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A robust fully Mixed Finite Element model for flow and transport in unsaturated fractured porous media Anis Younes<sup>1</sup>, Hussein Hoteit<sup>2</sup>, Rainer Helmig<sup>3</sup>, Marwan Fahs<sup>1</sup> <sup>1</sup>ITES, University of Strasbourg, CNRS, ENGEES, 67000, Strasbourg, France. <sup>2</sup> Physical Science and Engineering Division, King Abdullah University of Science and Technology (KAUST), 13 Thuwal, Saudi Arabia <sup>3</sup> Institute for Modelling Hydraulic and Environmental Systems, University of Stuttgart, Pfaffenwaldring 61, 70569 Stuttgart, Germany 21 23 24 25 26 27 28 29 Submitted to Advances in Water Resources Contact author: Marwan Fahs E-mail: fahs@unistra.fr 

# Abstract

A fully mixed finite element (MFE) model is developed for nonlinear flow and transport in
unsaturated fractured porous media with matrix-fracture and fracture-fracture fluid and mass
exchanges. The model is based on the discrete fracture matrix (DFM) approach and assumes
cross-flow equilibrium in the fractures. The MFE method is employed for the spatial
discretization of both flow and transport on the 2D-matrix elements as well as on the 1D-
fracture elements. An upwind scheme is employed to avoid unphysical oscillations in the case
of advection dominant transport. The temporal discretization is performed using high-order
time integration methods and efficient automatic time-stepping schemes via the MOL.
Two test problems dealing with flow and mass transport in saturated and unsaturated fractured
porous media are simulated to show the validity of the new model by comparison against (i) a
1D-2D Comsol finite element model and (ii) a 2D-2D Discontinuous Galerkin (DG) model
where both fractures and matrix continua are discretized with small 2D mesh elements. The
robustness and efficiency of the developed 1D-2D MFE model are then investigated for a
challenging problem dealing with infiltration of contaminated water into an initially dry soil
involving a fracture network.
The new model yields stable results for advection-dominated and advection-dispersion
transport configurations. Further, the results of the 1D-2D MFE model are in very good
agreement with those of the 2D-2D DG model for both configurations. The simulation of
infiltration of contaminated water into a dry fractured soil shows that the 1D-2D MFE model
is within 15 times more efficient than the 2D-2D DG model, which confirms the high benefit
of using robust and efficient DFM models for the simulation of flow and transport in fractured
porous media.

62 Key words:

- 63 Fractured porous media, discrete fracture matrix approach, unsaturated flow, advection-
- dispersion equation, mixed finite element, upwind scheme.

#### 1. Introduction

- 66 Flow and transport in fractured porous media are important in many applications such as
- 67 water resource management (Wireman 2003, Kavouri et al., 2017), contaminant transport
- 68 (Berkowitz, 2002; Brutz and Rajaram 2017, Klammler et al. 2016), nuclear waste
- 69 management (Follin and Stigsson 2014, Mattila and Tammisto 2012) and oil and gas
- 70 production (Li et al., 2015; Shen et al., 2016).
- 71 The flow and transport processes in fractured porous media can be significantly affected by 72 the characteristics of the fractures, such as location, size, orientation, and aperture. The 73 fractures can be empty, or contain a filling material (Berre et al., 2019). In this work, the 74 fractures are considered filled with a porous medium with different properties from the porous 75 matrix, as in Khoobor et al. (2020). Two approaches are commonly used for modeling flow in 76 fractured porous media (Berre et al., 2019). The first approach is based on an implicit 77 representation of the fractures and includes both single-continuum and multi-continuum 78 models. In single-continuum models, the fractures are taken into account by calculating an equivalent permeability of the porous medium, which depends on the properties of the 79 80 fractures and the fracture network (Durlofsky, 1991; Liu et al., 2016). In multi-continuum 81 models, the fractured porous medium is represented by two or more superimposed media with 82 their own flow and/or transport equations. Among these, the well-known dual porosity model 83 which considers superposition of a low permeability continuum representing the matrix with a 84 high permeability continuum representing the fractures (Jourde et al., 2002; Kordilla et al., 85 2012). The two continua are then linked by a linear exchange term. More sophisticated multi-86 continuum models have been developed for aquifers with high heterogeneities, such as karst

aquifers, to include different levels of porosities and cavities (Kuhlman *et al.*, 2015; Wu *et al.*, 88 2004).

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The second approach uses on an explicit representation of the fractures. Among this approach, the discrete fracture network (DFN) model. With DFN, the geometry and properties of discrete fractures are explicitly incorporated as a central component controlling flow and transport. Discrete fracture matrix (DFM) models consider that flow and transport processes occur through both, the porous matrix and the explicitly represented fractures. As a consequence, the DFM model is more appropriate for handling fractures in a permeable porous medium (Berre et al., 2019). Considering that the aperture of the fractures is small as compared to the matrix scale, the main idea of DFM is to use the cross-flow equilibrium concept across the fractures (Noorishad and Mehran, 1982; Baca et al., 1984; Granet et al., 1998; Hoteit et al., 2008). As a consequence, the fractures can be discretized with elements of co-dimension one with respect to the dimension of the surrounding matrix (Flemish et al., 2018; Martin et al., 2005), such as 1D fracture elements with 2D matrix elements. This simplification makes DFM models much more efficient than the single porosity 2D-2D model, where 2D elements are used for both matrix and fracture continua. Note that the applicability of the 2D-2D models is often hampered by their expansive computational cost since they require very fine mesh elements to correctly discretize the fractures with small apertures.

Hoteit and Firoozabadi (2005; 2006) employed DFM models assuming cross-flow equilibrium between the fractures and the adjacent matrix gridcells by imposing the pressure at a fracture and at the adjacent gridcells to be equal. Although efficient, this assumption still requires small mesh elements next to the fractures (Hoteit and Firoozabadi, 2008). To avoid this constraint, Hoteit and Firoozabadi (2008) proposed solving the flow equation with the hybrid formulation of the mixed finite element (MFE) method. This formulation has the

pressure at the gridcell interfaces as degrees of freedom (DOF), and hence, the cross-flow equilibrium can be directly assumed across the fractures (Hoteit and Firoozabadi, 2008). In this way, the matrix pressure at an element edge and the pressure at the fracture, which coincides with that edge, are assumed to be equal. As a consequence, no constraints are required for the mesh discretization near the fractures (Hoteit and Firoozabadi, 2008). This powerful feature is extended in this work by developing a fully MFE model for both unsaturated flow and transport in the porous matrix and in the fracture continuum.

The MFE (Raviart and Thomas, 1977; Chavent and Jaffré, 1986) is a robust numerical method for solving diffusion problems, which has recently received attention in geosciences. Indeed, with MFEs, the flux and the pressure unknowns are approximated simultaneously. The MFE method ensures local mass balance and can easily handle general unstructured meshes (Younes *et al.*, 2010). Further, it yields an accurate velocity field in highly heterogeneous and anisotropic media (Durlofsky, 1994). The hybridization procedure of the MFE method allows improving its efficiency by reducing the total number of unknowns and producing a final system with a positive symmetric definite matrix (Chavent and Jaffré, 1986). The unknowns, in this case, are the traces of the variable at the edges.

A lumped formulation of the MFE method has been developed by Younes *et al.* (2006) to improve the monotonicity of the solution and reduce the unphysical oscillations observed with transient problems. Belfort *et al.* (2009) showed that the lumped formulation is more efficient and more robust than the standard one for the simulation of water infiltration into initially dry soils. Further, contrarily to the standard MFE method, the lumped formulation maintains the time derivative continuous and thus, allows employment of high-order time integration methods via the method of lines (MOL), which can be very efficient for solving nonlinear problems (Fahs *et al.*, 2009 and Younes *et al.*, 2009).

