (b_o - b_g r_s) b_w}{b_o b_g (1 - r_s R_s)},$$

$$c_o = \frac{b'_o}{b_o} + \frac{R'_s (b_o - b_g r_s)}{b_g (1 - r_s R_s)},$$

$$c_g = \frac{b'_g}{b_g} + \frac{r'_s (b_g - b_o R_s)}{b_o (1 - r_s R_s)}.$$

Watts<sup>9</sup> gave these black oil compressibilities with  $r_s = R_{sw} = 0$ .

Eq. 13 gives various checks on black oil saturated PVT table data. Since the total compressibility must be positive for any saturations and  $c_r$  is 0 or positive,

$$(B_g - r_s B_o) R'_{sw} > B'_w (1 - r_s R_s), \quad (14a)$$

$$(B_g - r_s B_o) R'_s > B'_o (1 - r_s R_s), \quad (14b)$$

$$(B_o - R_s B_g) r'_s > B'_g (1 - r_s R_s). \quad (14c)$$

Additional requirements are

$$r_s R_s < 1, \quad (14d)$$

$$B_w (1 - r_s R_s) - R_{sw} (B_g - r_s B_o) > 0, \quad (14e)$$

$$B_g - r_s B_o > 0, \quad (14f)$$

$$B_o - R_s B_g > 0. \quad (14g)$$

Conditions 14e–14g follow from Eq. 14d and the requirement that the three-phase partial volumes be positive:

$$V_w = B_w - \frac{R_{sw}(B_g - r_s B_o)}{1 - r_s R_s} > 0, \quad (15a)$$

$$V_o = \frac{B_o - R_s B_g}{1 - r_s R_s} > 0, \quad (15b)$$

$$V_g = \frac{B_g - r_s B_o}{1 - r_s R_s} > 0. \quad (15c)$$

Normally  $R'_s$ ,  $r'_s$ ,  $R'_{sw}$ , and  $B'_o$  are positive, and  $B'_g$  and  $B'_w$  are negative.

Condition 14d arises as follows. A two-phase binary mixture must have  $K$  values  $K_1 < 1$  and  $K_2 > 1$ , where component 1 is the heavier component. The oil  $K$  value is

$$K_1 = \frac{r_s(\rho_o^* + R_s \rho_g^*)}{\rho_g^* + r_s \rho_o^*}, \quad (16)$$

and setting  $K_1 < 1$  gives  $r_s R_s < 1$ . The published SPE1 data<sup>14</sup> violate condition Eq. 14g at high pressure.

### Brief Descriptions of Three Isothermal IMPES Compositional Models

Young and Stephenson<sup>7</sup> (YS) chose  $n$  primary variables of  $z_1, z_2, \dots, z_{n_c-1}$ ,  $F$  and  $p$ , where  $F$  is  $\rho_o S_o + \rho_g S_g$ . Their secondary variables are  $y_1, y_2, \dots, y_{n_c-1}$ ,  $L$  and  $S_w$  (or  $\rho_w S_w$ ). Their  $n_c + 1$  constraint Eq. 3b are the  $n_c$  linearized fugacity constraints and the volume constraint  $S_w + S_o + S_g = 1$ . At the beginning of each Newton iteration, they perform the linear algebra of Eqs. 5 and 6 to obtain the pressure Eq. 7. For increased efficiency, they suggested partial or periodic update of the Jacobian as opposed to performing an equation of state (EOS) flash and Jacobian update each Newton iteration.

Acs *et al.*<sup>8</sup> (ADF) and Watts<sup>9</sup> derived the IMPES pressure Eq. 7 for their noniterative compositional models. They showed that the reduction factors  $X_i$  are single- or multiphase partial volumes  $V_i$ . Watts included a sequentially implicit calculation of saturations to allow larger time steps and greater efficiency. Linearization of their volume constraint  $V_f - \phi V_b = 0$  and combination with Eq. 2 above directly gives their pressure equation and shows that the  $X_i = V_i$ .

Wattenbarger<sup>15</sup> described use of a closure tolerance on the volume balance in IMPES models. Young and Stephenson *et al.*, and Watts extended that concept by carrying forward the volume balance discrepancy from one step to the next, thereby achieving exact mass balances with no permanent volume balance errors.

