



International Journal of Current Research and Academic Review

ISSN: 2347-3215 Volume 3 Number 7 (July-2015) pp. 231-252

www.ijcrar.com



Design of a simulator of a reservoir investigating the effect of surfactant mixture in an enhanced oil recovery process

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KEYWORDS

Chemical flooding,
Surfactant,
Multicomponent,
Multidimensional
and multiphase
system,
Orthogonal
collocation technique,
Finite
difference
method

A B S T R A C T

The present study deals with the development of a simulator for multidimensional, multiphase and multicomponent surfactant flooding concerned with the characteristics of the chemical slugs for an enhanced oil recovery process. The development starts with the description of the fluid flow in permeable media from the basic conservation laws and with linear constitutive theory. From this physical basis a mathematical formulation of the flow problem may be posed in the form of an initial-boundary value system of partial differential equations. This form is presented in detail for the general multicomponent, multiphase system and several special cases. A surfactant flood model for a two or three dimensions, two fluid phases (aqueous, oleic) and one adsorbent phase and four components (oil, water, surfactants 1 and 2) system is presented and analyzed. It is ruled by a system of non-linear, partial, differential equations; the continuity equation for the transport of each component, Darcy's equation for the flow of each phase and algebraic equations. This system is numerically solved in the one-dimensional case. The orthogonal collocation and finite difference techniques were used in solving the equations that characterized the multidimensional, multiphase and multicomponent flow problem. The orthogonal collocation solution in predicting the various concentration profiles is being presented here for the first time for the simulator design. The simulator is fed with the physical properties that are concentration dependent functions. The material transport equations are decoupled from the momentum transport equations and the complex, time changing flow-field requires a numerical solution. Matlab computer programs were used for the numerical solution of the model equations. The results of the orthogonal collocation solution were compared with those of finite difference solutions. The results indicate that the concentration of surfactants for orthogonal collocation show more features than the predictions of the finite difference, offering more opportunities for further understanding of the physical nature of the complex problem. Also, comparison of the orthogonal collocation solution with computations based on finite difference method offers possible explanation for the observed differences.

Introduction

In order to maximize oil recovery from reservoirs, operators consider enhanced oil

recovery as effective method. Also increasing high oil prices and declining

production in many regions around the globe makes this advance technologies called “Enhanced Oil Recovery” (EOR) of recovering trapped oil in reservoir attractive for exploration and production operations. This implies the injection of a fluid or fluids or materials into a reservoir to supplement the natural energy present in a reservoir, where the injected fluids interact with the reservoir rock /oil /brine system to create favourable conditions for maximum oil recovery (Bidner and Savioli, 2002; Ayirala, 2002).

The technical insights into enhanced oil recovery technologies are developed to increase the extraction of crude oil from reservoirs after primary production. Since not all the original oil in place can be recovered by the primary and secondary processes. Chemical enhanced oil recovery is used to mobilize the trapped oil in reservoir pores after a secondary recovery after water flooding. Surfactant flooding is a form of chemical flooding process. Surfactants are injected to decrease the interfacial tension between oil and water in order to mobilize the oil trapped after secondary recovery by water flooding. This is achieved by lowering the oil-water interfacial tension and allowing oil to flow within the pores of reservoir rock and into the well bores.

In a surfactant flood, a multi-component multiphase system is involved. The theory of multi- component, multiphase flow has been presented by several authors. The surfactant flooding is represented by a system of nonlinear partial differential equations: the continuity equation for the transport of the components and Darcy’s equation for the phase flow (Helfferich, 1981). The present work describes the development of a simulator for an Enhanced Oil Recovery process for surfactant assisted

water flooding by applying different mathematical methods, orthogonal collocation method and finite difference methods to solve the basic model transport equations.

The approach adopted here involves the use of different mathematical techniques; orthogonal collocation method and finite difference for the development and simulation of the relevant nonlinear partial differential equations. The two mathematical techniques further less the burden in this complex problem because of the multi-component, multiphase, multidimensional displacement phenomena in porous systems. The different mathematical techniques; orthogonal collocation method and finite difference are to be utilized to identify a particular type of physical behaviour and enable the understanding of the involved propagation phenomena in terms of cause and effects. More so, the techniques will in particular be utilized to predict what happens in EOR process and show the complexity of the problem can be reduced by intensive calculation.

This work applied different techniques; orthogonal collocation method and finite difference to solve the basic model transport equations. The approach is multidimensional. It involved at least three independent variables, which mean that the various composition path spaces required to map the composition routes of the system are at most two dimensional, allowing for a great simplification in complexity.

Systems of coupled, first-order, nonlinear hyperbolic partial differential equations (p.d.e.s) govern the transient evolution of a chemical flooding process for enhanced recovery. The method of characteristics (MOC) provides a way in which such systems of hyperbolic p.d.e.s can be solved

by converting them to an equivalent system of ordinary differential equations. In some cases, the characteristic solution has been used to track the flood-front in two-dimensional reservoir problems (Glimm *et al.*, 1983). The characteristic method was combined with a finite element approach to solve the problems (Ewing *et al.*, 1983). The MOC and an adjustable number of moving particles were used to track three-dimensional solute fronts in groundwater systems; adjusting the number of particles serves to maintain an accurate material balance and save computational time (Zheng, 1993).

At the simple level, the results of simulation using these techniques are analogous to the Buckley-Leverett theory for water flooding, the latter being evident in the work for polymer flooding (Patton *et al.*, 1971), for dilute surfactant flooding (Fayers and Perrine, 1959), for carbonated water flooding (Claridge and Bondor, 1974), and for miscible and immiscible surfactant flooding (Larson, 1979; Hirasaki, 1981), for isothermal, multiphase, multicomponent fluid flow in permeable media (Pope *et al.*, 1984). Also, Case studies for the feasibility of sweep improvement in surfactant-assisted water flooding (Harwell, 2012).

High oil prices and declining production in many regions around the globe, makes enhanced oil recovery (EOR) increasingly attractive for researchers. As evident in the work for a new class of viscoelastic surfactants for EOR (Siggel *et al.*, 2001), for microbially enhanced oil recovery at simulated reservoir conditions by use of engineered bacteria (Xu and Lu, 2001), for co-optimization of enhanced oil recovery and carbon sequestration (Leach and Mason, 2011), for development of improved surfactants and EOR methods for small operators (Harwell, 2012).

The present work describes the design of a simulator of reservoir using the effect of surfactant mixture assisted water flooding an Enhanced Oil Recovery process by applying two different mathematical methods, orthogonal collocation and finite difference method, to solve the basic model transport equations. The approach is multidimensional and involves at least three independent variables.

Methodology

This work considered the solution of a multidimensional, multicomponent and multiphase flow problem associated with enhanced oil recovery process in petroleum engineering. The process of interest involves the injection of surfactant of different concentrations and pore volume to displace oil from the reservoir.

The methodology used here is illustrated by the steps utilized in executing the solution using the developed mathematical models describing the physics of reservoir depletion and fluid flow in which one of the main aims is the determination of the areal distribution of fluids in the flooded reservoir. The system is for two or three dimensions, two fluid phases (aqueous, oleic) and one adsorbent phase, four components (oil, water, surfactants 1 and 2). The reservoir may be divided into discrete grid blocks which may each be characterized by having different reservoir properties. The flow of fluids from a block is governed by the principle of mass conservation coupled with Darcy's law. The following are taken into consideration in the modeling effort: (i) the simultaneous flow of oil, gas, and water in three dimensions, (ii) the effects of natural water influx, fluid compressibility, mass transfer between gas and liquid phases and (iii) the variation of such parameters as

porosity and permeability, as functions of pressure.

The model is developed from the basic law of conservation of mass with the following assumptions (Hankins and Harwell, 2004).

1. Fluid phases are incompressible, and individually obey Darcy's law. Fractional flows are unaffected by the presence of surfactants, due to their low concentrations.
2. Relative permeabilities are given by simple power law relationships. Fractional flow relationships are derived from relative permeability equations.
3. The effect of gravity and capillary forces are neglected. The effects of viscous fluid forces on the process will dominate by choosing a high oil viscosity, and by considering cases in which reservoir permeability variations are large.
4. The reservoir minerals are water wet, leading to complete contact between the solid phase and the aqueous phase. Local phase equilibrium (adsorption, solubility) is attained by virtue of a small mobile phase velocity. Adsorption of each surfactant component individually obeys the Trogus model. There is negligible partitioning of surfactant into the oleic phase, since the aqueous phase concentrations are relatively low, and hydrophobic chain lengths are relatively short.
5. Surfactant components react instantaneously and completely to form a pore blocking phase. Reaction occurs at a single interface; any solid or gel phase is deposited wherever it is formed. This leads to a permeability reduction of a fixed magnitude over the volume in which the phase separation occurs. The magnitude of this reduction is controllable by altering the concentrations at which the surfactants interact (and thus

the amount of precipitate formed per unit volume).