Although the MFE method is well adapted for diffusion type equations, when applied for the advection-dispersion transport equation, the solution can exhibit strong unphysical oscillations because of the hyperbolic nature of the advection operator. Therefore, the main objective of this work is to develop a stable MFE model for unsaturated flow and mass transport through both the 2D-matrix and the 1D-fracture elements. Both fluid and contaminant matrix-fracture and fracture-fracture exchanges are implicitly taken into account, without using any transfer functions, even for the case of several intersecting fractures. To avoid instabilities caused by the hyperbolic advection term, we use a robust monotonic upwind MFE scheme where the traces of concentration at edges are upwinded depending on the direction of the local velocity. An implicit scheme is used for the time discretization of the flow and transport equations. This alleviates restriction on the size of the time step from the CFL condition of explicit schemes. For the sake of brevity, the lumped hybrid MFE method employed in this work will also be denoted MFE.

Modeling flow and transport in unsaturated fractured porous media is likely to be highly CPU consuming due to (i) the strongly nonlinear Richards flow equation (RE), (ii) the high contrast of permeability between the conductive fractures and the low permeable matrix and (iii) the presence of sharp wetting and/or contaminant fronts. These difficulties make the commonly used, first-order backward Euler scheme combined with the heuristic time step management, inappropriate to obtain accurate solutions in a reasonable CPU time. To overcome these difficulties, time integration is performed using high-order time integration methods via the Method of Lines (MOL). The MOL allows versatile time step length and order of the temporal discretization to reduce the computational time while maintaining accuracy. The MOL was shown to be effective for the solution of the RE in the unsaturated zone (Fahs et al, 2009; Khoobor et al., 2020) and is used hereafter for the first time for coupled flow and transport through unsaturated fractured porous media.

This article is structured as follows. In section 2, we recall the nonlinear mathematical models governing flow and advection-dispersion transport processes in unsaturated porous media. In section 3, we develop a robust fully MFE formulation for the solution of flow and transport both in the porous matrix and in the fracture continuum. In section 4, numerical experiments are performed for flow and transport in saturated and unsaturated fractured porous media to investigate the validity and robustness of the new 1D-2D MFE model. Some conclusions are given in the last section of the article.

#### 2. Governing Equations

The porous matrix is assumed permeable, and the fractures are infilled by a porous medium whose physical characteristics are different from those of the porous matrix. Flow in variably saturated porous media, both in the matrix and through the fractures, is assumed to be ruled by the mass conservation of the fluid:

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$$\frac{\partial \theta}{\partial t} = \left(c(h) + S_S \frac{\theta}{\theta_S}\right) \frac{\partial H}{\partial t} = -\nabla \cdot \boldsymbol{q} = 0 \tag{1}$$

and the Darcy-Buckingham law:

$$q = -k_r K \nabla H \tag{2}$$

where  $c(h) = \partial \theta/\partial h$  is the specific moisture capacity  $[L^{-1}]$ ,  $S_s$  is the specific mass storativity related to head changes  $[L^{-1}]$ ,  $\theta$  is the current water content  $[L^3L^{-3}]$ ,  $\theta_s$  is the saturated water content  $[L^3L^{-3}]$ , H = h + y is the freshwater head [L], h is the pressure head [L], y is the upward vertical coordinate [L], t is the time [T], q is the Darcy velocity  $[LT^{-1}]$ ,  $k_r$  is the relative conductivity [-],  $K = \frac{\rho g}{\mu} k$  is the hydraulic conductivity tensor  $[LT^{-1}]$ ,  $\rho$  is the fluid

- density [ML<sup>-3</sup>], g is the gravity acceleration [LT<sup>-2</sup>],  $\mu$  is the fluid dynamic viscosity [ML<sup>-1</sup>T<sup>-1</sup>
- 182  $^{1}$ ] and k is the permeability of the rock matrix as a tensor, or that of the fracture, as a scalar
- 183  $[L^2]$ .
- The transport of contaminants in the unsaturated porous matrix and through the unsaturated
- fractures is ruled by the advection-dispersion equation:

186 
$$\frac{\partial (\theta C)}{\partial t} + \nabla \cdot (\mathbf{q}C) - \nabla \cdot (\mathbf{D}\nabla C) = 0$$
 (3)

where C [-] is the relative concentration [-] and D is the dispersion tensor given by:

188 
$$\mathbf{D} = D_{m} \mathbf{I} + (\alpha_{L} - \alpha_{T}) \mathbf{q} \otimes \mathbf{q} / |\mathbf{q}| + \alpha_{T} |\mathbf{q}| \mathbf{I}$$
 (4)

- In which  $\alpha_L$  and  $\alpha_T$  are the longitudinal and transverse dispersivities [L],  $D_m$  is the pore
- water diffusion coefficient [ $L^2T^{-1}$ ] and I is the unit tensor.
- 191 The standard van Genuchten (van Genuchten, 1980) model is used for the relationship
- between water content and pressure head:

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$$S_{e} = \frac{\theta(h) - \theta_{r}}{\theta_{s} - \theta_{r}} = \begin{cases} \frac{1}{\left(1 + \left|\alpha h\right|^{n}\right)^{m}} & h < 0\\ 1 & h \ge 0 \end{cases}$$
 (5)

- where  $\alpha$  [L<sup>-1</sup>] and n [-] are the van Genuchten parameters, m=1-1/n,  $S_e$  is the effective
- saturation [-], and  $\theta_r$  is the residual water content [L<sup>3</sup>L<sup>-3</sup>].
- 196 The conductivity-saturation relationship is analytically expressed from the Mualem (Mualem,
- 197 1976) model,

198 
$$k_r = S_e^{1/2} \left[ 1 - \left( 1 - S_e^{1/m} \right)^m \right]^2 \tag{6}$$

The nonlinear system (1)-(6) is solved numerically on (*i*) unstructured triangular 2D elements for the porous matrix and (*ii*) linear 1D elements for fracture branches. All hydraulic and transport parameters in the system (1)-(6) are defined elementwise, and therefore, they can be different for each matrix or fracture element.

## 3. The fully MFE numerical model

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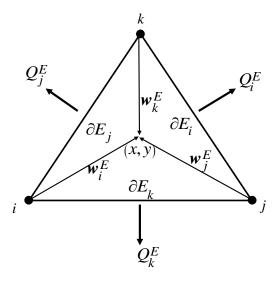
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- In this session, we recall the main stages for developing a robust MFE formulation for the solution of the flow and transport equations both in the porous matrix and in the fractures.
- 206 3.1 Discretization of the flow equation in the porous matrix
- 207 With the MFE method, the velocity q inside each triangular element E is approximated 208 using the linear Raviart-Thomas basis functions (see Figure 1):

$$q = \sum_{j=1}^{3} Q_j^E \mathbf{w}_j^E \tag{7}$$

- 210 where  $Q_j^E$  is the flux across the edge  $\partial E_j$  of E and  $\mathbf{w}_j^E = \frac{1}{2|E|} \begin{pmatrix} x x_j^E \\ y y_j^E \end{pmatrix}$  is the Raviart-
- Thomas basis functions (Raviart and Thomas, 1977) with  $(x_j^E, y_j^E)$  the coordinates of the
- 212 node j faced to the edge  $\partial E_i$  of E and |E| the area of E.



