The Effect of the Definition of Fractional Flow upon Grid Effects in a Numerical Model of Thermal Processes

by

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Abstract

In previous research regarding the numerical simulation of single phase miscible displacement, a numerical procedure which does not exhibit serious grid effects and is highly compatible with nine point finite difference models has been developed. To determine if this procedure could successfully deal with grid effects in general reservoir simulators, this numerical procedure has been implemented in a simplified thermal recovery model. In the initial implementation of this procedure in a complex setting, multiple phase mass transfer between the computational molecules associated with the discretization procedure utilized the well known concepts of fractional flow and total Darcy velocity. The resulting numerical model exhibits unrealistic phenomenon, which is unexpected in light of the realistic simulations earlier obtained for the model problem. By changing the model of multiple phase mass transfer, these physically unrealistic effects are eliminated. The new model uses the total molar flux instead of the total Darcy velocity. The fractional flows are defined in a fashion compatible with the total molar flux.
1. Introduction

Fractional flow curves were used by Buckley and Leverett [1] and Welge [2] for the prediction of the recovery efficiency of a linear waterflood. In the absence of capillary pressure and gravity, the continuity equation for the displacing phase used in these investigations takes the form

\[ \frac{\partial \phi^d}{\partial t} + \frac{\partial f^d v_T}{\partial x} = Q^d \]  

(1)

A similar equation is used to govern continuity of the resident phase. The fractional flow \( f^d \) of the displacing phase is defined as

\[ f^d = \frac{k^d}{k^d + k^r} \frac{\mu^d}{\mu^d + \mu^r} \]  

(2)

In the case of the linear, incompressible waterflood studied in [1] and [2], the total Darcy velocity \( v_T \) is related to the cross sectional area and the injection rate of the displacing fluid. Furthermore, the total Darcy velocity is a constant throughout the system, and hence can be eliminated from the equations by defining a dimensionless time and distance. After completing these manipulations, the continuity of the displacing phase before breakthrough of this phase is equivalently expressed as the boundary value problem

\[ \frac{\partial \phi^d}{\partial t} + \frac{\partial f^d v_T}{\partial x} = 0 \]  

(3)
This equation is solved analytically in [1] and [2] using the method of characteristics.

The concept of fractional flow is often used in numerical models of physical systems that do not possess a closed form mathematical representation. For example, fractional flow curves were used by Blair, Douglas, and Wagner [3] as a model of multiple phase mass transfer in an areal waterflood simulator. The total Darcy velocity is not constant in the general case, and cannot simply be factored out of the flow equations, as is done in [1] and [2]. For multiple phase mass transfer, however, the total Darcy velocity is expressed as the sum of the individual phase velocities, which are in turn related to the pressure distribution by Darcy's Law. The resulting expression for the total Darcy velocity takes the form

\[ v_T = - \sum_k K_k \frac{r_t}{\mu} v_P \]  \hspace{1cm} (4)

In the absence of capillary pressure and gravity, the fractional flow of any phase \( s \) is calculated from

\[ f^s = \frac{\frac{k^{rs}}{s}}{\frac{\mu}{r_t}} \setminus \frac{\sum_k K_k \frac{r_t}{\mu} v_P}{t} \]  \hspace{1cm} (5)

The purpose of this investigation is to examine the validity of a model of multiple phase mass transfer based upon (4) and (5) in a physical system where a component - water - is present in both a liquid and a vapor phase. After briefly describing a numerical discretization
technique which exhibits insignificant grid effects for a model test problem, this procedure is extended by material balance considerations as a model of multiple phase mass transfer which uses (4) and (5). The computed pressure distribution generated by the resulting model exhibits unphysical effects. By changing the model of multiple phase mass transfer, these effects are eliminated. The modified model of multiple phase mass transfer uses a total molar flux and a corresponding fractional flow which are similar to quantities defined in (4) and (5).

The primary purpose of this paper is not to present a new numerical model. The purpose is to study a model of multiple phase mass transfer which can be implemented using any numerical discretization procedure. For this reason, the numerical methods referred to in this paper are discussed in broad generalities. Many details are omitted in this discussion, however, references are made to more complete treatments of the discretization procedures outlined below.

