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**A Finite Element Material
Balance for Two Dimensional
Convection - Diffusion Equations ***

by

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Abstract

A consistent finite element material balance is developed for the two dimensional convection - diffusion equation. The resulting numerical scheme is an average of the conventional Galerkin procedures for both the divergence and nondivergence form of the continuity equations. This derivation is valid for finite dimensional approximating spaces having the property that the basis functions sum to unity. Computational molecules are associated with each basis function of the finite dimensional approximating space. The physical significance of coefficients appearing in the resulting material balance governing every computational molecule is discussed. The scheme is compared with standard finite difference procedures. Regularization of the resulting numerical scheme is accomplished by lumping and upstream weighting.

1. Introduction

Convection - diffusion equations arise frequently in transport phenomenon. Such equations serve as the differential equations of change governing the distribution of each component in multiple component systems. Closed form solutions to the equations of change governing many interesting physical systems are not known. Accurate numerical solutions to the equations of change are hence essential for proper simulation of the associated physical processes. For example, various nonlinear versions of the convection - diffusion equation arise frequently in the petroleum industry. Frontier tertiary recovery processes are described by these nonlinear versions of the convection - diffusion equation. Although both one, two, and three dimensional equations are in practice used to represent typical recovery processes, the two dimensional linear variant of the convection - diffusion equation is studied in this investigation.

Many state of the art reservoir simulation codes utilize upwinded five point finite difference procedures. The advantages enjoyed by these numerical schemes are manifold. The resulting procedures are easy to implement. The numerical procedures are computationally fast. A large amount of software compatible with five point finite difference procedures is readily available. The procedures are conceptually similar to the "shell balance" approach used to derive the corresponding equations of change. The disadvantages of this numerical scheme are twofold. The approximate solution depends on the orientation of the grid, as is illustrated by Nirasaki, O'Dell, and Todd [1]. The grid orientation effect associated with five point is significantly magnified in simulated displacements at extremely unfavorable mobility ratios, such as

steepflooding [2]. Front smearing is also a problem due to artificial dispersion that is added by upwinding.

McCracken and Yanosik [3] propose a nine point finite difference scheme that attempts to eliminate the grid orientation effect. This procedure is readily implemented in existing finite difference models. The procedure is quite successful in dealing with grid orientation effects [3] [4] [5], provided the upwinding is applied to a properly scaled partial differential equation [5] [6]. One major and one minor problem are associated with the procedure suggested by Yanosik and McCracken. The major problem is that the numerical dispersion is on the same order of magnitude as that encountered using five point finite difference procedures. A less significant problem is that the procedure is not readily extended to domains that do not have a rectangular underlying partition.

Both conventional and unconventional Galerkin techniques are proposed in the literature for obtaining approximate solutions to the convection - diffusion equation. Some of the numerous efforts include those of Dupont, Price and Settari [7], Darlow, Douglas, Kendall, and Wheeler [8], and Russell [9]. It is possible to eliminate grid orientation and dispersion effects using many of these codes, provided sufficient care is taken in choosing many of the important input parameters. One drawback of such models is that the models are not compatible with five point finite difference techniques. A second drawback is that the models often require fine tuning to obtain physically meaningful results, a luxury which is not practical in realistic studies. A final drawback is that the numerical methods are so complicated that the underlying physical principles are

easily obscured by the complexity of the numerical method.

Young [10] introduces a modified finite element Galerkin procedure in an investigation that addresses many of the criticisms regarding variational procedures. The scheme proposed by Young is simple to use and appears to converge to the true solution of the differential equation. Although numerical dispersion is not a problem with the scheme proposed by Young, the grid orientation effects are severe at practical discretization sizes for the procedure which resembles standard five point finite difference schemes. A secondary drawback of the scheme proposed by Young is that the method is based upon an approximating space that uses tensor product Lagrange functions as basis functions and hence is not defined on irregular domains.

Porempa [11] [12] introduces a finite element material balance for convection - diffusion equations. Regularization is accomplished through lumping and upwinding. This procedure has been previously developed using physical considerations. A mathematical basis for this procedure is indicated in this investigation. A consistent finite element material balance is developed. The procedure is based upon both the divergence and the nondivergence forms of the equation of the convection - diffusion equation. Regularization of this material balance is accomplished by lumping and a modification of the rate of mixing between computational molecules. Both the good and the bad properties of the resulting procedure are outlined.

