Journal of Computational Physics **149,** 148–167 (1999)
Article ID jcph.1998.6150, available online at http://www.idealibrary.com on IDEAL®

A New Formulation of the Mixed Finite Element Method for Solving Elliptic and Parabolic PDE with Triangular Elements

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Received May 21, 1998; revised September 22, 1998

For the groundwater flow problem (which corresponds to the Darcy flow model), we show how to produce a scheme with one unknown per element, starting from a mixed formulation discretized with the Raviart Thomas triangular elements of lowest order. The aim is here to obtain a new formulation with one unknown per element by elimination of the velocity variables $\mathbf{q} = -k$ grad P, without any restriction concerning the computation of the velocity field. In the first part, we describe the triangular mixed finite element method used for solving Darcy's and mass balance equations. In the second part, we study the elliptic–parabolic problem; we describe the new formulation of the problem in order to use mixed finite elements (MFE) with less unknowns without any specific numerical integration. Finally, we compare the computational effort of the MFE method with the new formulation for different triangulations using numerical experiments. In this work, we show that the new formulation can be seen as a general formulation which can be equivalent to the finite volume or the finite difference methods in some particular cases.

Key Words: mixed finite element method; finite volume method; elliptic–parabolic problem; triangular elements.

1. INTRODUCTION

The usual equations describing the flow in a porous medium are given by the mass balance equation and Darcy's law,

$$s\frac{\partial P}{\partial t} + \nabla \cdot (\mathbf{q}) = f, \tag{1}$$

$$\mathbf{q} = -k\nabla P, \tag{2}$$

0021-9991/99 $30.00

where s (L^{-1}) is the specific storativity of the porous material, k (LT^{-1}) is the so-called hydraulic conductivity, f (T^{-1}) is the source or sink term per unit area, P (L) and $\mathbf{q}$ (LT^{-1}) are the piezometric head and the Darcy's velocity, respectively.

This system is often modelled by finite difference or finite element methods of lower order. The finite difference method ensures an exact mass balance over each element but the finite element method is considered as more flexible because of its high capacity of discretizing complex geometry domains. However, with the finite element method we have discontinuous fluxes at the element's edge.

The idea of mixed finite element is to approximate simultaneously the piezometric head P and the velocity $\mathbf{q}$. This approximation gives velocity throughout the field and the normal component of the velocity is continuous across the inter-element boundaries. Moreover, with the mixed formulation, the velocity is defined with the help of Raviart Thomas basis functions [1, 2] and, therefore, a simple integration over the element gives the corresponding streamlines. The drawback of an indefinite stiffness matrix is circumvented by hybridization. The system is solved in this case for one unknown, the average piezometric head per element edge.

Several studies have shown the superiority of the mixed finite element method with regard to the other classical methods; Durlofsky [3] compared mixed and controlled volume finite element approximations for different contrasts of hydraulic conductivity. He showed that for very variable or discontinuous hydraulic conductivity fields the mixed finite element method approximates flow variables more accurately and more realistically than the control volume method with the same number of unknowns. Some comparisons between the mixed finite element method and other classical methods can be found in the works of [4–7]. For a triangular mesh, the mixed method requires about 3 times the number of unknowns, compared to finite differences and about 1.5 times, compared to finite volumes.

Because mixed finite element (MFE), finite volume (FV), and finite difference (FD) methods use an harmonic mean of the hydraulic conductivity to calculate the flux between two adjacent cells, one could show, in some conditions, a certain correspondence between the three methods. It has been reported that for rectangular meshes, mixed finite elements of lowest order reduce to the standard cell-centred finite volume method [8, 9], provided numerical integration is used. Recently, Cordes and Kinzelbach [10] showed equivalence between mixed finite element and (1) block-centred finite differences, when the triangulation is obtained by subdivision of rectangular elements, and (2) finite volumes, when general triangulation is used and without any numerical integration. This last connection was already noticed by Baranger *et al.* in 1994 [11].

Ackerer *et al.* [12] stated that such equivalence is restricted to divergence-free velocity (steady state flow field, no sink/source terms inside the domain). Moreover, the mixed finite element method does not require a Delaunay triangulation [9], unlike a finite volume scheme. Notice that imposing boundary conditions with finite volume or finite difference methods often poses nontrivial problems.

MFE is more accurate but uses more unknowns (number of edges) than the other methods (number of cells for FD or FV). Hence, the objective of this work is to reduce the number of unknowns for the MFE method using a new formulation in order to lead to a final system with the number of cells as unknowns without any approximation. In this paper one is interested in a general triangular grid.

In the first part, we describe briefly the triangular MFE method used for solving Darcy's and mass balance equations.

In the second part, we present the new formulation of the problem in order to use MFE with less unknowns. We show how we built the final system to solve. The new formulation is equivalent to the usual MFE method. However, the final system obtained with the new formulation leads to a symmetric matrix for the steady-state case and an unsymmetric matrix for the transient flow.

In the third part, we show connections between this formulation, the MFE, FD, and FV methods. The new formulation can indeed be seen as a general formulation equivalent to the FV or the FD methods in some particular cases. This shows also that we can design a FV method for a general triangulation (not necessarily Delaunay triangulation), being aware that the state variable for the FV method does not represent the average potential head inside the element.

The end of the paper is devoted to some numerical experiments. We show the efficiency of the new algorithm in some specific cases and we point out the correlation between the triangulation type and the definite positivity of the functional matrix of the new method.

2. THE TRIANGULAR MIXED FINITE ELEMENT METHOD

In the lowest-order MFE formulation for triangular elements, the velocity vector is approximated with vector basis functions that are piecewise linear along both coordinate directions. Velocity $\mathbf{q}_E$, in any point inside element E can be obtained by (e.g., [13])

$$\mathbf{q}_E = \mathbf{w}_1 Q_1 + \mathbf{w}_2 Q_2 + \mathbf{w}_3 Q_3, \tag{3}$$

where Q_i ($\mathrm{L}^2\mathrm{T}^{-1}$) are the fluxes across the element edges E_i and $\mathbf{w}_i$ (L^{-1}) are the three vector basis functions for the element E (Fig. 1) defined by

$$\int_{E_j} \mathbf{w}_i \cdot \mathbf{n}_{E_j} = \begin{cases} 1, & \text{if i} = \text{j} \\ 0, & \text{if i} \neq \text{j}. \end{cases} \tag{4}$$

For a triangular element these three vector basis functions are

$$\mathbf{w}_1 = \frac{1}{2|E|}\begin{pmatrix} x - x_1 \\ y - y_1 \end{pmatrix}, \quad \mathbf{w}_2 = \frac{1}{2|E|}\begin{pmatrix} x - x_2 \\ y - y_2 \end{pmatrix}, \quad \mathbf{w}_3 = \frac{1}{2|E|}\begin{pmatrix} x - x_3 \\ y - y_3 \end{pmatrix}, \tag{5}$$

where (x_i, y_i) are the coordinates of the vertices of E and $|E|$ is its area.

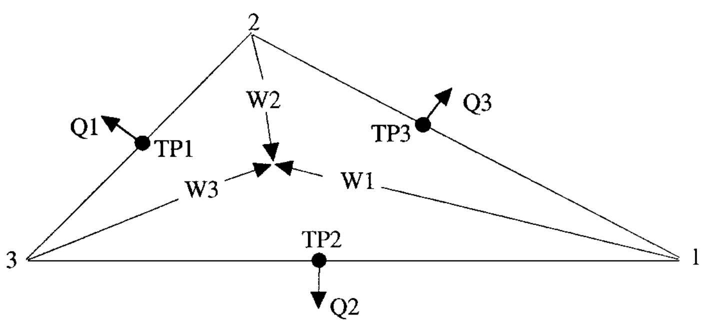

FIG. 1. Basis functions for the triangular MFE method.