2. A Model of Convective Mass Transfer

This section presents a brief overview of a method presented by Potempa [4] [5] for the simulation of single phase, two dimensional, two component miscible displacement. Consider a domain of interest Ω. Over every element of volume in the domain Ω, both total mass distribution and the distribution of the invading component satisfy

Accumulation = Flux + Sources

. . . (6)

The flux and the source terms appearing in (6) are considered positive quantities if mass is flowing into an arbitrary element of volume over a
specified time interval.

To satisfy exactly the mass conservation law, (6) must hold for every element of volume contained in the domain under consideration. Using a finite computing machine, it is only feasible to enforce (6) for a finite number of elements of volume. The elements of volume used by a numerical discretization procedure are known as computational molecules, and are denoted by $\Omega_i$. In five point finite difference procedures, the computational molecules correspond to the cells formed by the partition associated with the discretization. Complex finite dimensional methods, such as the finite element method and the procedure outlined below, do not possess a simple geometric interpretation of the computational molecules.

For each computational molecule $\Omega_i$, a continuous time mass balance of total fluid present in the molecule is

$$v_i \frac{\partial \rho_i}{\partial t} = \sum_j \Gamma_{ij} \rho_{ij} + Q_i$$

...(7)

The volumetric flow rate $\Gamma_{ij}$ between the computational molecules $\Omega_i$ and $\Omega_j$ is defined to be positive if fluid is entering $\Omega_i$. Similarly, the source term $Q_i$ is defined to be positive if fluid is entering $\Omega_i$. A similar material balance governs the distribution of the invading component. Let

$$v_i \frac{\partial \rho_i c_i}{\partial t} = \sum_j \Gamma_{ij} \rho_{ij} c_{ij} + Q_i \bar{c}_i$$

...(3)
Both finite difference procedures and the procedure used in this investigation are based upon (7) and (8). The total volume of a computational molecule is defined in a similar fashion for both procedures. The injection rates at production wells are calculated using either a Peaceman correction [6] or are set equal to specified values. Both the concentration of the invading component and the density coefficients appearing in the mass transfer terms linking the computational molecules are upwinded to insure that the computed solution obeys a maximum principle. Properties such as the fluid density and porosity within each computational molecule $\Omega_i$ are calculated the "average" value of the primary unknowns within $\Omega_i$.

The only major difference between the procedure used in this investigation and finite difference procedures lies in the approximation that is used to model the volumetric flow rates between neighboring computational molecules. In finite difference procedures, the flow rates between the computational molecules are calculated from an equation of the form

$$\Gamma_{ij} = \left| \begin{array}{c} i \cdot x - j \cdot x \\ i \cdot y - j \cdot y \end{array} \right| \frac{K_{ij}}{\mu_{ij}} (P_j - P_i) \frac{\Delta y_{ij}}{\Delta x_{ij}} +$$

This equation is obtained by substitution of a finite difference approximation to the pressure gradient into Darcy's Law. By comparison, the volumetric flow rates used in this discretization procedure take the form

- 5 -
\[
\Pi_{ij} = |i_x - j_x| \int \int v_x^T \frac{\partial W_i}{\partial x} v_y^T j_y \, dx \, dy + \\
|i_y - j_y| \int \int v_y^T \frac{\partial W_i}{\partial y} x_j \, dx \, dy
\]

. . . (10)

The functions \( Y_i \), \( X_j \), and \( W_i \) are continuous, differentiable, linear functions. A definition of these functions, as well as a broader treatment of (10), is found in [4] and [5]. An approximation to the volumetric flow rates can be calculated from (10) using any approximation to the velocity distribution, including, at least in principle, the exact velocity distribution. The procedure described in [4] and [5] uses a linear combination of the functions \( \Omega_i \) and the "average" values of the pressure distribution \( P_i \) in conjunction with Darcy's Law to obtain an approximation to the velocity distribution. Using this approximation to the Darcy velocity and an appropriate numerical integration rule, (10) is evaluated as a linear combination of a either four or six nodal pressure values \( P_i \). For linear flow, the flow rates calculated using (10) are equivalent to those generated by (9).