The following simplifications are also made:

- a. The presence of reservoir fractures is precluded, in order to investigate the effects of rock matrix heterogeneity unambiguously.
- b. The effects of molecular diffusion and fluid dynamic dispersion on the process are secondary and significant.
- c. Temperature and pressure changes have negligible effects on physico-chemical equilibrium relationships.
- d. The breakdown of plugs under high pressure gradients, or dissolution and weakening of the plugs, is ignored.
- e. No volume change occurs in the aqueous phase upon mixing or precipitation. Porosity relations are neglected. (The actual volume of precipitate formed is very small.)

The developed partial differential equation is converted to ordinary differential equation using finite difference and orthogonal collocation methods.

The finite difference method is a technique that converts partial differential equations into a system of linear equations. There are essentially three finite difference techniques. The explicit, finite difference method converts the partial differential equations into an algebraic equation which can be solved by stepping forward (forward difference), backward (backward difference) or centrally (central difference).

The orthogonal collocation method converts partial differential equations into a system of ordinary differential equations using the Lagrangian polynomial method. This set of ordinary differential equations generated is

then solved with appropriate numerical technique such as the Runge Kutta.

The rock and fluid properties such as density, porosity, viscosity, oil and water etc, and other parameters are listed in tables 1, 2, 3 and 4. Table 1 is the reservoir characteristics (Hankins and Harwell, 2004). Table 2 is the reservoir characteristics used for the simulation (Oyedeko, 2014). Parameter values used in Trogus adsorption model (Trogus *et al.*, 1979) for verification runs are shown in table 3, while table 4 contains additional reservoir parameters (Hankins and Harwell, 2004).

In considering the more general form of the multiphase, multicomponent problem, the explicit Runge-Kutta method is chosen for the solution of the problem. The motivation for this explicit method is its simplicity and computational efficiency with regard to the reduction of truncation errors more effectively than other methods. The MATLAB computer program was used to obtain the solutions.

The model encompasses two fluid phases (aqueous and oleic), one adsorbent phase (rock), and four components (oil, water, surfactants 1 and 2). The oil is displaced by water flooding. In-situ interaction of surfactant slugs may occur, with consequent phase separation and local permeability reduction. The model accommodates two (or three) physical dimensions and an arbitrary, nonisotropic description of absolute permeability variation and porosity.

For most of the simulated cases (Hankins and Harwell, 2004), the reservoir consisted of a rectangular composite of horizontal oil bearing strata, sandwiched above and below by two impervious rocks. Oil is produced from the reservoir by means of water injection at one end and a production well at

the other. Data for the hypothetical reservoir simulated are given in table 1 (Hankins and Harwell, 2004).

Momentum Transport Equations

According to Darcys' law, the flux of a phase j is:

$$q_{mj} = \frac{-(K_{abs,m} k_{rj})}{\mu_j} \frac{\partial p}{\partial m}$$

(1)

The total fluid flux in the *m*-direction is then:

$$q_{mj} = -K_{abs,m} \left\{ \sum_{j=1}^{j=2} \frac{k_{rj}}{\mu_j} \right\} \frac{\partial p}{\partial m}$$

(2)

Denoting

$$K_m = K_{abs,m} \left\{ \sum_{j=1}^{j=2} \frac{k_{rj}}{\mu_j} \right\}$$

(2a)

$$q_{mj} = -K_m \left\{ \frac{\partial p}{\partial m} \right\}$$

(3)

Where, the effective permeability K_m is a function of phase saturation through the dependence of relative permeability on the latter; q_m also represents the superficial fluid velocity:

$$q_m = \phi v_m$$

(3a)

Where, v_m is the interstitial velocity, and ϕ the porosity.

Hence from Eqn. 3

$$v_x = \frac{-K_x}{\phi} \frac{\partial p}{\partial x} \quad \text{and} \quad v_y = \frac{-K_y}{\phi} \frac{\partial p}{\partial y}$$

(4)

From the continuity equation for incompressibility fluids:

$$\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} = 0 \quad (5)$$

And substitution of eqn. (4) leads to:

$$\frac{\partial}{\partial x} \left\{ \frac{K_x}{\phi} \frac{\partial p}{\partial x} \right\} + \frac{\partial}{\partial y} \left\{ \frac{K_y}{\phi} \frac{\partial p}{\partial y} \right\} \quad (6)$$

Relative permeabilities are given by the following relationships [18]:

$$K_{ro} = \left\{ \frac{1 - S_w - S_{ro}}{1 - S_{iw} - S_{ro}} \right\}^4 \quad (7)$$

$$K_{rw} = \left\{ \frac{S_w - S_{iw}}{1 - S_{iw}} \right\}^4 \quad (8)$$

Where, S_w is the water saturation, S_{iw} is the connate water saturation, and S_{ro} is the residual oil saturation. The fractional flow of phase j , f_j is given by:

$$f_j = q_{mj} / \sum_{k=1}^2 q_{mk} \quad (9)$$

Substitution of Eqns. 1, 7, and 8 in Eqn.9, then yields the fractional flow of water [18]:

$$f_w = \frac{\left\{ \frac{S_w - S_{iw}}{1 - S_{iw}} \right\}^4}{\left\{ \frac{S_w - S_{iw}}{1 - S_{iw}} \right\}^4 + \frac{\mu_w}{\mu_o} \left\{ \frac{1 - S_w - S_{ro}}{1 - S_{iw} - S_{ro}} \right\}^4} \quad (10)$$

Assuming that $S_{iw} = 0.1, S_{ro} = 0.2,$
 $\mu_w = 1.0$ cp and $\mu_o = 5.0$ cp, then

$$f_w = \frac{(S_w - 0.1)^4}{(S_w - 0.1)^4 + 0.5465(0.8 - S_w)^4} \quad (11)$$

And

$$f_w = \frac{df_w}{dS_w} = \frac{1.5302(0.8 - S_w)^3 f_w^2}{(S_w - 0.1)^5} \quad (11a)$$

Note that:

$$\begin{aligned} \text{For } 0 \leq S_w \leq 0.1 \quad f_w = 0 \quad f_w' = 0 \\ \text{for } 0.1 \leq S_w \leq 0.8 \quad f_w = (11) \end{aligned}$$

$$f_w' = (11a)$$

for $0.8 \leq S_w$

$$f_w = 1.0$$

$$f_w' = 0$$

The effective permeability in Eqn. 2a may be calculated from Eqns. 7 and 8.

Material transport equations

In the following analysis, we assume ρ and ϕ to be constant. However, a slight modification allows these quantities to be variable. For simplicity, the corresponding analysis is not presented here. The general material conservation equation, in the absence of diffusion, for a component i is (Hankins. and Harwell, 2004):

$$\frac{\partial C_i}{\partial t} + \nabla \cdot \mathbf{J}_i = -r_i \quad (12)$$

where C_i is the concentration of i in moles per unit total volume.

\mathbf{J}_i is the flux of i in moles per unit area and time, and r_i is the net reactive loss of i in moles per unit volume and time.

Adsorbates

If the surfactants partition solely between the solid and aqueous phases, then.

$$C_i = S_w \phi C_{i,w} + \rho(1 - \phi) \bar{C}_i \quad (13)$$

And

$$\mathbf{J}_i = \mathbf{V} \phi f_w C_{i,w} \quad (14)$$

where \bar{C}_i is the adsorption density of i on the reservoir minerals, moles per unit mass;

$C_{i,w}$ is the concentration of surfactant i in the aqueous phase, moles per unit volume; \mathbf{V} is the interstitial fluid velocity vector.

Substituting Eqns. 13 and 14 in Eqn. 12 yields (Hankins. and Harwell, 2004):

$$\phi \frac{\partial}{\partial t} [S_w C_{i,w}] + \rho(1-\phi) \frac{\partial \bar{C}_i}{\partial t} + \phi \frac{\partial}{\partial x} [V_x f_j C_{i,w}] + \phi \frac{\partial}{\partial y} [V_y f_j C_{i,w}] = -r_i \quad (i=1,2) \quad (15)$$

Fluid Phases

For incompressible phases, we can work in terms of volumes rather than moles. Thus, in Eqn. 12, $C_j = \phi S_j$ and $\mathbf{J}_j = \mathbf{V} \phi f_j$ so that:

$$\phi \frac{\partial S_j}{\partial t} + \phi \frac{\partial}{\partial x} (V_x f_j) + \phi \frac{\partial}{\partial y} (V_y f_j) = 0 \quad (16)$$

Since there is no reactive fluid losses then eliminating of ϕ , carrying out the product differentiation by the chain rule, multiplying the continuity equation (Eqn. 5) by f_j , and subtracting from Eqn.16, we obtain:

$$\frac{\partial S_j}{\partial t} + v_x \frac{\partial f_j}{\partial x} + v_y \frac{\partial f_j}{\partial y} = 0 \quad (j = o, w) \quad (17)$$

Again, multiplying Eqn.17 (for $j = w$) by $\phi C_{i,w}$, Eqn.5 by $\phi f_w C_{i,w}$, and subtracting these from Eqn.15 with application of the triple chain-rule leads to [18];

$$\phi S_w \frac{\partial C_{i,w}}{\partial t} + \rho(1-\phi) \frac{\partial \bar{C}_i}{\partial t} + \phi v_x f_w \frac{\partial C_{i,w}}{\partial x} + \phi v_y f_w \frac{\partial C_{i,w}}{\partial y} = -r_i \quad (i=1,2) \quad (18)$$

The term r_i represents the rate of loss of surfactant due to precipitation: for a one-to-one reaction stoichiometry, $r_1 = r_2$. Since reaction occurs instantaneously at a sharp interface, this term may be ignored away from the singular region of the interface.