In addition they satisfy

$$\nabla \cdot \mathbf{w}_i = \frac{1}{|E|}. \tag{6}$$

On the edge E_j

$$\mathbf{w}_i \cdot \mathbf{n}_{E_j} = \begin{cases} \frac{1}{|E_i|}, & \text{if i = j} \\ 0, & \text{if i} \neq \text{j}, \end{cases} \tag{7}$$

where $|E_i|$ is the length of the edge E_i.

The mass balance equation (1) is discretized using a finite volume formulation in space,

$$\int_E s\frac{\partial P}{\partial t} + \int_E \nabla \cdot \mathbf{q}_E = \int_E f = Q_s, \tag{8}$$

and a finite difference scheme in time,

$$s\frac{P^n - P^{n-1}}{\Delta t} + \frac{(Q_1 + Q_2 + Q_3)}{|E|} = \frac{Q_s}{|E|}, \tag{9}$$

where Q_s ($\mathrm{L}^2\mathrm{T}^{-1}$) is the source or sink term associated with the element E and n is the index of the time step. The fluxes Q_i, $i = 1 \cdots 3$ are expressed at time n for an implicit scheme and at $n - 1$ for an explicit scheme.

We recall that Darcy's law is given by $\mathbf{q}_E = -k\nabla P$, k being the hydraulic conductivity in the element E. Using properties (6) and (7) of the vector basis functions $\mathbf{w}_i$, Darcy's law written in a variational form leads to

$$\int_E \left(k^{-1}\mathbf{q}_E\right) \cdot \mathbf{w}_i = -\int_E (\nabla P) \cdot \mathbf{w}_i = \int_E P\nabla \cdot \mathbf{w}_i - \sum_{j=1}^{3} \int_{E_j} P\mathbf{w}_i \cdot \mathbf{n}_{E_j} = \frac{1}{|E|}\int_E P - \frac{1}{|E_i|}\int_{E_i} P$$

which gives

$$\sum_{j=1}^{3} Q_{E_j} \int_E \left(k^{-1}\mathbf{w}_j\right) \cdot \mathbf{w}_i = P_E - TP_{E_i}. \tag{10}$$

P_E is the average potential head over E and TP_{E_i} are the average potential heads on each element edge E_i and will be denoted respectively P and TP_i for simplicity.

Darcy's law can then be written in the matrix form

$$\begin{pmatrix} B_{11} & B_{12} & B_{13} \\ B_{21} & B_{22} & B_{23} \\ B_{31} & B_{32} & B_{33} \end{pmatrix} \begin{bmatrix} Q_1 \\ Q_2 \\ Q_3 \end{bmatrix} = \begin{bmatrix} P - TP_1 \\ P - TP_2 \\ P - TP_3 \end{bmatrix}, \tag{11}$$

where

$$B_{ij} = \frac{1}{k}\int_E \mathbf{w}_i \cdot \mathbf{w}_j.$$

As shown in [10], if we define $\mathbf{r}_{ij}$ as the edge vector from node i toward node j, L_{ij} as its length ($L_{ij} = \|\mathbf{r}_{ij}\|$) and by applying the scalar product, $\mathbf{r}_{ij}\mathbf{r}_{ik} = \frac{1}{2}(L_{ij}^2 + L_{ik}^2 - L_{jk}^2)$, we find

$$B = \frac{1}{48k|E|}\begin{pmatrix} 3L_{12}^2 + 3L_{13}^2 - L_{23}^2 & -3L_{12}^2 + L_{13}^2 + L_{23}^2 & L_{12}^2 - 3L_{13}^2 + L_{23}^2 \\ -3L_{12}^2 + L_{13}^2 + L_{23}^2 & 3L_{12}^2 - L_{13}^2 + 3L_{23}^2 & L_{12}^2 + L_{13}^2 - 3L_{23}^2 \\ L_{12}^2 - 3L_{13}^2 + L_{23}^2 & L_{12}^2 + L_{13}^2 - 3L_{23}^2 & -L_{12}^2 + 3L_{13}^2 + 3L_{23}^2 \end{pmatrix}. \tag{12}$$

One notices that

$$B_{11} + B_{21} + B_{31} = B_{12} + B_{22} + B_{32} = B_{13} + B_{23} + B_{33} = L$$

with

$$L = \left(L_{12}^2 + L_{13}^2 + L_{32}^2\right)/48k|E|.$$

The system of equations (11) gives

$$L(Q_1 + Q_2 + Q_3) = 3P - (TP_1 + TP_2 + TP_3). \tag{13}$$

Defining $S = |E|L(s/\Delta t)$ and $F = LQ_s$ the substitution of Eq. (13) in the mass balance equation (9), expressed in an implicit scheme, gives

$$P^n = \frac{1}{S+3}\left(TP_1 + TP_2 + TP_3 + F + SP^{n-1}\right). \tag{14}$$

Equation (10) can also be solved for the corresponding fluxes across the element edges

$$\begin{aligned} Q_1 = -\frac{k}{|E|}\bigg[& L_1^{-1} \cdot P + \left(\mathbf{r}_{23}\mathbf{r}_{23} - \frac{L_1^{-1}}{3}\right)TP_1 + \left(\mathbf{r}_{23}\mathbf{r}_{31} - \frac{L_1^{-1}}{3}\right)TP_2 \\ & + \left(\mathbf{r}_{23}\mathbf{r}_{12} - \frac{L_1^{-1}}{3}\right)TP_3\bigg], \end{aligned} \tag{15}$$

where $L_1^{-1} = -|E|L^{-1}/k$.

Defining

$$\varsigma = \frac{L_1^{-1}}{3} - \frac{L_1^{-1}}{S+3}, \tag{16}$$

$$b = \frac{L_1^{-1}}{S+3}(F + SP^{n-1}). \tag{17}$$

The substitution of P in (15) by its expression in (14) leads to

$$\begin{aligned} Q_1 &= a_{11}TP_1 + a_{12}TP_2 + a_{13}TP_3 - \frac{kb}{|E|} \\ Q_2 &= a_{21}TP_1 + a_{22}TP_2 + a_{23}TP_3 - \frac{kb}{|E|} \\ Q_3 &= a_{31}TP_1 + a_{32}TP_2 + a_{33}TP_3 - \frac{kb}{|E|}, \end{aligned} \tag{18a}$$

where

$$a_{11} = -\frac{k}{|E|}(\mathbf{r}_{23}\mathbf{r}_{23} - \varsigma), \quad a_{12} = a_{21} = -\frac{k}{|E|}(\mathbf{r}_{23}\mathbf{r}_{31} - \varsigma), \quad a_{13} = a_{31} = -\frac{k}{|E|}(\mathbf{r}_{23}\mathbf{r}_{12} - \varsigma)$$

$$a_{22} = -\frac{k}{|E|}(\mathbf{r}_{31}\mathbf{r}_{31} - \varsigma), \quad a_{23} = a_{32} = -\frac{k}{|E|}(\mathbf{r}_{12}\mathbf{r}_{31} - \varsigma), \quad a_{33} = -\frac{k}{|E|}(\mathbf{r}_{12}\mathbf{r}_{12} - \varsigma). \tag{18b}$$

