Research

# Testing of New High-Order Finite Difference Methods for Solving the Convection-Diffusion Equation

Boyun Guo[1*§], Xiangwen Wang[2*]

Address: [1]University of Louisiana at Lafayette, P.O. Box 44690, Lafayette, LA 70504, USA, [2]Det Norske Veritas, 16340 Park Ten Place Suite 100, Houston, TX 77084, USA

Email: Boyun Guo - boyun.guo@lousiana.edu: Xiangwen Wang - maggie.wang@dnv.com
*These authors contributed equally to this work
[§]Corresponding author

Published: 05 October 2005 Received: 14 September 2005

*E-Journal of Reservoir Engineering* 2005, *ISSN: 1715-4677*. Accepted: 26 September 2005

This article is available from: http://www.petroleumjournals.com/



## Abstract

Numerical simulation has become a common means of predicting performance of oil and gas reservoirs in the petroleum industry. It is also a time-consuming task due to the large dimension of the simulation grids and computing time required to complete a simulation job. Commercial software packages used in the petroleum reservoir simulation employ the first-order-accuracy finite difference method to solve the convection-diffusion equation. This method introduces numerical dispersion because of truncation error caused by neglecting higher-order terms in Taylor's expansion.

This study focused on providing solutions to the above problems. We developed and tested two new algorithms to speed up computation and minimize numerical dispersion. In this research, we have derived the second- and third-order accuracy finite difference formulations to solve the convection-diffusion equation and applied a counter-error mechanism to reduce numerical dispersion. The results indicated that the use of the second- and third-order accuracy finite difference formulations can speed up numerical simulations and retain a sharp displacing front controlled by the physical diffusion coefficient.

## Introduction

Numerical simulation has become a common means of predicting performance of oil and gas reservoirs in the petroleum industry. It has been widely used for simulations of primary, secondary, and tertiary oil and gas recovery processes. However, even with modern computing technologies, numerical reservoir simulation is still a time-consuming task. Depending upon the dimension of the simulation grids, the computing time required to complete a simulation job varies from a few days to a few weeks. The low-speed simulation runs hinder the application of the technology to large-dimension reservoirs.

Commercial software packages used in the petroleum industry for reservoir simulation employ the first-order-accuracy finite difference method to solve the diffusivity equation for pressure and fluid saturation distributions in the reservoirs. The most widely used technique is the implicit-pressure explicit-saturation (IMPES) algorithm. For a given dimension of simulation grids, the speed of computation is controlled by timestep size ($\Delta t$). While large $\Delta t$ causes instability of algorithm, small $\Delta t$ induces high-level numerical dispersion.

The convection-diffusion equation exhibits many of the features of petroleum reservoir simulation equations. It can be written in the form of

$$\phi\frac{\partial C(x,t)}{\partial t}=D\frac{\partial^2 C(x,t)}{\partial x^2}-u\frac{\partial C(x,t)}{\partial x} \quad .....(1)$$

where $\phi$ is porosity of porous medium, $u$ is convective rate, $D$ is diffusion coefficient, $C(x,t)$ is normalized concentration, $x$ is location, and $t$ is time. In the real reservoir simulations, the function $C(x,t)$ can also represent pressure function and saturation function. The constant $D$ can also represent reservoir transmissibility $k/\mu$, where $k$ is effective formation permeability and $\mu$ is fluid viscosity.

The convection-diffusion equation can be extended for simulations of enhanced oil recovery (EOR) by miscible displacement,[1-5] immiscible displacement,[1-4] and thermal methods.[2,5] Therefore, most discussions on the effects of numerical dispersion and algorithm stability have adopted Equation (1) as an original equation.[1-3, 5-7]

Distortion of numerical solution of Equation (1) is most significant in the simulation of EOR processes[3] where sharp displacement, concentration or temperature fronts play important roles in the efficiency of the processes, and the artificial smearing as a result of numerical dispersion can render the simulation result meaningless. The numerical dispersion minimization has been an open problem in the petroleum reservoir simulation studies.

A number of investigators have studied the numerical dispersion problem, and several alternative solution techniques have been proposed to overcome the difficulties. These techniques include the method of characteristics,[8,9] modified random choice methods,[10,11] and various flux-updating schemes.[3] Although the method of characteristics is capable of producing exact solutions for certain simple problems, its use as a general simulation tool is limited by the complexity of the computer codes required to apply the method to general three-dimensional multiphase-flow problems. Both of the random choice and flux-updating methods are based on the method of characteristics, and the use of these two methods is also limited by their complexity. Although the variational methods[11-15] have been shown to produce solutions that are more accurate than those obtained with simple finite-difference techniques, their practical uses in reservoir engineering problems are again limited by their complexity and computational expense. The simplicity and generality of finite-difference techniques make them attractive. Thus the majority of commercial simulators still use the finite-difference form of approximation in the convection-diffusion equation.

Lantz[2] was the first to quantify numerical dispersion in one-dimensional equations such as Equation (1). His formulation was used by Peaceman[1] to characterize numerical solutions to such equations and proved useful in interpreting the results of a simple chemical-flood model,[16,17] where the predicted oil recovery was strongly dependent on gridblock size. Fanchi[18] generalized Lantz's formulation to three dimensions. Laumbach,[5] Price[19] and Todd[20] used second-order approximations to control numerical dispersion. Stone and Brian[4] used a Fourier analysis to improve the accuracy and stability of the numerical solution to Equation (1). Taggart and Pinczewski[21] proposed a uniformly second order finite-difference scheme capable of accurately simulating flows characterized by sharp fronts and low levels of physical dispersion. Fleming and Mansoori[22] proposed a solution method to the convection-diffusion equation, which combines the important parts of Lantz's formulation, Peaceman's[1] work, Stone and Brian's[4] method, and Laumbach's[5] technique. To the best of our knowledge, those methods and techniques either lack generality or are too complicated to be economically used on a commercial scale.