In their 1985 article, Acs *et al.* said previous methods were unable to eliminate correctly the saturation/concentration terms from the accumulation term of the pressure equation. This correct elimination was published in 1980 for compositional and more complex  $n$ -equation IMPES models,<sup>2</sup> as discussed above. Young and Stephenson<sup>7</sup> also correctly eliminated those terms in their 1983 article.

### Similarity of the Three Models

Young<sup>10</sup> states the YS, ADF, and Watts models are very similar. Wong *et al.*<sup>11,13</sup> find them less similar, describing the first as a coupled model and the latter two as decoupled models. Various authors distinguish the YS model from the ADF and Watts models as iterative versus noniterative.

The models are very similar with little or no significance to the terms iterative, noniterative, coupled, and decoupled. Since the ADF and Watts models (excluding the sequential step) are similar, the discussion here relates to the YS and ADF models and excludes the YS partial Jacobian update feature.

First, the terms iterative and noniterative are discussed. The need for or choice of Newton iteration in any type of model stems from the nonlinearity of the model equations. There is nothing in the ADF method that eliminates or reduces any of those nonlin-

earities. Their noniterative approach simply reflects their choice to perform only one iteration per time step. The YS or any other iterative model can be called noniterative, simply by constraining the timestep size (and cutting  $\Delta t$  and repeating steps when necessary) so that closure tolerances are met in one iteration. Results from the YS model, run without iteration, and the ADF model should be the same, assuming equal closure tolerances and the same logic of timestep selection.

Flow direction reversals, phase changes, negative mass, and other trauma can lead to unacceptable first-iterate results with any type of model. In such cases, Newton iteration is arguably a better response than timestep cutting or step sizing which guarantees first-iterate acceptability. The reservoir simulation literature overwhelmingly indicates a preference for iterative models. In agreement with Young's briefer assertion,<sup>10</sup> there is little significance to the terms iterative and noniterative.

A second point is that the YS and ADF models both obtain the same, correct pressure equation in similar or identical conceptual frameworks. They both begin the new iteration with the same information: EOS flash results are available along with values and derivatives of all fugacities and gas and oil densities (or equivalent terms in the ADF case). They both use those values to obtain coefficients in the pressure equation. YS use them in linearized phase equilibrium and volume constraints, Eq. 3b. They then perform the linear algebra of Eq. 5 and the minimal work of Eq. 6 to obtain the pressure Eq. 7. YS called this an analytical approach.

ADF have the form of the pressure equation directly but need to calculate the partial volumes which enter its coefficients. Several articles<sup>11-13</sup> describe the EOS-based linear algebra necessary for that. That linear algebra is no less analytical than the YS linear algebra just described.

Thus both YS and ADF perform linear algebra which couples EOS phase equilibrium and volume constraints to their conservation equations and gives the same pressure Eq. 7. They both (a) use a linear solver to solve the pressure equation for  $\delta p$ ; (b) calculate the right-hand side terms of Eq. 2 or 4; (c) calculate new  $M_i$  for  $i = 1, 2, \dots, n$ , from Eq. 2 or 4; (d) update all variables using in part an EOS flash.

Step (d) brings them to the point described at the beginning of the second paragraph above, ready for the next iteration or timestep. Both models accomplish one EOS flash iteration each Newton iteration because the phase equilibrium constraints are built into the pressure equation coefficients.

### Effects of Variable Choice and Partial Jacobian Update on Efficiency

The YS primary variables result in near-diagonal matrices  $B$  and  $A$  and a near-zero matrix  $C$ . The former reduces the work of determining  $\mathbf{X}$  from Eq. 6 from the order of  $n^3$  to the order of  $n$ . Coats<sup>16</sup> (Cs) used a set of primary variables which result in full matrices  $B$ ,  $C$ , and  $A$ . The ratio of work (multiplies and divides) related to Eqs. 5 and 6 in three-phase blocks is about

$$R_w = \frac{(16n_c^3 + 9n_c^2)/6}{(2n_c^3 + 45n_c^2)/6}. \quad (17)$$

For  $n_c = 12$ , the Cs variable choice results in a work count which is about three times larger than that using the YS variables. This work count includes the work of forming the coefficients  $g_{ij}$ . Those coefficients require an EOS flash and values of fugacities and gas and oil densities and their derivatives. That work is excluded from the counts.

