COMBINED MIXED FINITE ELEMENT AND FINITE VOLUME FOR FLOW AND TRANSPORT IN POROUS MEDIA

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Abstract. This paper is concerned with numerical methods for the modeling of flow and transport of contaminant in porous media. The numerical methods feature the mixed finite element method over triangles as a solver to the Darcy flow equation, and a conservative finite volume scheme for the concentration equation. A series of numerical examples demonstrates the effectiveness of the methodology for a coupled system which includes an elliptic equation and a diffusion-convection equation arising in modeling of flow and transport in heterogeneous porous media.

Keywords: Diffusion-Convection, Finite Volume Method, Mixed Finite Element, Porous Media.

AMS classification: 76M12, 65M12, 35K65.

§1. Introduction

In this paper, we focus our attention on the study and prediction of single phase flow of an incompressible fluid with a dissolved solute with an eye toward nuclear waste repository studies. The understanding and prediction of fluid flow through porous media is of great importance in various areas of research and industry. Petroleum engineers need to model multiphase and multicomponent flow for production of hydrocarbons from petroleum reservoirs. Hydrologists and soil scientists are concerned with underground water flow in connection with applications to civil and agricultural engineering, and, of course, the design and evaluation of remediation technologies in water quality control rely on the properties of underground fluid flow. More recently, modeling flow and transport of contaminant received an increasing attention in connection with the behavior of geological isolation of radioactive waste after the drilling of the wells of shafts.

The governing equations arise from the laws of conservation of mass of the fluid, along with a constitutive relation relating the fluid velocity which appear in the conservative law to the pressure gradient and gravitational effects. Traditionally, the standard Darcy equation provides this relation.

The mathematical nature of the flow and mass balance equations is different and specific methods for their approximations should be considered in numerical simulation. The method

that one chooses to numerically solve the balance equation should mimic the essence of the physics by preserving the corresponding conservation laws. Yet, discontinuity which presents should move at the correct speeds and should be well resolved by the numerics. One must also have accurate calculations of the velocity, even for highly heterogeneous media where there are large jumps in the flow capabilities and other physical properties.

Flow simulation in petroleum and environmental applications has been extensively studied using finite element methods in the last two decades (see, e.g., [15], [9] and the bibliographies therein). Also, discretizations using both finite element and finite volume methods are presented in [10]. More recently, finite volume methods were developed and analyzed for immiscible two-phase flow in porous media in the case where the diffusion term is neglected, (see [12] and the references therein). This approach leads to robust schemes applicable for unstructured grids and the approximate solution has various interesting properties which correspond to the properties of the physical solution. These methods have been useful for advective flow problems because they combine element by element conservation of mass with numerical stability and minimal numerical diffusion, (see [1], [2], [4], [8], [13], [17] and the references therein).

The purpose of this paper is to discuss the applicability of the mixed finite element methods and finite volume methods to flow and transport in porous media. We focus on miscible flow in heterogeneous porous media. The mathematical formulation of these types of flow leads to a coupled system of partial differential equations which includes an elliptic pressure-velocity equation and a diffusion-convection concentration equation. The concentration equation is convection dominated and thus special care should be taken in discretization. The diffusion-dispersion term is important in several cases and cannot be neglected.

The mixed finite element method is employed to discretize the Darcy flow equation. Not only do mixed methods provide a very accurate determination of the velocity field, but they also allow for a natural treatment of practical well conditions. A conservative finite volume method is then used for the mass balance law, i.e. the concentration equation. A Godunov-type method is used to treat the convective term and a P_1-finite element scheme is used for the discretization of the diffusion term.

The paper will be organized as follows. In the next section, we give a short description of the mathematical and physical model used in this study. In section 3, the numerical scheme for the flow equation is presented with emphasis on the mixed finite element method employed for the solution of the pressure-velocity equation. Section 4 contains the finite volume scheme developed for the transport equation. A vertex-centered finite volume method is used for the solution of the concentration equation. Section 5 is devoted to the presentation of the results of the COUPLEX1 Test case [6]. Additional conclusions are drawn in section 6.