In the current practice of reservoir simulation in the petroleum industry, Equation (1) is solved by finite difference approximation with the first-order of accuracy. The numerical formulation with an explicit scheme is expressed as:

$$\phi\frac{C_i^{n+1}-C_i^n}{\Delta t}=D\frac{C_{i-1}^n-2C_i^n+C_{i+1}^n}{\Delta x^2}-u\frac{C_i^n-C_{i-1}^n}{\Delta x} \quad .....(2)$$

where

$$C_i^n=C(x,t)$$

$$C_i^{n+1}=C(x,t+\Delta t)$$

$$C_{i-1}^n=C(x-\Delta x,t)$$

$$C_{i+1}^n=C(x+\Delta x,t)$$

As shown by Wang,[23] this scheme is stable under the following condition:

$$\Delta t \le \frac{(\Delta x)^2 \phi}{2D + u\Delta x} \quad . \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(3)$$

For typical values of parameters used in tracer flow simulation with local refinement of grids ($\phi$ = 0.3, $u$ = 0.001 cm/s, $D$ = 0.00006 cm$^2$/s, and $\Delta x$ = 10 cm) the maximum value of timestep size $\Delta t$ is only 2,964 seconds, or 0.034 day. Because of the low value of $\Delta t$ for the explicit scheme of numerical formulation, implicit schemes are normally used in commercial software packages. Numerical formulation with an implicit scheme is expressed as:

$$\phi \frac{C_i^{n+1} - C_i^n}{\Delta t} = D \frac{C_{i-1}^{n+1} - 2C_i^{n+1} + C_{i+1}^{n+1}}{\Delta x^2}$$
$$- u \frac{C_i^{n+1} - C_{i-1}^{n+1}}{\Delta x} \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(4)$$

where

$$C_{i-1}^{n+1} = C(x - \Delta x, t + \Delta t)$$

$$C_{i+1}^{n+1} = C(x + \Delta x, t + \Delta t) \quad .$$

Although this numerical formulation allows the use of much higher values of $\Delta$t to speed up computing while still maintaining numerical stability, the accuracy of the simulation results suffer due to numerical dispersion. This can make the simulation result meaningless.

With today's computing technologies, numerical reservoir simulation is still a time-consuming task and the accuracy of simulation results is often not satisfactory. Better numerical algorithms are needed to speed up simulation runs and improve simulation accuracy. The objective of this research was to develop a new finite difference method for improving the accuracy of reservoir simulation while still increasing the computing speed necessary for large-dimension simulation grids. The goal of this work was to formulate and test two new algorithms for solving the convection-diffusion equation, Equation (1), with reduced error by minimizing numerical dispersion.

## New Methods

Two numerical methods for solving the convection-diffusion equation were developed in this study. They are finite difference formulations with second-order and third-order accuracies. It is known that an implicit formulation will always produce more dispersion than an explicit formulation.[24] However, we used explicit formulations in this study to simplify the testing procedure. Testing of these two methods with implicit formulations are being carried out at time of this writing.

**Explicit Finite Difference Formulation with First–Order Accuracy.** The widely used finite difference form of Equation (1) with the first-order accuracy is expressed as:

$$\phi \frac{C_i^{n+1} - C_i^n}{\Delta t} = D \frac{C_{i-1}^n - 2C_i^n + C_{i+1}^n}{\Delta x^2}$$

$$- u \frac{C_i^n - C_{i-1}^n}{\Delta x} \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots..(5)$$

Equation (5) introduces numerical dispersion due to truncation error caused by neglecting higher-order terms in Taylor's expansion. The magnitude of the numerical dispersion can be revealed in the following sections where two new methods are presented.

**Explicit Finite Difference Formulation with Second–Order Accuracy**. Derivation of an explicit finite difference formulation with second-order accuracy is documented by Wang.[23] The result indicates that Equation (5) represents more closely the following partial differential equation rather than Equation (1):

$$\phi \frac{\partial C}{\partial t} = -u \frac{\partial C}{\partial x} + \left( D + \frac{\phi u \Delta x - u^2 \Delta t}{2\phi} \right) \frac{\partial^2 C}{\partial x^2}$$

$$+ \left( \frac{uD\Delta t}{\phi} \right) \frac{\partial^3 C}{\partial x^3} + \left( - \frac{D^2 \Delta t}{2\phi} \right) \frac{\partial^4 C}{\partial x^4} \qquad \ldots.(6)$$

Derivation of Eq. (6) is too lengthy to be included in this paper. It is available from the authors upon request.

Comparing Equation (1) and Equation (6) indicates that the latter has an additional term

$$\frac{\phi u \Delta x - u^2 \Delta t}{2\phi}$$

that will generate artificial (numerical) dispersion. Although this artificial dispersion can be eliminated by choosing an optimal value for the timestep size value $\Delta t$ so that

$$\frac{\phi u\Delta x - u^2\Delta t}{2\phi} = 0,$$

or $\Delta t = \frac{\phi\Delta x}{u}$, numerical stability at

$\Delta t = \frac{\phi\Delta x}{u}$ is not guaranteed. The additional terms

$$\left(\frac{uD\Delta t}{\phi}\right)\frac{\partial^3 C}{\partial x^3} \text{ and } \left(-\frac{D^2\Delta t}{2\phi}\right)\frac{\partial^4 C}{\partial x^4}$$

will also generate error. Since the physical diffusion coefficient *D* takes very low values in reservoir simulation, term

$\left(\frac{uD\Delta t}{\phi}\right)\frac{\partial^3 C}{\partial x^3}$ is more dominating than term

$$\left(-\frac{D^2\Delta t}{2\phi}\right)\frac{\partial^4 C}{\partial x^4}.$$

Obviously, the error caused by the term

$\left(\frac{uD\Delta t}{\phi}\right)\frac{\partial^3 C}{\partial x^3}$ is proportional to timestep size $\Delta t$.

In order to minimize the numerical dispersion caused by these additional terms that are created by discretization, a counter-error mechanism was used in this study. The counter-error mechanism involves arbitrarily subtracting those error-causing terms from the original differential equation before the equation is discretized. When applied to Eq. (1), the following equation is obtained:

$$\phi\frac{\partial C}{\partial t} = -u\frac{\partial C}{\partial x} + \left(D - \frac{\phi u\Delta x - u^2\Delta t}{2\phi}\right)\frac{\partial^2 C}{\partial x^2}$$

$$-\left(\frac{uD\Delta t}{\phi}\right)\frac{\partial^3 C}{\partial x^3} + \left(\frac{D^2\Delta t}{2\phi}\right)\frac{\partial^4 C}{\partial x^4} \qquad \text{.....(7)}$$

To simplify the equation, let

$$\alpha_1 = -u$$

$$\alpha_2 = D - \frac{\phi u\Delta x - u^2\Delta t}{2\phi}$$

$$\alpha_3 = -\frac{uD\Delta t}{\phi}$$

$$\alpha_4 = \frac{D^2\Delta t}{2\phi}$$

Equation (7) may be rewritten as:

$$\phi\frac{\partial C}{\partial t} = \alpha_1\frac{\partial C}{\partial x} + \alpha_2\frac{\partial^2 C}{\partial x^2} + \alpha_3\frac{\partial^3 C}{\partial x^3} + \alpha_4\frac{\partial^4 C}{\partial x^4} \qquad \text{.....(8)}$$

