A NEW MASS LUMPING SCHEME FOR THE MIXED HYBRID FINITE ELEMENT METHOD : *APPLICATION TO UNSATURATED WATER FLOW MODELLING*

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ABSTRACT

Groundwater flow modelling is of interest in many sciences and engineering applications for scientific understanding and/or technological management. Accurate numerical simulation of infiltration in the vadose zone remains a challenge, especially when very sharp fronts are present.

This study is focused principally on an alternatively numerical approaches referred to in the literature as the mixed hybrid finite element (MHFE) method. MHFE schemes simultaneously approximate both the pressure head and its gradient. For some problems of unsaturated water flow, the MHFE solutions contain oscillations. Various authors (see Farthing *et al.*, 2003) suggest the use of a mass lumping procedure to avoid this unphysical phenomenon. An analyse of the resulting matrix system shows that the recommended technique differs from the standard mass-lumping well-established for Galerkin finite element method.

A "new" effective mass-lumping scheme adapted from Younes *et al.* (2005) has been specially developed for the MHFE method. Its ability for eliminating oscillations have been tested in unsaturated conditions.

1. INTRODUCTION.

Prediction of accurate fluid movement in porous media is an important issue for scientists and engineers who are interested in the management of water resources. Computational simulations have received a great attention to achieve this predictive role. However, many assumptions have been formulated to translated the physical reality in an appropriate mathematical model. Then, the problem consists in solving (system of) ordinary or partial differential equation(s), with one of the various numerical techniques that have been developed. Whatever the way followed in this context, an important aspect of our work deals with the verification of codes and simulations (Roy, 2005).

Due to the fact that it produces accurate and mass-conservative velocity fields also for heterogeneous complex system, the mixed hybrid finite element (MHFE) method has been recently applied in many water flow applications. Hence, this numerical scheme has been generalized for variably-saturated flow and analyzed in terms of the temporal approximation involved (Farthing et al., 2003), the adopted linearization technique (Bergamaschi and Putti, 1999) or for adaptive grid refinement (Bause and Knabner, 2004).

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However, several studies have shown that the simulations of sharp infiltration front can lead to unphysical oscillations (Farthing *et al*, 2003; Belfort *et al*, 2005). This problem has still been encountered with the standard finite element (FE) method (Celia et al., 1990; Pan et al., 1996). A natural approach for solving this difficulty has been to generalize the FE mass-lumping technique for the MHFE scheme. In fact, the use of suitable quadrature formula allows to diagonalize the element matrices. This works nicely on rectangular meshes, where numerical quadrature makes mixed approximation equivalent to finite differences (Chavent and Roberts, 1991; Weiser and Wheeler, 1988; Arbogast *et al.*, 1998). The procedure has been extended to triangular grids with the constraint of a weakly acute triangulation (see ref in Younes *et al.,* 2005). Younes et al (2005) propose a new mass lumping procedure for the MHFE, and test it for advection-dispersion problems.

In this work, the new lumped MHFE method is briefly described and discussed in the specific context of unsaturated water flow. Then, some numerical experiments are run to compare the lumped formulation with the standard MHFE method.

2. THEORY.

2.1. **Unsaturated water flow**. The combination of the Darcy Buckingham law and the mass conservation equation, under the assumption of an incompressible porous media, leads to the Richards equation:

$$\frac{\partial\theta}{\partial t}+\nabla.\left(k\left(h\right)\nabla\left(h-z\right)\right)=f_v \qquad (1)$$

where θ refers to the volumetric water content, t is time, k is the hydraulic conductivity, h is the pressure head, z is the depth taken to be positive downward and f_v is a source-sink term.

This equation may be written in several forms with either the water content and/or the pressure head as main unknown. According to the chosen form, some care and specific adaptations have to be taken into account to conserve good mass balance or to simulate variably saturated flow.