§2. Governing Equations

We consider for simplicity a two-dimensional horizontal reservoir where the gravity effects are negligible. The single-phase flow of an incompressible fluid with a dissolved solute in a horizontal porous reservoir $\Omega \subset I\!R^2$ over a time period $]0, T[$, is given by [14]:

Pressure equation:

$$\begin{cases} \vec{q} = -\frac{K(x)}{\mu}\nabla p & \text{in } \Omega \\ div\, \vec{q} = 0 & \text{in } \Omega \\ \vec{q}.\vec{n}|\Gamma_{N1} = -q_0\ ;\ \vec{q}.\vec{n}|\Gamma_{N2} = 0\ ;\ p|\Gamma_D = p_0 \end{cases} \tag{1}$$

where the boundary Γ splits up into three parts such that $\Gamma = \overline{\Gamma}_{N1} \cup \overline{\Gamma}_{N2} \cup \overline{\Gamma}_D$.

Concentration equation:

$$\begin{cases} \Phi(x)\frac{\partial C}{\partial t} - div(D(x,\vec{q})\nabla C - C\vec{q}) + \lambda(x)C = f(x,t) & \text{in } \Omega\times]0,T[\\ C|\Gamma_1 = c_1;\ \ D\nabla C.\vec{n}|\Gamma_2 = 0;\ \ (D\nabla C - C\vec{q}).\vec{n}|\Gamma_3 = d_3 & \text{in }]0,T[\\ C(x,0) = C_0(x) & \text{in } \Omega \end{cases} \tag{2}$$

where the boundary Γ splits up into three parts such that $\Gamma = \overline{\Gamma}_1 \cup \overline{\Gamma}_2 \cup \overline{\Gamma}_3$, p and $\vec{q}$ are the pressure and Darcy velocity of the fluid mixture, Φ and K are the porosity and the permeability of the medium, μ is the viscosity of the mixture, C is the concentration of the contaminant solute, and f is the external rate of flow. λ is the latency retardation factor. q_0 is a flow rate specified at Γ_{N1} and p_0 is a given pressure at Γ_D. c_1 is a given concentration at Γ_1, d_3 is the total flux specified at Γ_3. In addition, an initial condition C_0 is specified. For more details on the assumptions on the data see [3].

The form of the diffusion-dispersion tensor D that we use in our simulator is given by:

$$D(x,\vec{q}) = d_m I + |\vec{q}|[\alpha_l E(\vec{q}) + \alpha_t(I - E(\vec{q}))]$$

with $E_{ij}(\vec{q}) = \frac{q_i q_j}{|\vec{q}|^2}$, d_m is the molecular diffusion coefficient, and α_l and α_t are the magnitudes of longitudinal and transverse dispersion respectively.

Before describing the numerical discretization of the coupled problem $(1)-(2)$, we give some notations. Let $\mathcal{T}$=$\{t_0, ..., t_N\}$ be a partition of $[0,T]$ and $\Delta t^n = t_{n+1} - t_n$ the time step size of $\mathcal{T}$. Furthermore, let $(\mathcal{T}_h)_{h>0}$ be an admissible triangulation of Ω, such that $\bar{\Omega} = \cup_{T\in\mathcal{T}_h}\bar{T}$ and I denotes the set of vertex indices of the triangulation. Let us note by E_h the set of the edges of the triangulation. We define for each vertex x_j, $j \in I$ of the triangulation $(\mathcal{T}_h)_{h>0}$ the corresponding dual cell M_j by connecting the barycenter with the medium of the edge (see Figure 1). The dual mesh $\Sigma_h = \{M_j,\ j \in I\}$ is a partition of our domain Ω.

Let us state the following notations and assumptions:

- Ω is a bounded open polygonal subset of IR^2. $Q = \Omega\times]0,T[$.
- $\Phi \in L^\infty(\Omega)$, $0 < \Phi_- \leq \Phi(x) \leq \Phi^+ \leq 1$ a.e. in Ω.
- $C_0 \in L^\infty(\Omega)$, $0 \leq C_0(x) \leq 1$ a.e. in Ω, $\lambda \in L^\infty(\Omega)$, $\lambda(x) \geq 0$ a.e. in Ω.
- D and K are bounded, uniformly positive definite symmetric tensors.
- $\vec{q} \in H(div,\Omega)$, $\vec{q} \in (L^\infty(\Omega))^2$ a.e. in $]0,T[$.
- $f \in L^2(Q)$, $f(x,t) \geq 0$ a.e. in Q.
- $(\mathcal{T}_h)_{h>0}$ is a regular triangulation of Ω.
- $\delta_{jl} = \delta(x_j, x_l)$ is the Euclidian distance between x_j and x_l.
- $N_j^0 =$ card $\{l \in \partial M_j\}$.
- $M^0 =$ card $\{M_j \in \Sigma_h\}$.
- $h =$ min $\{|l|,\ l \in \partial M_j,\ M_j \in \Sigma_h\}$.
- $H =$ max $\{|L|,\ L \in \partial T,\ T \in \mathcal{T}_h\}$.
- $\Phi_j = \frac{1}{|M_j|}\int_{M_j}\Phi(x)dx$ and $\lambda_j = \frac{1}{|M_j|}\int_{M_j}\lambda(x)dx$.

