XVIII International Conference on Water Resources
CMWR 2010
J. Carrera (Ed)
CIMNE, Barcelona 2010

A MODIFIED MASS LUMPING PROCEDURE FOR THE MIXED HYBRID FINITE ELEMENT METHOD APPLIED TO UNSATURATED WATER FLOW MODELLING

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Key words: unsaturated flow, mass lumping, mixed hybrid finite element

Summary. This article deals with variably saturated flow modeling. Mixed Hybrid Finite Element (MHFE) methods have become popular in recent years for modeling groundwater flow. A new procedure of mass lumping, suitable for various shapes of 2D elements, is developed to avoid unphysical oscillations obtained with the standard MHFE scheme. Efficiency of this formulation is demonstrated for the simulation of sharp infiltration fronts in the vadose zone.

1 INTRODUCTION

Numerical simulation of variably saturated flow in porous media is of interest in many applications including geotechnical engineering, ground water hydrology, soil science, and environmental technology. Based on the assumption that the air phase in soil can move without any appreciable pressure gradients in the air phase, the Richards Equation (RE) is a valuable model to predict water movement and solute transport in variably saturated media[1].

From a mathematical point of view, the RE can be a highly nonlinear parabolic equation under unsaturated conditions, or a partial differential equation (PDE) of elliptic type for a fluid-saturated incompressible porous media. Mixed Hybrid Finite Elements (MHFE) are a numerical method becoming more and more popular in Geosciences. The method is well suited for the discretization of elliptic and parabolic PDEs. MHFE allow a simultaneous approximation of both pressure head and velocity and can handle general irregular grids with highly heterogeneous permeability. Hence, this numerical scheme has been extensively used in the last few years [2,3,4,5].

However, when dealing with infiltration problem, especially sharp wetting fronts in dry soils, the MHFE results may exhibit solution with unphysical oscillations due to the non respect of the discrete maximum principle[5,6]. A technique commonly used in finite element methods is the so-called mass lumping technique : 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[7]. The procedure has been extended to triangular grids with the constraint of a weakly acute triangulation (see ref

in [4]). A new mass lumping procedure for the MHFE, suitable for various shapes of 2D elements, has been proposed and tested for advection-dispersion problems [4] and generalized for variably saturated flow [8].

This procedure allows to reduce the unphysical oscillations in many cases. However, when applied for distorted elements and/or anisotropic domains, the obtained solution is still exposed to strong unphysical oscillations and to convergence difficulties. To avoid this problem, we develop a new procedure that takes into account the anisotropy and the shape of the element during the masse distribution of the accumulation and sink/source terms at edges.

In this work, the modified mass lumping technique is briefly described and discussed in the specific context of variably saturated water flow. A 2D numerical experiments in homogeneous porous media is provided to illustrate the benefits of this procedure. Other numerical test in heterogeneous will be presented at the meeting.

2 THEORY

2.1 Variably saturated flow modeling

The combination of the Darcy Buckingham law and the mass conservation equation leads to the Jacob-Richards equation:

$$\frac{\partial \theta}{\partial t} + S_S S_w(\theta)\frac{\partial H}{\partial t} + \nabla.\left(K(h).\nabla H\right) = f \tag{1}$$

where H and h are the piezometric and pressure heads, respectively, such that H = h - z; z is the depth taken positive downward; S_s the specific storage coefficient; S_w (= θ / θ_s) is the relative saturation of the aqueous phase; θ is the volumetric water content; θs is the saturated water content; f is a source–sink term; and K is the hydraulic conductivity. Under unsaturated conditions, the porous media and the fluid are assumed to be incompressible ($S_s = 0$) and in this case, the Jacob–Richards equation reduces to the well-known RE. that will be considered in the rest of this article.

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 pressure head, hydraulic conductivity, and water content are characterized using constitutive relations. According to recent studies [9,10], the standard Mualem–van Genuchten model [11] has to be modified by adding an air-entry value (h_e). The effective saturation (S_e) is given by equation (2), where θ_s and θ_r are the saturated and residual volumetric water contents, respectively, α a parameter related to the mean pore size, n a parameter reflecting the uniformity of the pore-size distribution and $m = 1 - 1/n$.

$$S_e = \begin{cases} = \dfrac{\theta - \theta_r}{\theta_s - \theta_r} = \dfrac{1}{S_E^*}\left[1 + \left(\alpha |h|\right)^n\right]^{-m}, & h < -h_e \\ 1, & h \geq -h_e \end{cases} \tag{2}$$