Adsorption Model

It is possible to approximate the adsorption isotherm of a pure surfactant on a mineral oxide by use of a simple model. At low concentration the adsorption obeys Henry's law, while above the critical micelle concentration (CMC), the total adsorption remains constant. The Troguis adsorption model (Hankins and Harwell, 2004; Oyedeko, 2014) is used in this work. The following assumptions are made:

- (a) The composition and concentration of surfactant in the monomer and in the micelles can be approximated by assuming that these are separate phases in thermodynamic equilibrium.
- (b) Adsorption is a function of monomer composition only.
- (c) Adsorption of an individual surfactant component is a linear function of its monomer concentration (Henry's law), and is independent of micelle concentration and the other component monomer concentrations.

Application of Finite Difference to Solution of Model Equations

First-order, finite-difference expressions for the spatial derivatives were substituted into the hyperbolic chromatographic transport equations (Eq. 18), yielding 2 x m coupled ordinary differential equations which may then be integrated simultaneously (also known as the 'numerical method of lines').

$$S_w \frac{\partial C_{i,w}}{\partial \tau} + \sum_{j=1}^2 m_{ij} \frac{\partial C_{i,w}}{\partial \tau} + f_w(\tau, \epsilon_h) \times \left\{ \frac{C_{i,w}(\tau, \epsilon_h) - C_{i,w}(\tau, \epsilon_{h-1})}{\Delta \epsilon} \right\} = 0 \quad (19)$$

where $i = 1,2$ and $h = 1,2,.. m$.

Eqn. 19 is the finite-difference form of Eqn.18 written for one spatial dimension ε , where m_{ij} are the adsorption coefficients, τ is dimensionless time (injected volume/ pore volume), and ε is dimensionless distance (pore volumes travelled). In two dimensions, the finite-difference terms are multiplied by dimensionless velocities. The distortion of the solution in the τ direction may be neglected by using a 4th order Runge-Kutta method and a sufficiently small time step.

The above equation is now transformed to the original form of Eqns. 18 using the following defined variables:

$$C'_{i,w} = \phi C_{i,w} \quad (20)$$

$$\bar{C}'_i = \rho(1-\phi)\bar{C}'_i \quad (20)$$

$$m_{i,j} = \frac{\partial \bar{C}'_i}{\partial C'_{j,w}} \quad (21)$$

Again, recall that differentiation of a function of another function (chain rule) is of the form

$$\frac{\partial y}{\partial x} = \frac{\partial y}{\partial u} \times \frac{\partial u}{\partial x} \quad (22)$$

Applying the chain rule above, Eqn. 19 becomes:

$$S_w \frac{\partial C'_{i,w}}{\partial \tau} + \left(\frac{\partial \bar{C}'_i}{\partial C'_{1,w}} \cdot \frac{\partial C'_{1,w}}{\partial \tau} \right) + \left(\frac{\partial \bar{C}'_i}{\partial C'_{2,w}} \cdot \frac{\partial C'_{2,w}}{\partial \tau} \right) + f_w(\tau, \varepsilon_h) \times \left\{ \frac{C'_{i,w}(\tau, \varepsilon_h) - C'_{i,w}(\tau, \varepsilon_{h-1})}{\Delta \varepsilon} \right\} = 0$$

(24)

Eliminating the primes (') and bars (-) and introducing $m_{i,j}$ terms yield

$$(S_w + m_{11}) \frac{\partial C_{1,w}}{\partial \tau} + m_{12} \frac{\partial C_{2,w}}{\partial \tau} + f_w \frac{\partial C_{1,w}}{\partial \varepsilon} = 0 \quad (25)$$

$$(S_w + m_{22}) \frac{\partial C_{2,w}}{\partial \tau} + m_{21} \frac{\partial C_{1,w}}{\partial \tau} + f_w \frac{\partial C_{2,w}}{\partial \varepsilon} = 0 \quad (26)$$

Applying the method of lines, a partial transformation to a difference equation, to the equations above yield:

$$(S_w + m_{11}) \frac{\partial C_{1,w}}{\partial \tau} + m_{12} \frac{\partial C_{2,w}}{\partial \tau} + f_w \frac{C_{1,w(\tau,\varepsilon_h)} - C_{1,w(\tau,\varepsilon_{h-1})}}{\Delta \varepsilon} = 0 \quad (27)$$

$$(S_w + m_{22}) \frac{\partial C_{2,w}}{\partial \tau} + m_{21} \frac{\partial C_{1,w}}{\partial \tau} + f_w \frac{C_{2,w(\tau,\varepsilon_h)} - C_{2,w(\tau,\varepsilon_{h-1})}}{\Delta \varepsilon} = 0 \quad (28)$$

This can also be written as follows

$$(S_w + m_{11}) \frac{\partial C_{1,w(\tau,\varepsilon_h)}}{\partial \tau} + m_{12} \frac{\partial C_{2,w(\tau,\varepsilon_h)}}{\partial \tau} + \frac{f_w}{\Delta \varepsilon} [C_{1,w(\tau,\varepsilon_h)} - C_{1,w(\tau,\varepsilon_{h-1})}] = 0 \quad (29)$$

$$(S_w + m_{22}) \frac{\partial C_{2,w(\tau,\varepsilon_h)}}{\partial \tau} + m_{21} \frac{\partial C_{1,w(\tau,\varepsilon_h)}}{\partial \tau} + \frac{f_w}{\Delta \varepsilon} [C_{2,w(\tau,\varepsilon_h)} - C_{2,w(\tau,\varepsilon_{h-1})}] = 0 \quad (30)$$

Since we have a set of simultaneous ODE's, we will attempt to solve the equations

$$(S_w + m_{11}) \frac{\partial C_{1,w(\tau,\varepsilon_h)}}{\partial \tau} + m_{12} \frac{\partial C_{2,w(\tau,\varepsilon_h)}}{\partial \tau} + \frac{f_w}{\Delta \varepsilon} [C_{1,w(\tau,\varepsilon_h)} - C_{1,w(\tau,\varepsilon_{h-1})}] = 0 \quad (31)$$

$$(S_w + m_{22}) \frac{\partial C_{2,w(\tau,\varepsilon_h)}}{\partial \tau} + m_{21} \frac{\partial C_{1,w(\tau,\varepsilon_h)}}{\partial \tau} + \frac{f_w}{\Delta \varepsilon} [C_{2,w(\tau,\varepsilon_h)} - C_{2,w(\tau,\varepsilon_{h-1})}] = 0 \quad (32)$$

where

$$m_{11} = \frac{\partial \bar{C}_1}{\partial C_{1,w}}$$

$$m_{12} = \frac{\partial \bar{C}_1}{\partial C_{2,w}}$$

$$m_{21} = \frac{\partial \bar{C}_2}{\partial C_{1,w}}$$

$$m_{22} = \frac{\partial \bar{C}_2}{\partial C_{2,w}}$$

Substitution of these terms in Eqs. 31 and 32 (38)
yield:

$$\left(S_w + \frac{\bar{\alpha}_1}{\alpha_{1,w}} \right) \frac{\partial C_{1,w}(\tau, \varepsilon_h)}{\partial \tau} + \frac{\bar{\alpha}_1}{\alpha_{2,w}} \frac{\partial C_{2,w}(\tau, \varepsilon_h)}{\partial \tau} + \frac{f_w}{\Delta \varepsilon} [C_{1,w}(\tau, \varepsilon_h) - C_{1,w}(\tau, \varepsilon_{h-1})] = 0$$

(33)

And

$$\left(S_w + \frac{\bar{\alpha}_2}{\alpha_{2,w}} \right) \frac{\partial C_{2,w}(\tau, \varepsilon_h)}{\partial \tau} + \frac{\bar{\alpha}_2}{\alpha_{1,w}} \frac{\partial C_{1,w}(\tau, \varepsilon_h)}{\partial \tau} + \frac{f_w}{\Delta \varepsilon} [C_{2,w}(\tau, \varepsilon_h) - C_{2,w}(\tau, \varepsilon_{h-1})] = 0$$

(34)