2. The Model Problem

Let Ω denote a bounded domain in R^2 . Let f and g denote nonnegative scalar valued functions, \mathbf{v} denote a vector valued function with nonnegative components, and D denote a positive semidefinite matrix. A linear form of the convection - diffusion equation governing a distribution c on a region Ω that arises in petroleum engineering is the partial differential equation

$$\frac{\partial c}{\partial t} + \nabla \cdot \mathbf{v}c + fc = g + \nabla \cdot D \nabla c \quad . . . (1)$$

Let \mathbf{n} denote the outward normal to the boundary of the region $\partial\Omega$. If the coefficient functions appearing in (1) are smooth, c is assumed to obey boundary conditions of the form

$$\nabla c \cdot \mathbf{n} = 0 \quad . . . (2)$$

In practical applications, the coefficients appearing in (1) are not treated as smooth functions. In the more general case condition (2) is replaced by a more realistic reflection condition.

The vector function \mathbf{v} is a smooth function in practical applications. In many physical systems, the distribution of \mathbf{v} is assumed to obey an incompressibility condition of the form

$$\nabla \cdot \mathbf{v} + f = g \quad . . . (3)$$

The domain Ω is chosen in practice so that the vector function \mathbf{v} obeys boundary conditions on $\partial\Omega$ of the form

$$\mathbf{v} \cdot \mathbf{n} = 0$$

. . . (4)

The functions f and g appearing in (1) and (3) represent source and sink terms, respectively. The scalar functions f and g are both nonnegative. In many applications the source and sink terms act approximately as Dirac measures, as the areal extent of the region where these terms do not vanish is about one millionth of the areal extent of the domain under consideration. At practical discretization sizes these terms are hence written as a positive linear combination of Dirac measures.

The matrix D represents a physical diffusion and dispersion matrix. A first order approximation to this matrix is presented by Russell and Wheeler [13]. The physical matrix is in general composed of a dispersive part which depends upon the components of the vector function \mathbf{v} and a diffusive part which results from the application of Fick's Law to flow in a porous media. The physical dispersion matrix D is symmetric and positive semidefinite.

The equation of change (1) is presented in the divergence form of the continuity equation. By expanding the convective term of (1) using the product rule and replacing the divergence of \mathbf{v} using (3), a different form of the equation of change is obtained. The resulting equation is the nondivergence form of the continuity equation and is given by

$$\frac{\partial c}{\partial t} + \mathbf{v} \cdot \nabla c + gc = g + \nabla \cdot D \nabla c$$

. . . (5)

3. Material Balance Derivation

A conventional finite element Galerkin Method is applied to both (1) and (5). The domain D is partitioned by a triangulation τ into a finite number of polygonal elements. An approximating space H_τ with a finite

number of degrees of freedom is constructed. Continuity requirements are specified for M_τ . Functions contained in M_τ are required to be polynomials over every element of the triangulation. The number of degrees of freedom of M_τ is denoted by n . Let $w_i(x,y)$ denote elements of a basis for M_τ . In general, the basis functions $w_i(x,y)$ are nonvanishing only over a limited number of elements of the triangulation.

In addition to the standard requirements on the approximating space M_τ , it is assumed that for all (x,y) contained in \mathcal{B} the basis functions $w_i(x,y)$ obey

$$\sum_{j=1}^n w_j(x,y) = 1 \quad . . . (6)$$

Examples of triangulations τ and approximating spaces M_τ which obey (6) include C^0 linears on triangles, C^0 tensor product linears over rectangles, and C^1 tensor product quadratics over rectangles. Many other approximating spaces M_τ also satisfy the condition expressed by (6).

Every element contained in the approximating space M_τ is a linear combination of the basis functions $w_i(x,y)$. Let $C(x,y,t)$ denote a function contained in $M_\tau \times [0,T]$. The function C is represented as a linear combination of the form

$$C(x,y,t) = \sum_{j=1}^n c^j(t) w_j(x,y) \quad . . . (7)$$

The function C is used below to denote the approximation of the distribution of c which is obtained by a Galerkin procedure. For the sake of brevity, the functional dependence in C , c^j , and w_j is dropped. Lastly,

for either vector or scalar functions u and v let

$$\langle u, v \rangle = \int_{\Omega} u(x, y) v(x, y) dy dx \quad . . . (8)$$

Continuous time Galerkin procedures corresponding to (1) and (5) are defined using variational forms of the differential equations. Further manipulations are performed on the weak form of the differential equations by applying partial integration and substituting the zero flux conditions in the resulting line integrals over the boundary of the domain. The conventional Galerkin procedure determines the element C of M_{τ} which satisfies the resulting variational equation for every test function W contained in the space M_{τ} . This is equivalent to forcing the variational forms to hold for each basis function w_i of the approximating space M_{τ} . The application of the variational forms of (1) and (5) to each basis function w_i is considered a computational molecule Ω_i . For the divergence form (1) of the continuity equation, a continuous time Galerkin procedure for the computational molecule Ω_i is defined by

$$\left\langle \frac{\partial C}{\partial t}, w_i \right\rangle - \langle v, Cw_i \rangle + \langle DVC, Vw_i \rangle = \langle g, w_i \rangle - \langle f, Cw_i \rangle \quad . . . (9)$$

