A NEW APPROACH OF COMPOSITIONAL SIMULATION FOR A VOLATILE OIL RESERVOIR MODELING

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ABSTRACTS

This paper proposes a new compositional simulation approach for a volatile oil reservoir modelling. The proposed formulation has an implicit equation for the oil-phase pressure and water saturation, an explicit equation for the hydrocarbon saturation, and explicit equation for the overall composition of each hydrocarbon component that satisfies thermodynamic equilibrium. An Equation of State for phase equilibrium and property calculations is used in this new formulation. Interfacial tension effects are included in this approach to characterise the thermodynamically dynamic nature of the relative permeability. A two-dimensional relative permeability algorithm is included which handles lumped hydrocarbon phase hydrocarbon phase as well as individual phase flows. For each grid block two equations are required, namely total hydrocarbon and water-phase flow equations. These equations are highly non-linear and they are linearised by using Newton-Raphson method. The resulting equations are solved by an efficient Conjugate Gradient based iterative technique to obtain pressures and saturations simultaneously, and hydrocarbon-phase saturations are deduced from their respective equations.

The new compositional simulation approach is validated through analytical and numerical methods. It is demonstrated in this present paper that the results are compared favourably with analytical techniques and published numerical results. They also confirm that the proposed codified formulation is unconditionally stable and it is as stable as fully compositional model yet the computational cost reduction was substantial.

Keywords: *compositional, equation of state, volatile, unconditionally stable*

I. INTRODUCTION

A volatile oil is defined as a high shrinkage crude oil near its critical point (Moses, 1986). In a phase diagram, it is recognised as a type between a black-oil and a gas-condensate fluid. For the volatile oil, as the reservoir pressure drops below the bubble point, the reservoir flow stream becomes mostly gas and the effective permeability to oil can exhibit a rapid decline. This can often occur within a few tens or hundreds of psi below the bubble point. The thermodynamic behaviour of a volatile oil is very sensitive to pressure and temperature changes, and hence the treatment of compositional alterations is important.

During the late of 1960's, the use of numerical compositional methods increased significantly with the rapid evolution of large scale, high speed, digital computers and the development of numerical mathematical methods. Numerical simulators, in general, utilise finite difference approximations to the rather complex partial differential equations that mathematically describe the physics and the thermodynamics of fluid flow in porous media. Simultaneously solving the continuity equations (after applying Darcy's Law), and the Equations of State for each phase, under the prescribed initial and boundary equations has become a standard method of developing a model for two-phase fluid flow in a porous media. Black oil simulators are used to simulate and predict reservoir performance by considering hydrocarbon fluids as two lumped components (phases) namely oil and gas. In this ap-

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proach, inter-phase mass transfers were assumed to be a function of pressure only. For volatile oils, and gas condensates, this assumption may not be valid (Daltaban, 1986). Compositional models are used to simulate adequately the inter-phase mass transfer and predict reservoir performance when compositional effects cannot be neglected.

The development of compositional simulators can be classified into three categories. The first category concerns with the new formulations and efficient solution schemes for the mass conservation equations. In this category the formulations are divided into two basic schemes, namely non-fully implicit and fully implicit schemes. The primary difference between these two schemes is in the treatment of the flow coefficient. The second category concerns with the efficiency of the phase equilibrium calculation schemes. In this category, the formulation is differenced whether or not they use the Equations of State for phase equilibrium and property calculations. The last category concerns the representations of physical phenomena, such as the effect of interfacial tension to the shape of relative permeability curves.

With regard to the formulations used in compositional simulations, flow equations were obtained from three sources (here we use notation similar to that Kazemi *et al*. (1978)):

a. Differential material balances describing component flow of water and hydrocarbon phases:

$$\nabla\cdot(\xi_w\lambda_w\nabla\Phi_w)+q_w=\frac{\partial}{\partial t}(\phi\xi_w S_w) \tag{1}$$

$$\nabla\cdot\left(x_i\,\xi_o\lambda_o\nabla\Phi_o+y_i\,\xi_g\lambda_g\nabla\Phi_g\right)+q_i =\frac{\partial}{\partial t}\left[\phi\left(x_i\,\xi_o S_o+y_i\,\xi_g S_g\right)\right] \tag{2}$$

b. Phase equilibrium relationships:

$$K_i=\frac{y_i}{x_i} \tag{3}$$

c. Constraint equations that require the mole fraction in each phase to sum to unity and the phase saturations to sum to unity:

$$\sum_{i=1}^{n}x_i=\sum_{i=1}^{n}y_i=\sum_{i=1}^{n}z_i=1, \tag{4}$$

$$S_o+S_g+S_w=1. \tag{5}$$

In the above equation,

λ = $(k\,k_r/m)$ = phase mobility,
Φ = phase potential,
ϕ = porosity,
ξ = molar density,
S = phase saturation,
x_i = mole fraction of component *i* in the liquid phase,
y_i = mole fraction of component *i* in the vapour phase,
z_i = total mole fraction of component *i*,
K_i = equilibrium ration of component *i*,
q_i = injection or production rate of com ponent *i*.

Several formulations which became the bases for the current state-of-the-art compositional simulation procedures have been proposed. These include two fully implicit formulations (Coats, 1980; Chien *et al*., 1985), a sequential semi-implicit formulation (Watts, 1983), an adaptive implicit scheme (Collins *et al*., 1992), three IMPES formulations (Kazemi *et al*., 1978; Nghiem *et al*., 1981; Acs *et al*., 1985) and two formulations which solve for pressure and composition simultaneously, but use explicit flow coefficients (Fussell & Fussell, 1979; Young & Stephenson, 1983). Also, the other recent formulations that are essentially similar to these formulations have been commented on (*e.g*., Guehria *et al*., 1990; Guehria *et al*., 1991; Quandalle & Savary, 1989; Branco & Rodriguez, 1994; Rodriguez & Bonet, 1994; Rodriguez, Galindo-Nava & Guzman, 1994). In general, the differences between these formulations lie on the treatment of the left hand side of Eqs. (1) & (2) and the combination of the relationships between Eqs. (1) through (5) to obtain the primary variables.

The IMPES appears to be the cheapest simulation alternative. This is because only one equation per grid block is solved (the pressure equation). In terms of physics, however, there is an important inconsistency in that the fluid is transported in the porous media by using current pressure differences and old time level transmissibilities. Hence, the velocity terms contain temporal inconsistencies. This imposes severe restriction on the use of the IMPES technique. For example, in cases where there is high vertical stratification, the change in the capillary forces over a time step cannot be neglected. When there is a

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sharp pressure and saturation gradient (like in the case of coning problems and in general when the reservoir realisation includes complex vertical and horizontal rock and fluid heterogeneities) the use of IMPES can be computationally prohibitive. In coning problems, for example, the time steps of the simulation can go well below a fraction of a second.

Fully implicit simulation approaches may seem to be computationally expensive per time step but due to their unconditionally stable nature, they can solve the most complex problems with fewer iterations and at a lower overall computational cost than IMPES scheme. However, the computer memory and CPU time required for the fully implicit methods are their major disadvantages. Moreover, the program coding is more difficult than those of the IMPES type formulations.