These on simplification yield

$$S_w \frac{\partial C_{1,w}(\tau, \varepsilon_h)}{\partial \tau} + \frac{\bar{\alpha}_1}{\alpha_{1,w}} \frac{\partial C_{1,w}(\tau, \varepsilon_h)}{\partial \tau} + \frac{\bar{\alpha}_1}{\alpha_{2,w}} \frac{\partial C_{2,w}(\tau, \varepsilon_h)}{\partial \tau} + \frac{f_w}{\Delta \varepsilon} [C_{1,w}(\tau, \varepsilon_h) - C_{1,w}(\tau, \varepsilon_{h-1})] = 0$$

$$S_w \frac{\partial C_{1,w}(\tau, \varepsilon_h)}{\partial \tau} + \frac{\bar{\alpha}_1}{\partial \tau} + \frac{\bar{\alpha}_1}{\partial \tau} + \frac{f_w}{\Delta \varepsilon} [C_{1,w}(\tau, \varepsilon_h) - C_{1,w}(\tau, \varepsilon_{h-1})] = 0$$

$$S_w \frac{\partial C_{1,w}(\tau, \varepsilon_h)}{\partial \tau} + 2 \frac{\bar{\alpha}_1}{\partial \tau} + \frac{f_w}{\Delta \varepsilon} [C_{1,w}(\tau, \varepsilon_h) - C_{1,w}(\tau, \varepsilon_{h-1})] = 0$$

similarly

$$S_w \frac{\partial C_{2,w}(\tau, \varepsilon_h)}{\partial \tau} + 2 \frac{\bar{\alpha}_2}{\partial \tau} + \frac{f_w}{\Delta \varepsilon} [C_{2,w}(\tau, \varepsilon_h) - C_{2,w}(\tau, \varepsilon_{h-1})] = 0$$

(35)

(36)

From the Trogus model,

$$\bar{C}_1 = k_1 C_{1,w}$$

$$\bar{C}_2 = k_2 C_{2,w}$$

A final substitution results in the equation below:

$$S_w \frac{\partial C_{1,w}(\tau, \varepsilon_h)}{\partial \tau} + 2 \frac{\partial (k_1 C_{1,w})}{\partial \tau} + \frac{f_w}{\Delta \varepsilon} [C_{1,w}(\tau, \varepsilon_h) - C_{1,w}(\tau, \varepsilon_{h-1})] = 0$$

$$S_w \frac{\partial C_{1,w}(\tau, \varepsilon_h)}{\partial \tau} + 2k_1 \frac{\partial C_{1,w}}{\partial \tau} + \frac{f_w}{\Delta \varepsilon} [C_{1,w}(\tau, \varepsilon_h) - C_{1,w}(\tau, \varepsilon_{h-1})] = 0$$

$$(S_w + 2k_1) \frac{\partial C_{1,w}}{\partial \tau} + \frac{f_w}{\Delta \varepsilon} [C_{1,w}(\tau, \varepsilon_h) - C_{1,w}(\tau, \varepsilon_{h-1})] = 0$$

and

$$S_w \frac{\partial C_{2,w}(\tau, \varepsilon_h)}{\partial \tau} + 2 \frac{\partial (k_2 C_{2,w})}{\partial \tau} + \frac{f_w}{\Delta \varepsilon} [C_{2,w}(\tau, \varepsilon_h) - C_{2,w}(\tau, \varepsilon_{h-1})] = 0$$

$$(S_w + 2k_2) \frac{\partial C_{2,w}}{\partial \tau} + \frac{f_w}{\Delta \varepsilon} [C_{2,w}(\tau, \varepsilon_h) - C_{2,w}(\tau, \varepsilon_{h-1})] = 0$$

Application of Orthogonal Collocation to Solution of Model Equations

Equation 24 can be written as:

$$S_w \frac{\partial C_{i,w}}{\partial \tau} + 2 \frac{\partial \bar{C}_i}{\partial \tau} + f_w(\tau, \varepsilon_h) \times \left\{ \frac{C_{i,w}(\tau, \varepsilon_h) - C_{i,w}(\tau, \varepsilon_{h-1})}{\Delta \varepsilon} \right\} = 0$$

(39)

$$S_w \frac{\partial [C_{i,w}]}{\partial \tau} + 2 \frac{\partial [\alpha(1-\phi)\bar{C}_i]}{\partial \tau} + f_w(\tau, \varepsilon_h) \times \left\{ \frac{[C_{i,w}](\tau, \varepsilon_h) - [C_{i,w}](\tau, \varepsilon_{h-1})}{\Delta \varepsilon} \right\} = 0$$

(40)

$$\phi S_w \frac{\partial C_{i,w}}{\partial \tau} + 2\alpha(1-\phi) \frac{\partial \bar{C}_i}{\partial \tau} + \phi f_w(\tau, \varepsilon_h) \times \left\{ \frac{C_{i,w}(\tau, \varepsilon_h) - C_{i,w}(\tau, \varepsilon_{h-1})}{\Delta \varepsilon} \right\} = 0$$

(41)

Now, from the Trogus model,

$$\bar{C}_i = \kappa_i C_{i,w}$$

(42)

$$\phi S_w \frac{\partial C_{i,w}}{\partial \tau} + 2\alpha(1-\phi) \frac{\partial (\kappa_i C_{i,w})}{\partial \tau} + \phi f_w(\tau, \varepsilon_h) \times \left\{ \frac{C_{i,w}(\tau, \varepsilon_h) - C_{i,w}(\tau, \varepsilon_{h-1})}{\Delta \varepsilon} \right\} = 0$$

(43)

$$\phi S_w \frac{\partial C_{i,w}}{\partial \tau} + 2\kappa_i \alpha(1-\phi) \frac{\partial C_{i,w}}{\partial \tau} + \phi f_w(\tau, \varepsilon_h) \times \left\{ \frac{C_{i,w}(\tau, \varepsilon_h) - C_{i,w}(\tau, \varepsilon_{h-1})}{\Delta \varepsilon} \right\} = 0$$

(44)

$$\phi S_w \frac{\partial C_{i,w}}{\partial \tau} + 2\kappa_i \alpha(1-\phi) \frac{\partial C_{i,w}}{\partial \tau} + \phi f_w(\tau, \varepsilon_h) \frac{\partial C_{i,w}}{\partial \varepsilon} = 0$$

(45)

$$[\phi S_w + 2\kappa_i \alpha(1-\phi)] \frac{\partial C_{i,w}}{\partial \tau} + \phi f_w(\tau, \varepsilon_h) \frac{\partial C_{i,w}}{\partial \varepsilon} = 0$$

(46) (37)

Let

$$R = [\phi S_w + 2\kappa_i \alpha(1-\phi)]$$

$$B = \phi f_w$$

The above equations now become:

$$R \frac{\partial C}{\partial \tau} + B \frac{\partial C}{\partial \varepsilon} = 0 \quad (47)$$

where C is a function of both ε (dimensionless distance) and τ (dimensionless time).

Using the method of orthogonal collocation, let C be approximated by the expression

$$C(\tau, \varepsilon) = \sum_{I=1}^{N+1} C_I(\tau) X_J(\varepsilon_I) \quad (48)$$

Equation 47 can now be expressed as follows:

$$R \frac{\partial C}{\partial \tau} + B \frac{\partial}{\partial \varepsilon} \sum_{I=1}^{N+1} C_I(\tau) X_J(\varepsilon_I) = 0 \quad (48)$$

$$R \frac{\partial C}{\partial \tau} + B \sum_{I=1}^{N+1} \frac{\partial}{\partial \varepsilon} [C_I(\tau) X_J(\varepsilon_I)] = 0 \quad (49)$$

$$R \frac{\partial C}{\partial \tau} + B \sum_{I=1}^{N+1} \frac{\partial}{\partial \varepsilon} [X_J(\varepsilon_I)] \cdot C_I(\tau) = 0 \quad (50)$$

$$a_{JI} = \frac{\partial}{\partial \varepsilon} X_J(\varepsilon_I) \quad (51)$$

$$R \frac{\partial C_J}{\partial \tau} + B \sum_{I=1}^{N+1} a_{JI} C_I = 0 \quad (52)$$

$$\frac{\partial C_J}{\partial \tau} + \frac{B}{R} \sum_{I=1}^{N+1} a_{JI} C_I = 0 \quad (53)$$

$$\frac{\partial C_J}{\partial \tau} = -\frac{B}{R} \sum_{I=1}^{N+1} a_{JI} C_I \quad (54)$$

For $I = 1, 2, 3, 4 \dots N+1$

Therefore,

$$\frac{\partial C_J}{\partial \tau} = -\frac{B}{R} [a_{J1} C_1 + a_{J2} C_2 + a_{J3} C_3 + a_{J4} C_4 + \dots + a_{JN+1} C_{N+1}] \quad (55)$$

Again $J = 1, 2, 3, 4 \dots N+1$

Therefore the following system of ODE's can be generated

$$\frac{\partial C_1}{\partial \tau} = -\frac{B}{R} [a_{11} C_1 + a_{12} C_2 + a_{13} C_3 + a_{14} C_4 + \dots + a_{1N+1} C_{N+1}]$$

$$\frac{\partial C_2}{\partial \tau} = -\frac{B}{R} [a_{21} C_1 + a_{22} C_2 + a_{23} C_3 + a_{24} C_4 + \dots + a_{2N+1} C_{N+1}]$$

$$\frac{\partial C_3}{\partial \tau} = -\frac{B}{R} [a_{31} C_1 + a_{32} C_2 + a_{33} C_3 + a_{34} C_4 + \dots + a_{3N+1} C_{N+1}]$$

$$\frac{\partial C_4}{\partial \tau} = -\frac{B}{R} [a_{41} C_1 + a_{42} C_2 + a_{43} C_3 + a_{44} C_4 + \dots + a_{4N+1} C_{N+1}]$$