A corresponding continuous time Galerkin procedure is defined for the nondivergence form (5) of the continuity equation by

$$\left\langle \frac{\partial C}{\partial t}, w_i \right\rangle + \langle v, w_i VC \rangle + \langle DVC, Vw_i \rangle = \langle g, w_i \rangle - \langle g, Cw_i \rangle \quad . . . (10)$$

Finite difference procedures are generally viewed as material balances on computational molecules Ω_i^{fd} corresponding to regions in R^2 contained in Ω . Associated with every finite difference computational molecule Ω_i^{fd} is a volume V_i^{fd} , a source term G_i^{fd} , and a sink term F_i^{fd} . As a finite element

material balance on a computational molecule Ω_i corresponds to a material balance on the measure $w_i dx dy$ [13], similar volume, source, and sink terms are defined in terms of integrals involving the basis functions. Toward this end, let

$$V_{ij} = \langle w_i, w_j \rangle \quad . . . (11)$$

Let the volume V_i of each computational molecule Ω_i be given by

$$V_i = \sum_{j=1}^n V_{ij} \quad . . . (12)$$

To consistently treat the source terms, define

$$G_{ij} = \langle g w_i, w_j \rangle \quad . . . (13)$$

Let the source term G_i acting on a computational molecule Ω_i be given by

$$G_i = \sum_{j=1}^n G_{ij} \quad . . . (14)$$

To consistently treat production terms, define

$$F_{ij} = \langle f w_i, w_j \rangle \quad . . . (15)$$

Let the production term F_i acting on a computational molecule Ω_i be given by

$$F_i = \sum_{j=1}^n F_{ij} \quad . . . (16)$$

Interactions between computational molecules Ω_i^{fc} and Ω_j^{fc} which are associated with finite difference procedures are generally characterized in terms of a flow rate Γ_{ij}^{fd} and a mixing rate D_{ij}^{fd} . The mixing rate between two different finite element computational molecules Ω_i and Ω_j is defined by

$$D_{ij} = -\langle \mathbf{D} w_i, w_j \rangle \quad . . . (17)$$

The mixing rate D_{ij} is a nonnegative quantity if $i \neq j$. The mixing rate D_{ii} is defined only for convenience and has no physical significance. Since the basis is required to sum to unity, the mixing rates D_{ij} satisfy

$$\sum_{j=1}^n D_{ij} = 0 \quad . . . (18)$$

The flow rate between finite element computational molecules Ω_i and Ω_j is defined by

$$\Gamma_{ij} = \langle \mathbf{v}, w_i \nabla w_j - w_j \nabla w_i \rangle \quad . . . (19)$$

The flow rate Γ_{ij} is positive if the material is leaving the computational molecule Ω_i and entering the computational molecule Ω_j . Using the fact that the basis functions sum to unity, the incompressibility condition (3), and partial integration, one obtains that the flow rates satisfy

$$\sum_{j=1}^n \Gamma_{ij} = G_i - F_i \quad . . . (20)$$

By averaging the Galerkin procedures (9) and (10) which correspond to the divergence and nondivergence form of the continuity equation, one

obtains that

$$\sum_{j=1}^n \left[\frac{\partial c^j}{\partial t} v_{ij} + \frac{1}{2} c^j \Gamma_{ij} - c^j D_{ij} + \frac{1}{2} c^j G_{ij} + \frac{1}{2} c^j F_{ij} \right] = G_i \quad \dots (21)$$

If the identities (19) and (20) are multiplied by $\frac{1}{2}c^i$ and the resulting equations are combined with (21), the resulting identity is given by

$$\sum_{j=1}^n \left[\frac{\partial c^j}{\partial t} v_{ij} + \frac{1}{2} (c^i + c^j) \Gamma_{ij} + (c^i - c^j) D_{ij} \right] = G_i - \sum_{j=1}^n \left[\frac{1}{2} (c^j - c^i) G_{ij} + \frac{1}{2} (c^j + c^i) F_{ij} \right] \quad \dots (22)$$

Let the average μ_{ij} of c_i and c_j be denoted by

$$\mu^{ij} = \frac{1}{2} (c^i + c^j) \quad \dots (23)$$

Let the difference δ_{ij} of c_i and c_j be denoted by

$$\delta^{ij} = c^i - c^j \quad \dots (24)$$

A finite element material balance is obtained by combining (23) and (24) with (22). Let

$$\sum_{j=1}^n \left[\frac{\partial c^j}{\partial t} v_{ij} + \mu^{ij} \Gamma_{ij} + \mu^{ij} F_{ij} + \delta^{ij} D_{ij} - \frac{1}{2} \delta^{ij} G_{ij} \right] = G_i \quad \dots (25)$$

This finite element material balance (25) is consistent with the continuity equations. The resulting equation is conservative.