The adaptive implicit approach can partially solve the memory and CPU time problems exhibited by the fully implicit models while allowing the time step sizes that approach those of the fully implicit formulation. In addition, the other major drawback of this formulation is the complexity of the program since both fully implicit and IMPES type formulations are included. Finally, flash calculations are required to compute phase compositions.

In general, the IMPES is inherently unstable and the fully implicit can overkill the problem computationally. To realise the problems, it is therefore intended to propose a new formulation in order to minimise the cost of the computational simulation while maintaining the thermodynamic consistency of the prediction. The formulation must be able to model recovery from volatile oil reservoirs in the presence of heterogeneity under different recovery mechanisms. In summary, the main objective of this paper is to develop a new formulation for compositional simulation procedure to model, efficiently, the volatile oil reservoir behaviour. Then, validate the new formulation against both analytical and numerical methods.

II. GENERALIZED FLOW EQUATIONS

The continuity equation of multi-phase flow is given by Daltaban (1986):

$$\nabla\left[\sum_{m}^{M} C_{mn}\left(\frac{k k_{rm}}{\mu_m}\xi_m \nabla\Phi_m\right)\right]+\left[\sum_{m}^{M} C_{mn}\xi_m q_m\right]=\frac{\partial}{\partial}\phi\left[z_n\sum_{m}^{M} C_{mn}S_m\right] \quad (6)$$

where,

C = mass fraction,

m = phase,

n = composition.

Assuming that the hydrocarbon in phase equilibrium at all times, the remaining constraint relations are:

$$\sum_{i=1}^{N_c} x_i=\sum_{i=1}^{N_c} y_i=\sum_{i=1}^{N_c} z_i=1.0, \quad (7)$$

$$K_i=\frac{y_i}{x_i}, \quad (8)$$

$$z_i=y_i V+x_i L, \quad (9)$$

$$L+V=1.0, \quad (10)$$

$$x_i=\frac{z_i}{1+V(K_i-1)}, \quad (11)$$

$$y_i=\frac{K_i z_i}{1+V(K_i-1)}. \quad (12)$$

Capillary pressure and saturation definition are given by:

$$P_o-P_w=P_{cwo}(S_w), \quad (13)$$

$$P_g-P_o=P_{cog}(S_g), \quad (14)$$

$$S_w+S_o+S_g=1.0. \quad (15)$$

The general flow equation (Eq. (6)) can be split into water, oil and gas equations by summing up all the equations, applying mole constraint, and converting the resulting expressions into finite difference form namely:

- Water equation:

$$\Delta[T_w\Delta\Phi_w]+(\xi_w q_w)=\frac{V_r}{\Delta t}\left[(\phi\xi_w S_w)^{n+1}-(\phi\xi_w S_w)^n\right], \quad (16)$$

- Oil equation:

$$\Delta[T_o\Delta\Phi_o]+(\xi_o q_o)=\frac{V_r}{\Delta t}\left[(\phi\xi_o S_o)^{n+1}-(\phi\xi_o S_o)^n\right], \quad (17)$$

- Gas equation:

$$\Delta[T_g\Delta\Phi_g]+(\xi_g q_g)=\frac{V_r}{\Delta t}\left[(\phi\xi_g S_g)^{n+1}-(\phi\xi_g S_g)^n\right], \quad (18)$$

where,

$$T_o=\left(\frac{k A}{\Delta x}\right)\left(\frac{k_{ro}}{\mu_o}\xi_o\right),$$

$$T_g = \left(\frac{k\,A}{\Delta x}\right)\left(\frac{k_{rg}}{\mu_g}\xi_g\right),$$

$$T_w = \left(\frac{k\,A}{\Delta x}\right)\left(\frac{k_{rw}}{\mu_w}\xi_w\right),$$

In this formulation, all transmissibility term are treated implicitly. To obtain the hydrocarbon equation, both sides of oil and gas equations (Eqs. (17) & (18)) are multiplied by ξ_o^{n+1} and ξ_g^{n+1} and combined, hence (Syahrial & Daltaban, 1998):

- Hydrocarbon equation:

$$\begin{aligned}&\xi_g^{n+1}\Delta\left[T_o^{n+1}\Delta\Phi_o^{n+1}\right]+\xi_o^{n+1}\Delta\left[T_g^{n+1}\Delta\Phi_g^{n+1}\right]+\xi_g^{n+1}\left(\xi_o q_o\right)^n+\xi_o^{n+1}\left(\xi_g q_g\right)^n\\&=\frac{V_r}{\Delta t}\left[\left(\phi\xi_o\xi_g S_h\right)^{n+1}-\xi_g^{n+1}\left(\phi\xi_o S_o\right)^n-\xi_o^{n+1}\left(\phi\xi_g S_g\right)^n\right]\end{aligned} \quad (19)$$

where,

$$\left(S_h\right)^{n+1}=\left(S_o\right)^{n+1}+\left(S_g\right)^{n+1}$$

- Water equation:

$$\Delta\left[T_w^{n+1}\Delta\Phi_w^{n+1}\right]+\left(\xi_w q_w\right)^n=\frac{V_r}{\Delta t}\left[\left(\phi\xi_w S_w\right)^{n+1}-\left(\phi\xi_w S_w\right)^n\right] \quad (20)$$

Linearisation

It is clear that both water and hydrocarbon equation (Eqs. (19) & (20)) are highly non-linear and analytical solutions are not possible. Consequently, numerical methods are required. To implement numerical techniques, however, the flow equations must be linearised by using the following identities (Daltaban, 1986):

$$a^{k+1}\cong a^k+\delta a \quad , \quad (21)$$

$$\left(ab\right)^{k+1}\cong\left(ab\right)^k+a^k\delta b+b^k\delta a \quad , \quad (22)$$

where,

$$\delta a = a^{k+1}-a^k \quad ,$$

$$\delta b = b^{k+1}-b^k \quad ,$$

k = iteration level.

As a result, water and hydrocarbon equations are obtained as follows:

- Water equation in oil-phase pressure form:

$$\Delta\left[T_w\Delta\delta P_o\right]+\Delta\left[\left(T_w PC_w\right)^k\delta P_o\Delta\Phi_w^k\right]+C_{pw}\delta P_o=C_{rw} \quad , \quad (23)$$