⋮

⋮

⋮

$$\frac{\partial C_{N+1}}{\partial \tau} = -\frac{B}{R} [a_{N+11} C_1 + a_{N+12} C_2 + a_{N+13} C_3 + a_{N+14} C_4 + \dots + a_{N+1N+1} C_{N+1}] \quad (57)$$

In matrix form, we have the following expression:

$$\begin{bmatrix} \frac{\partial C_1}{\partial \tau} \\ \frac{\partial C_2}{\partial \tau} \\ \frac{\partial C_3}{\partial \tau} \\ \frac{\partial C_4}{\partial \tau} \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \frac{\partial C_{N+1}}{\partial \tau} \end{bmatrix} = -\frac{B}{R} \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} & \dots & \dots & \dots & \dots & a_{1N+1} \\ a_{21} & a_{22} & a_{23} & a_{24} & & & & & a_{2N+1} \\ a_{31} & : & & & & & & & a_{3N+1} \\ a_{41} & : & & & & & & & a_{4N+1} \\ : & : & & & & & & & : \\ : & : & & & & & & & : \\ : & : & & & & & & & : \\ : & : & & & & & & & : \\ : & : & & & & & & & : \\ a_{N+11} & a_{N+12} & \dots & \dots & \dots & \dots & \dots & \dots & a_{N+1N+1} \end{bmatrix} \begin{bmatrix} C_1(\tau) \\ C_2(\tau) \\ C_3(\tau) \\ C_4(\tau) \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ C_{N+1}(\tau) \end{bmatrix} \quad (58)$$

Similarly, the following expression defines a_{JI} (Villadsen and Stewart, 1967; Villadsen and Stewart, 1968).

$$a_{II} = \begin{cases} \frac{1 P_{N+1}^{(2)}(\epsilon_I)}{2 P_{N+1}^{(1)}(\epsilon_I)} & \text{For } J = I \\ \frac{1 P_{N+1}^{(1)}(\epsilon_I)}{\epsilon_I - \epsilon_J P_{N+1}^{(1)}(\epsilon_J)} & \text{For } I \neq J \end{cases} \quad (59)$$

Where

$$\begin{aligned} P_J(\epsilon) &= (\epsilon - \epsilon_J)P_{J-1}(\epsilon); J=1,2,3,\dots,N+1 \\ P_J^{(1)}(\epsilon) &= (\epsilon - \epsilon_J)P_{J-1}^{(1)}(\epsilon) + P_{J-1}(\epsilon) \\ P_J^{(2)}(\epsilon) &= (\epsilon - \epsilon_J)P_{J-1}^{(2)}(\epsilon) + 2P_{J-1}^{(1)}(\epsilon) \quad (60) \\ P_0^{(1)}(\epsilon) &= P_0^{(2)}(\epsilon) = 0 \\ P_0(\epsilon) &= 1 \end{aligned}$$

Recall that the elements of the matrix can be generated from the following Lagrange polynomial

$$a_{ij} = \frac{dl_j(x_i)}{dx} = \begin{cases} \frac{1 P_{N+1}^{(2)}(x_i)}{2 P_{N+1}^{(1)}(x_i)} & j=i \\ \frac{1 P_{N+1}^{(1)}(x_i)}{x_i - x_j P_{N+1}^{(1)}(x_j)} & i \neq j \end{cases} \quad (61)$$

For $i = j$, the elements here refer to the leading diagonal of the matrix to be generated

For $i \neq j$, the elements here refer to all other elements of the matrix

Also, the following recurrence relations are defined below.

$$\begin{aligned} p_o(x) &= 1 \\ P_j(x) &= (x - x_j)P_{j-1}(x) \\ P_j^{(1)}(x) &= (x - x_j)P_{j-1}^{(1)}(x) + P_{j-1}(x) \\ P_j^{(2)}(x) &= (x - x_j)P_{j-1}^{(2)}(x) + 2P_{j-1}^{(1)}(x) \end{aligned} \quad (62)$$

For $j = 2, 3, 4, \dots, N+1$

The following substitutions and manipulations will now be made to redefine Eqn.61.

Substituting the recurrence relations into Eqn.61 yields:

$$a_{ij} = \begin{cases} \frac{1}{2} \left[\frac{(x_i - x_j)P_{j-1}^{(2)}(x_i) + 2P_{j-1}^{(1)}(x_i)}{(x_i - x_j)P_{j-1}^{(1)}(x_i) + P_{j-1}(x_i)} \right] & j=i \\ \frac{1}{x_i - x_j} \left[\frac{(x_i - x_j)P_{j-1}^{(1)}(x_i) + P_{j-1}(x_i)}{(x_j - x_j)P_{j-1}^{(1)}(x_j) + P_{j-1}(x_j)} \right] & i \neq j \end{cases} \quad (63)$$

Now, some terms will be cancelled out.

Since $j = i$,

$$(x_i - x_j) = 0$$

And

$$(x_j - x_j) = 0$$

$$a_{ij} = \begin{cases} \frac{1}{2} \left[\frac{2P_{j-1}^{(1)}(x_i)}{P_{j-1}(x_i)} \right] & j=i \\ \frac{1}{x_i - x_j} \left[\frac{(x_i - x_j)P_{j-1}^{(1)}(x_i) + P_{j-1}(x_i)}{P_{j-1}(x_j)} \right] & i \neq j \end{cases} \quad (64)$$

The above becomes:

$$a_{ij} = \begin{cases} \left[\frac{P_{j-1}^{(1)}(x_i)}{P_{j-1}(x_i)} \right] & j=i \\ \frac{(x_i - x_j)P_{j-1}^{(1)}(x_i)}{(x_i - x_j)P_{j-1}(x_j)} + \frac{1}{x_i - x_j} \left[\frac{P_{j-1}(x_i)}{P_{j-1}(x_j)} \right] & i \neq j \end{cases} \quad (65)$$

This becomes:

$$a_{ij} = \begin{cases} \left[\frac{P_{j-1}^{(1)}(x_i)}{P_{j-1}(x_i)} \right] & j=i \\ \frac{P_{j-1}^{(1)}(x_i)}{P_{j-1}(x_j)} + \frac{1}{x_i - x_j} \left[\frac{P_{j-1}(x_i)}{P_{j-1}(x_j)} \right] & i \neq j \end{cases} \quad (66)$$

Rewriting the above in terms of epsilon, (ϵ):

$$a_{ij} = \begin{cases} \begin{bmatrix} P_{j-1}^{(1)}(\varepsilon_i) \\ P_{j-1}(\varepsilon_i) \end{bmatrix} & j=i \\ \frac{P_{j-1}^{(1)}(\varepsilon_i)}{P_{j-1}(\varepsilon_j)} + \frac{1}{\varepsilon_i - \varepsilon_j} \begin{bmatrix} P_{j-1}(\varepsilon_i) \\ P_{j-1}(\varepsilon_j) \end{bmatrix} & i \neq j \end{cases} \quad (67)$$

The matrix now looks like this:

$$\begin{aligned} a_{11} &= \frac{P_0^{(1)}(\varepsilon_1)}{P_0(\varepsilon_1)} \\ a_{12} &= \frac{P_1^{(1)}(\varepsilon_1)}{P_1(\varepsilon_2)} + \frac{1}{\varepsilon_1 - \varepsilon_2} \frac{P_1(\varepsilon_1)}{P_1(\varepsilon_2)} \\ a_{13} &= \frac{P_2^{(1)}(\varepsilon_1)}{P_2(\varepsilon_3)} + \frac{1}{\varepsilon_1 - \varepsilon_2} \frac{P_2(\varepsilon_1)}{P_2(\varepsilon_3)} \\ a_{21} &= \frac{P_0^{(1)}(\varepsilon_2)}{P_0(\varepsilon_1)} + \frac{1}{\varepsilon_2 - \varepsilon_1} \frac{P_0(\varepsilon_2)}{P_0(\varepsilon_1)} \\ a_{22} &= \frac{P_1^{(1)}(\varepsilon_2)}{P_1(\varepsilon_1)} \\ a_{23} &= \frac{P_2^{(1)}(\varepsilon_2)}{P_2(\varepsilon_3)} + \frac{1}{\varepsilon_2 - \varepsilon_3} \frac{P_2(\varepsilon_2)}{P_2(\varepsilon_3)} \\ a_{31} &= \frac{P_0^{(1)}(\varepsilon_3)}{P_0(\varepsilon_1)} + \frac{1}{\varepsilon_3 - \varepsilon_1} \frac{P_0(\varepsilon_3)}{P_0(\varepsilon_1)} \\ a_{32} &= \frac{P_1^{(1)}(\varepsilon_3)}{P_1(\varepsilon_2)} + \frac{1}{\varepsilon_3 - \varepsilon_2} \frac{P_1(\varepsilon_3)}{P_1(\varepsilon_2)} \\ a_{33} &= \frac{P_2^{(1)}(\varepsilon_3)}{P_2(\varepsilon_3)} \end{aligned} \quad (68)$$

The recurrence relations below will again be used to evaluate the terms of the matrix.