The Cs  $n$  primary and  $N$  secondary variables are  $x_2, x_3, \dots, x_{n_c-1}$ ,  $S_w$ ,  $S_g$ ,  $p$  and  $y_1, y_2, \dots, y_{n_c-1}$ ,  $x_1$ , respectively. For undersaturated gridblocks, the Cs primary variables are  $z_1, z_2, \dots, z_{n_c-1}$ ,  $S_w$ ,  $p$  and  $N = 0$ . Both the YS and Cs variable sets require no pivoting. All work count and efficiency discussion relate only to saturated (three-phase) blocks. The work for undersaturated blocks is very small in comparison, except for the  $n_c^3$  Eq. 6 work with the Cs variables, which is absent with the YS variables.

Runs using a generalized model<sup>17</sup> were made for a number of problems using: (1) the YS variables and (for  $n_c > 2$ ) partial Jacobian update; (2) the Cs variables, with EOS flash and Jacobian update each Newton.

For a 24-component IMPES problem, run (1) required 34% of the central processing unit (CPU) time of run (2). The 66% reduction was 39% due to the YS variables and 27% due to partial update of the Jacobian. Complete problem data are given elsewhere<sup>18</sup> and further discussion follows.

For black oil IMPES problems the run times were the same, and for compositional IMPES problems with small  $n_c$ , the runs (1) were 10 to 20% faster. The implicit model<sup>17</sup> runs are faster with the Cs variables than with the YS variables. The work of Eq. 6, which benefits from the YS variables in IMPES, is absent in the implicit case.

The one-dimensional (1D) 300-block 24-component problem serves two comparative purposes. First, the literature reflects a lack of consensus regarding the most efficient method for two-phase EOS flash calculations. The model here<sup>17</sup> uses the Newton-Raphson (NR) method<sup>19</sup> while many authors prefer accelerated direct substitution<sup>20</sup> or similar methods. The relative efficiency (vs. Newton) of the latter method might be expected to increase as  $n_c$  increases. Thus it would be of interest to learn which method gives lower flash-related CPU in this case where  $n_c = 24$ . Second, the IMPES timesteps are limited by Eq. 18 for the first 750 (of 1,200) days. Thus it would be of interest to learn whether the fewer steps of a sequential model lead to lower total CPU time.

Runs terminated at 1,201 days due to the economic limit of 0.1 STB/D oil. Recoveries of all components were 100% at that time and 3.23 hydrocarbon pore volume (HCPV) of gas were injected. About 1,721 steps and 1,730 iterations were taken. Component mass balances (1-error/cumulative production) were 1.000 000 and gas/oil ratio (GOR) monotonically increased after breakthrough.

With the YS variables and partial Jacobian update, run (1) results were as follows.

260 seconds IBM RS6000/590 total CPU time; 3.3 seconds spent in flash; 13.2 seconds spent in phase detection; 3,646 flashes with an average of 1.33 NR iterations per flash.

With EOS flash and Jacobian update each Newton iteration, run (2) results were as follows.

470 seconds total CPU time; 134 seconds spent in flash; 13.2 seconds spent in phase detection; 199,470 flashes with an average of 1.01 NR iteration per flash.

The flash CPU times include time spent in calculating fugacities and their derivatives. Solver CPU time was 10 seconds. Automatic timestep selection used Eqs. 18 and 19 below. The data file can be obtained from the author.

## Comparison of the ADF and YS Model Efficiencies

ADF say the computing work of one timestep of their method is less than that of one iteration of an iterative model. Young<sup>10</sup> says the YS work in obtaining the pressure equation is less than the ADF work.

The work comparison here assumes that EOS flash results and all fugacities and volume or density terms and their derivatives are available. The work count is only that necessary to obtain the pressure equation coefficients. The YS work is  $(2n_c^3 + 45n_c^2)/6$ , from Eq. 17. The ADF work is  $(8/6)n_c^3$ . Thus the ADF work required to form the pressure equation exceeds the YS work for large  $n_c$ —by about 23% for  $n_c = 10$  and 88% for  $n_c = 20$ . There are no reasons for significant differences in other one-iterate work by the two models, apart from differences in solvers, EOS flash methods, and implementation.