- Water equation in the water saturation form:

$$\Delta\left[\left\{\left(\frac{KA}{\Delta L}\right)\left(\frac{\xi_w}{\mu_w}\right)^k\left(\frac{\partial k_{rw}}{\partial S_w}\right)^k-\left(T_w PC_w\right)^k\left(\frac{\partial P_{cw}}{\partial S_w}\right)^k\right\}\delta S_w\Delta\Phi_w^k\right]-\Delta\left[T_w^k\left(\frac{\partial P_{cw}}{\partial S_w}\right)\Delta\delta S_w\right]+C_{sw}\delta S_w=C_{rw} \quad , \quad (24)$$

where,

$$PC_w^k=\left(\frac{1}{\xi_w}\frac{\partial\xi_w}{\partial P_w}-\frac{1}{\mu_w}\frac{\partial\mu_w}{\partial P_w}\right)^k \quad ,$$

$$C_{pw}=-\frac{V_r}{\Delta t}\left[\left(\phi S_w\right)^k\left(\frac{\partial\xi_w}{\partial P_w}\right)^k+\left(\xi_w S_w\right)^k\left(\phi_d C_r\right)^k\right] \quad ,$$

$$C_{sw}=-\frac{V_r}{\Delta t}\left[\left(\phi\xi_w\right)^k-\left\{\left(\phi S_w\right)^k\left(\frac{\partial\xi_w}{\partial P_w}\right)^k+\left(\xi_w S_w\right)^k\left(\phi_d C_r\right)^k\right\}\left(\frac{\partial P_{cw}}{\partial S_w}\right)\right] \quad ,$$

$$C_{rw}=-\Delta\left[T_w^k\Delta\Phi_w^k\right]-\left(\xi_w q_w\right)^k+\frac{V_r}{\Delta t}\left[\left(\phi\xi_w S_w\right)^k-\left(\phi\xi_w S_w\right)^n\right] \quad .$$

- Hydrocarbon equation in oil-phase pressure form:

$$\begin{aligned}&\xi_g^k\Delta\left[T_o^k\Delta\delta P_o\right]+\xi_o^k\Delta\left[T_g^k\Delta\delta P_o\right]+\xi_g^k\Delta\left[\left(T_o PC_o\right)^k\delta P_o\Delta\Phi_o^k\right]\\&+\xi_o^k\Delta\left[\left(T_g PC_g\right)^k\delta P_o\Delta\Phi_g^k\right]+C_{ph}\delta P_o=C_{rh} \quad ,\end{aligned} \quad (25)$$

- Hydrocarbon equation in water saturation form:

$$\begin{aligned}&-\xi_o^k\Delta\left[T_g^k\left(\frac{\partial P_{cg}}{\partial S_h}\right)^k\Delta\delta S_w\right]-\xi_g^k\Delta\left[\left(\frac{KA}{\Delta L}\right)\left(\frac{\xi_o}{\mu_o}\right)^k\left(\frac{\partial k_{ro}}{\partial S_h}\right)^k\delta S_w\Delta\Phi_o^k\right]\\&+\xi_o^k\Delta\left[\left(T_g PC_g\right)^k\delta P_o\Delta\Phi_g^k\right]+C_{ph}\delta P_o=C_{rh} \quad ,\end{aligned} \quad (26)$$

where,

$$PC_o^k=\left(\frac{1}{\xi_o}\frac{\partial\xi_o}{\partial P_o}-\frac{1}{\mu_o}\frac{\partial\mu_o}{\partial P_o}\right)^k \quad ,$$

$$PC_g^k=\left(\frac{1}{\xi_g}\frac{\partial\xi_g}{\partial P_g}-\frac{1}{\mu_g}\frac{\partial\mu_g}{\partial P_g}\right)^k \quad ,$$

$$\begin{aligned}C_{ph}=-\frac{V_r}{\Delta t}&\left[\left(\xi_o\xi_g S_h\phi_d C_r\right)^k+\left[\left(\phi\xi_o S_h\right)^k-\left(\phi\xi_o S_o\right)^k\left\{\left(\frac{\partial\xi_g}{\partial P_g}\right)^k+\left[\left(\phi\xi_g S_h\right)^k-\left(\phi\xi_g S_g\right)^k\left\{\left(\frac{\partial\xi_o}{\partial P_o}\right)^k\right\}\right]\right.\right.\\&\left.\left.+\left[\left(\xi_o q_o\right)^n+\Delta\left[T_o^k\Delta\Phi_o^k\right]\left\{\left(\frac{\partial\xi_g}{\partial P_g}\right)^k\right\}\right]+\left[\left(\xi_g q_g\right)^n+\Delta\left[T_g^k\Delta\Phi_g^k\right]\left\{\left(\frac{\partial\xi_o}{\partial P_o}\right)^k\right\}\right]\right] \quad ,\end{aligned}$$

$$C_{sh}=\frac{V_r}{\Delta t}\left[\left(\phi\xi_o\xi_g\right)^k+\left[\left(\phi\xi_o S_h\right)^k-\left(\phi\xi_o S_o\right)^n\left\{\left(\frac{\partial\xi_g}{\partial P_g}\right)^k\left(\frac{\partial P_{cg}}{\partial S_h}\right)^k\right\}\right]-\left[\left(\xi_o q_o\right)^n+\Delta\left[T_o^k\Delta\Phi_o^k\right]\left\{\left(\frac{\partial\xi_g}{\partial P_g}\right)^k\left(\frac{\partial P_{cg}}{\partial S_h}\right)^k\right\}\right] \quad ,$$

$$C_{rh}=-\xi_g^k\Delta\left[T_o^k\Delta\Phi_o^k\right]-\xi_o^k\Delta\left[T_g^k\Delta\Phi_g^k\right]-\xi_g^k\left(\xi_o q_o\right)^n-\xi_o^k\left(\xi_g q_g\right)^n+\frac{V_r}{\Delta t}\left[\left(\phi\xi_o\xi_g S_h\right)^k-\left(\phi\xi_o S_o\right)^n\xi_g^k-\left(\phi\xi_g S_g\right)^n\xi_o^k\right] \quad .$$

Discretisation

The discretisation of water and hydrocarbon equations (Eqs. (23), (24), (25), and (26)) is carried out by applying a finite difference scheme using backward difference in time and central difference in space (Peaceman, 1977). With this scheme, the continuous domain is represented by a mesh of grid blocks and the flow parameters are characterised at the centre of these grid blocks. Therefore, continuous variations

in the properties are replaced by step changes. This discretisation leads to a five-point finite difference scheme for areal domains and a seven point finite difference scheme for three dimensional domains. This results in water and hydrocarbon equations having the form:

- Water Equation:

$$\begin{aligned} &W_{P_{i,j,k-1}}\,\delta P_{o_{i,j,k-1}} + W_{P_{i,j-1,k}}\,\delta P_{o_{i,j-1,k}} + W_{P_{i-1,j,k}}\,\delta P_{o_{i-1,j,k}} + \\ &W_{P_{i,j,k}}\,\delta P_{o_{i,j,k}} + W_{P_{i+1,j,k}}\,\delta P_{o_{i+1,j,k}} + W_{P_{i,j+1,k}}\,\delta P_{o_{i,j+1,k}} + \\ &W_{P_{i,j,k+1}}\,\delta P_{o_{i,j,k+1}} + W_{S_{i,j,k-1}}\,\delta S_{w_{i,j,k-1}} + W_{S_{i,j-1,k}}\,\delta S_{w_{i,j-1,k}} + \\ &W_{S_{i-1,j,k}}\,\delta S_{w_{i-1,j,k}} + W_{S_{i,j,k}}\,\delta S_{w_{i,j,k}} + W_{S_{i+1,j,k}}\,\delta S_{w_{i+1,j,k}} + \\ &W_{S_{i,j+1,k}}\,\delta S_{w_{i,j+1,k}} + W_{S_{i,j,k+1}}\,\delta S_{w_{i,j,k+1}} = C_{rw} \end{aligned} \tag{27}$$