3. THE NEW FORMULATION FOR THE ELLIPTIC–PARABOLIC PROBLEM

The goal is now to eliminate state variables on the edges with the help of a new variable associated with an element for a general case (steady state or transient flow with or without sink/source terms). This new variable H is defined so that the three fluxes have the expressions

$$\begin{aligned} Q_1 &= \xi_1(H - \beta_1 T P_1) + \gamma_1, \\ Q_2 &= \xi_2(H - \beta_2 T P_2) + \gamma_2, \\ Q_3 &= \xi_3(H - \beta_3 T P_3) + \gamma_3, \end{aligned} \tag{19}$$

and

$$H = \pi_1 T P_1 + \pi_2 T P_2 + \pi_3 T P_3. \tag{20}$$

H does not represent necessarily the average potential head on the element. Replacing (20) in (19) and comparing with the MFE scheme (18), the coefficients $\gamma_1, \gamma_2, \gamma_3, \pi_1, \pi_2, \pi_3, \xi_1, \xi_2, \xi_3, \beta_1, \beta_2$, and β_3 are defined by the 12 equations

$$\gamma_1 = \gamma_2 = \gamma_3 = -\frac{k}{|E|}b, \tag{21}$$

$$\xi_1(\pi_1 - \beta_1) = -\frac{k}{|E|}(\mathbf{r}_{23}\mathbf{r}_{23} - \varsigma), \tag{22}$$

$$\xi_1 \cdot \pi_2 = -\frac{k}{|E|}(\mathbf{r}_{23}\mathbf{r}_{31} - \varsigma), \tag{23}$$

$$\xi_1 \cdot \pi_3 = -\frac{k}{|E|}(\mathbf{r}_{23}\mathbf{r}_{12} - \varsigma), \tag{24}$$

$$\xi_2 \cdot \pi_1 = -\frac{k}{|E|}(\mathbf{r}_{31}\mathbf{r}_{23} - \varsigma), \tag{25}$$

$$\xi_2(\pi_2 - \beta_2) = -\frac{k}{|E|}(\mathbf{r}_{31}\mathbf{r}_{31} - \varsigma), \tag{26}$$

$$\xi_2 \cdot \pi_3 = -\frac{k}{|E|}(\mathbf{r}_{31}\mathbf{r}_{12} - \varsigma), \tag{27}$$

$$\xi_3 \cdot \pi_1 = -\frac{k}{|E|}(\mathbf{r}_{12}\mathbf{r}_{23} - \varsigma), \tag{28}$$

$$\xi_3 \cdot \pi_2 = -\frac{k}{|E|}(\mathbf{r}_{12}\mathbf{r}_{31} - \varsigma), \tag{29}$$

$$\xi_3(\pi_3 - \beta_3) = -\frac{k}{|E|}(\mathbf{r}_{12}\mathbf{r}_{12} - \varsigma). \tag{30}$$

The nine coefficients ($\pi_1, \pi_2, \pi_3, \xi_1, \xi_2, \xi_3, \beta_1, \beta_2$, and β_3) are obtained by solving the system constituted by Eqs. (22) to (30), which are not linearly independent. Indeed, we have

$$\frac{(23)}{(24)} \Leftrightarrow \frac{\pi_2}{\pi_3} = \frac{\mathbf{r}_{23}\mathbf{r}_{31} - \varsigma}{\mathbf{r}_{23}\mathbf{r}_{12} - \varsigma} \tag{31}$$

$$\frac{(25)}{(27)} \Leftrightarrow \frac{\pi_1}{\pi_3} = \frac{\mathbf{r}_{31}\mathbf{r}_{23} - \varsigma}{\mathbf{r}_{31}\mathbf{r}_{12} - \varsigma} \tag{32}$$

$$\frac{(28)}{(29)} \Leftrightarrow \frac{\pi_1}{\pi_2} = \frac{\mathbf{r}_{12}\mathbf{r}_{23} - \varsigma}{\mathbf{r}_{12}\mathbf{r}_{31} - \varsigma}. \tag{33}$$

We see immediately that $(31) \times (33) = (32)$.

Therefore, we assume one of the unknowns, for example β_1, is a given parameter denoted τ hereafter. This parameter is defined at the element level and can be different for each element. The previous relations give

from $\frac{(22)}{(23)}$ and (33)

$$\pi_2 = \frac{(\mathbf{r}_{23}\mathbf{r}_{31} - \varsigma)(\mathbf{r}_{12}\mathbf{r}_{31} - \varsigma)}{(\mathbf{r}_{23}\mathbf{r}_{31} - \varsigma)(\mathbf{r}_{12}\mathbf{r}_{23} - \varsigma) - (\mathbf{r}_{23}\mathbf{r}_{23} - \varsigma)(\mathbf{r}_{12}\mathbf{r}_{31} - \varsigma)}\tau \tag{34}$$

from (33) and (34)

$$\pi_1 = \frac{(\mathbf{r}_{12}\mathbf{r}_{23} - \varsigma)}{(\mathbf{r}_{12}\mathbf{r}_{31} - \varsigma)}\pi_2 \tag{35}$$

from (32) and (34)

$$\pi_3 = \frac{(\mathbf{r}_{23}\mathbf{r}_{12} - \varsigma)}{(\mathbf{r}_{23}\mathbf{r}_{31} - \varsigma)}\pi_2 \tag{36}$$

from $\frac{(26)}{(27)}$

$$\beta_2 = \frac{(\mathbf{r}_{31}\mathbf{r}_{23} - \varsigma)\pi_2 - (\mathbf{r}_{31}\mathbf{r}_{31} - \varsigma)\pi_1}{(\mathbf{r}_{31}\mathbf{r}_{23} - \varsigma)} \tag{37}$$

from $\frac{(30)}{(29)}$

$$\beta_3 = \frac{(\mathbf{r}_{12}\mathbf{r}_{31} - \varsigma)\pi_3 - (\mathbf{r}_{12}\mathbf{r}_{12} - \varsigma)\pi_2}{(\mathbf{r}_{12}\mathbf{r}_{31} - \varsigma)} \tag{38}$$

from (24)

$$\xi_1 = -\frac{k}{|E|}\frac{(\mathbf{r}_{23}\mathbf{r}_{12} - \varsigma)}{\pi_3} \tag{39}$$

from (25)

$$\xi_2 = -\frac{k}{|E|}\frac{(\mathbf{r}_{31}\mathbf{r}_{23} - \varsigma)}{\pi_1} \tag{40}$$

and from (29)

$$\xi_3 = -\frac{k}{|E|}\frac{(\mathbf{r}_{12}\mathbf{r}_{31} - \varsigma)}{\pi_2}. \tag{41}$$

In the case of an elliptic problem (steady state flow with sink/source terms), Eq. (16) leads to $\varsigma = 0$. The relations (34, ..., 41) become

$$\pi_1 = \frac{(\mathbf{r}_{13}\mathbf{r}_{23})(\mathbf{r}_{12}\mathbf{r}_{32})}{4|E|^2}\tau \tag{42}$$

$$\pi_2 = \frac{(\mathbf{r}_{12}\mathbf{r}_{13})(\mathbf{r}_{13}\mathbf{r}_{23})}{4|E|^2}\tau \tag{43}$$

$$\pi_3 = \frac{(\mathbf{r}_{12}\mathbf{r}_{13})(\mathbf{r}_{12}\mathbf{r}_{32})}{4|E|^2}\tau \tag{44}$$

$$\beta_2 = \tau \tag{45}$$

$$\beta_3 = \tau \tag{46}$$

$$\xi_1 = \frac{4k|E|}{\mathbf{r}_{12}\mathbf{r}_{13}}\frac{1}{\tau} \tag{47}$$

$$\xi_2 = \frac{4k|E|}{\mathbf{r}_{23}\mathbf{r}_{21}}\frac{1}{\tau} \tag{48}$$

$$\xi_3 = \frac{4k|E|}{\mathbf{r}_{31}\mathbf{r}_{32}}\frac{1}{\tau}. \tag{49}$$

Substituting these relations in Eq. (20) leads to

$$H = \frac{\tau}{4|E|^2}(TP_1(\mathbf{r}_{13}\mathbf{r}_{23})(\mathbf{r}_{12}\mathbf{r}_{32}) + TP_2(\mathbf{r}_{12}\mathbf{r}_{13})(\mathbf{r}_{13}\mathbf{r}_{23}) + TP_3(\mathbf{r}_{12}\mathbf{r}_{13})(\mathbf{r}_{12}\mathbf{r}_{32})). \tag{50}$$

This relation shows that H is the linear interpolate of the three (edge) potential heads at the circumcentre of the cell, whatever its location (inside or outside the triangle). In the case of steady state flow if we take τ constant and equal to 1, these results are in agreement with those obtained by Cordes and Kinzelbach [10], where sink/source terms are zero. In this restrictive case, where the physical head also varies linearly in the element, H can be interpreted as the head at the circumcentre of the cell.