The ADF work of calculating the  $n_c$  partial volumes involves solving an equation of type  $A\mathbf{x} = \mathbf{b}$  for  $n_c$  right-hand sides, where  $A$  is an  $n_c \times n_c$  matrix.<sup>13</sup> That work is  $(8/6)n_c^3$ .

ADF mentions a numerical way of calculating pressure equation coefficients (their Eq. 33) and say it is more efficient than

calculating partial volumes from the EOS. They omit the description of the method and of the work necessary to evaluate the numerical derivatives.

## Effects of Fully Implicit Well Terms

Fully implicit well treatment increases IMPES model efficiency moderately to significantly, depending upon the problem. A theoretical maximum speedup factor of about six can be derived for the conventional Cartesian three-dimensional (3D) seven-point spatial difference scheme. In practice, the factor is far less than that. Young<sup>10</sup> found that the number of steps and CPU times for his model decreased by a factor of more than two for his 3D SPE5<sup>21</sup> runs when he implemented fully implicit well terms.

If the well terms  $q_i$  in  $Q_i$  of Eq. 1 are taken fully implicitly then the resulting implicit coefficients augment the coefficients  $g_{ij}$  of Eq. 3a. The resulting  $X_i$  are not partial volumes in these fully implicit well cells but are still given by Eq. 6, where the  $A^T$  matrix is now a full matrix. The resulting additional  $n_c^3/3$  work in these cells for the YS model adds relatively little work per iteration because the fraction of well cells is generally very small.

The use of  $X_i = V_i$  fails in the fully implicit well cells for the ADF and Watts models. However, they can adopt a procedure similar to that of YS with the  $X_i$  obeying Eq. 6 for such cells. This would render, again, all three models essentially the same, excluding partial Jacobian update, the Watts sequential step, and efficiency.

## Watts Sequential Step

IMPES is conditionally stable because of the explicit treatment in interblock flow terms of (a) saturations in mobilities and capillary pressure and (b) compositions. The stability condition for 1D two-phase gas-oil flow, due to explicit saturations, is

$$\Delta t < \frac{1}{\frac{2T_x \lambda_g \lambda_o (dP_{cgo}/dS_g)}{(\lambda_g + \lambda_o)V_b \phi} + \frac{q df_g/dS_g}{V_b \phi}}, \quad (18)$$

neglecting mass transfer and gravity and compressibility terms. The stability condition due to explicit compositions is

$$\Delta t < \frac{V_b \phi (1 - S_w)}{q}, \quad (19)$$

$T_x$  is the transmissibility  $k \Delta y \Delta z / \Delta x$ ,  $f_g$  is fractional flow of the gas phase, and  $q$  is the total flow rate of the gas and oil phases. Watts' sequential implicit saturation treatment can significantly reduce the number of time steps. Either or both of the denominator terms in Eq. 18 can be locally or persistently large in compositional simulations. His sequential treatment negates the  $\Delta t$  limit of Eq. 18 but not that of Eq. 19.

With exceptions, capillary pressure is usually unimportant in simulations. Compositional field studies are frequently performed with low or zero  $P_c$ . Eqs. 18 and 19 show that the sequential implicit saturation treatment increases the stable time step by a factor of  $(1 - S_w) df_g/dS_g - 1$  if  $P_c$  is 0. This apparent increase in step size ( $df_g/dS_g$  can be much greater than 1) can be mitigated in practice by several considerations. The stable step of Eq. 18 often can be exceeded by 50 to 100% with no ill effects.<sup>22</sup> In many gas condensate problems there is no displacement, which is required for Eq. 18 to apply, because liquid condensate mobility is small or zero. The SPE3 problem<sup>23</sup> involves cycling of a gas condensate reservoir at high pressure followed by blowdown. All of the time steps are determined by Eq. 19. Of course, gas-water instabilities can be controlling in such cases. Finally, the increased stable step size must be weighed against the additional work of the sequential treatment. Watts notes the desirability of sequentially implicit molar rates to negate the Eq. 19  $\Delta t$  limit.

In several compositional models from 1980 on, the writer has found that the  $P_c$  stability limit of Eq. 18 can be relaxed considerably by a nonpermanent time lagging in the gridblock's tracking of the data  $P_c$  curve.