- Hydrocarbon Equation:

$$\begin{aligned} &H_{P_{i,j,k-1}}\,\delta P_{o_{i,j,k-1}} + H_{P_{i,j-1,k}}\,\delta P_{o_{i,j-1,k}} + H_{P_{i-1,j,k}}\,\delta P_{o_{i-1,j,k}} + \\ &H_{P_{i,j,k}}\,\delta P_{o_{i,j,k}} + H_{P_{i+1,j,k}}\,\delta P_{o_{i+1,j,k}} + H_{P_{i,j+1,k}}\,\delta P_{o_{i,j+1,k}} + \\ &H_{P_{i,j,k+1}}\,\delta P_{o_{i,j,k+1}} + H_{S_{i,j,k-1}}\,\delta S_{w_{i,j,k-1}} + H_{S_{i,j-1,k}}\,\delta S_{w_{i,j-1,k}} + \\ &H_{S_{i-1,j,k}}\,\delta S_{w_{i-1,j,k}} + H_{S_{i,j,k}}\,\delta S_{w_{i,j,k}} + H_{S_{i+1,j,k}}\,\delta S_{w_{i+1,j,k}} + \\ &H_{S_{i,j+1,k}}\,\delta S_{w_{i,j+1,k}} + H_{S_{i,j,k+1}}\,\delta S_{w_{i,j,k+1}} = C_{rh} \end{aligned} \tag{28}$$

The system of equations above can be written in matrix form:

$$A\,\delta x^{k+1} = b^{k} \tag{29}$$

where,

A = Block Hepta-diagonal Jacobian Matrix containing the coefficients on the left-hand side of Eqs. (23), (24), (25) and (26),

δx = The sought solutions, $[\delta P_o, \delta S_w]$

b = Vector containing the right-hand side of Eqs. (23), (24), (25) and (26).

This particular matrix form can be solved in each Newtonian iteration by either direct, or iterative methods in order to obtain the required changes in pressure and saturation. The changes of pressure and saturation will be compared to a specified tolerance until the required criterion has been met. An efficient solution method is required in order to reduce the cost of computing time as the overall calculation inside the main iteration will increase with increasing numbers of grid blocks. Direct methods, such as Gaussian Elimination, are robust and require a fixed number of arithmetical operations to reach the solution. In this study direct-solution techniques described by Daltaban (1986) are used for the small reservoir simulation studies.

For large reservoir simulation studies, iterative methods are more favourable than direct methods since the calculations are directly proportional to the number of equations involved (n, say), whereas in direct methods it is proportional to n^2. In this study a semi-direct, semi-iterative, Conjugate Gradient Solver called ORTHOMIN (Vinsome, 1976) is used to solve pressure and saturation equations with Incomplete factorisation as Pre-conditioning (Daltaban, 1986). It is known that diagonal dominance in a matrix enhances the convergence rates of iterative solvers. In the simulator, pivoting is implemented between hydrocarbon and water equations in order to maintain diagonal dominance.

Composition and Saturation Equations

Once oil pressure and water saturation have been determined during the iteration, the compositions, oil and gas saturations can be calculated explicitly for the same iteration level. Also, all parameters inside pressure and water saturation equations that change within the iteration step are updated, such as molar densities and viscosities.

Compositions are computed explicitly by a method developed by Tsutsumi & Dixon (1972). The overall compositions of the components can be expressed as:

$$z_m^{n+1} = \left[\frac{\Delta\left[x_m^{n+1} T_o^{n+1} \Delta\Phi_o^{n+1} + y_m^{n+1} T_g^{n+1} \Delta\Phi_g^{n+1}\right] + \left(x_m \xi_o q_o + y_m \xi_g q_g\right)^n + \frac{V_r}{\Delta t}\left[z^n \left(\phi \xi_o S_o\right) + \left(\phi \xi_g S_g\right)\right]^n}{\Delta\left[T_o^{n+1} \Delta\Phi_o^{n+1} + T_g^{n+1} \Delta\Phi_g^{n+1}\right] + \left(\xi_o q_o + \xi_g q_g\right)^n + \frac{V_r}{\Delta t}\left[\left(\phi \xi_o S_o\right) + \left(\phi \xi_g S_g\right)\right]^n} \right] \tag{30}$$

Oil and gas saturations are calculated as the final result of a series of computations form:

$$S_o^{n+1} = \left[\frac{\Delta\left[T_o^{n+1} \Delta\Phi_o^{n+1}\right] + \left(\xi_o q_o\right)^n + \frac{V_r}{\Delta t}\left[\left(\phi \xi_o S_o\right)^n\right]}{\frac{V_r}{\Delta t}\left[\left(\phi \xi_o\right)^{n+1}\right]} \right], \tag{31}$$

$$S_g^{n+1} = \left[\frac{\Delta\left[T_g^{n+1} \Delta\Phi_g^{n+1}\right] + \left(\xi_g q_g\right)^n + \frac{V_r}{\Delta t}\left[\left(\phi \xi_g S_g\right)^n\right]}{\frac{V_r}{\Delta t}\left[\left(\phi \xi_g\right)^{n+1}\right]} \right]. \tag{32}$$

III. TWO-DIMENSIONAL INTERPOLATIONS OF RELATIVE PERMEABILITY

Linearisation of Eqs. (21) & (22) result in Eqs. (25) through (28). For two-phase oil and water, Eqs. (27) & (28) can be simplified to oil equations since

there is no gas in the system. Therefore, all derivatives of relative permeability with saturation are based on water saturation. However, for three-phase systems: oil, gas and water, hydrocarbon equations contain the derivative relative permeability to oil and gas with hydrocarbon saturations:

$$\frac{\partial k_{ro}}{\partial S_h} \quad \& \quad \frac{\partial k_{rg}}{\partial S_h}.$$

The main features of the new formulation exhibits relate to the derivative of the permeability to oil and gas with hydrocarbon saturations. The formulation used in this study are different with those reported previously in term of the treatment the relative permeability (*e.g.*, Kazemi *et al*. 1978; Coats, 1980; Daltaban, 1986). The authors treated relative permeability terms as a derivative to oil or gas and water saturation. After the new phase saturation has been determined, all properties of relative permeability are determined based on those new phase saturations.

In order to determine the derivative permeability to oil and gas for three-phase systems, an algorithm was written to determine the derivative of relative permeability to oil and gas with hydrocarbon saturation as a function of gas saturation. To illustrate this, Table (1) illustrates the process where the values of relative permeability to oil and gas are generated during the initialisation.

Table 1 shows that derivatives of oil and gas relative permeability with hydrocarbon are stored as a function of gas saturation. The specification of three-phase relative permeabilities are determined by the methods proposed by Stone (1970), Stone (1973) and Dietrich & Bondor (1976). As a results, during iteration of each time step, after the new phase saturation have been determined, the derivative of oil and gas relative permeability with hydrocarbon saturation are obtained by using two-dimensional interpolations.