Using the backward difference method, the concentration $C_i^{n+1}$ may be explicitly formulated as:

$$C_i^{n+1} = C_i^n + \frac{\alpha_1\Delta t}{\phi\Delta x}C_1^* + \frac{\alpha_2\Delta t}{\phi\Delta x^2}C_2^* + \frac{\alpha_3\Delta t}{\phi\Delta x^3}C_3^* + \frac{\alpha_4\Delta t}{\phi\Delta x^4}C_4^* \qquad \text{.....(9)}$$

where

$$C_1^* = C_i^n - C_{i-1}^n$$
$$C_2^* = C_{i+1}^n - 2C_i^n + C_{i-1}^n$$
$$C_3^* = C_{i+1}^n - 3C_i^n + 3C_{i-1}^n - C_{i-2}^n$$
$$C_4^* = C_{i+2}^n - 4C_{i+1}^n + 6C_i^n - 4C_{i-1}^n + C_{i-2}^n$$

**Explicit Finite Difference Formulation with Third–Order Accuracy.** Derivation of an explicit finite difference formulation with third–order accuracy was presented by Wang.[23] The result indicates that Equation (5) represents even more closely the following partial differential equation than Equation (1):

$$\phi\frac{\partial C}{\partial t} = -u\frac{\partial C}{\partial x} + \left(D + \frac{\phi u\Delta x - u^2\Delta t}{2\phi}\right)\frac{\partial^2 C}{\partial x^2} + \left(-\frac{u\Delta x^2}{6} + \frac{uD\Delta t}{\phi} + \frac{u^3\Delta t^2}{6\phi^2}\right)\frac{\partial^3 C}{\partial x^3}$$

$$+\left(\frac{D\Delta x^2}{12}-\frac{D^2\Delta t}{2\phi}-\frac{u^2D\Delta t^2}{2\phi^2}\right)\frac{\partial^4 C}{\partial x^4}$$
$$+\left(\frac{uD^2\Delta t^2}{2\phi^2}\right)\frac{\partial^5 C}{\partial x^5}+\left(-\frac{D^3\Delta t^2}{6\phi^2}\right)\frac{\partial^6 C}{\partial x^6}$$
$$\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(10)$$

Again, derivation of this equation is available from the authors upon request.

Comparing Equation (1) and Equation (10) indicates that the latter again has an additional term

$$\frac{\phi u\Delta x-u^2\Delta t}{2\phi}$$

that will generate artificial dispersion. Although this artificial dispersion can be eliminated by choosing

$$\Delta t=\frac{\phi\Delta x}{u},$$

numerical stability at

$$\Delta t=\frac{\phi\Delta x}{u}$$

is again not guaranteed. The additional terms will also generate error. The coefficient

$$\left(-\frac{u\Delta x^2}{6}+\frac{u^3\Delta t^2}{6\phi^2}\right)$$

should be a concern. Fortunately, choosing

$$\Delta t=\frac{\phi\Delta x}{u}$$

will also make this coefficient null.

Again, the counter-error mechanism can be used to reduce numerical dispersion due to these additional terms that are created during discretization of Eq. (1). Subtracting these error-causing terms from Eq. (1) results in:

$$\phi\frac{\partial C}{\partial t}=-u\frac{\partial C}{\partial x}+\left(D-\frac{\phi u\Delta x-u^2\Delta t}{2\phi}\right)\frac{\partial^2 C}{\partial x^2}$$
$$-\left(-\frac{u\Delta x^2}{6}+\frac{uD\Delta t}{\phi}+\frac{u^3\Delta t^2}{6\phi^2}\right)\frac{\partial^3 C}{\partial x^3}$$
$$-\left(\frac{D\Delta x^2}{12}-\frac{D^2\Delta t}{2\phi}-\frac{u^2D\Delta t^2}{2\phi^2}\right)\frac{\partial^4 C}{\partial x^4}$$
$$-\left(\frac{uD^2\Delta t^2}{2\phi^2}\right)\frac{\partial^5 C}{\partial x^5}-\left(-\frac{D^3\Delta t^2}{6\phi^2}\right)\frac{\partial^6 C}{\partial x^6}\qquad ..(11)$$

which is the equation to be discretized with minimum numerical dispersion. To simplify the equation, let

$$\alpha_1=-u$$
$$\alpha_2=D-\frac{\phi u\Delta x-u^2\Delta t}{2\phi}$$
$$\alpha_3=-\left(-\frac{u\Delta x^2}{6}+\frac{uD\Delta t}{\phi}+\frac{u^3\Delta t^2}{6\phi^2}\right)$$
$$\alpha_4=-\left(\frac{D\Delta x^2}{12}-\frac{D^2\Delta t}{2\phi}-\frac{u^2D\Delta t^2}{2\phi^2}\right)$$
$$\alpha_5=-\frac{uD^2\Delta t^2}{2\phi^2}$$
$$\alpha_6=\frac{D^3\Delta t^2}{6\phi^2}$$

Equation (11) may be rewritten as:

$$\phi\frac{\partial C}{\partial t}=\alpha_1\frac{\partial C}{\partial x}+\alpha_2\frac{\partial^2 C}{\partial x^2}+\alpha_3\frac{\partial^3 C}{\partial x^3}$$
$$+\alpha_4\frac{\partial^4 C}{\partial x^4}+\alpha_5\frac{\partial^5 C}{\partial x^5}+\alpha_6\frac{\partial^6 C}{\partial x^6}\qquad \ldots\ldots..(12)$$

Using the backward difference method, the concentration may be explicitly formulated as:

$$C_i^{n+1} = C_i^n + \frac{\alpha_1 \Delta t}{\phi \Delta x} C_1^* + \frac{\alpha_2 \Delta t}{\phi \Delta x^2} C_2^* + \frac{\alpha_3 \Delta t}{\phi \Delta x^3} C_3^* + \frac{\alpha_4 \Delta t}{\phi \Delta x^4} C_4^* + \frac{\alpha_5 \Delta t}{\phi \Delta x^5} C_5^* + \frac{\alpha_6 \Delta t}{\phi \Delta x^6} C_6^* \quad \text{.....(13)}$$

where

$$C_1^* = C_i^n - C_{i-1}^n$$

$$C_2^* = C_{i+1}^n - 2C_i^n + C_{i-1}^n$$

$$C_3^* = C_{i+1}^n - 3C_i^n + 3C_{i-1}^n - C_{i-2}^n$$

$$C_4^* = C_{i+2}^n - 4C_{i+1}^n + 6C_i^n - 4C_{i-1}^n + C_{i-2}^n$$

$$C_5^* = C_{i+2}^n - 5C_{i+1}^n + 10C_i^n - 10C_{i-1}^n + 5C_{i-2}^n - C_{i-3}^n$$

$$C_6^* = C_{i+3}^n - 6C_{i+2}^n + 15C_{i+1}^n - 20C_i^n + 15C_{i-1}^n - 6C_{i-2}^n + C_{i-3}^n$$