This new discretization procedure dramatically reduces the grid effects present in numerical simulations of this model problem. Shown in Figure 1 is an inverted seven spot pattern and a discretization of a domain that exhibits no flow boundary conditions. The computed compositional profiles from a numerical simulation of displacement in an inverted seven spot pattern should exhibit rotational symmetry through rotations of \( 60^\circ \). Any deviation from rotational symmetry is a manifestation of grid orientation. Data that are used in this study are
reported in [5]. The mobility ratio is taken to be 100. Shown in Figure 2 is a computed compositional profile of the invading component at one half pore volumes injected. These computations use an upstream weighted five point finite difference procedure on the grid illustrated in Figure 1. This computational profile clearly exhibits the serious grid effects present in upstream weighted five point finite difference procedures. The invading fluid is forced to follow the artificial channels formed by the discretization procedure, rather than the physical streamlines. Shown in Figure 3 is a similar compositional profile computed using this new procedure. This figure indicates the dramatic reduction in grid effects obtained using this numerical discretization procedure.

3. Incorporation into a Model of Multiple Phase Mass Transfer

The last section demonstrates that this new numerical procedure has two nice properties. First, the method clearly reduces the grid effects to an insignificant level for a model problem. Secondly, the material balances (7) and (8) which define the procedure are compatible with those used in finite difference procedures, modulo the definition of the total volumetric flow rates between two computational molecules. In this section, an outline of how this procedure is extended to a model of multiple phase displacement is presented. Details omitted in this discussion are found in Potempa [7].

For each component present in a general system, a molar balance (6) must hold for every element of volume in the system. As discussed previously, a numerical procedure only enforces (6) for a finite number of computational molecules $\Omega_i$. Consider any component of the system under consideration, e.g. water, n-octane, etc. The accumulation term
for this component in the computational molecule \( \Omega_i \) is written as

\[
\text{Accumulation} = V_i \frac{\partial \phi_i}{\partial t}
\]

. . . (11)

The source terms acting on \( \Omega_i \) for this component are denoted by \( Q_i \).

Consider the flux terms appearing in (6) in greater detail. Gravity and capillary pressure are ignored for the purposes of simplicity. Since the procedure outlined above based upon (10) performs adequately for the miscible displacement model problem, this approximation to the volumetric flow rates between computational molecules is used as a basis for modeling convective flux in the more general setting. Furthermore, the volumetric flow rates in the more general case are calculated using the total Darcy velocity (4). Fractional flow curves computed using (5) are used to model the volume fraction of the total volumetric flux that is due to flow in a particular phase. Using these quantities, the flux of any component in the system into a computational molecule \( \Omega_i \) is modeled as

\[
\text{Flux into } \Omega_i = \left\{ \begin{array}{l}
\text{sum over all} \\
\text{other } \Omega_j \\
\text{total volume flow} \\
\text{from } \Omega_j \text{ into } \Omega_i \\
\text{volume fraction of flow} \\
\text{that occurs in phase } t \\
\text{molar density} \\
\text{of phase } t \\
\text{mole fraction of phase } t \\
\text{that is this component}
\end{array} \right\} \text{ phases } t
\]

. . . (12)

In the simulation of dead oil reservoirs, as is undertaken in [7], the mole fraction of any component in each phase is either zero or unity. This term, however, is included for generality.
The total volumetric flow rates are calculated using (10), a differentiable approximation to the pressure distribution, and the total Darcy velocity (4). The fraction of the total flow that occurs in each phase is calculated using (5). The fractional flows, molar densities, and mole fractions appearing in (12) are upwinded to insure that the computed solution obeys a maximum principle.

The material balance on any component for a computational molecule \( \Omega_i \) takes the form

\[
\frac{\partial \phi_i}{\partial t} = \sum \sum \Gamma_{ij} f_{ij} \xi_{ij} x_{ij} + Q_i
\]

This continuous time material balance is discretized in time in an IMPES fashion [8]. The primary variables used in [7] are the total densities of each component and the pressure, although in principle there is no difficulty in defining the procedure using pressure, temperature, and saturations.