In addition to the treatment of the relative permeability curves, in compositional modelling, particularly in the miscible displacement where the two fluids are first-contact miscible, they can be mixed together in all proportions and all mixtures remain single-phase. Because only single-phase ensures, there is no interface and hence no interfacial tension between the fluids. This interfacial tension will become important for the fluid near the critical point, where interfacial tension approaches to zero, residual phase saturations also approach to zero as the relative permeability curves approach to straight lines.

Analytical representation of individual-phase relative permeabilities incorporating interfacial tensions for both two- and three-phases were derived by Coats (1980) and Nghiem *et al*. (1981). The formulation derived by Coats (1980) were fully implemented in this study. The gas/oil interfacial tension is calculated from the Macleod-Sugden correlation (Reid, Prausnitz & Sherwood, 1977):

$$\sqrt[4]{\sigma} = \sum_{i=1}^{N_c} P_{chi}\left(\xi_L\ x_i - \xi_V\ y_i\right) \qquad (33)$$

All parameters in Eq. (35) can be calculated using the Equations of State, except P_{chi}. If a gas cap is present initially in the reservoir, σ is calculated from Eq. (35) using the equilibrium phase densities and compositions. If the original reservoir is undersaturated, bubble point pressure is calculated and σ is calculated from Eq. (35) using the equilibrium phase densities and compositions at that pressure.

IV. EQUATIONS OF STATE AND VAPOUR-LIQUID EQUILIBRIA

Equations of State (EOS) offer the advantage of providing a single and consistent source of *K*-value predictions, phase densities and compositions at reservoir conditions. In the volatile oil reservoir, the Equations of State are used when either the process is depletion/cycling or miscible flooding with MCM generated *in situ*. In the latter process, Equations of State have become more important than the former since phase compositions and properties are converging at the critical point. It is, therefore, crucial to have a reasonable understanding of the Equations of State.

Many forms of Equations of State have been proposed since Van der Waals. The EOS types used in this study are Redlich-Kwong (1949) (R-K EOS), Soave-Redlich-Kwong (1972) (S-R-K EOS), Zudkevitch-Jofffe-Redlich-Kwong (1970) (ZJRK) and Peng-Robinson (1976)(P-R EOS). Many authors generalised the EOS in general forms (*e.g.*, Martin, 1979; Schmidt & Wenzel, 1980; Coats, 1982). Schmidt & Wenzel (1980) have shown that almost all cubic Equations of State can be expressed in a generalised form by the following four-constant expression:

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Table 1
Preparation of Relative Permeability Data During Initialisation

S_w	S_h	S_g	S_o	k_{row}	k_{rg}	k_{rw}	k_{rog}	k_{ro}
S_{wc}	1-S_{wc}	S_{gir}	1-S_g-S_o	..	..	..	..	..
..	..	..	..	..	..	..	..	..
1-S_{or}	S_{or}	S_{gir}	1-S_g-S_o	..	..	..	..	..
S_{wc}	1-S_{wc}	S_{gir}+0.01	1-S_g-S_o	..	..	..	..	..
..	..	..	..	..	..	..	..	..
1-S_{or}	S_{or}	S_{gir}+0.01	1-S_g-S_o	..	..	..	..	..
S_{wc}	1-S_{wc}	..	1-S_g-S_o	..	..	..	..	..
..	..	..	..	..	..	..	..	..
1-S_{or}	S_{or}	..	1-S_g-S_o	..	..	..	..	..
S_{wc}	1-S_{wc}	S_{gmax}-0.01	1-S_g-S_o	..	..	..	..	..
..	..	..	..	..	..	..	..	..
1-S_{or}	S_{or}	S_{gmax}-0.01	1-S_g-S_o	..	..	..	..	..
S_{wc}	1-S_{wc}	S_{gmax}	1-S_g-S_o	..	..	..	..	..
..	..	..	..	..	..	..	..	..
1-S_{or}	S_{or}	S_{gmax}	1-S_g-S_o	..	..	..	..	..

$$p=\frac{RT}{V-b}-\frac{a}{V^2+u\,b\,V+w\,b^2} \qquad (34)$$

where *a*, *b*, *u* and *w* are constant parameters and have different values for each types of Equation of State.

Due to semi-empirical nature of EOS, the prediction of liquid properties, especially liquid densities and volumes are usually lower than actual. In the S-R-K EOS, for example, the critical compressibility factor takes on the unrealistic universal critical compressibility of 0.333 (at the critical point) for all substances. As a result, the molar volumes are typically overestimated, *i.e.*, densities are underestimated. The concept of volume translation had been introduced after Soave's modification of the Redlich-Kwong equation. Volume translation attempts to alleviate one of the major deficiencies of the Redlich-Kwong EOS, *i.e.*, poor liquid volumetric prediction. Peneloux, Rauzy & Freze (1982) proposed a procedure for improving the volumetric predictions of the S-R-K EOS by introducing a volume correction parameter, into the equation. This parameter does not change the vapour-liquid equilibrium conditions determined by the unmodified S-R-K equation, but modifies the liquid and gas volumes by effecting the following translation along the volume axis. In this study, a volume correction parameter is tied into Equation of States.

Also in this study, a combination of a successive substitution method (Nghiem, Aziz & Li, 1983) and a Minimum Variable Newton-Raphson method (Fussell & Yanosik, 1978) are used to calculate flash composition and saturation points. The successive substitution methods can be used to detect the single phase region without having to compute the saturation pressure. However, this method converges very slowly (or not at all) near the critical region. In this study, when the successive substitution method is converging slowly, the computer program automatically switches to the more robust technique of Minimum Variable Newton-Raphson (MVNR). The MVNR method is a robust algorithm for solving the non-linear system of equations describing thermodynamic equilibrium.

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V. VALIDATION PROCEDURES

The equations presented in the previous section were coded into a computer program that provides a field-scale reservoir simulator which models the behaviour of compositional processes and in particular the behaviour of volatile oil reservoirs. The results from the simulation procedure are validated by comparing them against both analytical and numerical models.

The Buckley-Leverett method (Buckley & Leverett, 1942) was used as the analytical model. In this section, the Buckley-Leverett solution is used to validate the model since it can predict the exact solution for the one-dimensional immiscible displacement of two fluids and is well documented in the literatures (*e.g.*, Dake, 1978; Archer & Wall, 1986). Numerical validation was provided by *Eclipse300* (a fully compositional simulator that is the *de rigour* industry standard (GeoQuest, 1996)). For this purpose, fluid and relative permeability data are taken from a published paper (Killough & Kossak, 1987). To validate the simulation results, four test cases were considered:

1. Water injection in a one-dimensional reservoir,
2. Gas injection in a one-dimensional reservoir,
3. The fifth SPE comparison problem for three-dimensional reservoirs (Killough & Kossak, 1987),
4. Water coning model in a two-dimensional model.