## Some Properties of the Reduction Vector $\mathbf{X}$

The ADF and Watts volume balance models require that the IMPES reduction factors  $X_i$  equal partial volumes  $V_i$ . Their models are somewhat restricted in generality because of exceptions to that equality.

$\mathbf{X}$  is not the vector of partial volumes if porosity depends upon water saturation.<sup>24</sup> The resulting added complexity of the ADF and Watts methods depends upon whether the water phase contains hydrocarbons. The  $X_i$  are not partial volumes in fully implicit well cells. The  $X_i$  are not partial volumes in the thermal model, with the exception discussed next. The simple treatment of Eq. 6 gives the correct  $X_i$  in all cases.

ADF and Watts consider  $V_f$  as a function of  $M_i$ ,  $p$ , and  $T$ , where  $M_i$  are the component masses and partial volumes  $V_i$  are  $(dV_f/dM_i)_{p,T,M_j,j \neq i}$ . Now consider  $V_f$  a function of  $M_i$  and  $p$  where  $M_i$  is always the  $i$ th conserved species, not necessarily a mass, and  $\phi$  is dependent upon pressure only. Then combining the linearized volume balance  $V_f - V_b \phi = 0$  with Eq. 2 shows that the  $X_i$  are partial volumes satisfying the definition  $V_i = (dV_f/dM_i)_{p,M_j,j \neq i}$ . If  $M_n$  is internal energy  $U$  and the other  $M_i$  are conserved masses, then  $V_n$  is taken at constant mass and pressure while each component  $V_i$  is taken at constant energy, pressure, and masses of other components. For the simple thermal model  $n=2$ ,  $M_1 = \text{mass of H}_2\text{O}$ ,  $M_2 = U$ , the partial volumes are  $V_1 = X_1 = -0.38 \text{ ft}^3/\text{lbm}$  and  $V_2 = X_2 = 0.00074 \text{ ft}^3/\text{Btu}$  in a two-phase gridblock at 1,000 psia. Note the mixed signs of the  $X_i$ .

The  $X_i$  values can be of use in understanding or detecting abnormal model behavior. Eq. 7 gives  $\delta p = \mathbf{X} \cdot \mathbf{b}$ . The  $b_i$  are independent source terms and pressure should increase in response to a positive  $b_i$ . For example, envision the gridblock as a laboratory cell and the  $b_i$  as injected amounts of mass or energy, freely chosen. If the  $X_i$  are of mixed sign, a  $j$  always exists such that for  $b_j > 0$  and all other  $b_i = 0$ , the block pressure will fall. All  $X_i$  must have the same sign to guarantee against that abnormal response.

When the  $X_i$  are of mixed sign, the abnormal pressure response just mentioned may occur and cause computing difficulty. Two examples have been discussed<sup>2</sup> in both IMPES and implicit simulation. One is the abnormal response of a fully implicit production well cell in isothermal simulation of a gas condensate reservoir. This response can occur as pressure falls through the range of condensate revaporization. It is not physically real. A sufficiently small timestep rectifies the problem, contradicting the usual statement that a fully implicit model is unconditionally stable. The second example is the negative compressibility/transmissibility or steam collapse problem in thermal simulation. This phenomenon is physically real.

## Conclusions

The generalized IMPES pressure equation is easily and briefly derived and is unique. The associated IMPES reduction vector leads directly to the value of total compressibility  $c_t$  in multiphase gridblocks. This in turn gives several error checks for black oil PVT data.

The three IMPES-type compositional models of Young and Stephenson,<sup>7</sup> Acs *et al.*,<sup>8</sup> and Watts<sup>9</sup> are briefly compared. They are very similar, excluding the partial Jacobian update<sup>7</sup> and sequential implicit<sup>9</sup> features. The volume balance models<sup>8,9</sup> assume that the IMPES reduction factors  $X_i$  equal partial volumes  $V_i$ . Since that is not always the case, they are somewhat less general than the Young and Stephenson model.

All three models derive and solve the same correct IMPES pressure equation. The manner of its derivation is irrelevant except for efficiency. For large  $n_c$ , the volume balance method of Acs *et al.*<sup>8</sup> and Watts<sup>9</sup> requires more work in forming that equation than does the method of Young and Stephenson.<sup>7</sup>

An example 24-component problem serves two comparative purposes related to the efficiency of IMPES compositional models.