3.1. *The MFE Method with One Unknown per Element*

In this part we present the construction of the final system to solve with one unknown (H) per cell. We show that unlike the usual MFE method, the new formulation does not lead to a symmetric matrix in all cases.

Let us consider an element A with its three adjacent elements (Fig. 2), The mass balance equation for this element can be written as (substituting (14) in (13))

$$L\left(1 + \frac{S}{3}\right)(Q_1 + Q_2 + Q_3) + \frac{S}{3}(TP_1 + TP_2 + TP_3) = F + SP^{n-1}. \tag{51}$$

With the new formulation, the fluxes are given by

$$Q_i = \xi_i(H - \beta_i TP_i) + \gamma_i.$$

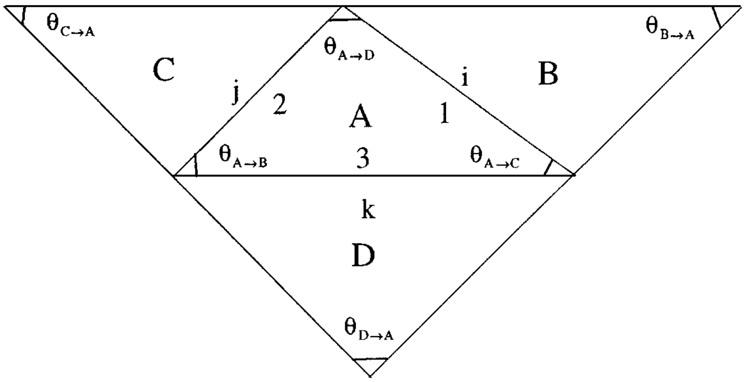

FIG. 2. Notation of edges and adjacent elements for the new formulation of the MFE method.

Substituting this last relation in Eq. (51) leads to

$$\left(1+\frac{S}{3}\right)\left(\sum_{i=1}^{3}\xi_i\right)H+\sum_{i=1}^{3}\left\{\frac{S}{3L}-\left(1+\frac{S}{3}\right)\xi_i\beta_i\right\}TP_i+\left(1+\frac{S}{3}\right)\sum_{i=1}^{3}\gamma_i=\frac{F}{L}+\frac{S}{L}P^{n-1}. \tag{52}$$

If we note $\lambda=(1+\frac{S}{3})\sum_{i=1}^{3}\xi_i$ and $\lambda_i=\{S/3L-(1+S/3)\xi_i\beta_i\}$, Eq. (52) becomes

$$\lambda H+\sum_{i=1}^{3}\lambda_i TP_i=\frac{F}{L}+\frac{S}{L}P^{n-1}+(3+S)\frac{kb}{|E|}=0. \tag{53}$$

Introducing the reference to element A in the notations by an index leads to

$$\lambda^A H^A+\lambda_1^A TP_1^A+\lambda_2^A TP_2^A+\lambda_3^A TP_3^A=0. \tag{54}$$

For this element if we define $b_i^A=\xi_i^A\beta_i^A$ and $\chi^A=-\frac{k^A}{|A|}b^A$, the fluxes across the element edges are

$$Q_i^A=\xi_i^A H_A-b_i^A TP_i^A+\chi^A. \tag{55}$$

In order to construct the final system to solve, we use the two properties of continuity between two adjacent elements A and B (Fig. 2):

The continuity of fluxes between two adjacent elements A and B is

$$Q_1^A+Q_i^B=0; \tag{56}$$

using (55) it leads to

$$\xi_1^A H^A-b_1^A TP_1^A+\chi^A+\xi_i^B H^B-b_i^B TP_i^B+\chi^B=0. \tag{57}$$

The continuity of piezometric head between two adjacent elements A and B,

$$TP_1^A=TP_i^B \tag{58}$$

which gives

$$TP_1^A = TP_i^B = \frac{\xi_1^A H^A + \xi_i^B H^B + \chi^A + \chi^B}{b_1^A + b_i^B}. \tag{59}$$

If we denote: $b_{AB} = b_1^A + b_i^B$, $b_{AC} = b_2^A + b_j^C$, and $b_{AD} = b_3^A + b_k^D$, substitution of Eq. (59) in (54) leads to the final system to solve

$$\begin{aligned} &H^A\left(\lambda^A + \frac{\lambda_1^A \xi_1^A}{b_{AB}} + \frac{\lambda_2^A \xi_2^A}{b_{AC}} + \frac{\lambda_3^A \xi_3^A}{b_{AD}}\right) + \left(\frac{\lambda_1^A \xi_i^B}{b_{AB}}\right) H^B + \left(\frac{\lambda_2^A \xi_j^C}{b_{AC}}\right) H^C + \left(\frac{\lambda_3^A \xi_k^D}{b_{AD}}\right) H^D \\ &\quad = -\lambda_1^A\left(\frac{\chi^A + \chi^B}{b_{AB}}\right) - \lambda_2^A\left(\frac{\chi^A + \chi^C}{b_{AC}}\right) - \lambda_3^A\left(\frac{\chi^A + \chi^D}{b_{AD}}\right). \end{aligned} \tag{60}$$

The solution H of Eq. (60) is proportional to τ. But the state variable on the edge (defined by Eq. (59)) is independent of τ (ξ_i^E (resp. β_i^E), being proportional to $1/\tau$ (resp. τ)).

The matrix associated to the system of Eqs. (60) is symmetric if

$$\frac{\lambda_1^A \xi_i^B}{b_{AB}} = \frac{\lambda_i^B \xi_1^A}{b_{BA}} \quad \text{or} \quad \frac{\left(\frac{S^A}{3L^A} - \left(1 + \frac{S^A}{3}\right)\beta_1^A \xi_1^A\right)\xi_i^B}{b_1^A + b_i^B} = \frac{\left(\frac{S^B}{3L^B} - \left(1 + \frac{S^B}{3}\right)\beta_i^B \xi_i^B\right)\xi_1^A}{b_1^A + b_i^B}. \tag{61}$$

Therefore, for an elliptic problem ($S=0$, $\beta=\tau$), the new formulation (60) leads to the resolution of a symmetric system if the parameter τ is constant over the domain. For the transient flow, the new formulation leads to an unsymmetric system for any kind of triangulation.

Like with standard MFE, the average head in the element is obtained by a local equation using Eqs. (59) and (14)

$$\begin{aligned} P^n = \frac{1}{S+3}\Bigg(&\frac{\xi_1^A H^A + \xi_i^B H^B + \chi^A + \chi^B}{b_{AB}} + \frac{\xi_2^A H^A + \xi_j^C H^C + \chi^A + \chi^C}{b_{AC}} \\ &+ \frac{\xi_3^A H^A + \xi_k^D H^D + \chi^A + \chi^D}{b_{AD}} + F + SP^{n-1}\Bigg). \end{aligned} \tag{62}$$

When we substitute Eq. (59) in (55), we obtain a relation which gives the flux between two adjacent elements A and B, functions of H_A and H_B for the general case (steady state, transient flow with or without sink source term)

$$Q_1^A = \xi_1^A H^A - b_1^A\left(\frac{\xi_1^A H^A + \xi_i^B H^B + \chi^A + \chi^B}{b_1^A + b_i^B}\right) + \chi^A. \tag{63}$$

3.2. *Imposing Boundary Conditions on Edges*

With the system (60) we have just one unknown H per element. In the case of steady state flow without sink/source terms, we have seen that H can be understood as the head at the circumcentre of the element. In order to impose boundary conditions, modelers usually add a layer of very thin cells. Indeed at the head boundary, elements with a right angle can be added to apply a head value directly at the center of each boundary edge [10].