4. Computational Results Using this Model

The model of convective mass transfer outlined above is used to simulate a representative steamflood in this section. The qualitative aspects of the computational results presented below are insensitive to the actual data used. A detailed description of the data is found in [7]. The qualitative aspects of the computed pressure solution are also insensitive to the coarseness of the discretization. For the purposes of simplicity, the results are presented using a 2x2x1 grid.
Shown in Figure 4 is the computed pressure solution at one-fifth the time between the start of steam injection and steam breakthrough for this representative steamflood. The injection well is located in the computational molecule shown at the lower left of this figure, and the production well is located at the upper right. A brief examination of the lines \(x=0\) or \(y=0\) reveals unrealistic effects in this computed pressure solution. The true pressure solution is monotonic along these lines, while the computed pressure solution is far from monotonic, showing considerable "wiggle".

This effect occurs in the vicinity of the steam front. If a finer discretization is employed, the computed pressure solution is monotonic except at the steam front. Using this procedure to model hot water floods results in both no grid orientation and no "wiggle" [4]. The phenomenon is also not present in one dimensional problems, where the numerical discretization procedure outlined above is equivalent to a finite difference procedure.

5. Discussion

Ce n'est pas possible! It is, to say the least, surprising that a procedure that works much better than finite difference procedures for single phase miscible displacement problems shows completely unrealistic behavior for multiple phase displacement. Furthermore, finite difference models have not been observed to exhibit this "wiggle". No attempt is made to rigorously explain the "wiggle" in this section. Instead, the discussion is undertaken only on a heuristic level.
There are two possible causes of this effect. First, the model approximating the volumetric flow rates between two computational molecules can be incorrect. Secondly, the model used to incorporate the volumetric flow rates into a model of multiple phase mass transfer can be incorrect. The second view is taken below.

The computational problems noted above are encountered only occur at a simulated phase boundary. Downstream of the steam front, the total Darcy velocity, i.e., the total volumetric flux, is due mainly to water flowing in a relatively dense liquid phase, and is relatively small. Upstream of the steam front, the most of the total volumetric flux is due to water in the form of steam, and is relatively large. The function representing the total volumetric flux is rough at the steam front, and is hard to approximate. Representations of the total Darcy velocity by functions such as discontinuous constants, which is the approximating space used when taking the finite difference gradient of the computed pressure solution, are able to better approximate the total volumetric flux than a smoother approximating space, such as that which is used by the procedure outlined above.

Use of the total volumetric flux results in an excellent model of multiple phase mass transfer in incompressible problems. In an incompressible problem, the total volumetric flux through any element of volume within a domain under consideration must be zero. Indeed, in the linear waterflood case, the total volumetric flux is a constant. Due to condensation effects at the steam front, the total volumetric flux is a rough function in a steamflood. The total volumetric flux is hard to approximate in a physical problem where mass transfer of a component
occurs in both a liquid phase and a vapor phase.

6. Modification of the Model of Multiple Phase Mass Transfer

The remarks in the previous section indicate that the unrealistic phenomenon noted above might be eliminated if the model of multiple phase mass transfer (12) is defined in terms of relatively smooth functions. Toward this end, let the total molar flux be defined as

\[ u^T = - \sum_k \frac{k^T \xi^T}{\mu^T} \nabla P \]

\[ \ldots \ldots \ldots (14) \]

In the absence of capillary pressure and gravity, the molar fractional flow of a phase \( s \) is expressed as

\[ m^s = \frac{k^s \xi^s}{\mu^s} \sum \frac{k^T \xi^T}{\mu^T} \]

\[ \ldots \ldots \ldots (15) \]

An approximation to the total molar flow rate between two computational molecules, still denoted as \( \Gamma_{ij}^T \), is calculated replacing the components of the total Darcy velocity appearing in (10) with the corresponding components of the total molar flux (14).