For the sake of comparison, any midpoint weighted finite difference material balance can be reduced to the form

$$\frac{\partial c^i}{\partial t} v_i^{fd} + c^i F_i^{fd} + \sum_{j=1}^n [\mu^{ij} \Gamma_{ij}^{fd} + \delta^{ij} D_{ij}^{fd}] = G_i^{fd} \quad \dots (26)$$

The treatment of material flux by both convection and diffusion is similar in (25) and (26). The treatment of the accumulation terms, the source terms, and the production terms acting on each computational molecule is significantly different in (25) and (26).

4. Lumping

The localization within a single computational molecule in finite difference procedures of accumulation terms, source terms, and production terms greatly simplifies the treatment of these terms with respect to the scheme which is indicated in (25). Young [10] considers the finite element treatment of the accumulation terms unacceptable for practical efforts. In particular, Young points out that IMPES [14] procedures are not possible for conventional finite element procedures.

Young addresses this particular problem by employing a special quadrature rule to evaluate the capacity terms. In the current investigation, a lumping procedure is used. Russell and Wheeler [13] illustrate that lumping corresponds to a $O(h^2)$ perturbation of the original differential system. By lumping the time derivatives and source terms appearing in (25), one obtains a modified finite element material balance that is given by

$$\frac{\partial c^i}{\partial t} v_i + c^i F_i + \sum_{j=1}^n [\mu^{ij} \Gamma_{ij} + \delta^{ij} D_{ij}] = G_i \quad \dots (27)$$

The form of the lumped finite element material balance (27) is exactly

analogous to that arising from the finite difference material balance (26). Similar data structures are used in practical computer implementations. Codes utilizing the finite element material balance are quite readily modified to incorporate five and nine point finite difference techniques [15].

5. Regularization

The lumping procedure is a convenient method for transforming the finite element material balance (25) into a scheme compatible with finite difference procedures. The lumping procedure also corresponds to a regularization of the original differential equation. In a single space variable, lumping corresponds to a long wave regularization of the continuity equations [16]. Examples of one space variable calculations where lumping is shown to be beneficial include numerical solutions of the Buckley-Leverette equations [16] [17] and numerical solutions of equations governing cap rock energy losses in a thermal model [18].

For many problems, the numerical solution generated by the lumped procedure (27) exhibits oscillatory behavior. This behavior is observed if material transfer due to convective flow dominates material transfer due to mixing. If it is not possible to use sufficiently fine mesh, which is often the case in practical calculations, the computed solution exhibits serious overshoot. A similar phenomenon is associated with finite difference procedures that employ midpoint weighting. A standard method of regularization which is utilized in finite difference techniques is the upwinding procedure. In finite difference procedures, upwinding is equivalent to a modification of the physical mixing rate that is determined by

$$\bar{D}_{ij} = \max(\frac{1}{2} |T_{ij}|, D_{ij}) \quad \dots (26)$$

A similar procedure is used to regularize the finite element material balance (27). The resulting procedure readily satisfies a maximum principle [19]. The upwinding procedure is equivalent to adding mesh dependent dispersion [19]. Numerical dispersion matrices for the upwinded five point finite differences, nine point [3] finite differences, and the finite element material balance are calculated by Bell and Shubin [20].

6. Discussion

Analogs of the finite element material balance derived above are implemented in models of incompressible and compressible single phase miscible displacement [11] [12] and in a steamflood model [21]. The procedure is implemented for nonrectangular domains [22]. A theoretical convergence proof under certain assumptions is undertaken by Bell, Shubin, and Wheeler [19]. This analysis is extended to slightly compressible problems by Potempa and Wheeler [22].

The scheme successfully eliminates grid effects in simulations of adverse mobility displacements. The procedure is compatible with the scheme employed by McCracken and Yanosik, as the two procedures computationally differ only in the calculation of the flow rates between two computational molecules. Provided sufficient care is taken in the mobility weighting [5], results obtained by the upstream weighted and lumped finite element material balance are extremely similar to those obtained by the procedure used by McCracken and Yanosik. This result is true for both incompressible miscible displacement problems and for steamflood problems [5]. This result is not surprising in view of the

result that the numerical dispersion matrices associated with the application of upwinding the two procedures are equivalent to within $O(h^2)$. The major advantage enjoyed by the upstream weighted and lumped finite element material balance procedure over the nine point finite difference scheme is that of applicability over arbitrary triangulations. Simulated displacements over triangular domains using the upstream weighted and lumped finite element material balance are reported [6] [22].

The major problem encountered by the upstream weighted and lumped finite element material balance procedure results from the magnitude of the numerical dispersion [20]. The numerical dispersion is too severe, resulting in smeared fronts, although the magnitude of the numerical dispersion is no more severe than that encountered when using either the five point or nine point finite difference procedures. Difficulties are also reported for simulations involving irregular mesh sizes.

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