For easy formulation, the coefficients in the $C^*$ expressions may be given by the Pascol's Triangle:

| | Point | | | | | | |
|---|---|---|---|---|---|---|---|
| Time (n): | *i-3* | *i-2* | *i-1* | *i* | *i+1* | *i+2* | *i+3* |
| 1 | | | -1 | 1 | | | |
| 2 | | | 1 | -2 | 1 | | |
| 3 | | -1 | 3 | -3 | 1 | | |
| 4 | | 1 | -4 | 6 | -4 | 1 | |
| 5 | -1 | 5 | -10 | 10 | -5 | 1 | |
| 6 | 1 | -6 | 15 | -20 | 15 | -6 | 1 |

## Testing Criteria

The new methods were tested using three criteria: 1) numerical stability, 2) truncation error, and (3) front slope.

**Numerical Stability.** Wang[23] shows that the finite difference approximation of first-order accuracy shown in Equation (5) is stable for

$$\Delta t \le \frac{(\Delta x)^2 \phi}{2D + u\Delta x} \quad \text{.....(14)}$$

For the finite difference approximations of second- and third-order accuracies represented by Eqs. (9) and (13), the stability is apparently governed by the value of $\alpha_2$. The condition of stability for these two formulations may be expressed as:

$$\frac{\phi u \Delta x - u^2 \Delta t}{2\phi} \ge 0 \quad \text{.....(15)}$$

which results in

$$\Delta t \le \frac{\Delta x \phi}{u}. \quad \text{.....(16)}$$

Dividing Equation (16) by Equation (14) gives the ratio of the maximum stable timestep size for finite difference approximation of first-order accuracy to that for the finite difference approximations of second- and third-order accuracies as

$$\frac{(\Delta t)_{2,3}}{(\Delta t)_1} = \frac{\frac{\Delta x \phi}{u}}{\frac{(\Delta x)^2 \phi}{2D + u\Delta x}} \quad \text{.....(17)}$$

or

$$\frac{(\Delta t)_{2,3}}{(\Delta t)_1} = 1 + \frac{2D}{u\Delta x} \quad \text{.....(18)}$$

which yields

$$(\Delta t)_{2,3} = (\Delta t)_1\left(1+\frac{2D}{u\Delta x}\right) \quad \text{.....(19)}$$

This relation indicates that the maximum stable timestep size for the second- and third-order accuracy formulations is larger than that for the first-order accuracy formulation by $\left(1+\frac{2D}{u\Delta x}\right)$ fold.

**Truncation Error.** Comparison of Equation (1) and Equation (7) indicates that the truncation error given by the second-order accuracy formulation can be expressed as

$$E_{tr} = \frac{\Delta t}{\phi}\left[(\alpha_2 - D)\frac{C_2^*}{\Delta x^2} + \frac{\alpha_3 C_3^*}{\Delta x^3} + \frac{\alpha_4 C_4^*}{\Delta x^4}\right] \quad \text{.....(20)}$$

where the $\alpha$'s are those for the second-order accuracy formulation.

Comparison of Equation (1) and Equation (11) indicates that the truncation error given by the third-order accuracy formulation can be expressed as

$$E_{tr} = \frac{\Delta t}{\phi}\left[(\alpha_2 - D)\frac{C_2^*}{\Delta x^2} + \frac{\alpha_3 C_3^*}{\Delta x^3} + \frac{\alpha_4 C_4^*}{\Delta x^4} + \frac{\alpha_5 C_5^*}{\Delta x^5} + \frac{\alpha_6 C_6^*}{\Delta x^6}\right] \quad \text{.....(21)}$$

where the $\alpha$'s are those for the third-order accuracy formulation. Although the second- and third-order accuracy formulations are stable with $\Delta t \le \phi\Delta x / u$, according to Equations. (20) and (21), decreasing $\Delta t$ in the stable range may cause truncation error to increase. Therefore, a factor called Dispersion Factor (DF) is introduced into the analysis. The DF is defined as

$$DF = (\phi\Delta x / u) / \Delta t \quad \text{.....(22)}$$

When DF = 1, one should obtain the stable scheme with minimum truncation error, which gives the least numerical dispersion effect. When DF < 1, the scheme is unstable. With values of DF being greater than unity, numerical dispersion increases.

**Front Slope.** Frontal behavior was evaluated with a parameter called front slope (FS) in this study. It is defined as:

$$FS = -\left(\frac{dC}{dx}\right)_{\text{front}} \quad \text{.....(23)}$$

## Results and Discussion

The derived second- and third-order accuracy formulations modified with the counter-error mechanism were tested in this study. This section presents results of testing in terms of numerical stability, truncation error, and front sharpening effect.

**Numerical Stability.** The following parameter values were used in the testing:

| | |
|---|---|
| Length of porous medium: | L = 1,000 cm |
| Porosity: | $\phi$ = 0.30 |
| Convective velocity: | $u$ = 0.05 cm/s |
| Physical diffusivity coefficient: | D = 0.1 cm$^2$/s |
| Grid block length: | $\Delta x$ = 10 cm |
| Total injection time: | $t_{inj}$ = 0.20 pore volume |

**Fig. 1** presents a calculated concentration profile with the first-order accuracy approximation, i.e., Equation (5), using $\Delta t$ = 43.5 seconds. It clearly indicates that the numerical instability has developed. **Fig. 2** shows a calculated concentration profile with the first–order accuracy approximation using $\Delta t$ = 42 seconds. It clearly demonstrates that the numerical algorithm was stable. The total CPU time consumed for the stable computation case is 3.5 seconds with the author's Pentium 4 PC. Thus the maximum stable timestep size for the first–order accuracy approximation may be between 42 seconds and 43.5 seconds (average 42.75 seconds). The analytical expression of the maximum stable timestep size for the first–order accuracy approximation, i.e., Equation (3), gives:

$$\Delta t = \frac{(\Delta x)^2\phi}{2D + u\Delta x} = \frac{(10)^2(0.3)}{2(0.1)+(0.05)(10)} = 42.86 \text{ seconds}$$

which is very consistent with the numerical result of 42.75 seconds.