- Figure 1: RT0 vectorial basis functions and orientation of fluxes for a 2D triangular element.
- Using  $\mathbf{w}_{i}^{E}$  as a test function, the variational formulation of the Darcy law Eq. (2) writes

216 
$$\int_{E} \left(k_r^{-1} \mathbf{K}^{-1} \mathbf{q}\right) . \mathbf{w}_i^E = -\int_{E} \nabla H . \mathbf{w}_i^E = \int_{E} H \nabla . \mathbf{w}_i^E - \sum_{j} \int_{\partial E_j} H \mathbf{w}_i^E . \mathbf{\eta}_j^E$$
 (8)

- where  $\eta_j^E$  is the outward unit normal vector to the edge  $E_j$ .
- Defining  $\mathbf{B}^{E}$  the elemental matrix of terms  $B_{i,j}^{E} = \int_{E} (k_r^{-1,E} \mathbf{K}^{-1,E} \mathbf{w}_j^{E}) . \mathbf{w}_i^{E}$ , we obtain (see
- 219 Younes et al., 2004 for details)

220 
$$\mathbf{B}^{E} = \frac{1}{48|E|} \begin{pmatrix} 3\ell_{ij} + 3\ell_{ik} - \ell_{jk} & -3\ell_{ij} + \ell_{ik} + \ell_{jk} & \ell_{ij} - 3\ell_{ik} + \ell_{jk} \\ -3\ell_{ij} + \ell_{ik} + \ell_{jk} & 3\ell_{ij} - \ell_{ik} + 3\ell_{jk} & \ell_{ij} + \ell_{ik} - 3\ell_{jk} \\ \ell_{ij} - 3\ell_{ik} + \ell_{jk} & \ell_{ij} + \ell_{ik} - 3\ell_{jk} & -\ell_{ij} + 3\ell_{ik} + 3\ell_{jk} \end{pmatrix}$$
(9)

- with  $\ell_{ij} = \mathbf{r}_{ij}^T \left( k_r^{-1,E} \mathbf{K}^{-1,E} \right)^{-1} \mathbf{r}_{ij}$  and  $\mathbf{r}_{ij}$  is the edge vector from the node i to the node j.
- Using Eq. (7) and properties of  $w_i^E$ , the Darcy Eq. (8) becomes

$$\sum_{j} B_{i,j}^{E} Q_{j}^{E} = \frac{1}{|E|} \int_{E} H - \frac{1}{|\partial E_{i}|} \int_{\partial E_{i}} H$$

$$= H_{E} - TH_{i}^{E}$$
(10)

- where  $H_E$  is the mean head at the element E and  $TH_i^E$  is the mean head at the edge  $\partial E_i$ .
- Inverting Eq. (10) provides the water flux  $Q_i^E$  across the edge  $\partial E_i$  as

$$Q_{i}^{E} = \delta_{i}^{E} H_{E} - \sum_{j} B_{i,j}^{-1,E} T H_{j}^{E}$$
(11)

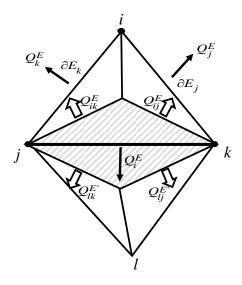
- 227 where  $\delta_{i}^{E} = \sum_{i} B_{i,j}^{-1,E}$ .
- The lumped formulation of MFE is then used in the following steps
- In a first step, integration of the mass conservation Eq. (1) over the element E,
- assuming a steady-state flow  $(\partial \theta / \partial t = 0)$  and substituting Eq. (11), yields

$$H_{E} = \sum_{i} \frac{\delta_{i}^{E}}{\delta^{E}} T H_{i}^{E}$$
 (12)

- where  $\delta^E = \sum_i \delta_i^E$
- Hence, the steady-state flux  $Q_i^E$  across the edge  $\partial E_i$  writes

$$\underline{Q}_{i}^{E} = \sum_{j} \left( \frac{\delta_{i}^{E} \delta_{j}^{E}}{\delta^{E}} - B_{i,j}^{-1,E} \right) T H_{j}^{E}$$
(13)

In a second step, a lumped region  $R_i$  is constructed around each edge  $\partial E_i$  by joining the two nodes of  $\partial E_i$  to the element centers  $\mathbf{x}_E$  and  $\mathbf{x}_{E'}$  of the elements E and E' sharing the edge i (Figure 2).



**Figure 2**: The lumping region  $R_i$  associated to the edge i sharing the elements E and E' and formed by the two simplex regions  $S_i^E$  and  $S_i^{E'}$ .

The domain is now partitioned into lumping regions  $R_i$  (hatched area in Figure 2) assigned to the edge i formed by the two simplex regions  $S_i^E$  and  $S_i^{E'}$  for an inner edge i and by the sole simplex region  $S_i^E$  for a boundary edge. The simplex region  $S_i^E$  is defined by joining the centre of E with the nodes E and E forming the edge E. The area of E is E is E area of E.

• In a third step, the integration of the transient mass conservation Eq. (1) over the lumped region  $R_i$  yields (see Figure 2 for notations):

$$\frac{|E|}{3} r_E \frac{dTH_i^E}{dt} + \frac{|E'|}{3} r_{E'} \frac{dTH_i^E}{dt} + \underline{Q}_{ij}^E + \underline{Q}_{ik}^E + \underline{Q}_{lj}^{E'} + \underline{Q}_{lk}^{E'} = 0$$
 (14)

where  $r_E = c(h_E) + S_S \theta(h_E)/\theta_S$  is the accumulation coefficient in Richards' 250 equation and  $Q_{ij}^E$  the interior flux, evaluated using the RTO approximation of the 251 velocity inside the element E given by Eq. (7), which yields

$$\underline{Q}_{ij}^{E} = \frac{1}{3} \left( \underline{Q}_{j}^{E} - \underline{Q}_{i}^{E} \right) \tag{15}$$

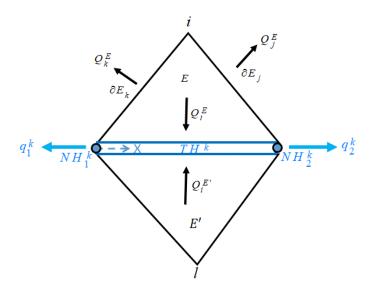
Substituting Eq. (13) and Eq. (15) into Eq. (14), allows to write the mass conservation Eq. (14) over the lumping regions  $R_i$  assigned to the edge i as a continuity of fluxes between two adjacent elements E and E' sharing the edge i as follows

$$\begin{cases}
Q_i^E + Q_i^{E'} = 0 \\
Q_i^E = \sum_j \left(\frac{\delta_i^E \delta_j^E}{\delta^E} - B_{i,j}^{-1,E}\right) TH_j^E - \frac{|E|}{3} r_E \frac{dTH_i^E}{dt}
\end{cases}$$
(16)

The flow system is formed by Eq. (16) for all the mesh edges which do not coincide with a fracture and solved for the mean head at edges  $TH_i$  by imposing continuity of the head at the interface of the elements  $\left(TH_i = TH_i^E = TH_i^{E'}\right)$ . The obtained system is highly nonlinear since the local matrix  $\boldsymbol{B}$ , and the accumulation term r depend on the pressure head. In the case of a Dirichlet condition with a prescribed head  $H_{imp}$  at the boundary edge i, Eq. (16) is replaced by  $TH_i = H_{imp}$ . If the boundary edge i has a prescribed flux  $Q_{imp}$  (Neumann boundary condition), Eq. (16) becomes  $Q_i^E + Q_{imp} = 0$ .

- Note that, contrarily to the standard MFE method, the time derivative remains continuous in Eq. (16), which facilitates employment of high-order methods for the time discretization.
- 3.2 Spatial discretization of the flow in the presence of a fracture

Let's consider a fracture k of length  $\ell_k$  and aperture  $e_k$ . The fracture k coincides with the edge i shared by the adjacent matrix-elements E and E' (see Figure 3). The flow through the fracture occurs between it's two nodes of pressures  $NH_1^k$  and  $NH_2^k$ . The flux  $Q_i^E$  (respectively  $Q_i^{E'}$ ) represents the matrix-fracture fluid exchange between E (respectively E') and the fracture k.



**Figure 3**: Schematic representation of the one-dimensional fracture k, which coincides with the edge i shared by the matrix elements E and E'. The flux  $Q_i^E$  (respectively  $Q_i^{E'}$ ) represents the matrix-fracture fluid exchange between E (respectively E') and k.