Using a modification of (12), the total flux of any component into a computational molecule \( \Omega \) is modeled by
Flux into $\Omega_i = \left\{ \sum_{\text{other } \Omega_j} \right\} \times \left\{ \sum_{\text{phases } t} \right\} \left\{ \text{total molar flow from } \Omega_j \text{ into } \Omega_i \right\} \times \left\{ \text{mole fraction of flow that occurs in phase } t \right\} \times \left\{ \text{mole fraction of phase } t \right\} \left\{ \text{that is this component} \right\} \quad \ldots \quad (16)

The continuity equation that is enforced over all computational molecules $\Omega_i$ for any component takes the form

$$\frac{\partial \phi_i}{\partial t} + \sum_j \sum_l \Gamma_{ij} \mu_{ij}^t x_{ij}^t + Q_i \quad \ldots \quad (17)$$

Further details concerning this discretization scheme are discussed in [7].

7. Computational Results

The computed pressure solution at one-fifth of the time between initial steam injection and steam breakthrough using the model of multiple phase mass transfer presented above is illustrated in Figure 5. The data used in this run is exactly the same as that used earlier. The unrealistic phenomenon noticed earlier are eliminated. The computed pressure solution is monotonically decreasing between the injection well and the production well.

8. Concluding Remarks

This paper raises the following questions. First, can the importance of the grid orientation effect present in finite difference models of steam displacement be diminished by incorporation of the ideas discussed above in these models? In particular, does the procedure of
McCracken and Yanosik [9] exhibit a serious grid effect when modeling a steamflood in an inverted seven spot pattern [10] if incorporated into a steamflood model using the above considerations? Secondly, it is conjectured above that the molar flux is a considerably smoother function than the volumetric flux near the steam front. Does experimental data measuring both the molar and volumetric flux for a linear laboratory steamflood support this conclusion? Lastly, are these ideas important to consider when modeling some other process where mass transfer of some component occurs in both a liquid and a vapor phase, i.e., in multiple phase miscible displacement?

9. Acknowledgements

I would like to acknowledge that this work was supported in part by the Internation Business Machines Corporation, Palo Alto Scientific Center. Also, I would like to thank Dr. Mary Wheeler and Dr. Trond Steihaug of Rice for their useful suggestions concerning this work. Lastly, I would like to especially thank Dr. John Dennis of Rice, whose question "What is a phase?" planted the seed for the ideas presented above.

10. Nomenclature

c_i Average concentration of the invading fluid in the computational molecule \( \Omega_i \).

\( \bar{c}_i \) Average concentration for well terms of the invading fluid in the computational molecule \( \Omega_i \).

\( c_{ij} \) Upwinded concentration between computational molecules \( \Omega_i \) and \( \Omega_j \).

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\( f^d \) Fractional flow of the displacing phase.

\( f^s \) Fractional flow of a phase \( s \).

\( f^t_{ij} \) Upwinded fractional flow of phase \( t \) between the computational molecules \( \Omega_i \) and \( \Omega_j \).

\( i_x \) Index in the \( x \) coordinate of the computational molecule \( \Omega_i \).

\( i_y \) Index in the \( y \) coordinate of the computational molecule \( \Omega_i \).

\( j_x \) Index in the \( x \) coordinate of the computational molecule \( \Omega_j \).

\( j_y \) Index in the \( y \) coordinate of the computational molecule \( \Omega_j \).

\( k^{rd} \) Relative permeability of the displacing phase.

\( k^{rr} \) Relative permeability of the resident phase.

\( k^{rs} \) Relative permeability of a phase \( s \).

\( k^{rt} \) Relative permeability of a phase \( t \).

\( m^s \) Molar fractional flow of a phase \( s \).

\( m^t_{ij} \) Upwinded molar fractional flow between the computational molecules \( \Omega_i \) and \( \Omega_j \).

\( t \) Time, days.

\( u^T \) Total molar flux, lb moles / day.

\( v^T \) Total Darcy velocity, ft / day.

\( v_x^T \) X component of the total Darcy velocity, ft / day.

\( v_y^T \) Y component of the total Darcy velocity, ft / day.

\( x \) Position in the \( x \) coordinate, ft.
- Dimensionless distance.

- \( \bar{x} \) Average total molar density of any component in the computational molecule \( \Omega_i \), lb moles / cu ft.