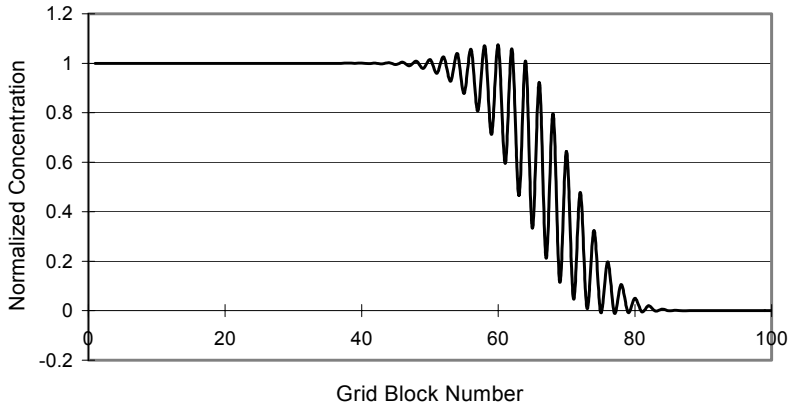


**Fig. 1 – Concentration profile given by the first-order formulation for Δt = 43.5 seconds**

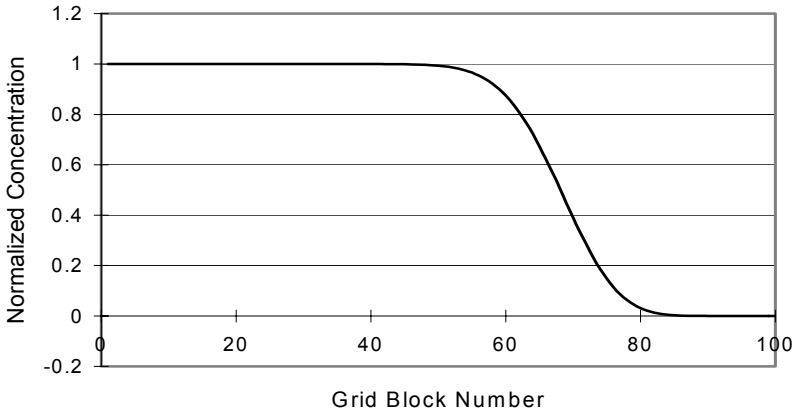


**Fig. 2 – Concentration profile given by the first-order formulation for Δt = 42 seconds**

**Fig. 3** shows a calculated concentration profile with the third-order accuracy approximation, i.e., Equation (13), using $\Delta t$ = 72 seconds. It clearly indicates that the numerical instability has developed. **Fig. 4** shows a calculated concentration profile with the third–order accuracy approximation using $\Delta t$ = 63 seconds. It clearly demonstrates that the numerical algorithm was stable. The total CPU time consumed for the stable computation case is 2.2 seconds with the author's Pentium 4 PC. Thus the maximum stable time step size for the third-order accuracy approximation may be between 63 seconds and 72 seconds (average 67.5 seconds). The analytical expression of the maximum stable time step size for the third-order accuracy approximation, i.e., Equation (16), gives:

$$\Delta t = \frac{\Delta x \phi}{u} = \frac{(10)(0.3)}{(0.05)} = 60 \text{ seconds}$$

which is close to the numerical result of 67.5 seconds.

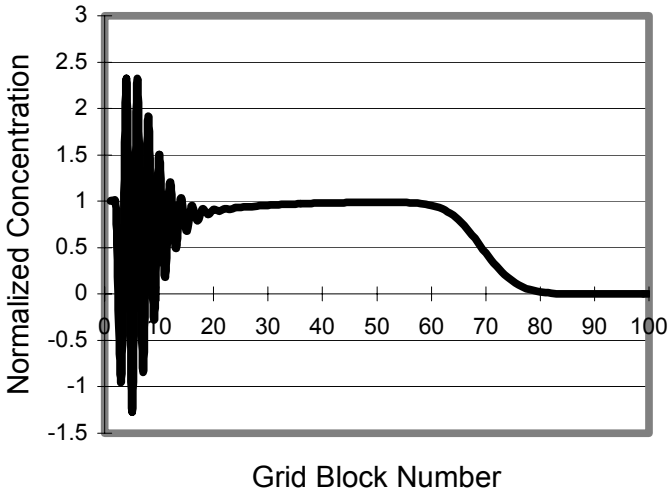


**Fig. 3 – Concentration profile given by the third-order formulation for Δt = 72 seconds**

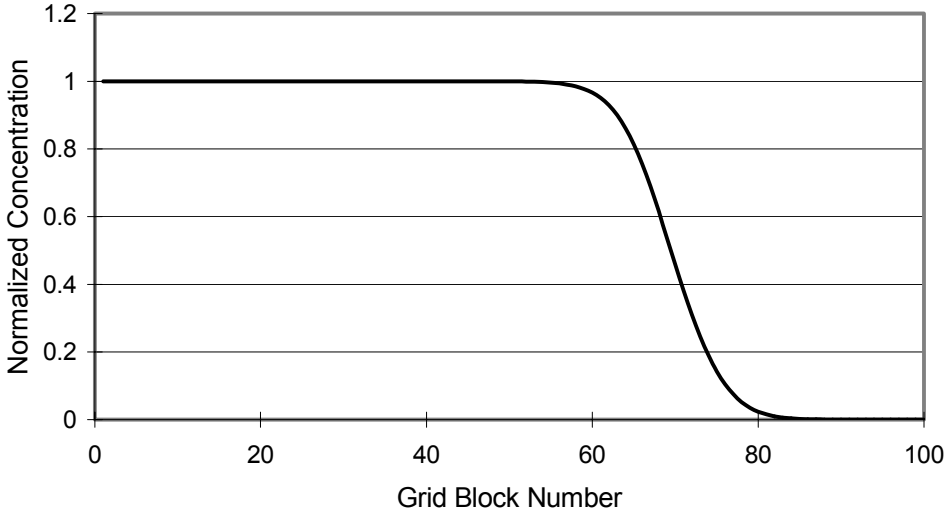


**Fig. 4 – Concentration profile given by the third-order formulation for Δt = 63 seconds**

Based on the numerical results, the timestep size improvement ($\Delta t_{imp}$) with the third-order accuracy approximation over the first-order accuracy approximation is

$$\Delta t_{imp} = \frac{67.5}{42.75} = 1.52 \text{ fold.}$$

The theoretical improvement can be calculated with Equation (18) as

$$\frac{(\Delta t)_{2,3}}{(\Delta t)_1} = 1 + \frac{2D}{u\Delta x} = 1 + \frac{2(0.1)}{(0.05)(10)} = 1.4 \text{ fold}$$

which is consistent with, but on the safe side of, the numerical result of 1.52 fold. This is consistent with the CPU time reduction of being from 3.5 seconds to 2.2 seconds.