The one-dimensional flow through the fracture k is discretized with the MFE method, which assumes a linear variation of the velocity  $q^k$  inside k,

$$q^{k} = q_{1}^{k} w_{1}^{k} + q_{2}^{k} w_{2}^{k}$$

$$\tag{17}$$

with  $q_{j=1,2}^k$  the flux leaving the node j=1,2 of the fracture k,  $w_1^k = \frac{x-\ell_k}{e_k\ell_k}$  and  $w_2^k = \frac{x}{e_k\ell_k}$ 

are the one-dimensional velocity interpolation functions using the local coordinate  $x \in [0, \ell_k]$ .

The mass conservation Eq. (1) integrated over the fracture k of length  $\ell_k$  and aperture  $e_k$  yields

$$e_{k}\ell_{k}r_{k}\frac{dTH^{k}}{dt} + q_{1}^{k} + q_{2}^{k} - Q_{i}^{E} - Q_{i}^{E'} = 0$$
(18)

- with  $TH^k$  the mean head in the fracture k and  $r_k = c(h_k) + S_S^k \frac{\theta_k}{\theta_S}$  the accumulation coefficient
- related to k,  $Q_i^E$  and  $Q_i^{E'}$  are the water fluxes from the element E and E' representing matrix-
- 287 fracture exchange.
- The variational formulation of the Darcy law Eq. (2) on the fracture k writes

$$\sum_{j} q_{j}^{k} \int_{0}^{\ell_{k}} w_{i}^{k} w_{j}^{k} = -k_{r}^{k} K_{f}^{k} \int_{0}^{\ell_{k}} (\nabla H) w_{i}^{k}$$
(19)

290 Integration by part leads to

$$\sum_{j} q_{j}^{k} \int_{0}^{\ell_{k}} w_{i}^{k} w_{j}^{k} = \frac{k_{r}^{k} K_{f}^{k}}{e_{k}} \left( TH^{k} - NH_{i}^{k} \right)$$
 (20)

- where  $NH_i^k$  corresponds to the head at the node *i* located at the extremity of the fracture k.
- Using numerical integration, based on the trapezoidal rule, for the calculation of the left term
- 294 (see Koohbor et al., 2020) yields

$$q_i^k = e_k k_r^k \frac{2K_f^k}{\ell_k} \left( TH^k - NH_i^k \right) \tag{21}$$

The cross-flow equilibrium assumption is then employed by prescribing equality of the matrix edge head and the fracture head  $\left(TH_i^E = TH_i^{E'} = TH^k\right)$ . Thus, substituting Eq. (21) and Eq. (16) into Eq. (18) yields

$$\sum_{j} \left( \frac{\delta_{i}^{E} \delta_{j}^{E}}{\delta^{E}} - B_{i,j}^{-1,E} \right) TH_{j}^{E} + \sum_{j} \left( \frac{\delta_{i}^{E'} \delta_{j}^{E'}}{\delta^{E'}} - B_{i,j}^{-1,E'} \right) TH_{j}^{E'} - e_{k} k_{r}^{k} \frac{2K_{f}^{k}}{\ell_{k}} \left( 2TH_{i}^{E} - NH_{1}^{k} - NH_{2}^{k} \right) - \left( \frac{|E|}{3} r_{E} + \frac{|E'|}{3} r_{E'} + e_{k} \ell_{k} r_{k} \right) \frac{dTH_{i}^{E}}{dt} = 0$$
(22)

To close the system of Eq. (22), the mass conservation is written at each intersection of fracture branches. At the node i shared by k fracture branches, we impose

$$\sum_{k} q_i^k = 0 \tag{23}$$

303 Using Eq. (21), we obtain

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$$\sum_{k} e_{k} k_{r}^{k} \frac{2K_{f}^{k}}{\ell_{k}} \left( TH^{k} - NH_{i}^{k} \right) = 0$$
 (24)

Finally, the global flow system is formed by Eq. (16) for all the edges which do not coincide with a fracture and by Eq. (22) else. This system is supplemented by Eq. (24) for all the nodes of the fracture branches and assuming the continuity of the head  $\left(NH_i = NH_i^k\right)$  at the node i, intersection of k fracture branches. Therefore, the final flow system has the heads at the edges of the mesh plus the heads at the nodes of the fracture branches as unknowns.

- 3.3 Discretization of the advection-dispersion transport equation in the porous matrix
- 311 The transport of contaminants in the unsaturated porous matrix described by Eq. (3) writes:

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$$C\left(\frac{\partial\theta}{\partial t} + \nabla \cdot \mathbf{q}\right) + \theta \frac{\partial C}{\partial t} + \mathbf{q}\nabla C - \nabla \cdot \left(\mathbf{D}\nabla C\right) = 0$$
 (25)

- 313 Using the fluid mass conservation Eq. (1), the transport equation can be written in the
- 314 following form:

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$$\begin{cases} \theta \frac{\partial C}{\partial t} + \mathbf{q} \nabla C + \nabla \tilde{\mathbf{q}} = 0 \\ \tilde{\mathbf{q}} = -\mathbf{D} \nabla C \end{cases}$$
 (26)

- 316 The MFE method is now used for the spatial discretization of the transport equation. To this
- 317 aim, the dispersion vector  $\tilde{q}$  is approximated inside each triangular element E with the
- 318 Raviart Thomas vectorial basis functions as:

$$\tilde{\boldsymbol{q}} = \sum_{j} \tilde{Q}_{j}^{E} \boldsymbol{w}_{j}^{E} \tag{27}$$

- where  $\tilde{Q}_{j}^{E} = \int_{\partial E_{j}} \tilde{q}_{d} . \eta_{j}^{E}$  is the dispersive flux across the edge  $\partial E_{j}$  of the element E.
- The variational formulation of Eq. (26) is written as

322 
$$\int_{E} \left( \boldsymbol{D}_{E}^{-1} \tilde{\boldsymbol{q}} \right) . \boldsymbol{w}_{i}^{E} = -\int_{E} \nabla C . \boldsymbol{w}_{i}^{E}$$
 (28)

which can take the following form

$$\sum_{j} \tilde{B}_{i,j}^{E} \tilde{Q}_{j}^{E} = C_{E} - TC_{i}^{E}$$

$$\tag{29}$$

- where  $C_E$  is the mean concentration at the element E and  $TC_i^E$  is the trace of concentration
- 326 at the edge  $\partial E_i$  of the element E and  $\tilde{\bf B}$  is the elemental matrix of terms

327 
$$\tilde{B}_{i,j}^E = \int_E \left( D_E^{-1} \mathbf{w}_j^E \right) . \mathbf{w}_i^E$$

328 Inverting Eq. (29) yields the dispersive flux across  $\partial E_i$  as

329 
$$\tilde{Q}_i^E = \sum_j \tilde{\boldsymbol{B}}_{i,j}^{-1,E} \left( C_E - T C_j^E \right)$$
 (30)

- 330 An upwind lumped MFE scheme is used to avoid unphysical oscillations caused by the
- 331 hyperbolic advection part of the transport equation. The main steps of this scheme are as
- 332 follows:
- In a first step, both advective and transient terms are removed from the first equation
- 334 in the system of Eq. (26), yielding a steady-state dispersive flux  $\tilde{Q}_i^E$  expressed by
- 335 (similarly to Eq. (12)):

336 
$$\underline{\tilde{Q}}_{i}^{E} = \sum_{j} \frac{\tilde{\delta}_{i}^{E} \tilde{\delta}_{j}^{E}}{\tilde{\delta}^{E}} T C_{j}^{E} - \sum_{j} \tilde{B}_{i,j}^{-1,E} T C_{j}^{E}$$
(31)

with 
$$\tilde{\delta}_i^E = \sum_i \tilde{B}_{i,j}^{-1,E}$$
 and  $\tilde{\delta}^E = \sum_i \tilde{\delta}_i^E$ .