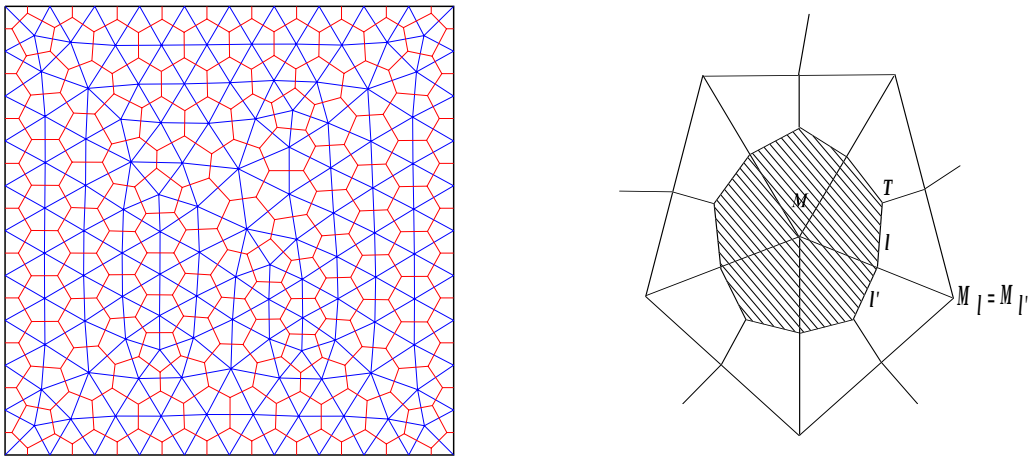

Figure 1: Vertex-centered mesh.

- $f_j^n = \frac{1}{\Delta t^n |M_j|} \int_{t_n}^{t_{n+1}} \int_{M_j} f(x,t)dxdt$ and $C_j^0 = \frac{1}{|M_j|} \int_{M_j} C_0(x)dx$.
- $\gamma H^2 \leq |M_j| \leq \beta h^2, \forall j \in I$, where $\beta \geq \gamma > 0$ are constants independent of h.
- $h^2 \leq |T| \leq H^2, \forall T \in \mathcal{T}_h$.

§3. Numerical Method for the Flow Equation

In this section, we describe a mixed finite element method for the accurate approximation of the pressure-velocity equation (see, e.g., [7]). This method conserves mass cell by cell and produces a direct approximation of the two variables pressure and velocity. Since the transport term in (2) is governed by the fluid velocity, accurate simulation requires an accurate approximation of the velocity $\vec{q}$. Because the lithology in the reservoir can change abruptly, causing rapid changes in the flow capabilities of the rock, the coefficient K in (1) can be discontinuous.

We introduce the following finite element spaces (see, e.g., [7], [18]): $T \in \mathcal{T}_h$: triangle, $T' \subset T$ edge of T.

$$RT_0(T) = \left\{\vec{\alpha} + \beta x, \text{ with } \vec{\alpha} \in \mathbb{R}^2 \; and \; \beta \in \mathbb{R}\right\}$$

RT_0 is the lowest Raviart-Thomas space.

$$X_{0,N}^h = \left\{\vec{q_h} \in L^2(\Omega),\ \vec{q_h}.\vec{n} = 0 \; on \; \Gamma_{N_1},\ q_h|T \in \ RT_0(T)\ ;\ \forall T \in \mathcal{T}_h\right\}$$

$$P_0^h = \left\{v^h \in L^2(\Omega),\ v^h|T = Cte\ ;\ \forall T \in \mathcal{T}_h\right\}$$

$$L_h^{p_0} = \left\{\lambda_h \in L^2(E_h)\ ;\ \lambda_h|T' = Cte\ ; \forall T' \in E_h,\ \lambda_h|\Gamma_D = p_0\right\}.$$

A Lagrangian multiplier λ is introduced in order to get the continuity of the normal component of the velocity across the inter-element boundaries (see [7]).