**Truncation Error.** Truncation error for the formulation of the third-order was calculated with Equation (21) and the following parameter values:

Length of porous medium: L = 1,000 cm
Porosity: $\phi$ = 0.30
Convective velocity: u = 1 cm/s
Physical diffusivity coefficient: D = 0.01 cm2/s
Total injection time: $t_{inj}$ = 0.20 pore volume

Grid block size $\Delta x$ and time step size $\Delta t$ were used as sensitizing parameters. **Fig. 5** presents a plot of calculated truncation error against grid block size with $\Delta t$ = 0.75 second. It shows that the truncation error increases with grid block size, so we have to pay attention to the selection of grid block size. **Fig. 6** shows a plot of calculated truncation error against time step size with $\Delta x$ = 10 cm. It shows that the truncation error decreases with time step size. Here we noticed that whether the truncation error is positive or negative depends on several parameter values such as time step size and diffusion coefficient.

**Frontal Slope.** The following data were used for evaluating the behavior of the displacing front:

Length of porous medium: L = 1,000 cm
Porosity: $\phi$ = 0.30
Convective velocity: $u$ = 1 cm/s
Physical diffusivity coefficient: D = 0.001, 0.01, 0.1, 1 cm2/s
Grid block length: $\Delta$x = 10 cm
Time step size: $\Delta$t = 1.5 second
Total injection time: $t_{inj}$ = 0.20 pore volume

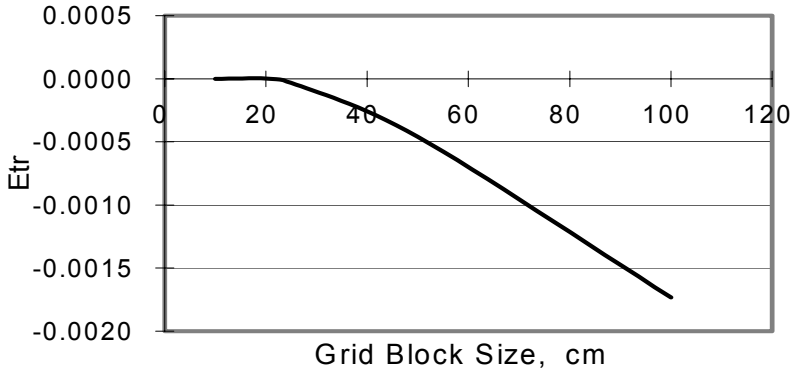


**Fig. 5 – Truncation error given by the third-order formulation for $\Delta$t = 0.75 seconds**

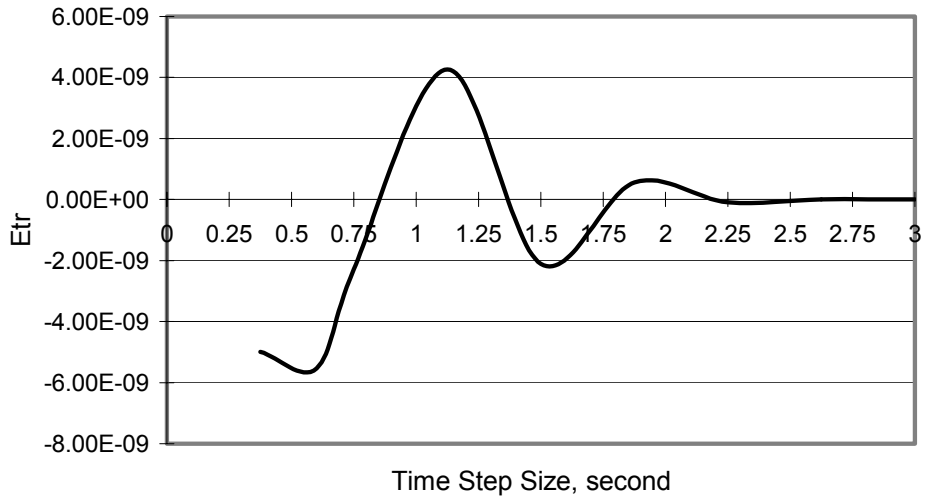


**Fig. 6 – Truncation error given by the third-order formulation for $\Delta$x =10 cm**

**Figs. 7 and 8** show calculated concentration profiles near the displacing front for $\Delta t$ = 1.5 second and different diffusion coefficient values. These figures demonstrate that the formulations with second– and third–order accuracies calculate displacing fronts that are much steeper than that given by the formulation with first–order accuracy. They also indicate that the formulations with second– and third–order accuracies yield similar displacing fronts.