- In a second step, the integration of the advection-dispersion equation (26) over the
- lumped region  $R_i$  writes (see Figure 2):

$$\left\{ \frac{|E|}{3} \theta_{E} \frac{\partial TC_{i}^{E}}{\partial t} + Q_{ij}^{E}TC_{ij}^{E} + Q_{ik}^{E}TC_{ik}^{E} - \left(Q_{ij}^{E} + Q_{ik}^{E}\right)TC_{i}^{E} - \underline{\tilde{Q}}_{i}^{E} \right\} + \left\{ \right\}' = 0$$
(32)

- where  $Q_{ij}^{E} = \frac{1}{3} (Q_{j}^{E} Q_{i}^{E})$  is the interior flux between edges i and j (see Eq. (15)).
- The interior concentration  $TC_{ij}^{E}$  is calculated using the upstream edge concentration
- 343 as:

$$TC_{ij}^{E} = \tau_{ij}^{E}TC_{i}^{E} + (1 - \tau_{ij}^{E})TC_{j}^{E}$$
(33)

with  $\tau_{ij}^E = 1$  for an outward flux  $(Q_{ij}^E \ge 0)$ , else  $\tau_{ij}^E = 0$ .

- Thus, if we note  $Qt_i^E$  the total (advection + dispersion) flux leaving the element E from the edge i, Eq. (32) can be rewritten as the continuity of the total flux between two adjacent elements E and E' sharing the edge i as
- $\begin{cases}
  Qt_{i}^{E} + Qt_{i}^{E'} = 0 \\
  Qt_{i}^{E} = \sum_{j} \left(\frac{\tilde{\delta}_{i}^{E} \tilde{\delta}_{j}^{E}}{\tilde{\delta}^{E}} \tilde{B}_{i,j}^{-1,E}\right) TC_{j}^{E} + Q_{ij}^{E} \left(1 \tau_{ij}^{E}\right) \left(TC_{i}^{E} TC_{j}^{E}\right) + Q_{ik}^{E} \left(1 \tau_{ik}^{E}\right) \left(TC_{i}^{E} TC_{k}^{E}\right) \theta_{E} \frac{|E|}{3} \frac{\partial TC_{i}^{E}}{\partial t}
  \end{cases}$   $350 \qquad (34)$
- 351 3.4 Spatial discretization of the advection-dispersion transport equation through a fracture
- 352 Let's consider a fracture k of length  $\ell_k$  and aperture  $e_k$  and x the local coordinate along k
- 353 with x = 0 at the first node of k and  $x = \ell_k$  at the second node of k.
- 354 The diffusion coefficient  $D_k$  through the fracture k is approximated by

$$D_k = \alpha_L^k |\overline{q}_k| + D_m^k \tag{35}$$

- 356 where  $\alpha_L^k$  is the longitudinal dispersivity through the fracture k,  $D_m^k$  is the molecular diffusion
- 357 through k, and  $\overline{q}_k = \frac{\left(q_2^k q_1^k\right)}{2e_k}$  is the mean velocity in the fracture k.
- 358 The dispersive flux  $\tilde{q} = -D\nabla C$  through the fracture is approximated using the MFE method.
- Similarly to Eq. (21), the dispersive flux  $\tilde{q}_i^k$  at the extremity i = 1, 2 of the fracture k writes

$$\tilde{q}_i^k = \frac{2e_k D_k}{\ell_k} \left( TC^k - N\tilde{C}_i \right) \tag{36}$$

361 where  $N\tilde{C}_i$  is the concentration at the node *i*.

362  $TC^{l+3}$ 363  $TC^{k} = TC^{l} \qquad N\tilde{C}_{i}$ 365  $TC^{l+2} \qquad TC^{l+1}$ 366

**Figure 4:** Intersection of multiple fracture branches.

Imposing the continuity of the dispersive fluxes arriving from all fracture branches sharing thenode *i* (see Figure 4) writes

$$\sum_{l} \frac{2e_{l}D_{l}}{\ell_{l}} \left( TC^{l} - N\tilde{C}_{j} \right) = 0 \tag{37}$$

Which yields

367

368

$$N\tilde{C}_{i} = \frac{\sum_{l} \frac{e_{l}}{\ell_{l}} D_{l} T C^{l}}{\sum_{l} \frac{e_{l}}{\ell_{l}} D_{l}}$$
(38)

374 Substituting Eq. (38) into the flux Eq. (36) yields

375 
$$\tilde{q}_{i}^{k} = \frac{2e_{k}D_{k}}{\ell_{k}} \left( TC^{k} - \frac{\sum_{l} \frac{e_{l}}{\ell_{l}} D_{l} TC^{l}}{\sum_{l} \frac{e_{l}}{\ell_{l}} D_{l}} \right)$$
(39)

- 376 The integration of the mass conservation equation over the fracture k which coincides with the
- 377 edge i shared by the two matrix elements E and E', writes

378 
$$\theta_{k}e_{k}\int_{0}^{\ell_{k}}\frac{\partial C}{\partial t}+e_{k}\int_{0}^{\ell_{k}}\nabla \cdot (\boldsymbol{q}C)-e_{k}\int_{0}^{\ell_{k}}C\nabla \cdot \boldsymbol{q}+e_{k}\int_{0}^{\ell_{k}}\nabla \cdot \tilde{\boldsymbol{q}}-Qt_{i}^{E}-Qt_{i}^{E'}=0$$
 (40)

379 The calculation of the different integrals yields

380 
$$\theta_{k}e_{k}\ell_{k}\frac{\partial TC^{k}}{\partial t} + q_{1}^{k}C_{1}^{k,*} + q_{2}^{k}C_{2}^{k,*} - (q_{1}^{k} + q_{2}^{k})TC^{k} + \tilde{q}_{1}^{k} + \tilde{q}_{2}^{k} = Qt_{i}^{E} + Qt_{i}^{E'}$$
(41)

381 where  $C_i^{k,*}$  is the concentration at the node *i* of the fracture *k* given by

$$C_i^{k,*} = \lambda_i^k N C_{i,in}^k + \left(1 - \lambda_i^k\right) \overline{NC}_{i,out}$$
(42)

- 383 in which  $NC_{i,in}^k = TC^k$  is the interior concentration and the parameter  $\lambda_i^k$  is used to select the
- 384 upstream concentration, it depends on the sign of  $q_i^k$  as

385 
$$\lambda_i^k = \begin{cases} 1 & \text{if} & q_i^k \ge 0\\ 0 & \text{if} & q_i^k < 0 \end{cases}$$
 (43)

- Hence, in the case of an outflow at the node *i* of *k*, the nodal concentration is  $C_i^{k,*} = TC^k$ ,
- whereas, in the case of an inflow at the node i of the fracture k, the nodal concentration is
- $\overline{NC}_{i,out}$ .