But in the case of steady state flow with sink/source terms or transient flow, the piezometric head does not vary linearly anymore in the element and, therefore, H does not represent the head at the circumcentre of the cell.

We construct the approximation of the boundary condition with the help of the mixed formulation. Indeed, we derive equations with Dirichlet or Neumann boundary conditions on the edges.

If we assume a Dirichlet boundary condition on edge 2, for example, of element A, Eq. (60) must be replaced by

$$H^A\left(\lambda^A + \frac{\lambda_1^A \xi_1^A}{b_{AB}} + \frac{\lambda_3^A \xi_3^A}{b_{AD}}\right) + \left(\frac{\lambda_1^A \xi_i^B}{b_{AB}}\right) H^B + \left(\frac{\lambda_3^A \xi_k^D}{b_{AD}}\right) H^D$$
$$= -\lambda_1^A\left(\frac{\chi^A + \chi^B}{b_{AB}}\right) - \lambda_2^A T P_2 - \lambda_3^A\left(\frac{\chi^A + \chi^D}{b_{AD}}\right). \tag{64}$$

If we assume now that we have a Neumann boundary condition on edge 2 of element A, then Eq. (60) must be replaced by

$$H^A\left(\lambda^A + \frac{\lambda_1^A \xi_1^A}{b_{AB}} + \frac{\lambda_2^A \xi_2^A}{b_2^A} + \frac{\lambda_3^A \xi_3^A}{b_{AD}}\right) + \left(\frac{\lambda_1^A \xi_i^B}{b_{AB}}\right) H^B + \left(\frac{\lambda_3^A \xi_k^D}{b_{AD}}\right) H^D$$
$$= -\lambda_1^A\left(\frac{\chi^A + \chi^B}{b_{AB}}\right) - \lambda_2^A\left(\frac{\chi^A + Q_2}{b_2^A}\right) - \lambda_3^A\left(\frac{\chi^A + \chi^D}{b_{AD}}\right). \tag{65}$$

4. THE NEW FORMULATION VERSUS FV AND FD METHODS

In the following we present some comments about the MFE approximation.

In the case of a steady state flow field with no sink/source terms, the velocity vector is constant; hence the potential head varies linearly inside each element and H may be interpreted as the potential head located at the circumcentre of the element. We notice a complete analogy between the MFE and FV methods which gives us a new perception of the FV method. The new variable H is not the average potential head on the element but it allows us to calculate the average potential heads on edges, fluxes on edges, and the average potential head on the element. Therefore, one can impose boundary conditions on the edges and the circumcentre may be even located outside the element. A misinterpretation of the significance of H can be at the origin of wrong statements. If a rhombus is divided into two triangles by its longer diagonal, the circumcentres lie outside of their respective elements (Fig. 3). By setting $\tau = 1$ and simplifying Eq. (60), the flux across the common edge of two arbitrarily shaped elements can be expressed by

$$Q_{AB} = L_{23}\frac{H_A - H_B}{\frac{L_A}{k_A} + \frac{L_B}{k_B}}, \tag{66}$$

where L_{23} is the length of the common edge 23,

$$L_A = L_{23}\frac{\mathbf{r}_{12}\mathbf{r}_{13}}{4|E_A|} \quad \text{and} \quad L_B = L_{23}\frac{\mathbf{r}_{42}\mathbf{r}_{43}}{4|E_B|},$$

$|E_A|$ (resp. $|E_B|$) is the area of the element A (resp. B), $\mathbf{r}_{ij}$ is the vector ij, and k_A (resp. k_B) is the hydraulic conductivity of the element A (resp. B)). In the present case, L_A and L_B in Eq. (66) become negative.

If we consider a flow from cell A to cell B, the flux Q_{AB} from the element A to the element B is positive and the average head on A is greater than the average head on B. One could

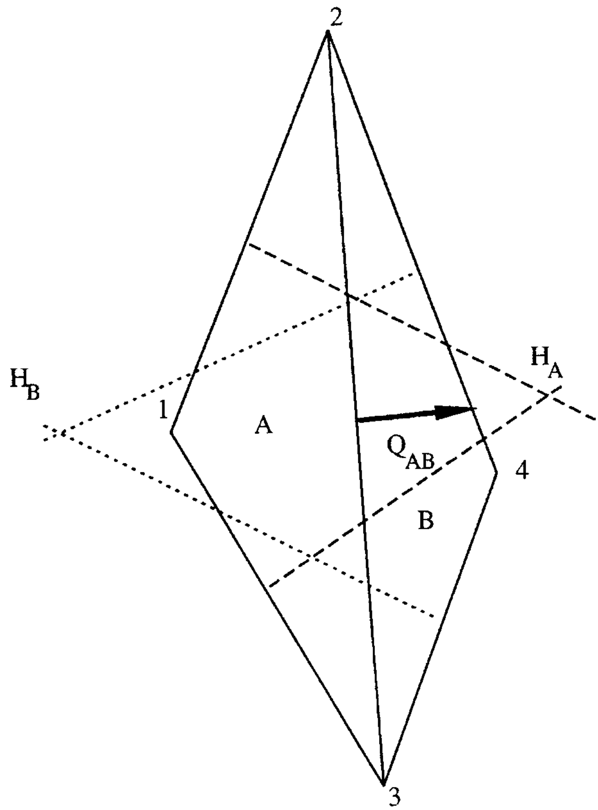

FIG. 3. Calculation of the flux in the case of a rhombus divided into triangles.

interpret this by $H_A > H_B$ and Eq. (66) gives in that case a negative flux Q_{AB}, i.e. a flow from B toward A. Furthermore, one could explain this with local minima and maxima in the head field and nonphysical orientation of fluxes and velocities. In fact there is no nonphysical orientation of fluxes because H_A and H_B are located outside their corresponding cells (at the circumcentres) and are not the average potential head inside their corresponding elements (Fig. 3). From a mathematical point of view, the triangular FV method does not require Delaunay triangulation. The average potential head over each element has to be calculated from values at the circumcentres using Eq. (62). When triangulation is obtained by subdivision of rectangles, the MFE method is equal to the FD method because H corresponds to the potential head at the circumcentre of each element of the rectangle which corresponds to the potential head in the center of the rectangle.

In the case of steady state flow field with sink/source terms, the velocity vector is not constant any longer. Unlike the FV method, the contribution of sink/source terms of the neighboring elements in the expression of fluxes is taken into account with the new formulation (χ^A and χ^B in Eq. (60)). In the case of transient flow, H is just the unknown cell and it cannot be interpreted as the average potential head in the element or the potential head at the circumcentre of the element.