The saturation at the cut-off point h_e is:

$$S_E^* = \left[1+(\alpha h_e)^n\right]^{-m} \tag{3}$$

The conductivity - saturation relationship becomes:

$$K(S_e) = \begin{cases} K_s S_e^{1/2}\left[\dfrac{1-\left(1-\left(S_E^* S_e\right)^{1/m}\right)^m}{1-\left(1-S_E^{*1/m}\right)^m}\right]^2, & S_e < S_E^* \\ K_s, & S_e \geq S_E^* \end{cases} \tag{4}$$

where S_e is given by equation (2) and $n > 1$. K_s is the saturated conductivity (usually assumed as a scalar but could be a tensor for the general case).

2.2 Lumped MHFE

The basic idea of the new mass lumping procedure is firstly to calculate steady-state fluxes by using the classical MHFE method [7,12] and then to add the accumulation and sink/source terms directly on the edges (2D) / faces (3D). Hence, the process to get the lumped MHFE system associated with equation (1) involves the following steps:

- The mean water flux $\overrightarrow{q_E}$ over the element E is defined via the lowest-order Raviart-Thomas space:

$$\overrightarrow{q_E} = \sum_{i=1}^{n_f} Q_{E,i}\overrightarrow{\omega_{E,i}} \tag{5}$$

  where $\overrightarrow{\omega_{E,i}}$ are the vectorial basis functions [12] and n_f refers to the number of edges or faces.

- $Q_{E,i}$ denotes the flux leaving E through the i^{th} edge / face. It is defined by:

$$Q_{E,i} = \overline{Q}_{E,i} + \beta_{E,i}\times\left[Q_{E,s} - |E|\left(\frac{\partial T\theta_{E,i}}{\partial t} + S_{s,E}S_{w,E}\frac{\partial TH_{E,i}}{\partial t}\right)\right] \tag{6}$$

  where $\overline{Q}_{E,i}$ is the flux corresponding to the stationary problem without sink/source terms, $\beta_{E,i}$ a pounding coefficient referred to as lumped coefficient, $Q_{E,s}$ is the sink/source term over the element E defined by $Q_{E,s} = \int_E f.dE$ and $|E|$ refers to the area of the element in 2D or volume in 3D. $T\theta_{E,i}$ and $TH_{E,i}$ are the mean values of the water content and the piezometric head respectively over the i^{th} edge / face of E (also called Traces of water content or piezometric head).

- The stationary part of the flux $\overline{Q}_{E,i}$ is expressed as

$$\overline{Q}_{E,i} = \sum_{j=1}^{n_f} \left(\frac{\alpha_{E,i}\alpha_{E,j}}{\alpha_E} - B^{-1}_{E,ij} \right) TH_{E,j} \tag{7}$$

The following notations are used: $B_{E,ij} = \int_E \overrightarrow{\omega_{E,i}}.K_E.\overrightarrow{\omega_{E,j}}$, $\alpha_{E,i} = \sum_{j=1}^{nf} B^{-1}_{E,ij}$, $\alpha_E = \sum_{i=1}^{nf} \alpha_{E,i}$, where K_E is the value of the conductivity in element E.

- Due to the (high) non-linearities of the relations between h - θ - k (equations (2) to (4)), the water content is expanded by means of a first-order Taylor series with respect to the traces of piezometric head [13]. According to this linearization strategy, equation (6) becomes:

$$Q^{n+1,k+1}_{E,i} = \sum_{j=1}^{ne} \widetilde{N}^{n+1,k}_{E,ij} TH^{n+1,k+1}_{E,j} + \beta_{E,i} \times F^{n+1,k}_{E,i} \tag{8}$$

where the local matrix $\left[\widetilde{N}_E \right]$ obtained with the lumped formulation is given by,

$$\widetilde{N}^{n+1,k}_{E,ij} = \frac{\alpha^{n+1,k}_{E,i}\alpha^{n+1,k}_{E,j}}{\alpha^{n+1,k}_{E}} - \left(B^{n+1,k}_{E,ij} \right)^{-1} - \lambda^{n+1,k}_{E,i} \times \beta_{E,i} \times \delta_{ij} \tag{9}$$

$$\text{with } \lambda^{n+1,k}_{E,i} = \frac{|E|}{\Delta t^n} \left(TC^{n+1,k}_{E,i} + S_{S,E} S^{n+1,k}_{w,E,i} \right) \text{ and } \delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$$

$$F^{n+1,k}_{E,i} = Q_{E,s} - \frac{|E|}{\Delta t^n} \left(T\theta^{n+1,k}_{E,i} - TC^{n+1,k}_{E,i} TH^{n+1,k}_{E,i} - T\theta^{n}_{E,i} - S_{S,E} S^{n+1,k}_{w,E,i} TH^{n}_{E,i} \right) \tag{10}$$