To calculate  $\overline{NC}_{i,out}$ , we use the contaminant conservation at the node i, shared by l fractures, which writes

$$\sum_{k=1}^{l} q_i^k C_i^{k,*} = 0 (44)$$

392 Using Eq. (42) and Eq. (43), we obtain

$$\overline{NC}_{i,out} = \frac{\sum_{k=1}^{l} q_i^k \lambda_i^k TC^k}{\sum_{k=1}^{l} q_i^k \left(\lambda_i^k - 1\right)}$$

$$(45)$$

- Note that the number of unknowns for the transport system to be solved does not depend on the number of fractures in the domain. Indeed, the final transport system has the concentration at edges as unknowns and is constructed as follows
- For all edges i sharing two matrix elements E and E' such that i does not coincide with a fracture k, Eq. (34) is solved for the unknown edge concentration  $TC_i$  assuming continuity of edge concentration  $\left(TC_i = TC_i^E = TC_i^{E'}\right)$ .
- 400 For all edges i sharing two matrix elements E and E' such that i coincides with a 401 fracture k, Eq. (41), in which we substitute Eq. (34), Eq. (39), Eq. (42), Eq. (43) and Eq. (45), is solved for the unknown edge concentration  $TC_i$  assuming that the 402 403 concentration edge matrix the fracture at the and at are equal  $\left(TC_{i} = TC_{i}^{E} = TC_{i}^{E'} = TC^{k}\right).$ 404
- 405 3.5 The temporal discretization of the nonlinear flow-transport system
- The final nonlinear flow-transport system, formed by Eq. (16), Eq. (22), and Eq. (24) for the

flow and by Eq. (34) and Eq. (41) for the transport, is written in a single implicit system of ordinary differential equations (ODEs) of the general form

$$F(t, \mathbf{y}, \mathbf{y}') = 0 \tag{46}$$

Where  $\mathbf{y} = \left[ \left( TH_i \right)_{i=1,...,nb\_edges}, \left( NH_i \right)_{i=1,...,nb\_nodefractures}, \left( TC_i \right)_{i=1,...,nb\_edges} \right]$  is the vector of unknowns formed by (i) the head traces at all the edges of the mesh (except boundary edges with prescribed head), (ii) the head at all the nodes corresponding to the extremity of fracture branches, and (iii) the concentration traces at all edges of the mesh (except boundary edges with prescribed concentration). Thus, the number of unknowns for the flow-transport system is approximately twice the number of edges plus the number of fractures.

For the time discretization, we use high-order methods, which are known to be more efficient and require less effort in the nonlinear solver compared to the lowest order methods (Farthing et al., 2002). An efficient automatic time-stepping scheme is employed to improve the computational efficiency while maintaining accuracy (Tocci et al., 1997; Kavetski et al., 2001). The time integration is performed with the DASPK time solver, which uses the preconditioned Krylov iterative method to solve the linear systems arising at each time step. DASPK is based on the Fixed Leading Coefficient Backward Difference Formulas (FLCBDF), which has good stability properties and is well adapted for time integration of stiff problems (Kees and Miller, 2002). The nonlinear problem is linearized using the Newton method with a numerical approximation of the Jacobian matrix. To improve efficiency, the Jacobian is reused for several time steps and is calculated by the solver only when necessary. Furthermore, the column grouping technique (Hindmarsh, 1982) is employed to reduce the computational time for the evaluation of the Jacobian matrix by perturbing variables by group, knowing the structure and sparsity of the Jacobian.

During calculation, the order (up to fifth order) of the time discretization and the time step size are adapted to improve efficiency while the relative and absolute convergence criteria are maintained under a fixed tolerance ( $10^{-6}$  in this work).

# 4. Numerical experiments

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In this section, three test problems dealing with flow and mass transport in saturated and unsaturated fractured porous media are simulated to investigate the robustness of the new MFE code. The first test case deals with flow and transport in a saturated porous medium involving a single fracture. This test case is used to validate the developed 1D-2D MFE code against the solution obtained with Comsol multiphysics 1D-2D model. Comosl uses the standard finite element (FE) method and an adaptive time stepping scheme. The test problem is also simulated with a 2D-2D model where 2D triangular elements are employed for the spatial discretization of both the matrix and the fractures continua using a very fine mesh in order to correctly discretize the fracture branches with a small aperture. We use the advanced 2D-2D DG model developed by Younes et al. (2021), based on the discontinuous Galerkin (DG) finite element and the multipoint flux approximation methods and high-order time integration techniques via the method of lines (MOL). The second test case deals with flow and transport in a fractured unsaturated-saturated porous medium. The porous medium has initially wet conditions and involves a single fracture. This test case is used to validate the developed 1D-2D MFE model against the solution obtained with the 2D-2D DG model in the case of unsaturated flow. The last test case is a challenging problem dealing with flow and transport into an initially dry soil containing a fracture network. This last problem is simulated to highlight the efficiency and robustness of the developed 1D-2D MFE model compared to the 2D-2D DG model.

## 4.1 Fractured saturated quarter-five-spot problem

We consider a quadratic 2D domain (quarter-five-spot configuration) of size [0,1m]×[0,1m] with impermeable walls except at the lower-left and the upper-right corners. The source at the lower-left corner is represented by a boundary flux  $q_{ini} = 10^{-3} \,\mathrm{m/s}$ at  $(0 \le x \le 0.03\text{m}) \cap (y=0) \cup (x=0) \cap (0 \le y \le 0.03\text{m})$ . The sink at the right-upper corner is Dirichlet boundary condition with represented by a a zero head at  $(0.97 \text{m} \le x \le 1 \text{m}) \cap (y=1) \cup (x=1) \cap (0.97 \text{m} \le y \le 1 \text{m})$ . The porous medium is formed by a homogeneous material with a diagonal fracture of 1mm aperture, located between (0.2m, 0.2m) and (0.8m, 0.8m). The hydraulic and transport properties of the porous matrix and the fracture continuum are depicted in Table 1. The initial conditions correspond to a domain free from pollutants. The simulation is performed for a time of 3456s.

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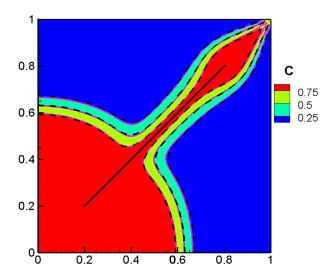
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	$K_s$ (m/s)	$S_s$ (1/m)	$ heta_{\scriptscriptstyle s}$	$\alpha_L(\mathbf{m})$	$\alpha_{T}(\mathbf{m})$	$D_m (m^2/s)$
Matrix	10 <sup>-6</sup>	10-10	0.4	0.0	0.0	10-6
Fracture	10-3	10-10	0.4	0.0	0.0	10-6

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**Table 1**: Hydraulic and transport parameters for the fractured saturated quarter-five-spot problem.



**Figure 5**: Concentration distribution for the fractured saturated quarter-five-spot problem.

Results of the new 1D-2D MFE model (dashed lines), the 1D-2D Comsol FE model (purple lines), and 2D-2D DG model (color map).

The problem is simulated with the new 1D-2D MFE model as well as with the 1D-2D Comsol FE model and the 2D-2D DG model of Younes *et al.* (2021). In the latter, the hydraulic and transport parameters used for the fractures in the 1D-2D approach are attributed to the 2D triangular elements located inside the fractures. The 2D-2D DG model is used with a fine mesh with local mesh refinement around fractures. The three models were used with the MOL and a variable high-order (up to 5) time integration BDF method. Figure 5 shows that the three models yield almost similar concentration distributions, which demonstrates the validity of the developed 1D-2D MFE model for simulating flow and transport in fractured saturated porous media.

4.2 Infiltration of contaminated water in a fractured unsaturated-saturated porous medium.

This test case, inspired by the laboratory experiments of Vauclin *et al.*, (1979), was proposed by Koohbor *et al.* (2020) to investigate unsaturated flow in fractured porous media. The problem is extended hereafter to tackle both flow and transport in the case of a homogeneous porous medium, including a single inclined fracture. The domain has a rectangular shape of

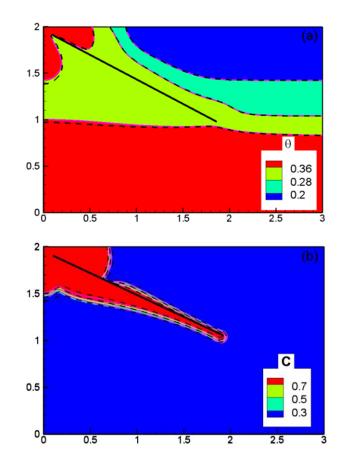
300cm×200 cm with a water table located at 65cm from the bottom. Initial conditions correspond to a hydrostatic pressure distribution and a zero concentration in the domain. Boundary conditions are as follows: contaminated water is infiltrated under a constant flux of 335cm/day over the first 50cm of the soil surface. The lower 65cm of the right side of the domain has a Dirichlet boundary condition with a fixed head of 65cm. A no-flow boundary is prescribed for the rest of the boundaries. The homogeneous porous medium includes an inclined fracture of 1cm aperture and 2m length, located near the infiltration zone. The hydraulic and transport parameters are depicted in Table 2.