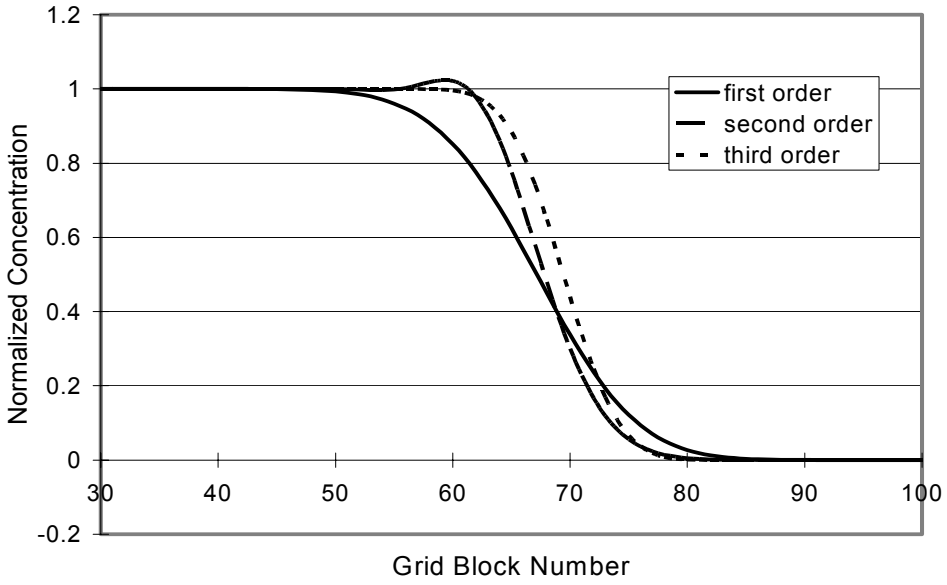


**Fig. 7 – Concentration profiles for $\Delta t$ = 1.5 seconds, D = 1 cm2/s**

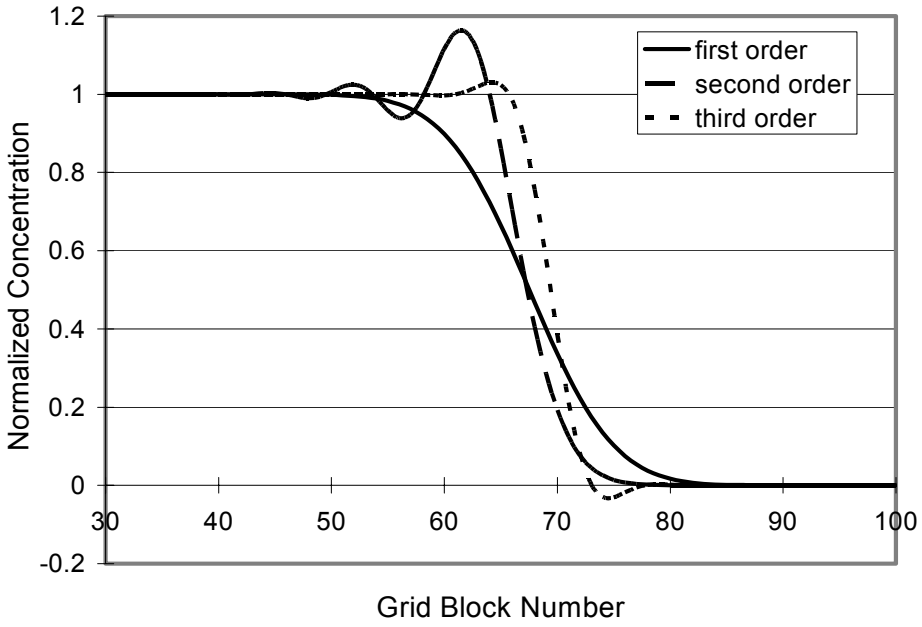


**Fig. 8 – Concentration profiles for $\Delta t$ = 1.5 seconds, D =0. 1 cm2/s**

**Fig. 9** plots the frontal slopes versus timestep size for the concentration profiles. It indicates that the frontal slope increases with timestep size for all the formulations. This is expected because use of small timestep size creates more numerical dispersion. Moreover, it is noticed that the curve presenting the first-order accuracy approximation stops between 1.875 seconds and 2.25 seconds; that is because of the numerical dispersion developed during that period. This further demonstrates that the high-order approximations are much better than the first-order approximation in this aspect.

**Fig. 10** illustrates the frontal slopes versus diffusion coefficient for the same concentration profiles. It demonstrates that the frontal slope decreases with diffusion coefficient for all the formulations. This is also expected because the diffusion coefficient creates more molecular diffusion.

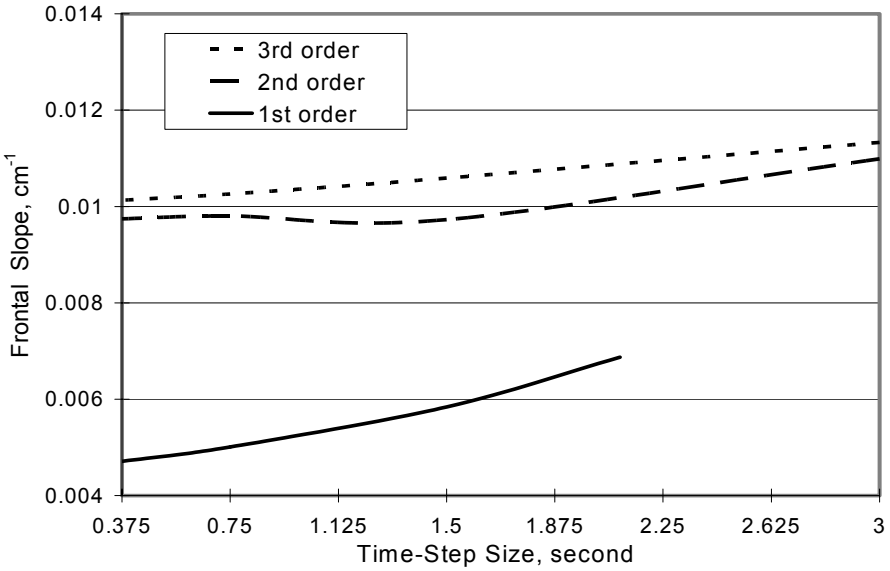


**Fig. 9 – Frontal slope for D = 1 cm2/s**

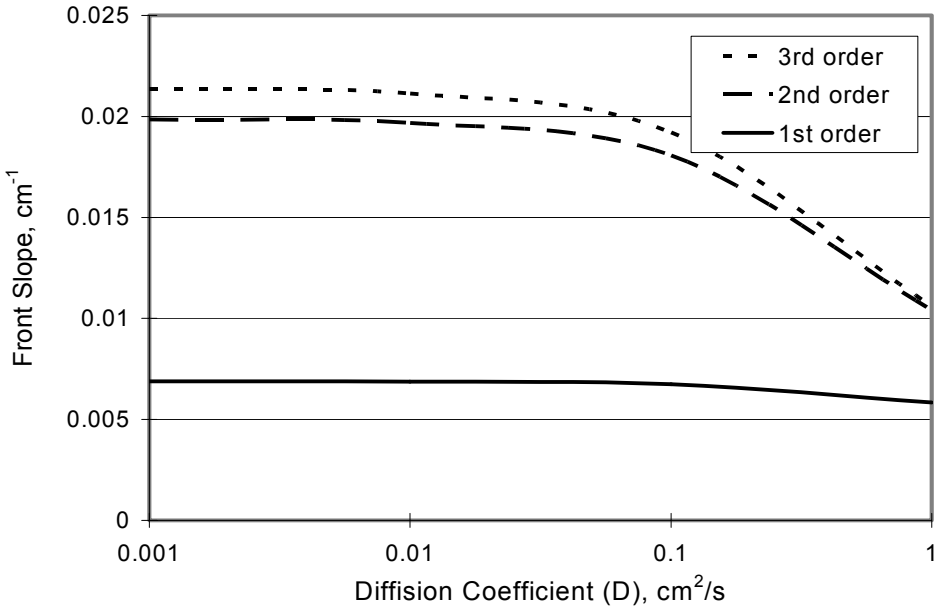


**Fig. 10 – Frontal slope for $\Delta t$ = 1.5 second**

## Conclusions

Finite difference formulations with second- and third-order accuracies have been developed and modified with a counter-error mechanism in this investigation. Numerical testing allows the following conclusions to be drawn:

The second- and third-order accuracy finite difference formulations are numerically stable for time step size

$$\Delta t \le \frac{\Delta x \phi}{u},$$

which is

$$\left(1+\frac{2D}{u\Delta x}\right)$$

times the maximum stable-timestep size for the first-order accuracy finite difference formulation. This mean that use of the second- and third-order accuracy finite difference formulations will speed up numerical reservoir simulation by

$$\left(1+\frac{2D}{u\Delta x}\right) \text{ times.}$$

Numerical diffusion and dispersion can be minimized using the second- and third-order accuracy finite difference formulations with time step size

$$\Delta t = \frac{\Delta x \phi}{u}.$$

Numerical dispersion due to truncation error increases with grid block size and decreases with timestep size.