In equation (8), (9) and (10), n refers to the time level, k to the iteration level and Δt^n to the time step size between the new and the old time levels $\left(\Delta t^n = t^{n+1} - t^n \right)$. $TC_{E,i}$ is the mean value of the capillary capacity at i^{th} edge / face.

- The final system to solve is obtained by writing the continuity of edge state variables $TH_{E,i} = TH_{E',j}$ and fluxes $Q_{E,i} + Q_{E',j} = 0$ between two adjacent cells A and B.

2.3 Analysis of matrix system and proposition of lumped coefficient

The comparison of the flux obtained with the standard and the lumped formulations of the MHFE method can be interesting to illustrate the effect of the new procedure. Hence, the expression of the flux for the standard MHFE approach is given by equation (11). Notice that

$\lambda_E^{n+1,k}$ and $F_E^{n+1,k}$ of equation (11) can be computed through equations (9) and (10) by using mean value of the variable (i.e. on the cell) instead of traces of state variable (i.e. edge state variable).

$$Q_{E,i}^{n+1,k+1} = \frac{\alpha_{E,i}^{n+1,k}}{\alpha_E^{n+1,k} + \lambda_E^{n+1,k}} \sum_{j=1}^{ne} \alpha_{E,j}^{n+1,k} TH_{E,j}^{n+1,k+1} - \sum_{j=1}^{ne} \left(B_{E,ij}^{n+1,k} \right)^{-1} TH_{E,j}^{n+1,k+1} + \frac{\alpha_{E,i}^{n+1,k}}{\alpha_E^{n+1,k} + \lambda_E^{n+1,k}} \times F_E^{n+1,k} \qquad (11)$$

Combining equations (8), (9) and (10) leads to the following expression of flux for the lumped MHFE method:

$$Q_{E,i}^{n+1,k+1} = \frac{\alpha_{E,i}^{n+1,k}}{\alpha_E^{n+1,k}} \sum_{j=1}^{ne} \alpha_{E,j}^{n+1,k} TH_{E,j}^{n+1,k+1} - \sum_{j=1}^{ne} \left(B_{E,ij}^{n+1,k} \right)^{-1} TH_{E,j}^{n+1,k+1} - \lambda_{E,i}^{n+1,k} \times \beta_{E,i} \times TH_{E,j}^{n+1,k+1} + \beta_{E,i} \times F_{E,i}^{n+1,k} \qquad (12)$$

In previous studies [4,8], a simple formula $\beta_{E,i} = 1 / n_f$ has been considered to define the lumped coefficient. Comparison of equation (11) and (12) shows that this strategy fails to take into account the specific geometry of each cell of the discretized domain. Moreover, the efficiency of the lumped method to avoid oscillation can be affected by this choice as it will be illustrated in the next part, dedicated to numerical simulations.

Consequently, the new formulation is based on a following definition of the lumped coefficient:

$$\beta_{E,i} = \frac{\alpha_{E,i}^{n+1,k}}{\alpha_E^{n+1,k}} = \frac{\hat{\alpha}_{E,i}}{\hat{\alpha}_E} \qquad (12)$$

$$\text{with } \hat{\alpha}_{E,i} = \sum_{j=1}^{n_f} \hat{B}_{E,ij}^{-1}, \ \hat{B}_{E,ij} = \int_E \overrightarrow{\omega_{E,i}} . \overrightarrow{\omega_{E,j}} \text{ and } \hat{\alpha}_E = \sum_{i=1}^{nf} \alpha_{E,i}$$

Equation (12) indicates that only the diagonal term of the final matrix system is affected by the choice of the lumped coefficient. The analysis of the matrix system according to the M-matrix criterion, which specifies the mathematical condition to respect the maximum principle, has shown that off-diagonal coefficients raise the main difficulties [4,8]. Then, the new mass lumping formulation will maintain the global properties of the previous one (see [8]), in summary:

- for 1D problem and contrary to the standard MHFE scheme, the new solution does not contain any unphysical oscillation;
- for triangular dsicretization, oscillation are strongly reduced and in case of an accurte triangulation they are totally removed;
- for quadrangular meshes, a subdiscretization technique [8] is advised to improved the monotonicity of the solution.