$$\begin{aligned} p_o(\varepsilon) &= 1 \\ P_j(\varepsilon) &= (\varepsilon - \varepsilon_j)P_{j-1}(\varepsilon) \\ P_j^{(1)}(\varepsilon) &= (\varepsilon - \varepsilon_j)P_{j-1}^{(1)}(\varepsilon) + P_{j-1}(\varepsilon) \\ P_0^{(1)}(\varepsilon) &= 0 \end{aligned} \quad (69)$$

Let \square assume the range:

$$\square = [0:0.01:0.09]$$

Where

$$\square_1 = 0 \quad (70)$$

$$\square_2 = 0.01 \quad (71)$$

$$\square_3 = 0.02 \quad (72)$$

Results and Discussion

The reservoir response, as predicted by the simulation on the basis of the theory of coherence, is compared with the numerical predictions obtained using traditional finite difference method and orthogonal collocation. The case studies are chosen to be both hypothetical and using of existing Nigerian well data with simple representative of the important elements of the simulator. The main objective of these case studies has been to demonstrate that the mathematical techniques of orthogonal collocation, finite difference and coherent theory in the context of application of the simulator can be used to obtain wave behaviour in a reservoir. A gradually increasing level of complexity is introduced, representing a range of systems from aqueous phase flow, to surfactant chromatography in two phase flow, to surfactant chromatography in two dimensional porous medium. The initial and injected surfactant compositions corresponding to cases 1, and 2 are shown in table 5 in appendix. The rock and fluid properties are listed in tables 1, 2, 3, 4 in appendix. These were taken as uniform for convenience.

The two fluid phases consisted of a water phase and an oil phase, which, for convenience are considered incompressible. The density of oil, the viscosity of oil, the salinity of water, and the formation volume factor of oil and water are listed in table 3 in appendix. All cases mentioned above were run by using anionic sodium dodecyl sulfate (SDS) and cationic dodecyl pyridinium chloride (DPC) as surfactants.

The system of equations is complete with the equations representing physical properties of the fluids and the rock. From a physical-chemical point of view, there are three components - water, petroleum and chemical. They are in fact, pseudo-components, since each one consists of several pure components. Petroleum is a complex mixture of many hydrocarbons. Water is actually brine, and contains dissolved salts. Finally, the chemical contains different kinds of surfactants.

These three pseudo-components are distributed between two phases –the oleic phase and the aqueous phase. The chemical has an amphiphilic character. It makes the oleic phase at least partially miscible with water or the aqueous phase at partially miscible with petroleum.

Interfacial tension depends on the surfactant partition between the two phases, and hence of phase behaviour. Residual phase saturation decrease as interfacial tension decreases. Relative permeability parameters depend on residual phase saturations. Phase viscosities are functions of the volume fraction of the components in each fluid phase. Therefore, the success or failure of surfactant flooding processes depends on phase behaviour. Phase behaviour influences all other physical properties, and each of them, in turn influences oil recovery.

Results of Reservoir Prediction in an Aqueous Phase Chromatographic Flow in One Dimension

Figure 1a is the result obtained for solving Equation 19 using the numerical technique for both orthogonal collocation and finite difference. The graph is for the bed composition profile for one dimensional aqueous-phase chromatography (case 1) at one half pore volume injected.

If a one-dimensional, adsorbing porous medium is initially equilibrated with an aqueous composition $C_1 = 0.21$, $C_2 = 0.181$ (concentrations normalized as moles in solution per m^3 of bed) and is then injected with a composition $C_1 = 0.17$, $C_2 = 0.013$ (Riemann-type problem: case 1, refer to table 5), the composition upstream of this injected fluid and composition downstream of the initial or previously injected fluid follows the slow “path” from the injected composition to the junction with the “fast path” from the final composition, where it switches to this “fast” path. In figure 1a, the profile C_1 of finite difference (FD) shows a steady rise from $C_1 = 0.17$ to $C_1 = 0.21$ and then attained a constant state. Also the profile C_1 of the orthogonal collocation (OC) increased steadily from $C_1 = 0.17$ to $C_1 = 0.21$ after which it started depressing from $C_1 = 0.2$ at distance 0.3 epsilon to $C_1 = 0.07$ at distance 0.5 epsilon before rising back to attain a constant state with the finite difference method. Similarly, the C_2 of finite difference (FD) increased steadily from $C_2 = 0.017$ to a constant state as for C_1 . The constant state is at $C_2 = 0.18$. The orthogonal collocation (OC) for C_2 first moves at constant state before rising steadily to $C_2 = 0.18$ and then declined from $C_2 = 0.18$ to a minimum of $C_2 = 0.08$ before rising to a constant state. The profiles for finite difference (FD) and that of orthogonal collocation (OC) agree except for the depressions of the orthogonal collocation profiles.

Figure 1b shows the result obtained for solving Equation 19 by using orthogonal collocation (OC) and finite difference (FD) as the numerical technique. The graph is for the bed composition profile for one dimensional aqueous phase chromatography for case 1 at one pore volume injected.

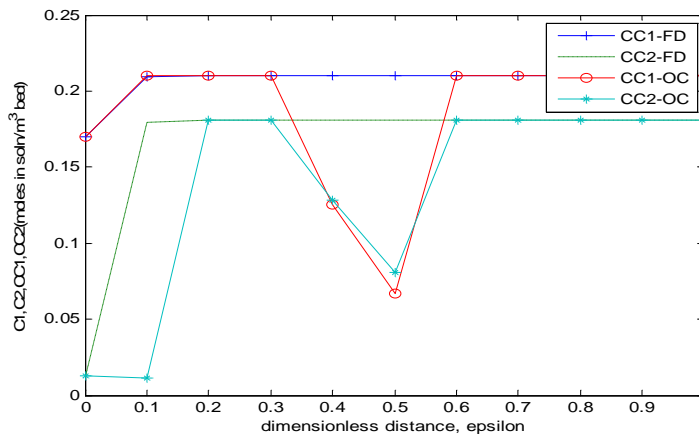
In this case also, the adsorbing porous medium is initially equilibrated with an aqueous composition. $C_1 = 0.21$, $C_2 = 0.181$ (concentrations normalized as moles in solution per m^3 off bed) and is then injected with a composition $C_1 = 0.17$, $C_2 = 0.013$ (Riemann-type problem: case 1, (refer to table 5)). The profile C_1 of finite difference (FD) indicates rise in concentration from $C_1 = 0.17$ to 0.21 after which the concentration maintained a constant state. The profile of C_1 of the orthogonal collocation (OC) also rise from $C_1 = 0.17$ to $C_1 = 0.21$ but falls to 0.03 at distance 0.4 epsilon and then increased steadily to constant state as for C_1 finite difference (FD). The C_2 of finite difference increased steadily from $C_2 = 0.02$ to attain constant state at 0.18 . Also the profile of C_2 of the orthogonal collocation (OC) increase gradually from $C_2 = 0.02$ to $C_1 = 0.18$ at distance 0.2 epsilon for short constant state and then decline to $C_2 = 0.02$ at distance 0.4 epsilon before rising back to reach constant state with the finite difference.

The bed composition profile for one dimensional aqueous phase chromatography for case 1 at two pore volume injected is

shown in figure 1c. This is the result obtained for solving Equation 19 by using numerical technique for both the orthogonal collocation (OC) and finite difference (FD). The adsorbing porous medium is initially equilibrated with an aqueous composition. $C_1 = 0.21$, $C_2 = 0.181$ (concentrations normalized as moles in solution per m^3 off bed) and is then injected with a composition $C_1 = 0.17$, $C_2 = 0.013$ (Riemann-type problem: case 1, (refer to table 5 in appendix).

The profile C_1 of finite difference (FD) and the profile C_1 of orthogonal collocation (OC) indicate that there is steady increase from $C_1 = 0.17$ to $C_1 = 0.21$ at distance 0.1 epsilon and then attained a constant state for both profiles. Similarly, the profile C_2 of finite difference (FD) shows a steady rise from $C_2 = 0.02$ to $C_2 = 0.18$ and then maintained a constant state. Also, the profile C_2 for orthogonal collocation (OC), follows the same pattern, which indicate an increase from $C_2 = 0.02$ to $C_2 = 0.18$ and then attained a constant state. The orthogonal collocation (OC) profiles match the finite difference (FD) profiles.

Figure.1a CASE 1 $C_1, C_2, CC1, CC2$ vs epsilon at $\tau = 0.5$. Bed composition profile for one-dimensional aqueous-phase chromatography; case 1, at one-half pore volume injected. The plots are for two methods: Orthogonal collocation (OC), and finite difference (FD).