The second- and third-order accuracy finite difference formulations retain the sharp displacing front controlled by the physical diffusion coefficient *D*.

## Acknowledgements

The authors are grateful to Chevron and API for providing Board of Regents Chevron I Endowed Professorship and API Endowed Professorship in Petroleum Engineering throughout this study. Financial support from the University of Louisiana at Lafayette CACS UCoMS Project is acknowledged.

## Nomenclature

| | |
|---|---|
| $C_i^n$ | = concentration at point *i*, time *n* |
| $C^*$ | = finite difference combined constant |
| $D$ | = diffusion coefficient, $cm^2/s$ |
| $n$ | = a general level of time spots |
| $t_{inj}$ | = pore volume injected, fraction |
| $t$ | = coordinate of time in 1-D flow, s |
| $\Delta t$ | = length of timestep, s |
| $u$ | = convective rate, cm/s |
| $x$ | = coordinate of location in 1-D flow, cm |
| $x_i$ | = location of point i |
| $x_k$ | = location of point k |
| $\Delta x$ | = grid block length in x direction, cm |

*Greek Symbols*

| | |
|---|---|
| $\alpha$ | = Constant in discretization equation. |
| $\phi$ | = Porosity of porous medium. |

## References

1. Peaceman, D.W.: **Fundamentals of Numerical Reservoir Simulation**. Elsevier Science Publishing Co., New York (1977).
2. Lantz, R.B.: **Quantitative Evaluation of Numerical Diffusion (Truncation Error)**. *SPEJ* (Sept. 1991) 315-20, *Trans*. AIME 251.
3. Larson, R.G.: **Controlling Numerical Dispersion by Variably Timed Flux Updating in One Dimension**. *SPEJ* (June 1982) 399-408.
4. Stone, H.L. and Brian, P.L.T.: **Numerical Solution of Convective Transport Problems**. *AIChE J*. (1963) 9, 681-688.
5. Laumbach, D.D.: **A High-Accuracy Finite-Difference Technique for Treating the Convection-Diffusion Equation**. *SPEJ* (Dec. 1975), 517-531.
6. Richtmyer, R.D.: **Difference Methods for Initial-Value Problems**. Interscience Publishers, Inc., New York (1957).
7. Brenner, H.: L**ongitudinal Diffusion in Packed Beds of Finite Length-Numerical Values.** *Chem. Eng. Sci.* (1962) Vol. 17, 229-243.
8. Garder, A.O. Jr., Peaceman, D.W. and Pozzi, A.L.Jr.: **Numerical Calculation of Multidimensional Miscible Displacement by the Method of Characteristics**. *SPEJ*. (March, 1964) 26-36.

9. Nolen, J.S.: **Numerical Simulation of Compositional Phenomena in Petroleum Reservoirs**. Paper SPE 4274 presented at the *1973 SPE Symposium on Numerical Simulation*, Houston, Jan. 11-12.
10. Concus, P. and Proskurowski, W.: **Numerical Solution of Non-Linear Hyperbolic Equation by the Random Choice Method**. *J. Comp. Phys.* (1979) 30, 153-166.
11. Sethian, J.A., Chorin, A.J., and Concus, P.: **Numerical Solution of the Buckley-Leverett Equations**. SPE 12254 presented at the *1983 SPE Reservoir Simulation Symposium*, San Francisco, Nov. 15-18.
12. Spivak, A., Price, H.S., and Settari, A.: **Solution of Equations for Multidimensional Two-Phase Immiscible Flow by Variational Methods**. *SPEJ* (Feb. 1977) 27-41.
13. Settari, A., Price, H.S., and Dupont, T.: **Development and Application of Variational Methods for Simulation of Miscible Displacement in Porous Media**. paper SPE 5721 presented at the *1976 SPE Symposium on Numerical Simulation*, Los Angeles, Feb. 19-20.
14. Mercer, J.W. and Faust, C.R.: **The Application of Finite Element Techniques to Immiscible Flow in Porous Media.** Proc., *First Intl. Conference on Finite Elements in Water Resources*, Princeton U. (July 1976) 1.2-1.57.
15. Allen, M.B. and Pinder, G.F.: **The Convergence of Upstream Collocation in the Buckley-Leverett Problem**. **SPEJ** (June 1985) 363-370.
16. Fleming, P.D., Thomas, C.P., and Winter, W.K.: **Application of a General Multiphase, Multicomponent Chemical Flood Model to Ternary, Two-Phase Surfactant Systems**. paper SPE 6727 presented at the *1977 SPE Annual Technical Conference and Exhibition*, Denver, Oct. 9-12.
17. Thomas, C.P. Fleming, P.D., and Winter, W.K.: **A Ternary, Two-Phase, Mathematical Model of Oil Recovery with Surfactant Systems**. *SPEJ* (Dec. 1984) 606-616.
18. Fanchi, J.R.: **Multidimensional Numerical Dispersion**. *SPEJ* (Feb. 1983) 143-151.
19. Price, H.S., Cavondish, J.C., and Varga, R.S.: **Numerical Methods of Higher-order Accuracy for Diffusion-Convection Equations**. *SPEJ* (Sept. 1968) 293-303; *Trans*., AIME, 243.
20. Todd, M.R., O'Dell, P.M., and Hirasaki, G.J.: **Methods for Increased Accuracy in Numerical Reservoir Simulators**. *SPEJ* (Dec. 1972) 515-30; *Trans*., AIME, 253.
21. Taggart, I.J., Pinczewski, W.V.: **The Use of Higher-order Differencing Techniques in Reservoir Simulation**. *SPEJ* (Aug. 1987) 360-372.
22. Fleming, P.D. and Mansoori, J.: **An Accurate Numerical Technique for Solution of Convection-Diffusion Equations without Numerical Dispersion**. *SPEJ* (Aug. 1987) 373-383.
23. Wang, X.: **New High-Order Finite Difference Methods for Increasing Speed and Reducing Numerical Dispersion in Petroleum Reservoir Simulations**. M.S. *Thesis*, University of Louisiana at Lafayette (2005).
24. Mattax, C.C. and Dalton, L.R.: **Reservoir Simulation**. *SPE Monograph* Volume 13, 60-61.