We focus now on the equivalence between the new formulation and block-centered finite differences when the triangulation is obtained by subdivision of rectangular elements. In the case of steady state flow ($\varsigma = 0$), with or without sink source terms, we cannot define all relations (42) $\cdots$ (49), because we have $\mathbf{r}_{ij}\mathbf{r}_{ik}$ equal to zero. If the triangle of Fig. 1 has

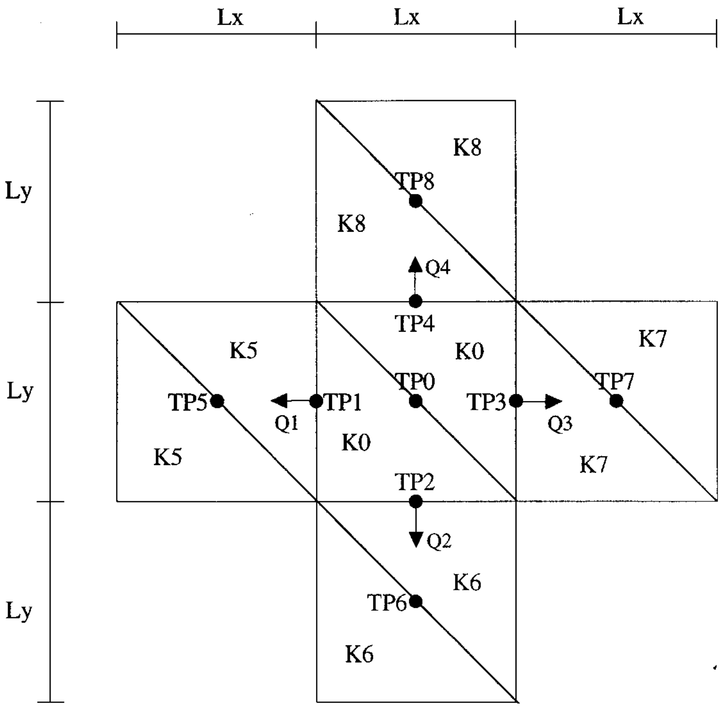

FIG. 4. Rectangular mesh subdivided into triangles.

a right angle at node 3 ($\mathbf{r}_{31}\mathbf{r}_{32} = 0$) and Eq. (18) leads to

$$\begin{aligned} Q_1 &= -\frac{k}{|E|}[r_{23}r_{23}TP_1 + r_{23}r_{12}TP_3 + b] = -\frac{k}{|E|}[r_{23}r_{23}(TP_1 - TP_3) + b] \\ Q_2 &= -\frac{k}{|E|}[r_{31}r_{31}TP_2 + r_{12}r_{31}TP_3 + b] = \frac{k}{|E|}[r_{31}r_{31}(TP_2 - TP_3) + b]. \end{aligned} \tag{67}$$

When the triangulation is obtained by subdivision of rectangular elements (Fig. 4) with a constant hydraulic conductivity k in each rectangle and a accumulation term Q_{s0} in each rectangle equally distributed ($Q_{s0}/2$ for each triangle), the previous relations (67) become

$$\begin{aligned} Q_1 &= -2k_0\frac{L_y}{L_x}[TP_1 - TP_0] + \frac{Q_{s0}}{6} \\ Q_2 &= -2k_0\frac{L_x}{L_y}[TP_2 - TP_0] + \frac{Q_{s0}}{6}. \end{aligned} \tag{68}$$

It is obvious that for this case the new variable H is equal to TP_0. By using the same approach as in Section 3.1, we can formulate the problem in order to find a final system of unknowns for the average head on the diagonals. This system is obviously the size of the number of rectangles.

In the case of steady state flow without sink source terms, this formulation is equal to the block-centred finite difference discretization. However, in the case of steady state flow with sink source terms, [14] stated that the two formulations were similar. We show that the mixed and block-centred finite difference discretizations are different.

The mass balance equation using the block-centered finite difference discretization leads to

$$-2\frac{L_y}{L_x}\frac{1}{\left(\frac{1}{k_0}+\frac{1}{k_5}\right)}[TP_5-TP_0]-2\frac{L_x}{L_y}\frac{1}{\left(\frac{1}{k_0}+\frac{1}{k_6}\right)}[TP_6-TP_0]$$
$$-2\frac{L_y}{L_x}\frac{1}{\left(\frac{1}{k_0}+\frac{1}{k_7}\right)}[TP_7-TP_0]-2\frac{L_x}{L_y}\frac{1}{\left(\frac{1}{k_0}+\frac{1}{k_8}\right)}[TP_8-TP_0]=Q_{s0}. \quad (69)$$

Using continuity of fluxes and the piezometric head between two adjacent elements, the MFE method leads to

$$-2\frac{L_y}{L_x}\frac{1}{\left(\frac{1}{k_0}+\frac{1}{k_5}\right)}[TP_5-TP_0]-2\frac{L_x}{L_y}\frac{1}{\left(\frac{1}{k_0}+\frac{1}{k_6}\right)}[TP_6-TP_0]$$
$$-2\frac{L_y}{L_x}\frac{1}{\left(\frac{1}{k_0}+\frac{1}{k_7}\right)}[TP_7-TP_0]-2\frac{L_x}{L_y}\frac{1}{\left(\frac{1}{k_0}+\frac{1}{k_8}\right)}[TP_8-TP_0]$$
$$=Q_{s0}+\frac{Q_{s0}k_5-k_0Q_{s5}}{6(k_5+k_0)}+\frac{Q_{s0}k_6-k_0Q_{s6}}{6(k_6+k_0)}+\frac{Q_{s0}k_7-k_0Q_{s7}}{6(k_7+k_0)}+\frac{Q_{s0}k_8-k_0Q_{s8}}{6(k_8+k_0)}. \quad (70)$$

This equation is different from the earlier one (69) obtained with the block-centred finite difference method. With the MFE method the right-hand term of this equation represents the contribution of the sink/source term, not only from the element but also from all adjacent elements weighted with hydraulic conductivity. For transient flow or steady state flow with sink/source terms, the head variation inside the element is no longer linear. Therefore, an additional term appears in the calculation of the fluxes (Eq. (18)) which leads to the additional sink/source terms in Eq. (70). Of course, one could use (69), instead of (70), for steady state flow with sink/source terms or transient flow. However, there is no equivalence between (69) and standard MFE method.

In the case of transient flow, there is no correspondence between FD and MFE methods since H is defined by triangular element.

5. NUMERICAL EXPERIMENTS

We have seen previously that we can formulate the MFE method in order to solve the problem for only one unknown H per element for both steady state and transient flow. The final system is given by Eq. (60) written for each element. For a general triangulation, this system leads to a symmetric matrix for steady-state flow with or without sink source terms. For transient flow, the system (60) leads to an unsymmetric matrix. However, no idea is available about the computational effort required for the new formulation in comparison with the usual MFE method. With the new formulation, the number of unknowns is reduced (the number of elements, instead of the number of edges), but the computational effort depends, not only on the number of unknowns, but also on the sparseness and on the positive definiteness of the matrix which can be affected by the kind of triangulation used.

The last part of this paper is aimed at a comparison of the computational effort with the new formulation and the MFE method for different triangulations. Chavent *et al.* [16] show that, in the case an elliptic problem, the matrix obtained with the new formulation is positive definite, if and only if, for each element A with its three adjacent elements (Fig. 2) we have

$$\frac{2}{\frac{\cot g\theta_{A\to B}}{k_A}+\frac{\cot g\theta_{B\to A}}{k_B}}+\frac{2}{\frac{\cot g\theta_{A\to C}}{k_A}+\frac{\cot g\theta_{C\to A}}{k_C}}+\frac{2}{\frac{\cot g\theta_{A\to D}}{k_A}+\frac{\cot g\theta_{D\to A}}{k_D}}>0, \tag{71}$$

where $\theta_{A\to B}$ is the angle of the element A face to the element B (Fig. 2).

If we assume a Dirichlet boundary condition on edge 2 of element A, then Eq. (71) must be replaced by

$$\frac{2}{\frac{\cot g\theta_{A\to B}}{k_A}+\frac{\cot g\theta_{B\to A}}{k_B}}+\frac{2}{\frac{\cot g\theta_{A\to C}}{k_A}+\frac{\cot g\theta_{C\to A}}{k_C}}+\frac{2}{\frac{\cot g\theta_{A\to D}}{k_A}}>0, \tag{72}$$

where $\theta_{A\to bc}$ is the angle face to the Dirichlet edge.