The mixed hybrid finite element approximation $(\vec{q}_h, p_h, \lambda_h) \in X^h_{0,N} \times P^h_0 \times L^{p_0}_h$ of $(\vec{q}, p, \lambda)$ is the solution of the following problem:

$$\begin{cases} \int_T \mu K^{-1}\vec{q}_h \cdot \vec{s}\, dT - \int_T p_h div\vec{s}\, dT + \sum_{T'\in T} \int_{T'} \lambda_h \vec{s}\cdot\vec{n}\, dT' = 0 & \forall \vec{s} \in RT_0 \\ \int_T w div\vec{q}_h\, dT = 0 & \forall w \in P^h_0 \\ \sum_{T\in\mathcal{T}_h}\sum_{T'\in T}\int_{T'} \mu\vec{q}_h\cdot\vec{n}\, dT' = \sum_{T'\in\Gamma_{N_1}}\int_{T'}\ q_0\ \mu\ dT' & \forall \mu \in L^0_h \end{cases} \tag{3}$$

Once the approximate formulation has been written, the resulting system of equations is very large and the next step is to choose the most efficient way to implement it. It is possible (see, e.g., [7], [5]) to reduce the solution of the system (3) to the solution of a linear system involving only the Lagrangian multipliers vector λ_h, with a symmetric positive definite and sparse matrix. Once this system is solved, $\vec{q}_h$ and p_h are obtained through a simple post-process at the element level.

§4. Approximation Method for the Transport Equation

In this section, we describe the finite volume method used for the approximation of the concentration equation. A Godunov scheme is used for the convection term and a P_1-finite element scheme is used for the discretization of the diffusion-dispersion term. We will define a semi-implicit finite volume scheme: explicit approximation of the convection term and implicit approximation of the diffusion-dispersion term. Only a short description of the method employed in this work will be given. The interested reader is reffered to [1], [2] and [3] for more details.

Integrating the equation (2) in $M_j \times [t_n, t_{n+1}]$, we obtain the following scheme:

$$\begin{aligned} &C_j^{n+1} - \tfrac{\Delta t^n}{|M_j|\Phi_j}\sum_{l\in\partial M_j\setminus\Gamma}(C_l^{n+1} - C_j^{n+1})\tfrac{D_{jl}^n}{\delta_{jl}}|l| + \tfrac{\Delta t^n}{\Phi_j}\lambda_j C_j^{n+1} \\ &= C_j^n + \tfrac{\Delta t^n}{|M_j|\Phi_j}\sum_{l\in\partial M_j}(C_l^n - C_j^n)(-\vec{q}_l^n.\vec{n}_{jl})^+|l| + \tfrac{\Delta t^n}{\Phi_j} f_j^n \end{aligned} \tag{4}$$

where

$$D_{jl}^n = -\frac{|T|}{|l|}\delta_{jl}\nabla\chi_{M_{l,T}} D_T(\vec{q}).\nabla\chi_{M_{j,T}} \tag{5}$$

with

$$D_T(\vec{q}) = \frac{1}{|T|\Delta t^n}\int_{t_n}^{t_{n+1}}\int_T D(x,\vec{q})dxdt \tag{6}$$

$\chi_{M_{j,T}}$ is the standard P_1-finite element basis associated to the triangle T.

In [3] we proved that this scheme satisfies a discrete maximum principle under appropriate CFL condition, L^∞ stability and BV estimates and some convergence results are derived.

§5. Numerical Experiments

In this section, we present some numerical results in 2D based on the schemes presented in this paper. We present the results obtained for the simulation of the COUPLEX1 Test case [6]. It is a benchmark of numerical techniques designed for the simulation of the transport

of contaminants by the water flowing through a porous medium. The goal is to compute a simplified far field model used in nuclear waste management simulation. The repository lies at a depth of 450m(meters) inside a clay layer which has above it a layer of limestone and a layer of marl and below it is a layer of dogger limestone. Water flows slowly through these porous media and convects the radioactive elements leak from containers. The computational domain is in a rectangle $[0, 25000] \times [0, 695]$ in meters. The layers of dogger, clay, limestone, and marl are located as in Figure 2, for this domain the computation should be carried for $t \in [0, T]$ with $T = 10^7$ years. The permeability tensor K, assumed constant in each layer is given in Table 1.