The interdependencies of the pressure head, the hydraulic conductivity and the water content must be characterized using constitutive relations. The standard van Genuchten model (1980) was used here for the pressure - saturation relationship as follows,

$$S_e\left(h\right)=\frac{\theta\left(h\right)-\theta_r}{\theta_s-\theta_r}=\begin{cases}\dfrac{1}{\left(1+\left(\alpha\left|h\right|\right)^n\right)^{1-(1/n)}} & h<0\\ 1 & h\geq 0\end{cases} \qquad (2)$$

where θ_s and θ_r are the saturated and residual volumetric water contents, respectively, α is a parameter related to the mean pore size and n a parameter reflecting the uniformity of the pore-size distribution. Mualem's model (1976) was chosen for the conductivity - saturation relationship, leading to (van Genuchten, 1980) :

$$K\left(S_e\right)=K_s S_e^{1/2}\left[1-\left(1-S_e^{\left(n/(n-1)\right)}\right)^{\left(1-(1/n)\right)}\right]^2 \qquad (3)$$

in which S_e is given by Eq. (2) and $n > 1$.
Finally, the mathematical description is closed with initial and boundary conditions.

2.2. **Numerical methods**. When the considered 2D or 3D domain is discretized with general shape elements, the procedure, that can be followed to get the lumped MHFE system associated with Eq. (1), could be described with the successive steps:

- For the element A with n_f edges (2D) or faces (3D), we define the mean water flux $\overrightarrow{q_A}$ over the element A via the lowest-order Raviart-Thomas space:

$$\overrightarrow{q_A} = \sum_{i=1}^{n_f} Q_i^A \overrightarrow{\omega_i^A} \tag{4}$$

  where $\overrightarrow{\omega_i^A}$ are the vectorial basis functions (Raviart and Thomas, 1997).

- Q_i^A denotes the flux leaving A through the i^{th} edge. It is defined by:

$$Q_i^A = \overline{Q}_i^A + \frac{|A|}{n_f} f_{v,A} - \frac{|A|}{n_f}\frac{\partial \theta_i^A}{\partial t} \tag{5}$$

  where $|A|$ refers to the area of the element in 2D or volume in 3D.

- $\overline{Q}_i^A$ is the flux corresponding to the stationary problem without sink/source terms

$$\overline{Q}_i^A = K^A \sum_{j=1}^{n_f}\left(\frac{\alpha_i \alpha_j}{\alpha} - B_{ij}^{-1}\right) Th_j^A \tag{6}$$

  where k^A is the value of the conductivity in element A, Th_j^A is the mean value of the pressure head over the edge A_i (also called Traces of pressure head). The following notations are used: $B_{ij} = \int_A \overrightarrow{\omega_i}.\overrightarrow{\omega_j}$, $\alpha_i = \sum_{j=1}^{nf} B_{ij}^{-1}$, $\alpha = \sum_{i=1}^{nf} \alpha_i$.

- Due to the (high) non-linearities of the relation between h - θ - k, the water content is expanded by means of a first-order Taylor series with respect to the traces of pressure head. According to this linearization strategy, Eq. (5) becomes:

$$\begin{aligned} Q_i^{A,n+1,k+1} &= K^A \sum_{j=1}^{n_f}\left(\frac{\alpha_i \alpha_j}{\alpha} - B_{ij}^{-1}\right) Th_j^{A,n+1,k+1} - \frac{|A|}{n_f \Delta t} TC_i^{A,n+1,k} Th_i^{A,n+1,k+1} \\ &+ \frac{|A|}{n_f}\left[f_{v,A}^{n+1} - \frac{1}{\Delta t}\left(T\theta_i^{A,n+1,k} - TC_i^{A,n+1,k} Th_i^{A,n+1,k} - T\theta_i^{A,n} \right)\right] \end{aligned} \tag{7}$$

  where n indicates the time level (unknown at n + 1), k is the non-linear iteration level and C is the capillary capacity. The prefix T describes edges variables.

- The final system to solve is obtained by writing the continuity of edge state variables $\left(Th_i^{A,n+1} = Th_i^{B,n+1}\right)$ and fluxes between two adjacent elements A and B $\left(Q_i^{A,n+1,k+1} + Q_i^{B,n+1,k+1} = 0\right)$.

It could be interesting, especially for the considerations of the next section, to detail the components of the final system: $[M]\{Th^{n+1,k+1}\}=\{R^{n+1,k}\}$. Table 1 describes the coefficients of the matrix M and B^{-1} in order to make easier the analyze of the system. The old procedure, incorrectly referred as mass-lumping, consists in using a quadrature rule to express the matrix B of Eq. (6). The formulation classically used is (Chavent and Roberts, 1991):

$$\int_A \varphi(x)\,dx \approx \frac{|A|}{n_f}\sum_{i=1}^{n_f}\varphi(M_i) \tag{8}$$

In fact, the water content is expressed on the element A rather than at its edges. Consequently, the quadrature modifies the coefficients of the matrix M without changing the mass-distributed form of the scheme, whereas the off-diagonal coefficients of the matrix M are independent of the time step size for the new mass-lumping procedure.