Table 2
Data used in the Analytical Buckley-Leverett for Comparison

Property	Field Units	SI Units
Reservoir Length, L	2000 ft	609.60 m
Grid Block Length, Δx	100 ft	30.48 m
Area of Cross-section	1000 ft^2	92.9 m^2
Grid System	40x1x1	40x1x1
Dip Angle, θ	0	0
Porosity, ϕ	30%	30%
Absolute Permeability, k	500 mD	4.93×10^{-13} m^2
Viscosity of Water, m_w	0.70 cp	0.0007 Pa×s
Initial Water Saturation, S_{wi}	20%	20%
Initial Oil Saturation, S_{oi}	80%	80%
Initial Gas Saturation, S_{gi}	0%	0%
Production Rate, q_{TOT}	80 RB/Day	12.72 m^3/Day
Production Rate, q_{inj}	80 RB/Day	12.72 m^3/Day
Production Point, Block No.	1	1
Injection Point, Block No.	40	40
Rock Compressibility, c_r	4×10^{-6} psi^{-1}	5.80×10^{-7} kPa^{-1}
Water Compressibility, c_w	3×10^{-6} psi^{-1}	4.35×10^{-7} kPa^{-1}

Buckley-Leverett Method

A one dimensional system of 40 grid blocks was constructed with an injector and producer at the extremas. Tables 2 & 3 contain the basic reservoir data and reservoir fluid properties for validating the model against analytical and numerical models. Initial reservoir pressure was set up to 4000 psia, with bubble point pressure and temperature at 2303 psia and 160°F respectively. Figure 1 shows the water-oil relative permeability curves. In order to keep the reservoir pressure always above the bubble point, the injection water and production rates are set to 80 RB/Day.

Reservoir Fluid Properties

Figure 3 shows a comparison of the water saturation profiles obtained after 300 days of simulation by the Buckley-Leverett method, *Eclipse* and this study respectively. It can be seen that this study provides almost identical results with *Eclipse* and gives sufficiently close approximations to the Buckley-Leverett solution, except for numerical dispersion at the water front due to the use of single point upstream mobility weighting. In addition to the accuracy of this formulation with analytical and other numerical method, this formulation only need one to two iterations per time step. With the less number equations to be solved per time step than fully implicit method, this formulation is as cheap as IMPES.

Gas Injection

For the system described in previous section, a gas injector well was introduced while the same basic reservoir data and properties were retained. Table

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Table 3
Reservoir Fluid Properties

Comp.	Mole Frac.	T_c (°R)	P_c (psia)	Z_c	MW	●
C_1	0.50	343.0	667.8	0.290	16.01	0.0130
C_3	0.03	665.7	616.3	0.277	44.10	0.1524
C_6	0.07	913.4	436.9	0.264	86.18	0.3007
C_{10}	0.20	1111.8	304.0	0.257	149.29	0.4885
C_{15}	0.15	1270.0	200.0	0.245	206.00	0.6500
C_{20}	0.05	1380.0	162.0	0.235	282.00	0.8500

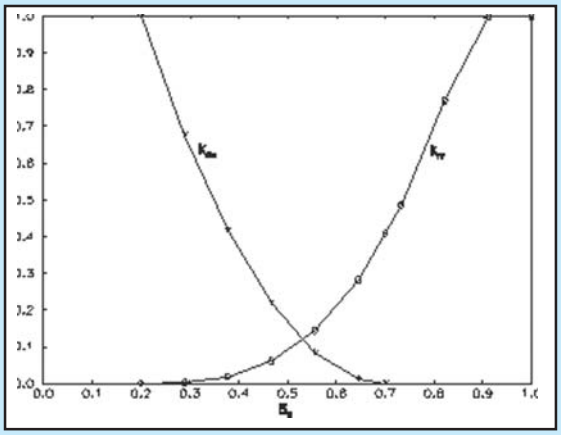

Figure 1
Water-Oil Relative Permeability Curves

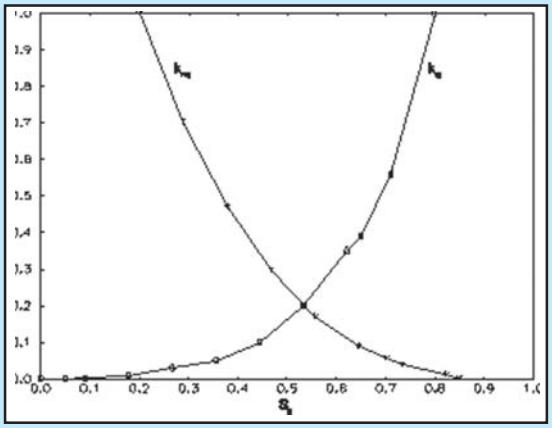

Figure 2
Gas-Oil Relative Permeability Curves

4 shows the composition of gas injection. Also, a one-dimensional system of 40 grid blocks was constructed with an injector and producer at the extremes. In this case, initial reservoir pressure was set at 2000 psia with initial oil, gas and water saturation distributions of 71.3%, 8.7% and 20% respectively in each grid block. Figure 2 shows gas-oil relative permeability curves. With gas injection and production rates of 80 RB/Day, reservoir pressure can be kept close to original reservoir pressure of 2000 psia.

Figure 4 shows a comparison of the gas saturation profiles obtained after 300 days of simulation by this study and *Eclipse*. Similarly with the case of water injection, this case only need one to two iterations per time step.

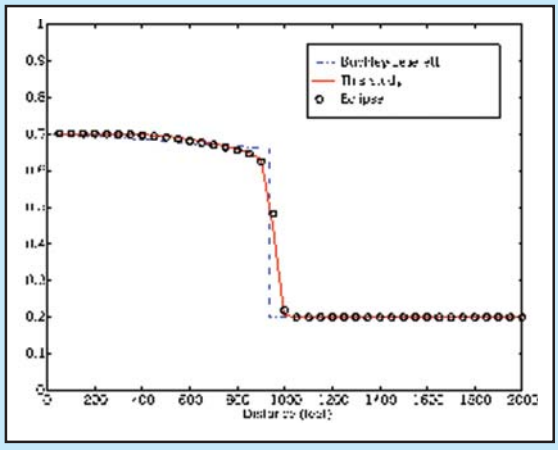

Figure 3
Water Injection in a One-Dimensional Reservoir

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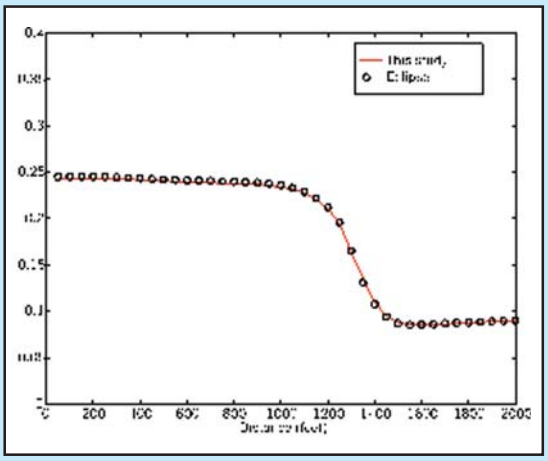