- \( x_{ij} \) Mole fraction of any component in phase \( t \).

- \( y \) Position in the \( y \) coordinate, ft.

- \( K \) Permeability, md * .006336.

- \( K_{xij} \) Average permeability in the \( x \) direction linking the computational molecules \( \Omega_i \) and \( \Omega_j \) for a five point finite difference procedure, md * .006336.

- \( K_{yij} \) Average permeability in the \( y \) direction linking the computational molecules \( \Omega_i \) and \( \Omega_j \) for a five point finite difference procedure, md * .006336.

- \( P \) Pressure, psi.

- \( P_i \) Average pressure in the computational molecule \( \Omega_i \), psi.

- \( P_j \) Average pressure in the computational molecule \( \Omega_j \), psi.

- \( Q_d \) Volumetric injection rate of the displacing phase, cu ft / day.

- \( Q_i \) Mass or molar injection rate into the computational molecule \( \Omega_i \), lbs / day or lb moles / day.

- \( S_d \) Saturation of the displacing phase.

- \( V_i \) Total volume of the computational molecule \( \Omega_i \), cu ft.

- \( W_i \) A function associated with the computational molecule \( \Omega_i \).
\( x \)  
A function associated with the computational molecule \( \Omega_i \).

\( y \)  
A function associated with the computational molecule \( \Omega_j \).

\( \mu_d \)  
Viscosity of the displacing phase, cp.

\( \mu_r \)  
Viscosity of the resident phase, cp.

\( \mu_s \)  
Viscosity of a phase \( s \), cp.

\( \mu_t \)  
Viscosity of a phase \( t \), cp.

\( \mu_{ij} \)  
Linking viscosity between the computational molecules \( \Omega_i \) and \( \Omega_j \) in a finite difference procedure, cp.

\( \xi_s \)  
Molar density of phase \( s \), lb moles / cu ft.

\( \xi_t \)  
Molar density of phase \( t \), lb moles / cu ft.

\( \xi_{ij} \)  
Upwinded molar density of phase \( t \) between the computational molecules \( \Omega_i \) and \( \Omega_j \), lb moles / cu ft.

\( \rho_i \)  
Average density in computational molecule \( \Omega_i \), lbs / cu ft.

\( \rho_{ij} \)  
Upwinded density between computational molecules \( \Omega_i \) and \( \Omega_j \), lbs / cu ft.

\( \tau \)  
Dimensionless time.

\( \phi \)  
Porosity.

\( \Delta x_i \)  
Width in the \( x \) direction of the computational molecule \( \Omega_i \) in a finite difference procedure, ft.

\( \Delta x_{ij} \)  
Distance between the computational molecules \( \Omega_i \) and \( \Omega_j \) in a finite difference procedure, ft.

\( \Delta y_i \)  
Width in the \( y \) direction of the computational molecule \( \Omega_i \) in a finite difference procedure, ft.
\( \Delta y_{ij} \) Distance between the computational molecules \( \Omega_i \) and \( \Omega_j \) in a finite difference procedure, ft.

\( \Gamma_{ij} \) Approximate volumetric or molar flow rate between the computational molecules \( \Omega_i \) and \( \Omega_j \), cu ft / day or lb moles / day.

\( \Omega \) Domain of interest.

\( \Omega_i \) An individual computational molecule with index \( i \).

\( \Omega_j \) An individual computational molecule with index \( j \).

11. References


FIGURE 1
DISCRETIZATION OF THE INVERTED SEVEN SPOT

- INJECTION WELL
- PRODUCTION WELL
FIGURE 2
COMPUTED COMPOSITIONAL
PROFILES AT .5 PV
SEVEN SPOT PATTERN
FINITE DIFFERENCES
FIGURE 3
COMPUTED COMPOSITIONAL
PROFILES AT .5 PPU
SEVEN SPOT PATTERN
NEW PROCEDURE
### FIGURE 4
COMPUTED PRESSURE SOLUTION USING VOLUMETRIC FLUX MODEL AT 300 DAYS

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### FIGURE 5
COMPUTED PRESSURE SOLUTION USING MOLAR FLUX MODEL AT 300 DAYS

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