	Marle	Limestone	Clay	Dogger
$K(m/year)$	$3.1536e-5$	6.3072	$3.1536e-6$	25.2288

Table 1: Permeability in the four rock layers.

The boundary conditions are:

$$\begin{cases} H = 289 & \text{on } \{25000\} \times \{0, 200\} \\ H = 310 & \text{on } \{25000\} \times \{350, 595\} \\ H = 180 + 160x/25000 & \text{on } \{0, 25000\} \times \{695\} \\ H = 200 & \text{on } \{0\} \times \{295, 595\} \\ H = 286 & \text{on } \{0\} \times \{0, 200\} \\ \frac{\partial H}{\partial n} = 0 & \text{elsewhere on the boundary.} \end{cases} \tag{7}$$

where H is the hydraulic head such as $H = p/\rho g + z$, g is Newton's constant, ρ is the density and z is the depth.

Table 2 contains the data corresponding to the convection-diffusion-reaction equation for the Iodine 129.

	$d_m(m^2/year)$	α_l	α_t	Φ	λ
Dogger	$5.0e-4$	50	1	0.1	$Log(2)/1.57e-7$
Clay	$9.48e-7$	0	0	0.001	$Log(2)/1.57e-7$
Limestone	$5.0e-4$	50	1	0.1	$Log(2)/1.57e-7$
Marl	$5.0e-4$	0	0	0.1	$Log(2)/1.57e-7$

Table 2: Diffusion/dispersion parameters in the four layers.

The values of the source term in the repository are given in tabulated form in separately provided data files [6]. It is assumed that there is no source outside the repository. The initial values of the concentration C are zero at time zero.

Boundary conditions for the transport are:

$$\begin{cases} \frac{\partial C}{\partial n} = 0 & \text{on } \{0\} \times (0, 200) \\ \frac{\partial C}{\partial n} = 0 & \text{on } \{0\} \times (350, 595) \\ (D\nabla C - C\vec{q}) \,.\vec{n} = 0 & \text{on } (0, 25000) \times \{0\} \\ C = 0 & \text{elsewhere on the boundary.} \end{cases} \tag{8}$$

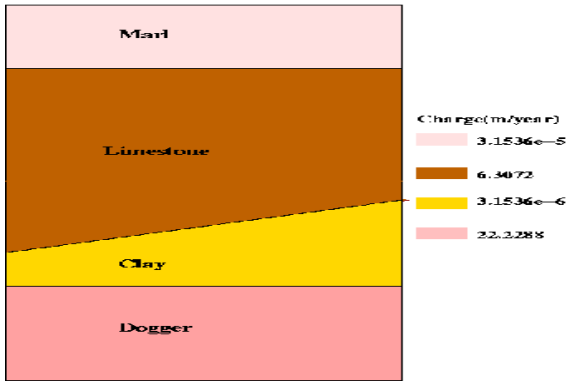

Figure 2: Permeability distribution.

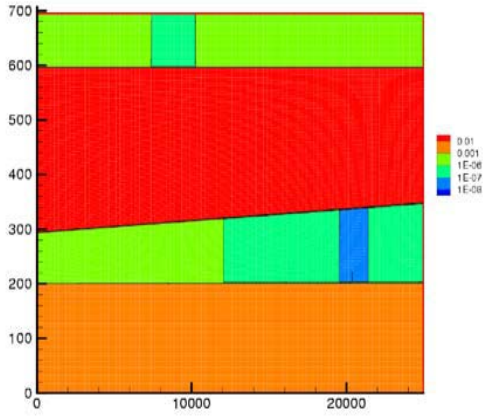

Figure 3: Velocity field.

Several authors tested COUPLEX1 by using various numerical schemes [6], (see, e.g., [11], [16], [19]). We present hereafter the main results concerning the hydraulic head field and the Iodine transport. Figure 3 shows the fluid flux. The hydraulic head contours are presented in Figure 4. In Figures 5, 6 and 7, we show the concentration contours at three times step. The significant result that one can retains is that the Iodine concentration reaches the left boundary of the domain. This is mainly due to the fact that the concentration equation is convection dominated what makes the dispersion of the Iodine follows the mouvement of the flow. One can also say that the transfer time of the radionucleides is very important around the geologic formation. After 10^7 years, a great quantity of the Iodine still remains in the repository.