These two criteria depend not only on the spatial discretisation but also on the distribution of the conductivity in the domain. In the case of homogenous porous media, if we verify the Delaunay criteria, we verify necessarily the criteria (71) and (72). These results cannot be extended to the parabolic problem.

Five-domain discretizations will be studied. The first mesh (Fig. 5a) is composed of only equilateral triangles; in the second one (Fig. 5b) we have equilateral elements with some deformed triangles. In the third mesh (Fig. 5c) all triangles present angles very close to $\pi/2$. The fourth mesh (Fig. 5d) presents some triangles with angles greater than $\pi/2$. The last mesh (Fig. 5e) is similar to the third mesh (Fig. 5c) but all triangles present angles greater than $\pi/2$. For the meshes (a), (b), and (c), all angles are strictly less than $\pi/2$; criteria (71) and (72) are verified and the system obtained with the H solution is therefore positive definite.

The five heterogeneous domains are presented with their corresponding meshes in Fig. 5. The boundary conditions for these domains are similar; a constant head (100 m) is imposed at the top and the bottom and a sink term (with a rate of $-100\,\mathrm{m}^3/\mathrm{d}$) is localized in the center of the domain. Their thickness is 1 m.

Both steady-state and transient flow (with a storativity coefficient $s = 0.2\,\mathrm{m}^{-1}$) will be studied. The CPU time will be assessed at various levels of refinement for the different domains. To refine a mesh, each element is divided into four elements by joining the three edge midpoints. In this way, the resulting meshes have the same properties as the previous one.

To solve the symmetric steady state flow equations, we use the *preconditioned conjugate gradient* method. For the unsymmetric transient flow equations, we use the *preconditioned biconjugate gradient stabilised* method [15].

For steady state flow with sink/source terms, Table I gives the CPU time (on a Digital PW 600 workstation), condition number, and the number of iterations to reach solver convergence versus the number of unknowns corresponding to each mesh. Since the MFE method uses 1.5 times more unknowns than the new formulation, this last one requires 45 to 50% less CPU time than the classical MFE formulation. For the third mesh composed of triangles having angles very close to $\pi/2$, the calculations are still in favor of the new formulation since the mesh verifies (71) and (72).

For mesh (d), we have a triangular element with a Dirichlet edge with an angle greater than $\pi/2$ (Fig. 6) which does not verify the criterion (72). In this case the matrix obtained with the H solution is not positive definite. It is well known that in this case the solution of the system is difficult and time consuming even with specific solvers. The same kind of results are obtained for the mesh in Fig. 5e.

Table II gives the CPU time and the number of iterations for the solver to reach convergence for the unsteady state flow. In this case, the following conclusions can be drawn.

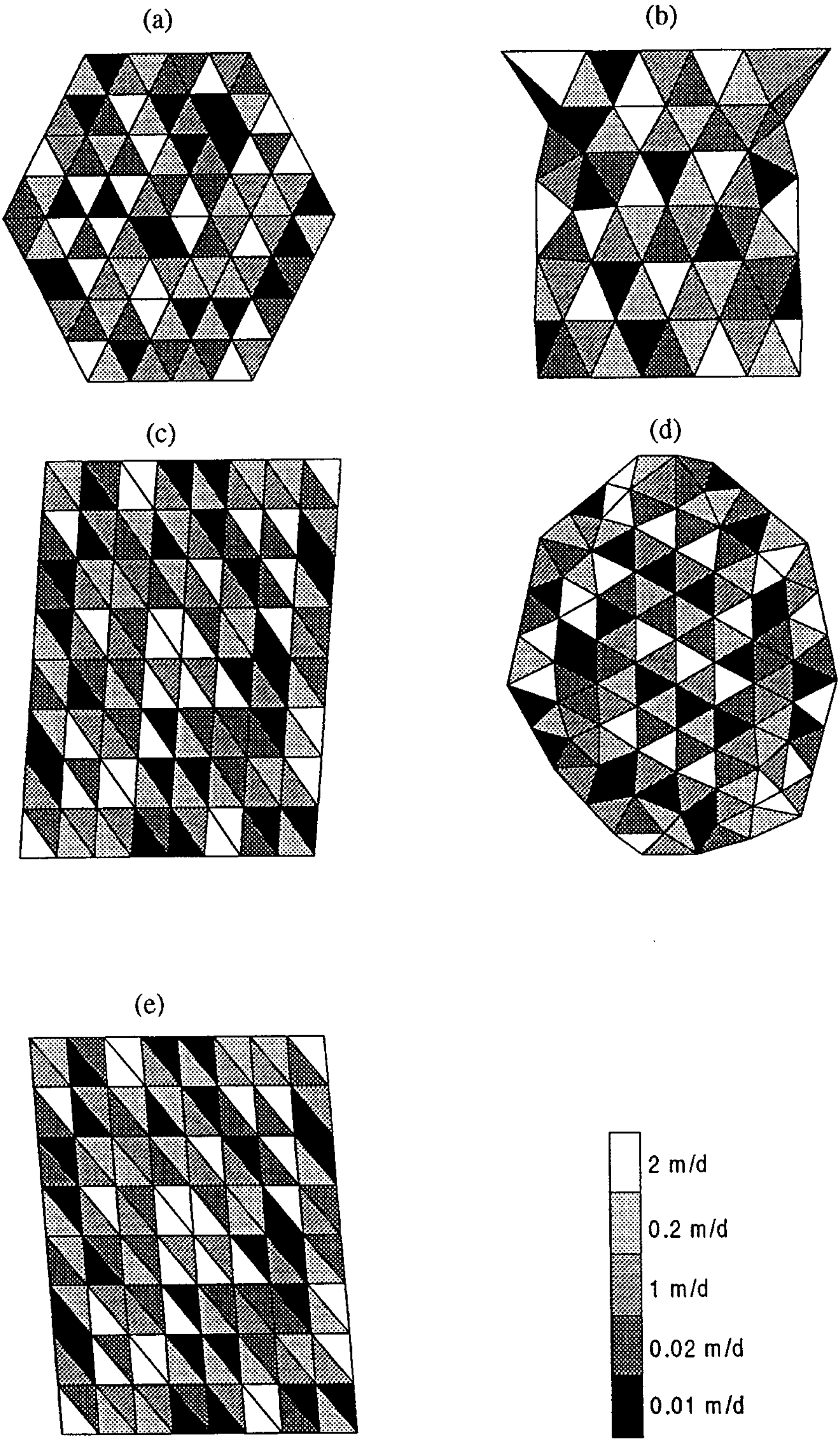

FIG. 5. Mesh and distribution of conductivity for each domain.