## Nomenclature

$a_{ij}$	= elements of matrix $A$
$B$	= phase formation volume factor, res bbl/STB or res bbl/scf
$b$	= $1/B$
$\mathbf{b}$	= see Eq. 4
$c$	= arbitrary constant
$c_t$	= total compressibility, 1/psi
$c_r$	= rock compressibility, $(1/\phi)d\phi/dp$
$\mathbf{e}$	= vector $\{e_i\}$ where $e_i = c \delta_{in}$
$\mathbf{f}$	= see Eq. 5
$f_g$	= gas phase fractional flow, $\lambda_g/(\lambda_g + \lambda_o)$
$f_{gi}$	= fugacity of component $i$ in the gas phase
$f_{oi}$	= fugacity of component $i$ in the oil phase
$\mathbf{h}$	= see Eq. 5
$k$	= absolute permeability
$L$	= mol fraction liquid in a two-phase mixture
$m_i$	= amount of species $i$ per unit bulk volume
$M_i$	= amount of species $i$ in a gridblock, $V_b m_i$
$\partial M_i / \partial p$	= partial derivative when other primary variables are held constant
$\mathbf{m}, \mathbf{M}$	= vectors $\{m_i\}$ and $\{M_i\}$ , respectively
$n$	= number of conserved species, including water
$n_c$	= number of nonaqueous components
$N$	= number of constraint equations
$p$	= gridblock pressure
$P_{cgo}$	= gas-oil capillary pressure
$p_k$	= neighbor block pressure
$P_j$	= $j$ th dependent variable
$\mathbf{P}$	= vector of $n$ primary variables $P_j$
$Q_i$	= see Eq. 1
$\mathbf{Q}$	= vector $\{Q_i\}$
$q_i$	= production rate of species $i$ , amount per day
$\mathbf{q}$	= vector with elements $q_i$
$r_s$	= STB oil/scf
$\mathbf{R}$	= see Eq. 5
$R_w$	= work ratio
$R_g$	= scf/STB oil, dissolved gas
$R_{sw}$	= scf/STB water, dissolved gas
$S$	= phase saturation
$t$	= time
$T$	= temperature
$T_{ik}$	= transmissibility for flow of species $i$ between a gridblock and its neighbor $k$ , amount per day per unit pressure difference, dated at time level $n$ for IMPES
$\Delta t$	= timestep
$U$	= internal energy
$V_b$	= gridblock bulk volume
$V_f$	= fluid volume in a gridblock
$V_i$	= partial volume, $(dV_f/dM_i)_{p,T,M_j,j \neq i}$
$w_i$	= mol fraction of component $i$ in the water phase
$X_i$	= IMPES reduction factor
$\mathbf{X}$	= IMPES reduction vector $\{X_i\}$
$x_i$	= mol fraction of component $i$ in the oil phase
$y_i$	= mol fraction of component $i$ in the gas phase
$z_i$	= overall mol fraction of component $i$

## Greek Letters

$\delta$	= $\delta x = x^{l+1} - x^l$ for $x$ any quantity
$\lambda$	= phase mobility, $k_r/\mu$
$\lambda_t$	= total mobility of all phases
$\rho$	= phase molar density, mol/res bbl
$\rho_g^*$	= surface gas density, mol/scf
$\rho_o^*$	= surface oil density, mol/STB oil
$\phi$	= porosity, fraction
$\mu$	= phase viscosity
$\delta_{in}$	= Kronecker delta function equals 1 if $i=n$ and equals 0 if $i \neq n$

## Subscripts

- $g$  = gas phase
- $o$  = oil phase
- $w$  = water phase

## Superscripts

- ' =  $x'$  denotes  $dx/dp$  for  $x$  any quantity, unless otherwise noted
- $T$  = transpose
- $-1$  = inverse
- $l$  = Newton iteration number
- $n$  = time step