The obtained results are very close to those obtained by [11], [19]. As can be seen, the method has captured the flow of the system very accurately. This demonstrates the excellent schock-capturing properties of the finite volume scheme for the solution of the concentration equation.

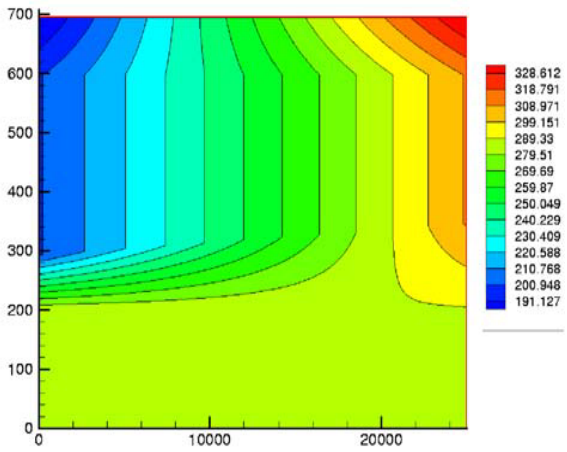

Figure 4: Hydraulic head profile.

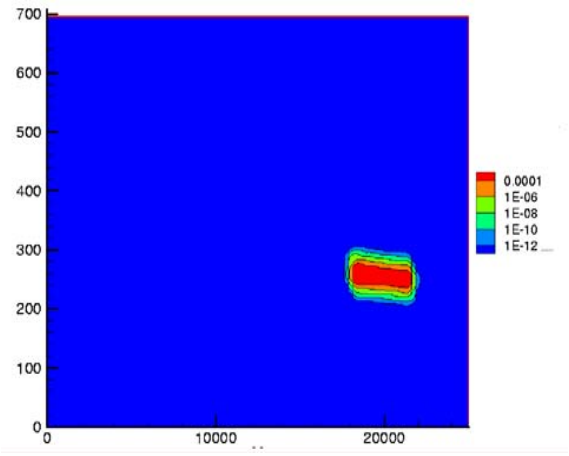

Figure 5: Concentration contours at T=50110.

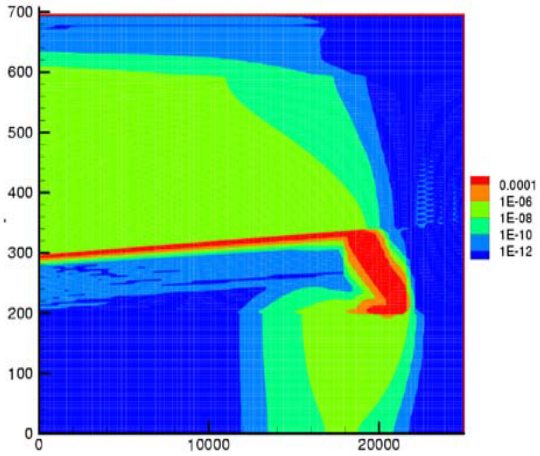

Figure 6: Concentration contours at T=501100.

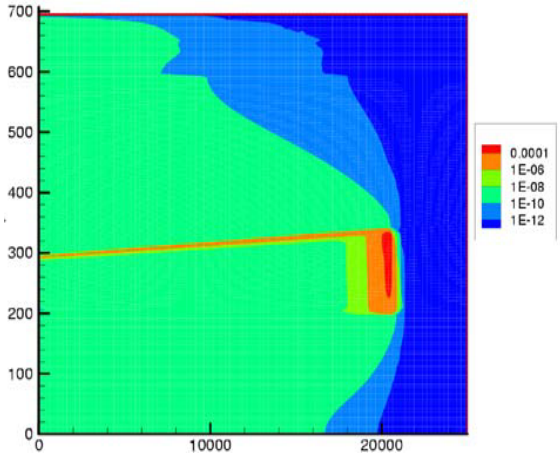

Figure 7: Concentration contours at T=1e+07.

§6. Conclusion

A mixed finite element method was used to obtain an accurate approximation of the flow equation and a vertex-centered finite volume method for the concentration equation. Numerical simulations from 2D tests show that this approach leads to a set of robust schemes. In the future, we will consider the extension of the approach described in this paper to 3D problems.