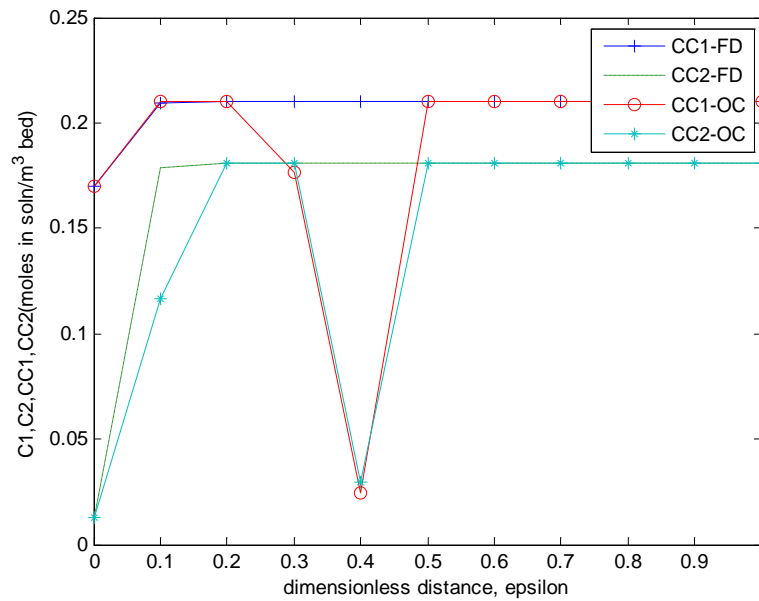


Figure.1b CASE 1 $C_1, C_2, CC1, CC2$ vs epsilon at $\tau = 1.0$. Bed composition profile for one-dimensional aqueous-phase chromatography; case 1, at one pore volume injected. The plots are for two methods: Orthogonal collocation (OC), and finite difference (FD).

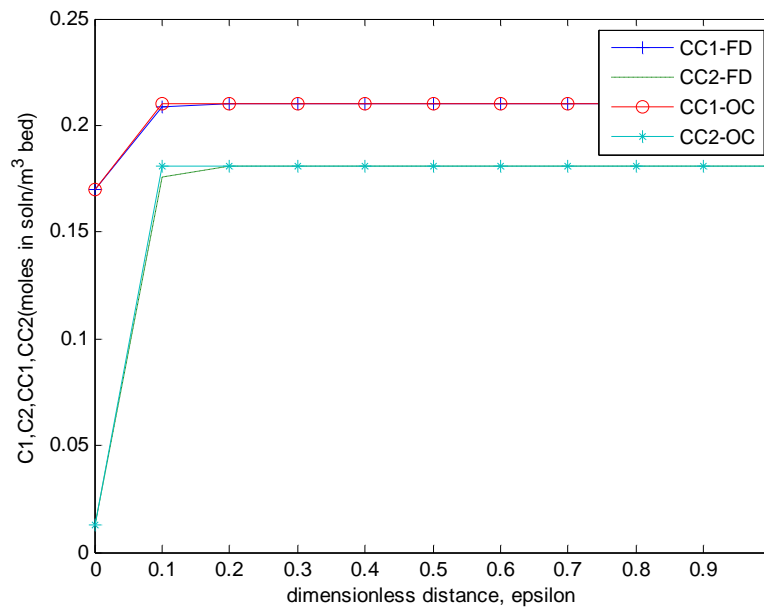


Figure.1c CASE 1 $C_1, C_2, CC1, CC2$ vs epsilon at $\tau = 2.0$. Bed composition profile for one-dimensional aqueous-phase chromatography; case 1, at two pore volumes injected. The plots are for two methods: Orthogonal collocation (OC), and finite difference (FD).

Figure 2a shows the bed concentration profiles for one dimensional aqueous phase chromatography for case 2 at one-half pore

volume injected in the adsorbing porous medium initially devoid of surfactant and then injected with a mixture $C_1 = 0.042, C_2$

= 0.115 (Riemann-type problem: case 2 (refer to table 5), with the numerical result obtained for solving Equation 19 by using orthogonal collocation (OC) and finite difference (FD) as the numerical technique. The profile C_1 of finite difference (FD) indicates a steady fall from in concentration from $C_1 = 0.04$ to a constant state of zero. The profile of C_1 of the orthogonal collocation (OC) falls steadily from $C_1 = 0.04$ but however oscillates between 0.01 and 0.04 jumping to its injection value before attaining constant state with the finite difference (FD). Similarly the C_2 of finite difference (FD) decreased steadily from $C_2 = 0.119$ to a constant state as for C_1 . Also the profile C_2 of orthogonal collocation (OC) decreases steadily from $C_2 = 0.119$ but however gives a more pronounced oscillation from $C_2 = 0.02$ and $C_2 = 0.119$ jumping to its injection value before attaining constant state with the finite difference (FD).

Figures 2b and 2c compare the bed concentration profiles expected at one and two pore volume injected with a mixture C_1

= 0.042, $C_2 = 0.115$ in the adsorbing porous medium initially devoid of surfactant [Riemann-type problem: case 2, (refer to table 5)]. The graph shows the results obtained using the numerical technique; finite difference (FD) and orthogonal collocation (OC)

In figure 2b, the profile C_1 of finite difference (FD) shows steady decline from $C_1 = 0.04$ to a constant state. Also the C_1 of orthogonal collocation falls steadily from $C_1 = 0.04$ to a constant state as for finite difference (FD). The profile C_2 of finite difference decreased steadily from $C_2 = 0.119$ to a constant state as for C_1 . Similarly, the C_2 of orthogonal collocation (OC) falls steadily from $C_2 = 0.119$ to a constant state.

In figure 2c, the profiles C_1 of orthogonal collocation (OC) follow the same pattern as that in figure 2b. Similarly, the profiles C_2 of finite difference (FD) and orthogonal collocation (OC) have the same pattern as in figure 2b.

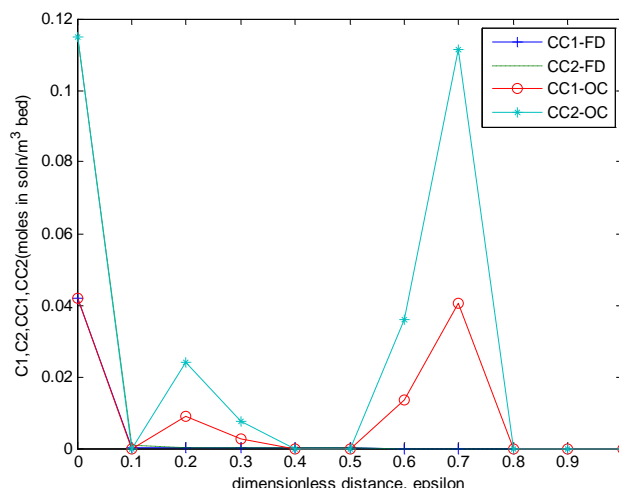


Figure.2a CASE 2 $C_1, C_2, CC1, CC2$ vs epsilon at $\tau = 0.5$. Bed composition profile for one-dimensional aqueous-phase chromatography; case 2, at one-half pore volume injected. The plots are for two methods: Orthogonal collocation (OC), and finite difference (FD)

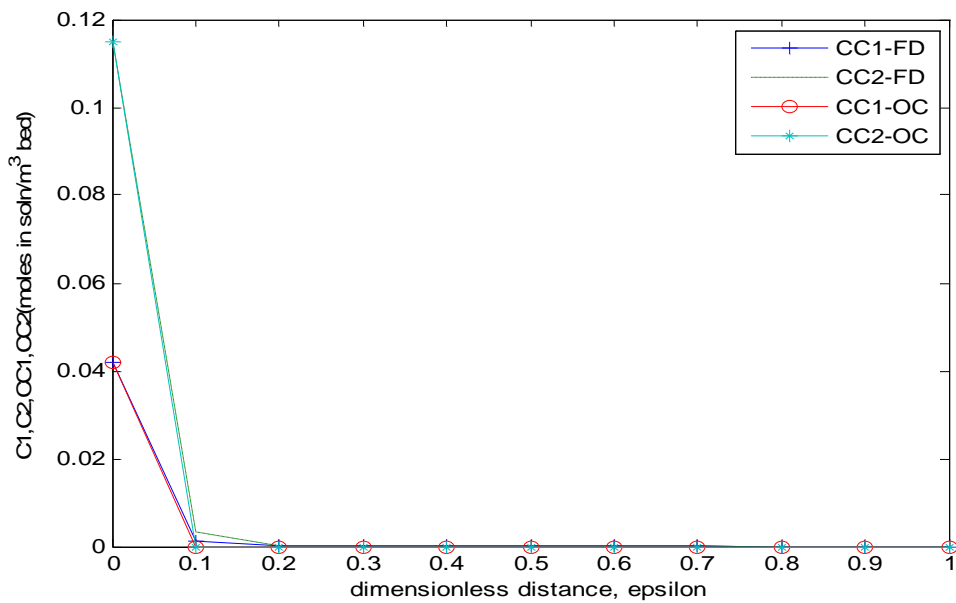


Figure.2b CASE 2 $C_1, C_2, CC1, CC2$ vs epsilon at $\tau = 1.0$. Bed composition profile for one-dimensional aqueous-phase chromatography; case 2, at one pore volume injected. The plots are for two methods: Orthogonal collocation (OC), and finite difference (FD).