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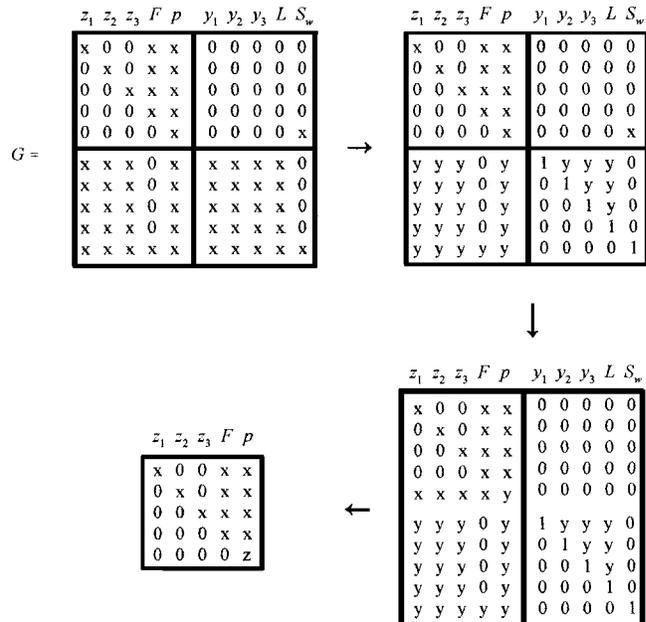
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## Appendix—Illustration of Model Reduction and Pressure Equation

The four frames below represent the steps of Eqs. 3, 5, 4, and 6 for the YS model<sup>7</sup> with  $c_r > 0$  and  $n_c = 4$ ,  $n = N = 5$ . The  $n$  conservation equations conserve mass of components 1 to 3, total mass of components 1 to 4, and mass of water, respectively. The next  $n_c$  equations are the phase equilibrium constraints  $f_{gi} - f_{oi} = 0$ , and the last  $n + N$ th equation is the volume constraint  $S_w + S_o + S_g = 1$ . The YS primary and secondary variables are listed in order as matrix column headings. The last frame represents the use of Eq. 6 and application of the  $X_i$  to eliminate nonpressure variables from the pressure equation which is the  $n$ th. See Eq. 5.



Acs *et al.*<sup>8</sup> and Watts<sup>9</sup> chose the variables  $p$  and  $M_i, i=1, n$ . Their volume constraint  $\Delta V = V_j - V_b \phi = 0$  gives

$$\sum_{i=1}^n V_i \delta M_i + \Delta V' \delta p + \Delta V^l = 0,$$

where  $\Delta V'$  is  $\partial(\Delta V)/\partial p$ . For the case  $n=4$ , choosing the four primary variables as  $M_1, M_2, M_3, p$  and the one secondary variable as  $M_4$  gives the  $G$  matrix as

$$G = \begin{matrix} & M_1 & M_2 & M_3 & p & M_4 \\ \begin{matrix} 1 \\ 0 \\ 0 \\ 0 \end{matrix} & \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} & \begin{matrix} 0 \\ 0 \\ 0 \\ 1 \end{matrix} \end{matrix}$$

The  $E$  matrix is the scalar  $V_4$  and  $E^{-1}D$  is the row vector  $\{V_1/V_4, V_2/V_4, V_3/V_4, \Delta V'/V_4\}$ . The  $4 \times 4$  matrix  $C(E^{-1}D)$  has this vector as its last row and all other elements 0. The matrix  $A = B - C(E^{-1}D)$  is then

$$A = \begin{matrix} & M_1 & M_2 & M_3 & p \\ \begin{matrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ -V_1/V_4 & -V_2/V_4 & -V_3/V_4 & -\Delta V'/V_4 \end{matrix} \end{matrix}$$

Choosing  $X_n = X_4 = 1$ , the  $X_i$  are  $V_i/V_4$  for  $i = 1, 3$ . The reduction vector  $\mathbf{X}$  is then  $\{V_1/V_4, V_2/V_4, V_3/V_4, 1\}$ , a multiple of the vector of partial volumes.

#### SI Metric Conversion Factors

bbbl $\times$ 1.589 873	E-01 = m <sup>3</sup>
Btu $\times$ 1.055 056	E+00 = kJ
ft <sup>3</sup> $\times$ 2.831 685	E-02 = m <sup>3</sup>
lbm $\times$ 4.535 924	E-01 = kg
psi $\times$ 6.894 757	E+00 = kPa

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