TABLE 1. Expression of the matrix coefficients for 1D and 2D elements: comparison of the standard, the lumped and the quadratured MHFE schemes.

	Quadratured MHFE	Standard MHFE	Lumped MHFE
m_{ii}^A	$K^A\left(B_{ii}^{-1}-\dfrac{K^A\alpha_i^2}{K^A\alpha+\dfrac{C^A\lvert A\rvert}{\Delta t}}\right)$		$K^A\left(B_{ii}^{-1}-\dfrac{\alpha_i^2}{\alpha}\right)+\dfrac{\lvert A\rvert TC_i^A}{n_f\Delta t}$
m_{ij}^A	$K^A\left(B_{ij}^{-1}-\dfrac{K^A\alpha_i\alpha_j}{K^A\alpha+\dfrac{C^A\lvert A\rvert}{\Delta t}}\right)$		$K^A\left(B_{ij}^{-1}-\dfrac{\alpha_i\alpha_j}{\alpha}\right)$
1D	$B^{-1}=\dfrac{2}{\Delta z}\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}$	$B^{-1}=\dfrac{2}{\Delta z}\begin{bmatrix}2 & 1\\ 1 & 2\end{bmatrix}$	
2D rectangles	$B^{-1}=2\begin{bmatrix}2\beta & 0 & 0 & 0\\ 0 & 2\beta & 0 & 0\\ 0 & 0 & 2/\beta & 0\\ 0 & 0 & 0 & 2/\beta\end{bmatrix}$	$B^{-1}=2\begin{bmatrix}2\beta & \beta & 0 & 0\\ \beta & 2\beta & 0 & 0\\ 0 & 0 & 2/\beta & 1/\beta\\ 0 & 0 & 1/\beta & 2/\beta\end{bmatrix}$	
	$\beta=\Delta z/\Delta x$		
2D triangles	$B^{-1}=\dfrac{1}{\lvert A\rvert}\begin{bmatrix}r_{23}r_{23} & r_{23}r_{31} & r_{23}r_{12}\\ r_{23}r_{31} & r_{31}r_{31} & r_{12}r_{31}\\ r_{23}r_{12} & r_{12}r_{31} & r_{12}r_{12}\end{bmatrix}+\dfrac{1}{3\ell}\begin{bmatrix}1 & 1 & 1\\ 1 & 1 & 1\\ 1 & 1 & 1\end{bmatrix}$		
	$\ell=\sum_{j=1}^{3}B_{ij}=\dfrac{\lVert r_{12}\rVert^2+\lVert r_{23}\rVert^2+\lVert r_{31}\rVert^2}{12\lvert A\rvert}\geq\dfrac{\sqrt{3}}{3}$	$\ell=\sum_{j=1}^{3}B_{ij}=\dfrac{\lVert r_{12}\rVert^2+\lVert r_{23}\rVert^2+\lVert r_{31}\rVert^2}{48\lvert A\rvert}\geq\dfrac{\sqrt{3}}{12}$	

where r_{ij} is the edge vector from node i toward node j and ℓ refers to a dimensionless shape coefficient.

2.3. **Analyse of the system**. An M-matrix can be defined as a non singular matrix with two conditions on its coefficients,

$$m_{ii} > 0 \ \ (1) \quad \text{and} \quad m_{ij} \le 0 \ \ (2) \tag{9}$$

This property guaranties the respect of the discrete maximum principle, *i.e.*, local maxima or minima will not appear for the main variable solution in a domain without local sources or sinks. Therefore it ensures that the resulting numerical state variable h and its related fluxes $\vec{q}$ are consistent with the physics. In order to show the advantages of the lumped scheme an analyze of the resulting system is performed for the various declinations of the MHFE method.

For our parabolic equation and according to the coefficients of Table 1, it can be easily shown that condition (1) of Eq. (9) is respected for all the MHFE schemes. Condition on the off-diagonal coefficients is more restrictive.