Furthermore, the new formulation allows to handle complex mesh geometry and to increase local monotonicity (between traces and mean pressure head) compared to our first proposition.

3 RESULTS AND DISCUSSION

The infiltration of a sharp wetting front has been simulated in this test case which is completely characterized by table 1. In fact, this 2D example reduces to a 1D problem because of the homogeneous porous media and uniform boundary conditions along each border. However, several mesh discretization are compared to illustrate the impact of mesh size ratio ($\Delta z / \Delta x$) which is an important issue when more complex geometry (small depth and large width - length) and evolution are considered.

Parameters	**value**
Dimensions of the domain	$x \in [0 ;3\ m], z \in [0 ;3\ m]$
Soil characteristics	$\theta_r = 0.102$ (-) $\theta_s = 0.368$ (-) $\alpha = 3.3\ (m^{-1})$ $n = 2$ (-) $he = 2\ 10^{-2}$ (m) $K_s = 9.22\ 10^{-5}\ (m.s^{-1})$
Initial pressure head	$Th_{(t=0)} = -1.15$ m
Top boundary condition	$TH_{(z=0\ m\ ,\ t)} = 0$ m
Bottom boundary condition	$TH_{(z=3\ m\ ,\ t)} = -4.15$ m
Lateral boundary condition	$Q_{(x=0\ m\ and\ x=1\ m,\ t)} = 0\ m.s^{-1}$
Final time	1800 s
Mesh size ration $\Delta z / \Delta x$	1 (mesh-1); 10^{-1} (mesh-2); 10^{-2} (mesh-3)
Fixed time step, Δt	10 s

Table 1 : Simulation's characteristics

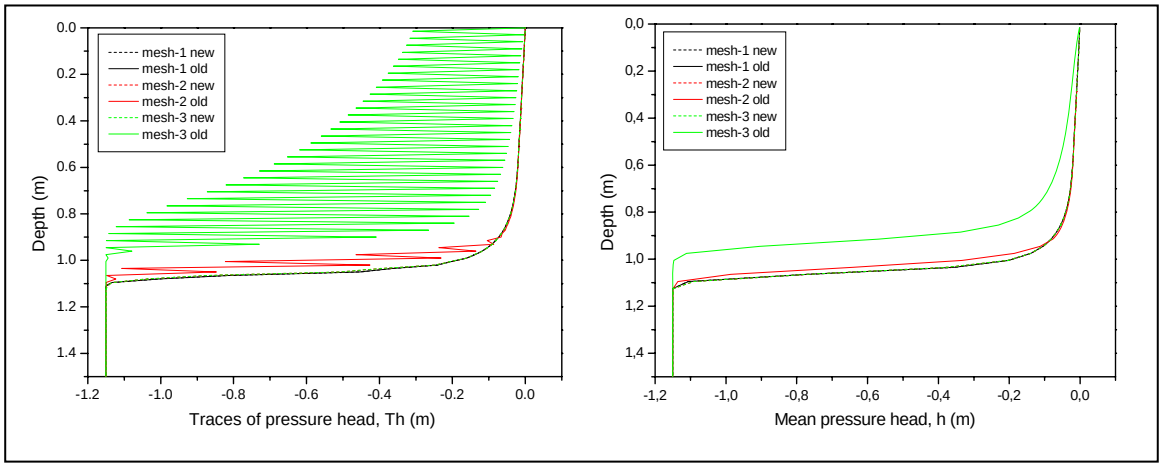

Figure 1: Evolution of the infiltration front (mean pressure head and traces of pressure head) for both LMHFE approaches after 1800 s.

Figure 1 shows that the decrease of the mesh size ratio produces two main effects on the old lumped MHFE formulation. Firstly, it significantly reduces the accuracy of the mean pressure head solution. On the other hand it causes oscillations between the different traces of pressure head. Notice that these unphysical oscillations disappear from the mean pressure head solution and that mass-balances are correct for all the simulations, which could mask this problem. However, this numerical failure amplifies with the decrease of the mesh size ratio. This simple example shows that the definition of the lumped coefficient is a crucial point. The modified mass lumping scheme is more stable for both traces and mean pressure head. Consequently, it is a better formulation to handle more complex shape of elements.

Results of other investigations in heterogeneous media will be presented at the next CMWR meeting to illustrate the benefits of the new mass-lumping method.

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