TABLE I

Steady State Flow with Sink/Source Terms: CPU Time, Condition Number and Iterations Number versus the Number of Unknowns for Each Mesh

	MFE				H resolution				
Mesh	Unkn	CPU	Nb iter	Condition	Unkn	CPU	Nb iter	Condition	Matrix
(a)	156	0.014	104	17042	96	0.006	54	9185	Pos. def
	600	0.045	176	53540	384	0.02	140	41518	Pos. def
	2362	0.38	364	171182	1536	0.19	318	156634	Pos. def
	9312	4.65	713	—	6144	2.41	685	—	Pos. def
(b)	106	0.011	62	2005	64	0.006	32	2777	Pos. def
	404	0.018	97	9197	256	0.014	80	17603	Pos. def
	1576	0.146	223	33229	1024	0.08	190	62338	Pos. def
	6224	2.11	487	—	4096	1.05	396	—	Pos. def
(c)	208	0.014	94	10840	128	0.009	58	19405	Pos. def
	800	0.052	175	35201	512	0.035	166	62263	Pos. def
	3136	0.56	389	118706	2048	0.32	376	211983	Pos. def
	12416	6.73	787	—	8192	3.37	775	—	Pos. def
(d)	200	0.016	56	1097	125	0.014	56	3667	Indefinite
	775	0.08	256	108322	500	0.1	535	1659733	Indefinite
	3050	0.73	516	3788620	2000	3.13	3997	5463773	Indefinite
	12100	10.5	1250	—	8000	197.52	47208	—	Indefinite
(e)	208	0.015	134	11415	128	0.02	355	18421	Indefinite
	800	0.08	262	37143	512	0.96	5483	56067	Indefinite
	3136	0.6	425	125212	2048	17.01	21284	187516	Indefinite
	12416	7.36	871	—	8192	[a]	50000	—	Indefinite

[a] Convergence not reached after 50000 iterations.

TABLE II

Transient Flow with Sink/Source Terms: CPU Time, and Iterations Number versus the Number of Unknowns for Each Mesh

	MFE			H resolution			
Mesh	Unkn	CPU	Nb iter.	Unkn	CPU	Nb iter	Matrix
(a)	156	0.007	57	96	0.001	28	Pos. def
	600	0.027	95	384	0.018	72	Pos. def
	2362	0.2	192	1536	0.18	149	Pos. def
	9312	2.54	389	6144	1.78	323	Pos. def
(b)	106	0.008	16	64	0.001	10	Indefinite
	404	0.01	27	256	0.007	40	Indefinite
	1576	0.046	56	1024	0.77	1139	Indefinite
	6224	0.52	117	4096	2.31	655	Indefinite
(c)	208	0.01	32	128	0.007	82	Indefinite
	800	0.025	54	512	0.53	1725	Indefinite
	3136	0.16	108	2048	2.52	1594	Indefinite
	12416	1.9	223	8192	[a]	50000	Indefinite
(d)	200	0.01	30	125	0.002	19	Indefinite
	775	0.023	58	500	0.09	276	Indefinite
	3050	0.2	138	2000	75	49434	Indefinite
	12100	2.44	287	8000	[a]	50000	Indefinite
(e)	208	0.008	36	128	0.01	132	Indefinite
	800	0.026	62	512	[a]	50000	Indefinite
	3136	0.18	119	2048	[a]	50000	Indefinite
	12416	2.14	250	8192	[a]	50000	Indefinite

[a] Convergence not reached after 50000 iterations.

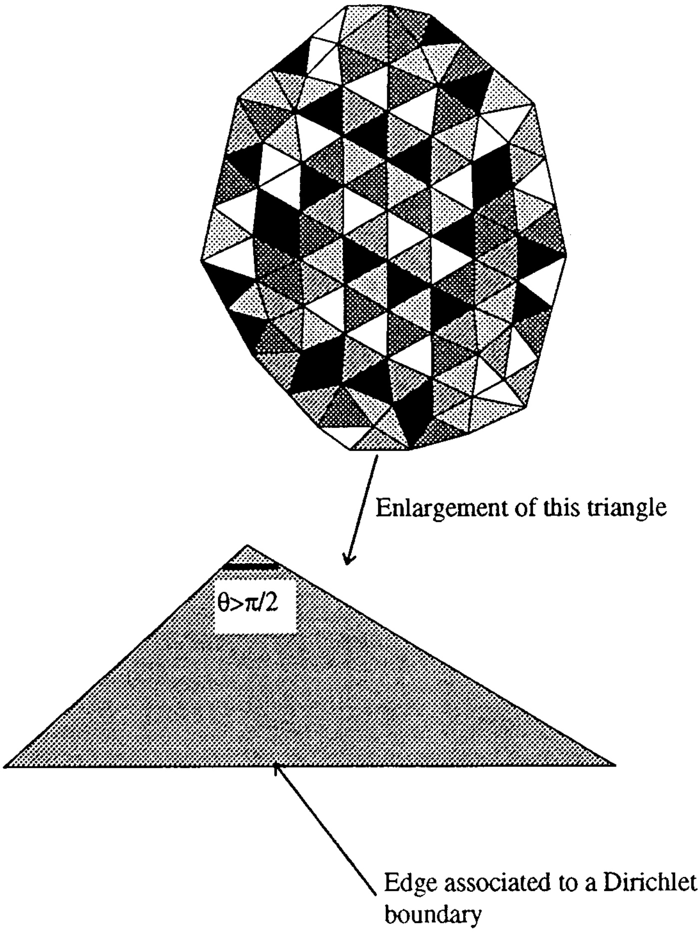

FIG. 6. Triangular element with an edge associated with a Dirichlet boundary and with an angle greater then $\pi/2$.

For the mesh in Fig. 5a, although the matrix is not symmetric but positive definite, the calculation is still in favor of the new formulation. For more general triangulation (meshes in Figs. 5b–5e), the new formulation gives an unsymmetric and not a positive definite matrix. CPU time is of course not favored for the algorithm presented here. An alternative to the "inversion" of an unsymmetric and indefinite matrix is to solve the normal form of the system (i.e. $({}^tA \cdot A)H = {}^tA \cdot B$) and, therefore, to obtain a symmetric, positive definite form of the system. But the normal matrix ${}^tA \cdot A$ is dense, in comparison with the matrix obtained by the usual MFE approximation. The convergence becomes slow, since the condition number of the normal equations matrix is less favorable than the condition number of the original matrix. For example, for the mesh (d) with 12,100 unknowns, the MFE approximation requires 2.44 s of CPU time and 287 iterations. With the new formulation, we could not converge without the use of the normal form of the system. This form of the new formulation requires 43.54 s of CPU time and 7792 iterations which are huge numbers, in comparison with those referring to the original MFE system.

6. CONCLUSION

The aim of this work was to obtain a new formulation of the MFE approximation in order to decrease the number of unknowns and to understand connections between the MFE, FV, and FD methods. We have shown how to build such a form of the mixed approximation and this without any simplification for the general problem (steady or transient flow, with or without sink/source terms). The number of unknowns with the new algorithm is now the number of elements, instead of the number of edges. A new variable is defined by a linear combination of the average head on element edges and a parameter denoted τ. The choice of this parameter has no impact on the calculation of the average head on element edges, on the average head inside the element, nor on the fluxes across element edges. The new formulation can indeed be seen as a general formulation equivalent to the FV or the FD methods in some particular cases.

This shows that, from a mathematical point of view, the FV method can be applied for whatever triangulation (circumcentre not necessarily inside the element). However, the final system can lead to a nonpositive definite matrix.

In the case of steady state flow with no sinks or sources, the new formulation is equivalent to the FV method which was already mentioned by some other authors.

In the case of steady state flow with sink/source terms or transient flow, there is no longer equivalence between MFE and FV or FD methods. The new formulation for an elliptic partial differential equation leads to the resolution of a symmetric matrix. This matrix is always positive definite if the inner angle of each element is less than $\pi/2$. For an arbitrary triangulation, the matrix can still be positive definite, depending on the hydraulic conductivity. For a positive definite matrix, the new formulation is very attractive in terms of CPU costs.

For transient flow, the new formulation leads to the resolution of an indefinite unsymmetric system for a general triangulation. In that case, the standard MFE approximation is preferable, because it leads to a symmetric positive definite matrix.

The extension of the new formulation to 3D elliptic problems is an ongoing work. It is an interesting challenge due to strong reduction of the number of unknowns.

ACKNOWLEDGMENTS

The helpful comments and the relevant questions of the anonymous reviewers are acknowledged. Funding for this work was provided by the French National Research Centre (CNRS).

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