- For 1D domain, condition (2) of Eq. (9) is also directly verified for the quadratured and the lumped MHFE scheme, whereas the standard scheme is conditioned by the following criterion,

  $$\frac{C^A \Delta z^2}{6 K^A \Delta t} \le 1 \tag{10}$$

  to respect the M-matrix condition.
- For 2D rectangular elements, the matrix system of the lumped and standard MHFE schemes are never M-matrix. On the contrary, the scheme using a quadrature rule respects the conditions of Eq. (9).
- For 2D triangular elements, the off-diagonal coefficients of the resulting system can be expressed as:

  $$m_{ij}^A = -2\cot(\theta_k) + \frac{\phi}{3}\frac{\lambda}{3K^A + \lambda \ell} \tag{11}$$

  with $\lambda = |A|\, C^A / \Delta t$; $\phi = 1$ for the standard and quadratured schemes and $\phi = 0$ for the lumped one. θ_k refers to the angle k of the element A.

  Specific criteria either on angles or on simulations parameters have to be verified to have an M-matrix, as indicates in Table 2. Condition on angles is sufficient whereas this on time step length is necessary.

TABLE 2. Conditions on angles and time step to enforce M-matrix system for the various MHFE schemes developed in 2D triangular discretization.

MHFE schemes	Conditions on angles	Condition on time step size
Quadratured	$0 \le \theta_k \le 73.90°$	$\tan(\theta_k) - 6\ell \le \frac{18 K^A \Delta t}{C^A \lvert A \rvert}$
Standard	$0 \le \theta_k \le 40.89°$	
Lumped	$0° \le \theta_k \le 90°$	-

Finally, the use of a quadrature rule is potentially efficient for rectangular elements. The condition to have an M-matrix is less restrictive for the lumped scheme than for the corresponding MHFE one, which makes easier the respect of the maximum principle.

3. RESULTS AND DISCUSSION.

The first test case deals with the vertical infiltration of a sharp wetting front. The simulations are characterized by parameters specified in table 3. A comparison of the various MHFE schemes have been performed to show the efficiency of the lumped method. Therefore, Figure 1 depicts the global error versus the required CPU time for different nodal spacing. The lumped formulation appears clearly as the more accurate and efficient method for the MHFE scheme.

TABLE 3. Simulations' characteristics.

Parameters	**value**
Length of the column	100 cm
Soil characteristics	$\theta_r = 0.102$ (-) ; $\theta_s = 0.368$ (-)
	$\alpha = 0.033$ (cm^{-1}) ; n = 2 (-)
Celia *et al.* (1990)	$K_s = 9.22\times10^{-3}$ (cm.s^{-1})
Initial conditions	$Th_{init} = -1000$ cm
Top boundary condition	$Th_{sup} = -75$ cm
Bottom boundary condition	$Th_{inf} = -1000$ cm
Simulation length	21600 s
Nodal spacing, Δz	0.1 cm (reference) 0.5-1-1.5-2-3-4-5-5.5-6cm
Time step, Δt	0.1s (reference), 1s
Global error	$GErr = \int_{z=0}^{z=L} \left\| Th_{cal}(z) - Th_{ref}(z) \right\| dz \Big/ \int_{z=0}^{z=L} \left\| Th_{ref}(z) \right\| dz$

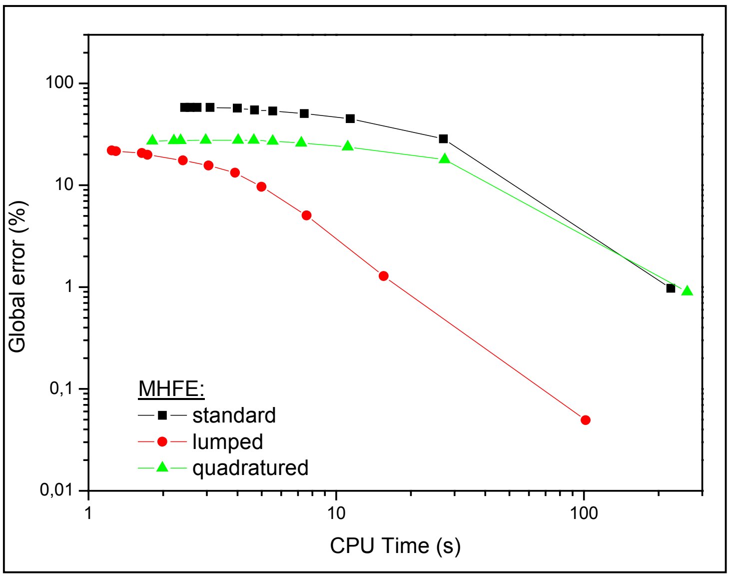

FIGURE 1. Global error versus CPU time for various MHFE schemes and nodal spacing.