Figure 4
Gas Injection in a One-Dimensional Reservoir

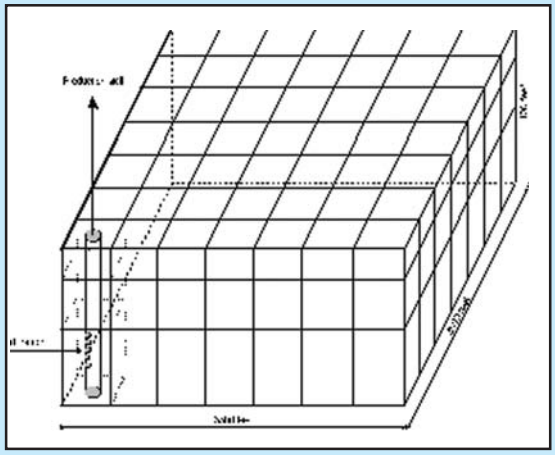

Figure 5
Location of Production Well in the Three-Dimensional Model

Table 4
Composition of the Injection Gas

Dry Gas	C_1	C_3	C_6	C_{10}	C_{15}	C_{20}
Mole Fraction	0.70	0.03	0.07	0.10	0.05	0.05

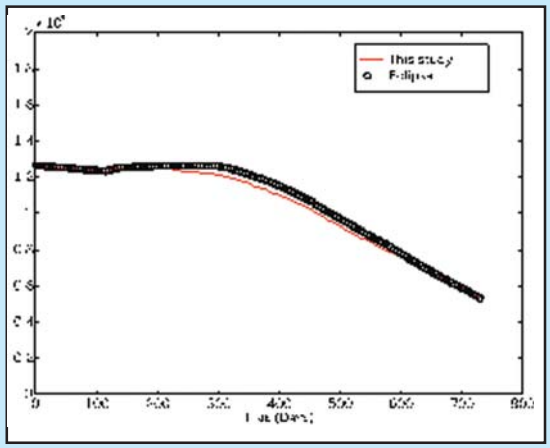

Figure 6
Comparison of Oil Production Rates from This Study and Eclipse

The Fifth SPE Comparison Problem

The numerical simulator developed in this study was compared with *Eclipse* in a three-dimensional reservoir, using data shown in Table 5 (Killough & Kossack, 1987). Table 3 shows the fluid properties employed as used in the case of water injection. A set of relative permeability curves for oil-water and gas-oil systems are shown in Figures 1 & 2. A production well is situated in layer 3 in in grid block 5 in block *x* and *y* directions as shown in Figure 5. The well is produced for two years with oil producing rate of 120000 STB/Day. Figure 6 shows that oil production predicted from this study and *Eclipse* are in excellent agreement.

Radial Models

To illustrate the validation of a numerical coning model utilising the method described in the previous chapter, a two-dimensional water coning problem was selected. Using similar data taken from published paper (Blair & Weinaug, 1969), a 10´20 block model was constructed. The system being considered is of a cylindrical shape having radius of 1300 ft and a thickness of 610 ft, of which the top 110 ft contained oil and connate water as shown in Figure 7. The radii at block boundaries are set at 2.5, 3.9, 9.0, 18.5, 38.1, 78.3, 332.0, 663.9, 1131.5, and 1300.0 ft. The data is similar to that of the Blair & Weinaug (1969) study except in the thickness of the water zone which was increased to facilitate earlier water breakthrough. The radial permeability is 1000 mD in the oil zone and 5000 mD in the water zone. The ratio of vertical to radial permeability for oil and water zones is 0.1. The water permeability zone and their ratio of vertical to horizontal permeability have been chosen by

the authors (Blair & Weinaug, 1969) to be unrealisticly high to accelerate the cone development and to test the ability of simulation approach to cope with this situation.

A description of the layering model is given in Table 7. In this study, a least volatile oil reservoir (Coats & Smart, 1982), with properties shown in Table 8 was chosen. This type of oil has the bubble point at 1661 psia and 131°F. A set of water-oil relative permeability curves is shown in Table 6. The bottom-water drive system produced 6000 RB/Day from layers 2 and 3.

Calculations were made for the case which predicted the model performance at 1000 days. Table 9 shows the calculated performance for the example case. The comparison of the water saturation at the bottom of the producing interval from *Eclipse* and this study is shown in Figure 8. Figure 9 shows the comparison of water-oil ratio from *Eclipse* and this study.

Table 5
Data used in the Fifth SPE Comparison Problem

Property	Field Units	SI Units
Grid System	7x7x3	7x7x3
Areal Dimensions	3500x3500 ft^2	1067x1067 m^2
Thickness Layer 1, h_1	20 ft	6.10 m
Thickness Layer 2, h_2	30 ft	9.14 m
Thickness Layer 3, h_3	50 ft	15.24 m
Reservoir Depth	8325 ft	2537.5 m
Permeability Layer 1, kx_1	500 mD	$4.93x10^{-13}$ m^2
Permeability Layer 2, kx_2	50 mD	$4.93x10^{-13}$ m^2
Permeability Layer 3, kx_3	200 mD	$1.97x10^{-13}$ m^2
Permeability Layer 1, ky_1	500 mD	$4.93x10^{-13}$ m^2
Permeability Layer 2, ky_2	50 mD	$4.93x10^{-13}$ m^2
Permeability Layer 3, ky_3	200 mD	$1.97x10^{-13}$ m^2
Permeability Layer 1, kz_1	50 mD	$4.93x10^{-13}$ m^2
Permeability Layer 2, kz_2	50 mD	$4.93x10^{-13}$ m^2
Permeability Layer 3, kz_3	25 mD	$2.47x10^{-13}$ m^2
Porosity, ϕ	30%	30%
Initial Oil Saturation, S_{oi}	80%	80%
Initial Gas Saturation, S_{gi}	0%	0%
Initial Water Saturation, S_{wi}	20%	20%
Residual Oil Saturation, S_{or}	30%	30%
Residual Gas Saturation, S_{gr}	5%	5%
Initial Reservoir Pressure, P_i	4000 psia	27.5 Mpa
Datum	8400 ft	2560 m
Oil Production Rate, q_o	120000 STB/Day	19000 sm^3/Day
Rock Compressibility, c_r	$4x10^{-6}$ psi^{-1}	$5.80x10^{-7}$ kPa^{-1}
Water Compressibility, c_w	$3x10^{-6}$ psi^{-1}	$5.80x10^{-7}$ kPa^{-1}
ςισχοσιτψ οφ Ωατερ, μ_ω	0.70 cp	0.0007 Pa×s

V. CONCLUSIONS

1. Volatile oil is generally defined as high shrinkage crude oil and near critical oil with high initial solution gas oil ratio (ranges between 2000 and 3500 SCF/STB), its formation volume factor is usually greater than 2 res BBL/STB and stock-tank oil gravity is usually 45°API or more.
2. As reservoir pressure goes below the bubble point pressure, the effective permeability to oil shows rapid decline and the reservoir flow stream becomes mostly gas within a few hundred psi below the bubble point.
3. The model formulation developed has an implicit transmissibility term, an implicit for oil-phase pressure and water saturation and explicit equation for the overall composition of each hydrocarbon