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References

[1] M. Afif and B. Amaziane, Convergence of Finite Volume Schemes for a Degenerate Convection-Diffusion Equation Arising in Flow in Porous Media. *Comput. Methods in Appl. Mech. Engrg. 191,* (2002), 5265–5286.

[2] M. Afif and B. Amaziane, Numerical Simulation of Two-Phase Flow through Heterogeneous Porous Media. *Numerical Algorithms 34*, (2003), 117–125.

[3] B. Amaziane and M. El Ossmani, Convergence of a Mixed Finite Element-Finite Volume Scheme for Flow and Transport of Contaminant in Porous Media. *In Preparation.*

[4] Y. Amirat, D. Bates and A. Ziani, Convergence of a Mixed Finite Element-Finite Volume Scheme for a Parabolic-Hyperbolic System Modeling a Compressible Miscible Flow in Porous Media. *To appear in Numer. Math.*, (2004).

[5] A. Bendali, N. Raynaud and J.M. Thomas, New Decomposition of Shape Functions Spaces of Mixed Finite Element Methods. *Appl. Math. Lett. 9*, (1996), 33–38.

[6] A. Bourgeat, M. Kern, S. Schumacher and J. Talandier, The COUPLEX Test Cases: Nuclear Waste Disposal Simulation. *http://www.andra.fr/couplex/*, (2002).

[7] F. Brezzi and M. Fortin, *Mixed and Hybrid Finite Element Method*. Springer-Verlag, New York, 1991.

[8] D. BURKLE AND M. OHLBERGER, Adaptative Finite Volume Methods for Displacement Problems in Porous Media. *Comput. Visuel Sci. 5*, (2002), 95–106.

[9] Z. CHEN AND R. E. EWING, EDITORS, *Fluid Flow and Transport in Porous Media: Mathematical and Numerical Treatment*. American Mathematical Society, Providence, Rhode Island, 2002.

[10] G. CHAVENT, J. JAFFRÉ AND J. E. ROBERTS, Mixed-Hybrid Finite Elements and Cell-Centred Finite Volumes for Two-Phase Flow in Porous Media. In *Mathematical Modeling of Flow Through Porous Media*, A. P. Bourgeat et al., Eds. World Scientific, London, 1995, pp. 100–114.

[11] E. CHÉNIER, R. EYMARD AND X. NICOLAS, A Finite Volume Scheme for the Transport of Radionucleides in Porous Media. *To appear in Computational Geosciences*, (2004).

[12] R. EYMARD, T. GALLOUET AND R. HERBIN, The Finite Volume Method. In *Handbook of Numerical Analysis, Vol. 7*, P.G. Ciarlet and J.L. Lions, Eds. North Holland, Amsterdam, 2000, pp. 715–1022.

[13] R. EYMARD, T. GALLOUET, R. HERBIN AND A. MICHEL, Convergence of a Finite Volume Scheme for Nonlinear Degenerate Parabolic Equations. *Numer. Math. 92*, (2002), 41–82.

[14] R. E. EWING, *The Mathematics of Reservoir Simulation*. Frontiers in Applied Mathematics, SIAM, Philadelphia, 1983.

[15] R. E. EWING, Computational Sciences in Environmental Applications. In *Computational Science for the 21st Century*, M-O. Bristeau et al., Eds. Wiley, New York, 1997, pp. 250–259.

[16] H. HOTEIT, *Simulation d'Écoulements et de Transports de Polluants en Milieux Poreux : Application à la Modélisation de la Sûreté des Dépôts de Déchets Radioactifs.* Thèse de Doctorat de l'Université de Rennes 1, 2002.

[17] M. OHLBERGER, Convergence of a Mixed Finite Element-Finite Volume Methods for Two Phase Flow in Porous Media. *East-West J. Numer. Math. 5*, 3 (1997), 183–210.

[18] J. E. ROBERTS AND J. M. THOMAS, Mixed and Hybrid Methods. In *Handbook of Numerical Analysis, Vol. 2*, P.G. Ciarlet and J.L. Lions, Eds. North Holland, Amsterdam, 2000, pp. 523–639.

[19] D. TRUJILLO, Mixed Primal-Dual Method for Nuclear Waste Disposal Far Field Simulation. *To appear in Computational Geosciences*, (2004).

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