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	$K_{s}$	$S_s$	$ heta_{\!\scriptscriptstyle S}$	$ heta_{\!\scriptscriptstyle r}$	α	n	$lpha_{\scriptscriptstyle L}$	$lpha_{\scriptscriptstyle T}$	$D_{\scriptscriptstyle m}$
	(m/s)	(1/m)			(1/m)		(m)	(m)	(m <sup>2</sup> /s)
Matrix	5 10-5	10-10	0.4	0.1	3.31	2.1	0	0	10-7
Fracture	10-2	10-10	0.4	0.01	3.31	2.1	0	0	10-7

**Table 2**: Hydraulic and transport parameters for the problem of infiltration of contaminated water into a fractured unsaturated-saturated porous medium.

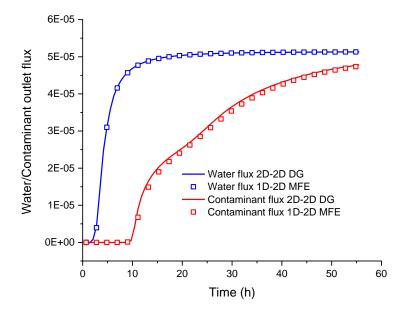
The simulation of this problem cannot be performed with the 1D-2D Comsol FE model since Comsol cannot treat unsaturated flow in the fractures. The problem is simulated with the 1D-2D MFE model as well as with the 2D-2D DG model and the 2D-2D FE model of Comsol. Figure 6 depicts the water content and the concentration distributions at t = 1000s obtained with the three models. A good agreement is observed between the results of the three models for the volumetric water content as well as for the concentration contours (Figure 6).



**Figure 6**: Water content (a) and concentration (b) distributions for the problem of infiltration of contaminated water in a fractured unsaturated-saturated porous medium. Results of the new 1D-2D MFE model (dashed lines), 2D-2D DG model (purple lines), and 2D-2D FE Comsol model (color map).

A more in-depth comparison is then performed between the new 1D-2D MFE model and the 2D-2D DG model. To this aim, the fluid and contaminant mass fluxes at the outlet are calculated with both models over the simulation time of 55 hours. The results of the Figure 7 show that the outlet fluid flux is almost constant after around 15 hours which indicates that an almost steady state water content distribution is reached at this time. A first contaminant front, caused by the fast mobility of the contaminated water through the fractures, is observed in the Figure 7 after around 10 hours. A second slower and more dispersed contaminant front was occurred, which was caused by the transport of the contaminant through the rock matrix. The

results of Fgure 7 show a very good agreement between the 1D-2D MFE and the 2D-2D DG models for both fluid and contaminant outlet mass fluxes. These results demonstrate the validity of the new 1D-2D MFE model for the simulation of flow and transport in fractured unsaturated porous media.

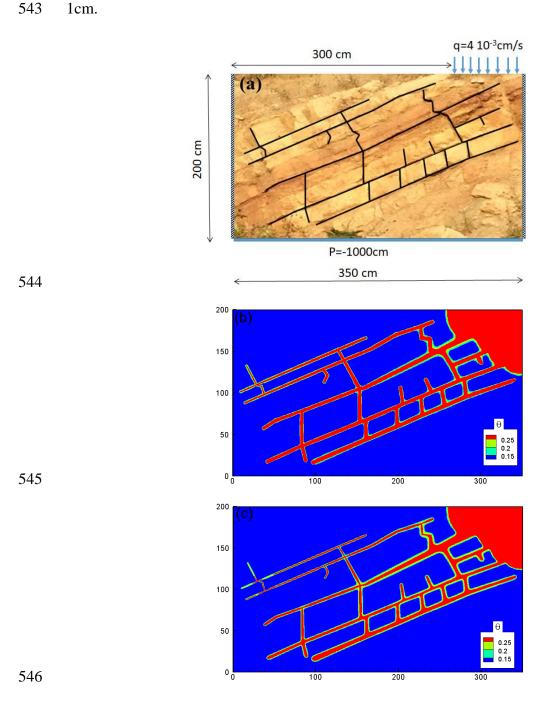


**Figure 7**: Outlet fluid and contaminant mass fluxes obtained with the 1D-2D MFE and the 2D-2D DG models for the problem of infiltration of contaminated water in a fractured unsaturated-saturated porous medium.

4.3 Infiltration of contaminated water in a fractured dry soil.

Simulation of the infiltration of contaminated water into initially dry soils is known to be challenging because of the presence of sharp wetting fronts (Zha *et al.*, 2017). Sharp fronts are often the origin of unphysical oscillations, which can cause several convergence issues. To investigate the efficiency of the developed model for such situations, we simulate an infiltration problem, adapted from Koohbor *et al.* (2020). The fractured porous medium has a rectangular shape of 350cm in length and 200cm in height (Figure 8a). Left and right vertical boundaries are impermeable. A pressure head of -1000 cm is imposed at the bottom of the

domain. Water is injected at the right part of the surface  $(300cm \le x \le 350cm)$  with a constant flow rate of  $4 \times 10^{-4}$  cm/s. The simulation is performed for a period of  $2 \times 10^{5}$  s. Clean water is injected for the first half period  $(C = 0 \ if \ t \le 10^{5} s)$ , and contaminated water is injected for the second half period  $(C = 1 \ if \ t > 10^{5} s)$ . Initial conditions correspond to a highly dry soil with a head of -1000cm in both matrix and fracture continua. All fractures have an aperture of 1cm.



**Figure 8**: The problem of infiltration of contaminated water in a fractured initially dry soil:

(a) domain and boundary conditions, (b) final water content distribution obtained with the 1D
2D MFE model and with the 2D-2D DG model (c).

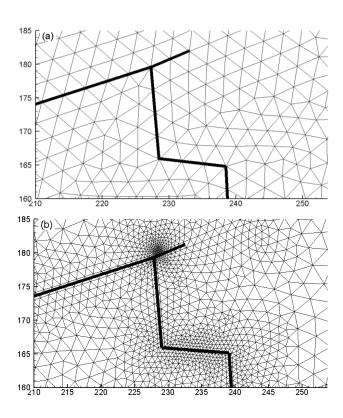
The hydraulic parameters of the two continua are depicted in Table 3.

	K <sub>s</sub> (cm/s)	S <sub>s</sub> (1/cm)	$ heta_{s}$	$ heta_{r}$	α (1/cm)	n
Matrix	5.25 10 <sup>-6</sup>	10 <sup>-8</sup>	0.34	0.01	0.0139	1.6
Fracture	1.16 10 <sup>-2</sup>	10-8	0.8	0.001	0.0139	1.6

**Table 3**: Hydraulic parameters for the problem of infiltration of contaminated water in a fracture initially dry soil.