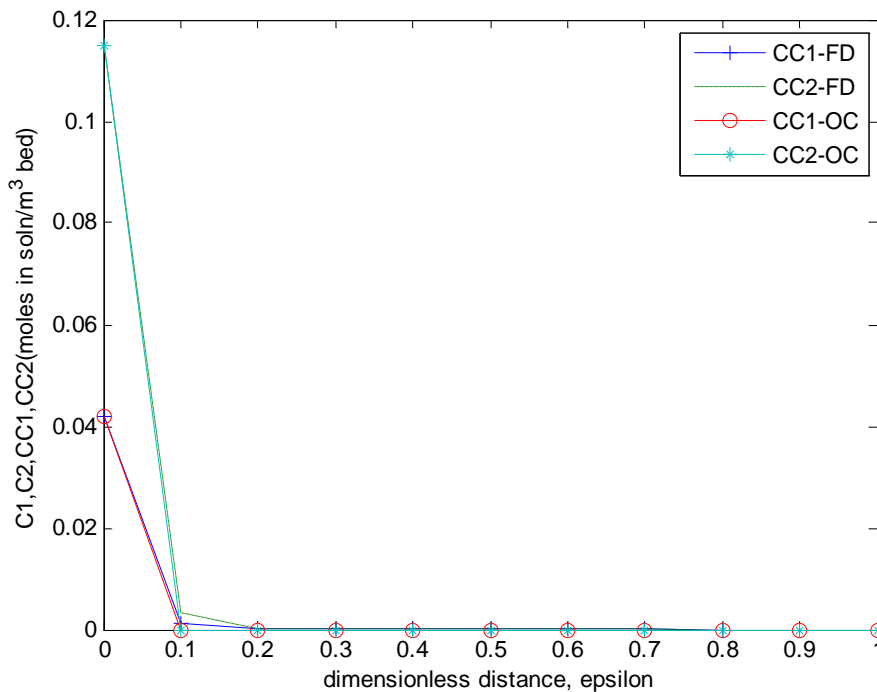


Figure.2c CASE 2 $C_1, C_2, CC1, CC2$ vs epsilon at $\tau = 2.0$. Bed composition profile for one-dimensional aqueous-phase chromatography; case 2, at two pore volumes injected. The plots are for two methods: Orthogonal collocation (OC) and finite difference (FD)

Table.1 Reservoir characteristics from the work of Hankins and Harwell (2004)

Parameter	Value
Rock density	2.65 g/cm ³
Porosity	0.2
Oil viscosity	5.0 cp
Water viscosity	1.0 cp
Injection pressure gradient (maintained constant)	1.5 psi/ft
Fluid densities	1.0 g/cm ³
Width of injection face	50 ft
Width of central high permeability streak	10 ft
Length of reservoir	100 or 5000 ft
Residual oil saturation	0.2
Connate water saturation	0.1
First injected surfactant	SDS
Second injected surfactant	DPC
Henry's law constant SDS DPC	2.71×10 ⁻⁴ l/g 8.30×10 ⁻⁵ l/g
CMC Values SDS DPC	800 μmol/l 4000 μmol/l
Injected concentration SDS DPC	10 CMC 10 CMC
Brine spacer (typical)	≈ 0.05 pore volumes
Slug volumes	≈ 0.10 pore volumes

Table.2 Reservoir Characteristics used for the Simulation work by Oyedeko (2012)

Parameter	Value
Rock density	2.65 g/cm ³
Porosity	0.2
Oil viscosity	0.40 cp
Water viscosity	0.30 cp
Injection pressure gradient (maintained constant)	1.5 psi/ft
Fluid densities	1.0 g/cm ³
Width of injection face	50 ft
Width of central high permeability streak	10 ft
Length of reservoir	100 or 5000 ft
Residual oil saturation	0.2
Connate water saturation	0.2
First injected surfactant	SDS

Second injected surfactant	DPC
Henry's law constant SDS DPC	2.71×10^{-4} l/g 8.30×10^{-5} l/g
CMC Values SDS DPC	800 $\mu\text{mol/l}$ 4000 $\mu\text{mol/l}$
Injected concentration SDS DPC	10 CMC 10 CMC
Brine spacer (typical)	≈ 0.05 pore volumes
Slug volumes	≈ 0.10 pore volumes

Table.3 Parameter values used in Trogu's adsorption model for verification runs

Parameter	Value
Pure component CMCs	$C_1^* = 1.0 \text{ mol/m}^3$ $C_2^* = 0.35 \text{ mol/m}^3$
Phase separation model parameter	$\theta = 1.8$
Henry's law constants for adsorption	$\bar{C}_i = k_i C_{i,w}$ ($C_{i,w}$ = aqueous monomer concentration) $k_1 = 0.21 \times 10^{-3} \text{ m}^3/\text{kg}$ $k_2 = 0.80 \times 10^{-3} \text{ m}^3/\text{kg}$
Henry's law constant for oleic partitioning	$C_{i,o} = q_i C_{i,w}$ ($C_{i,w}$ = aqueous monomer concentration) $q_1 = 7.1$ $q_2 = 1.3$
Adsorbent properties	$\rho_s = 2.1 \times 10^3 \text{ m}^3/\text{kg}$ $\phi = 0.2$

Table.4 Additional Reservoir Parameters for the coherence work by Hankin and Harwell (2004)

Model designation	A	B
Grid points in the horizontal direction (m+1)	21	21
Grid points in the vertical direction (n+1)	11	21
Coherent waves of water saturation	28	28
Initial number of points per coherent wave		
Water	41	41
Surfactant	81	81
Maximum number of points required per coherent wave	≈ 300	≈ 300
Average time step size (days)		
Short reservoir (100 ft)		
200 mD streak	3.47	3.47

1000 mD streak Long reservoir (5000ft)	0.69	0.69
200 mD streak	174.0	174.0
1000 mD streak	34.7	34.7
Typical number of time steps required to inject first pore volume		
Short reservoir	33	33
Long reservoir	75	75

Table.5 Conditions for case studies of surfactant chromatography (Hankins and Harwell, 2004)

Case	Injected composition: CC1(mol/m ³ bed)	Injected composition: CC2(mol/m ³ bed)	Initial composition: C1(mol/m ³ bed)	Initial composition: C2(mol/m ³ bed)
1	0.17	0.013	0.21	0.181
2	0.042	0.115	0	0
3	0.66	0.875	0.35	0.15

The prediction of the appropriate surfactant concentration necessary for the required enhanced oil recovery from reservoirs and the basic physical principle employed by the simulator is that of mass conservation. Usually those quantities are conserved at stock tank conditions and related to reservoir fluid quantities through the pressure dependent parameters. The profiles of two cases 1 and 2, one dimensional aqueous phase chromatography and two-phase chromatography for one, one-half, and two pore volume injected were developed using simulated solutions to model equations. These equations are solved by finite difference (FD) and orthogonal collocation (OC). The use of these methods permit the determination of the relative efficiency of the methods and how well they predicts the complex characteristics of the enhanced oil recovery process.

Injecting a mixture of low concentration aqueous surfactant composition into adsorbing porous medium that is initially injected with high concentration aqueous surfactant composition. This variation may exist in the initial profile or be generated by

injection. The initial fluid or previously injected fluid has the composition downstream of the change in amount while the newly injected fluid has the composition upstream of the original variation. The composition route along the bed follows the slow path from the injected composition and then switches to the fast path which leads to the previously injected composition. The route passes along paths and follows the paths in the sequence of increasing wave velocities.

Injecting a mixture of an aqueous composition into a porous medium, initially devoid of surfactant, the expected composition is a self-sharpening shock wave. The steepness in all the profiles generated by finite difference (FD), and orthogonal collocation (OC), confirms the self sharpening behaviour. It may be noted in all cases of these natures the waves trajectories gradually fall, as a result of a gradual increase in the associated eigenvalues of the waves as salinity increases. The consequence of this steepening is that the flows are sharpening, so that they break through both earlier and

over a smaller injected volume. For the dependent variables such as component concentration, common velocity exists at each point in the wave, and the associated composition route remains unchanged and the same during relative shifts of waves associated with other dependent variable waves as shown in the methods. This is in agreement with other work (Helfferich, 1981).

The complexities could not have been detected by using only the coherent technique (Hankins and Harwell, 2004). This is a major accomplishment of this work. Not only was the discontinuities discovered by this work, it also provides an insight into the complex behaviour of enhanced oil recovery process.

Conclusions

The applicability of the simulator for the solution of the model equations of multiphase, multicomponent flow and transport in a reservoir has been demonstrated using orthogonal collocation solution and finite difference. The results of the orthogonal collocation solution were compared with those of finite difference. The results obtained using this methodology revealed certain features unobserved by previous investigators (Hankins and Harwell, 2004). The results indicate that the concentration of surfactants (C_1 , C_2) for orthogonal collocation appear to show more features than the predictions of finite difference. The reason for the difference is the subject of continuing study.

It is obvious that the routes for the compositions of adsorbing surfactants correspond to the simpler case of aqueous phase chromatography, with modified eigenvalue. The route passes along the paths and follows the paths in the sequence of

increasing wave velocities. The steepness in the profiles generated by finite difference and orthogonal collocation confirms the self sharpening behaviour. The consequence of this steepening is that the flows are sharpening, so that they break through both earlier and over a smaller injected volume. This observation also holds for “shock” waves. Therein lies the possibility of the differences in the concentration profiles predicted by the two numerical techniques. Again, the use of the orthogonal collocation and finite difference solution provide easier solution to future possible problems that may arise as the simulator is being used.

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