Then, this example has been extended for a two dimensional domain (100x100 cm) with impermeable lateral boundary condition. Table 4 describes the properties of the meshes that have been used to analyse oscillations' phenomena.

TABLE 4. Mesh properties.

Mesh	Rec-1	Rec-2	Quad-1	Quad-2	3ang-1	3ang-2	U3ang-1	U3ang-2
type	Rectangles		Quadrangles		Triangles		Unstruct. triangles	
Nb nodes	10201	1681	10201	1681	5101	841	5134	855
Nb cells	10000	1600	10000	1600	10000	1600	9990	1600
Nb edges	20200	3280	20200	3280	15100	2440	15123	2454

TABLE 5. Error analysis.

	Δt	1s			10			100s		
		P_{min} (cm)	Over (%)	Extr (%)	P_{min} (cm)	Over (%)	Ext (%)	P_{min} (cm)	Over (%)	Ext (%)
Rec-1	MHFE	-1038.09	16.91	4.00	-1035.26	15.70	4.00	-1023.53	11.01	4.00
	LMHFE	-1000.14	$1.50E^{-2}$	1.00	-1000.42	$4.59E^{-2}$	1.00	-1000.13	$1.40E^{-2}$	1.00
Quad-1	MHFE	-1047.74	14.00	4.14	-1044.61	12.31	4.26	No conv.		
	LMHFE	-1001.80	$6.03E^{-2}$	1.02	-1003.76	0.11	0.97	No conv.		
3ang-1	MHFE	-1000.90	0.21	2.00	-1000.74	$4.11E^{-2}$	1.00	-1063.51	7.64	2.00
	LMHFE	-1000.00	0.00	0.00	-1000.00	0.00	0.00	-1000.00	0.00	0.00
U3ang-1	MHFE	-1033.93	0.85	1.59	-1029.56	0.86	1.61	No conv.		
	LMHFE	-1000.00	0.00	0.00	-1000.00	0.00	0.00	No conv.		
Rec-2	MHFE	-1015.59	5.52	7.50	-1015.65	5.54	7.50	-1016.30	5.76	7.50
	LMHFE	-1001.09	0.12	2.50	-1000.94	0.10	2.50	-1000.00	0.00	0.00
Quad-2	MHFE	-1033.72	6.90	8.69	-1033.81	7.03	8.81	-1034.63	7.51	9.00
	LMHFE	-1007.51	$6.61E^{-2}$	1.69	-1007.44	0.13	1.69	-1006.31	$2.63E^{-2}$	1.69
3ang-2	MHFE	-1058.55	7.65	5.00	-1058.37	7.63	5.00	-1056.44	7.43	5.00
	LMHFE	-1000.00	0.00	0.00	-1000.00	0.00	0.00	-1000.00	0.00	0.00
U3ang-2	MHFE	-1032.84	1.29	4.13	-1032.87	1.29	4.13	-1033.24	1.28	4.13
	MHFE	-1000.00	0.00	0.00	-1000.00	0.00	0.00	-1000.00	0.00	0.00

P_{min} should be -1000cm; Ext is the % of extremum; $\text{Over}(\%) = \sum_{i=1}^{\text{Nb cells}} \min\left(P_i + 1000, 0\right) \div 1000 \times \text{Ext}$

For this specific issue too, the lumped formulation is very efficient, as the statistical analysis of table 5 demonstrates it. This second test case shows firstly that for a given type of mesh, oscillations decrease using the lumped formulation. Besides, triangles are advantageous in this context.

Other test cases in a 2D domain, for homogeneous and heterogeneous dry porous media and subject to different boundary conditions have been performed. Although they are not reported in this paper, previous conclusions are confirmed.

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