The simulation of this last test case with the 2D-2D FE Comsol model encountered several convergence issues because of the initial high dry conditions. Indeed, the initial dry conditions are responsible of the appearance of several unphysical oscillations leading to the non-convergence of the nonlinear flow-transport model. These difficulties are avoided with the 2D-2D DG model thanks to the incorporated advanced numerical methods (see Younes et al. (2021) for more details). As a consequence, the results of the new 1D-2D MFE model are only compared to those of the 2D-2D DG model. The final water content distribution obtained with the two models is depicted in Figure 8. Similar distributions are obtained with the two models. As expected, the infiltrated water invades the fracture network, and high water saturation is observed in almost all fracture branches (Figure 8) because of their high saturated hydraulic conductivity, which is around 2200 times higher than that of the matrix continuum. Two configurations are investigated. The first configuration corresponds to a

highly advective transport problem. In this case, all dispersivities of the matrix and the fractures are zero  $\left(\alpha_L^m = \alpha_T^m = \alpha_L^f = 0\right)$ , and a small molecular diffusion occurs in both continua  $\left(D_m^m = D_m^f = 10^{-6} \ cm^2/s\right)$ . In the second configuration, a more significant dispersion is considered for both continua with longitudinal and transverse dispersivities in the matrix, respectively  $\alpha_L^m = 5m$ , and  $\alpha_T^m = 2m$ . The longitudinal dispersivity in the fractures is  $\alpha_L^f = 5m$ . The molecular diffusion in both continua is  $10^{-5} \ cm^2/s$ . For the 1D-2D model, the domain is discretized using 15400 triangles for the matrix continuum and 853 lines for the fracture branches without any constraint on the size of mesh elements next to the fractures (Figure 9a). The 2D-2D model is used on a fine mesh of 76000 elements with local mesh refinement in the fractures in order to correctly discretize the flow and transport through the fracture branches with a small aperture of 1cm (Figure 9b).



**Figure 9**: Spatial discretization for the 1D-2D MFE (a) model (fractures are represented by mesh edges) and for the 2D-2D DG (b) model (fractures are represented by small mesh elements).

Two versions of the 1D-2D MFE model are employed for the simulations: (*i*) the upwind scheme described above and (*ii*) a centered scheme where no upwinding is used for the advection operator in the matrix nor in the fractures. The results of Figure 10 show that the centered scheme provides similar results to the upwind scheme in the case of high dispersion (Figures 10d and 10e). However, in the case of advection-dominated transport, the centered scheme fails to provide accurate results and generates strong unphysical concentrations both in the matrix and in the fracture continuum (Figure 10b). The results of the upwind 1D-2D MFE model are exempted from unphysical oscillations (negative concentration are completely avoided) for both advection dominated and advection-dispersion configurations which demonstrates the robustness of the developed upwind 1D-2D MFE scheme. Furthermore, the solution of the upwind 1D-2D MFE model is in good agreement with the solution of the 2D-2D DG model both in the case of advection-dominated transport (Figure 10a vs 10c) and in the case of advection-dispersion transport (Figure 10d vs. 10f).

The advantage of using a high-order time discretization scheme is investgated by comparison against the first-order (conventional) scheme. The simulation using the upwind 1D-2D MFE model with a first-order time discretization scheme requires 20902 time steps and needs 6566s, whereas the high-order scheme requires only 3401 time steps and needs 375s. Thus, the high-order method is around four times faster than the first order method. Concerning the efficiency of the 1D-2D approach in comparison to the 2D-2D approach, the 2D-2D DG model required 5259s for the whole simulation, whereas the new 1D-2D MFE model requires only 375s. Thus, the new 1D-2D MFE model is around 15 times more efficient than the 2D-

2D DG model, which highlights the great benefit of robust and accurate 1D-2D models to simulate flow and transport processes in unsaturated and saturated fractured porous media.

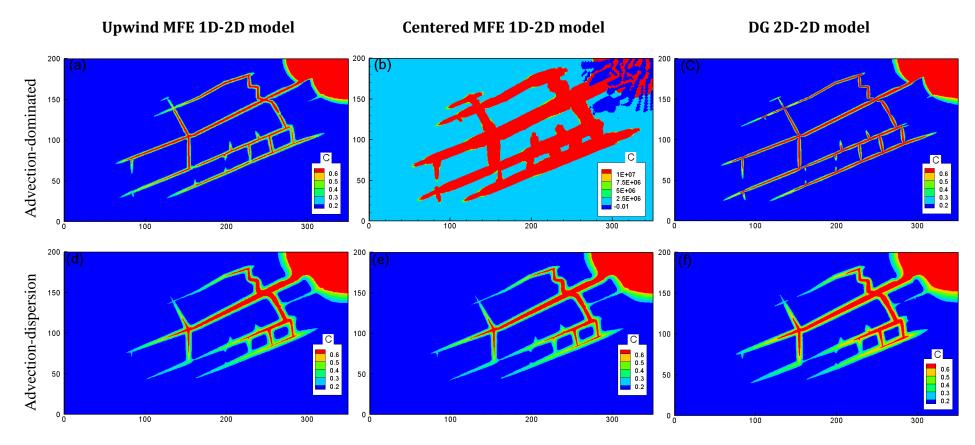


Figure 10: Infiltration of contaminated water in a fractured initially dry soil: Results of the upwind 1D-2D MFE model, the centered 1D-2D MFE model and the 2D-2D DG model in the case of advection dominated transport  $\left(\alpha_L^m = \alpha_T^m = \alpha_L^f = 0 \text{ and } D_m^m = D_m^f = 10^{-6} \text{ cm}^2/\text{s}\right)$  and in the case of advection-dispersion transport  $\left(\alpha_L^m = \alpha_L^f = 5m, \, \alpha_T^m = 2m, \, \text{and } D_m^m = D_m^f = 10^{-5} \, \text{cm}^2/\text{s}\right)$ .

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#### 5. Conclusion

A new model has been developed for nonlinear flow and transport in unsaturated fractured porous media with implicit matrix-fracture and fracture-fracture fluid and contaminant exchanges. The model is based on the DFM approach, which describes fractures and matrix explicitly. Cross-flow equilibrium is assumed only across the fractures thanks to the MFE method which has been employed for the full spatial discretization of the flow and transport in both the matrix and the fracture continua. The MFE method avoids the constraints on the mesh size next to the fractures and allows to approximate the matrix-fracture and fracturefracture exchange without any transfer functions. An upwind scheme is employed to avoid unphysical oscillations in the case of advection dominant transport. The time integration is performed with variable high-order methods via the MOL. An efficient automatic timestepping scheme is used to improve the computational efficiency while maintaining accuracy of the nonlinear solver. Three test problems dealing with flow and mass transport in saturated and unsaturated fractured porous media have been simulated to investigate the validity and robustness of the new 1D-2D MFE model. The first test case deals with the fractured quarter-five-spot problem and concerns flow and transport in a saturated porous medium involving a single fracture. The results of this test case with the 1D-2D MFE model were similar to those of the 1D-2D FE Comsol model and that of the 2D-2D DG model, which demonstrates the validity of the new model to simulate flow and transport in fractured saturated porous media. The second test case deals with flow and transport in an unsaturated-saturated porous medium, including a single inclined fracture. This test case has been simulated with the 1D-2D MFE model as well as with the 2D-2D DG model and the 2D-2D FE model of Comsol

since the 1D-2D FE model of Comsol cannot treat unsaturated flow in fractures. A very good agreement is obtained between the three models for both the volumetric water content and the concentration contours, which demonstrates the validity of the new model for unsaturated fractured porous media. The last test case is a challenging problem dealing with flow and transport in an initially dry soil containing a fracture network. For this problem, the 2D-2D FE Comsol model encountered several convergence issues because of the initial high dry soil conditions. The problem has been simulated using the 1D-2D MFE model using upwind and centered schemes. The results show that both schemes yield accurate results in the case of high dispersion. However, in the case of advection-dominated transport, only the upwind scheme provides stable results. The solution of the upwind 1D-2D MFE model is in good agreement with the solution of the 2D-2D DG model both in the case of advection-dominated transport and in the case of advection-dispersion transport. The new 1D-2D MFE model is much more efficient than the 2D-2D DG model. The new model allows a speedup of around 15, which confirms the usefulness of efficient and accurate models based on the DFM approach for the simulation of flow and transport in fractured porous media.

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