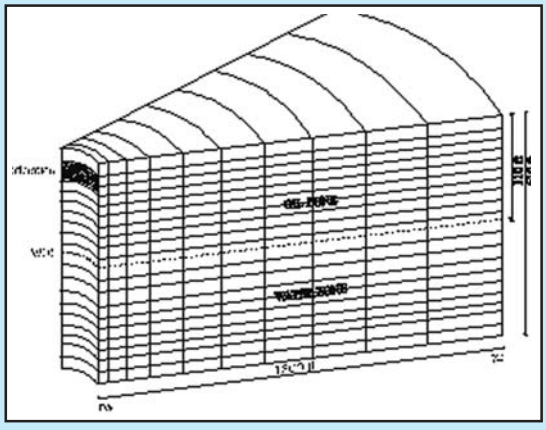

Figure 7
Two-Dimensional Single Well Model

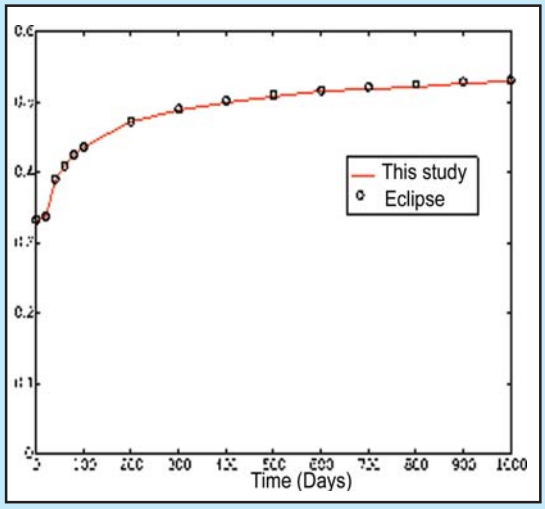

Figure 8
Calculated Water Saturation at Bottom Producing Block

Table 6
Water-Oil Relative Permeabilities and Capillary Pressures

S_w	k_{rw}	k_{row}	P_{cow}
0.2000	0.0000	1.0000	45.0000
0.2899	0.0022	0.6769	19.0300
0.3778	0.0180	0.4153	10.0700
0.4667	0.0607	0.2178	4.9000
0.5556	0.1438	0.0835	1.8000
0.6444	0.2809	0.0123	0.5000
0.7000	0.4089	0.0000	0.0500
0.7333	0.4855	0.0000	0.0100
0.8222	0.7709	0.0000	0.0000
0.9111	10.000	0.0000	0.0000
10.000	10.000	0.0000	0.0000

component that satisfies thermodynamic equilibrium. For each grid block, only two equations are required in simultaneous algebraic form, namely the pressure and water saturations. It is unconditionally stable like the Fully Implicit approach and can be as cheap as IMPES.

4. The validation tests have shown that this formulation gives sufficiently close approximations to the analytical Buckley-Leverett solution and other numerical methods. The new model requires less number of equations to be solved per time step than the fully implicit method and only needs one to two iterations per time step, this formulation is as cheap as IMPES and is as accurate as fully implicit methods.
5. An algorithm for handling

Table 7
Properties by Each Layer

Layer No.	Thickness (ft)	◆ (frac.)	k_h (mD)	k_v (mD)
1	3.75	0.207	1000	100
2	8.75	0.207	1000	100
3	7.50	0.207	1000	100
4	6.25	0.207	1000	100
5	8.75	0.207	1000	100
6	10.00	0.207	1000	100
7	11.25	0.207	1000	100
8	15.00	0.207	1000	100
9	18.75	0.207	1000	100
10	20.00	0.207	1000	100
11	50.00	0.207	5000	500
12	50.00	0.207	5000	500
13	50.00	0.207	5000	500
14	50.00	0.207	5000	500
15	50.00	0.207	5000	500
16	50.00	0.207	5000	500
17	50.00	0.207	5000	500
18	50.00	0.207	5000	500
19	50.00	0.207	5000	500
20	50.00	0.207	5000	500

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Table 8
Fluid Compositions and Properties at Reservoir Conditions

Comp	Mole Frac.	T_c (°F)	p_c (psia)	Z_c	MW	ω	P_{ch}
CO_2	0.0008	88.79	1071.33	0.2741	44.01	0.225	78.0
N_2	0.0164	-232.51	492.31	0.2912	28.01	0.040	41.0
C_1	0.2840	-116.59	667.78	0.2847	16.04	0.013	77.0
C_2	0.0716	90.10	708.34	0.2846	30.07	0.099	108.0
C_3	0.1048	205.97	618.70	0.2775	44.10	0.152	150.3
C_4	0.0840	295.43	543.45	0.2772	58.12	0.196	187.2
C_5	0.0382	378.95	487.17	0.2688	72.15	0.241	228.9
C_6	0.0405	461.93	484.38	0.2754	84.00	0.250	271.0
C_7^+	0.3597	923.00	201.61	0.2178	252.00	0.822	648.3

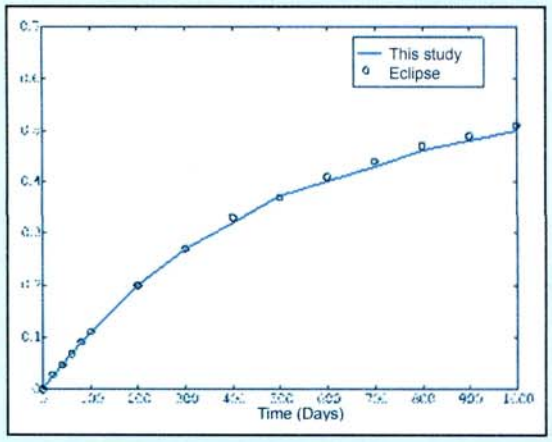

Figure 9
Calculated Water-Oil Ratio

oil and gas relative permeability as a function of total hydrocarbon saturation were incorporated in the formulation. It enables the model to simulate the reservoir behaviour under different recovery mechanisms.

6. Equations of State are the consistent source of parameter estimations for describing the thermodynamic behaviour of volatile oils by providing a

Table 9
Coning Model Performance - Sw : Water Saturation at Bottom Producing Block

Time (Days)	Q_o (STB/Day)	Q_w (STB/Day)	*WOR* (frac.)	S_w (frac.)
0	0	0	0.000	0.000
20	4740	134	0.028	0.337
40	4669	221	0.047	0.390
60	4594	312	0.068	0.409
80	4514	410	0.091	0.425
100	4416	493	0.110	0.436
200	4149	825	0.200	0.471
300	3949	1073	0.270	0.489
400	3821	1231	0.320	0.499
500	3715	1361	0.370	0.508
600	3630	1466	0.400	0.514
700	3567	1541	0.430	0.518
800	3512	1606	0.460	0.522
900	3465	1662	0.480	0.525
1000	3427	1707	0.500	0.528

single and consistent source of K-value predictions, phase densities and compositions at reservoir conditions.

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