

A robust fully Mixed Finite Element model for flow and transport in unsaturated fractured porous media

Anis A. Younes, Hussein Hoteit, Rainer Helmig, Marwan Fahs

► To cite this version:

Anis A. Younes, Hussein Hoteit, Rainer Helmig, Marwan Fahs. A robust fully Mixed Finite Element model for flow and transport in unsaturated fractured porous media. Advances in Water Resources, 2022, 166, pp.104259. 10.1016/j.advwatres.2022.104259. hal-04300425

HAL Id: hal-04300425 https://hal.science/hal-04300425v1

Submitted on 22 Nov 2023

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers. L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

1	
2	
3	A robust fully Mixed Finite Element model for flow and transport in
4	unsaturated fractured porous media
5	
6	
7	
8	Anis Younes ¹ , Hussein Hoteit ² , Rainer Helmig ³ , Marwan Fahs ¹
9	
10	¹ ITES, University of Strasbourg, CNRS, ENGEES, 67000, Strasbourg, France.
11 12 13 14 15 16 17 18 20 21 22 23 24 25 26 27 28 29 30 31	 ² Physical Science and Engineering Division, King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia ³ Institute for Modelling Hydraulic and Environmental Systems, University of Stuttgart, Pfaffenwaldring 61, 70569 Stuttgart, Germany
32	Submitted to Advances in Water Resources
33	Contact author: Marwan Fahs
34	E-mail: fahs@unistra.fr
35	
36	
37	

38 Abstract

39 A fully mixed finite element (MFE) model is developed for nonlinear flow and transport in 40 unsaturated fractured porous media with matrix-fracture and fracture-fracture fluid and mass 41 exchanges. The model is based on the discrete fracture matrix (DFM) approach and assumes 42 cross-flow equilibrium in the fractures. The MFE method is employed for the spatial 43 discretization of both flow and transport on the 2D-matrix elements as well as on the 1D-44 fracture elements. An upwind scheme is employed to avoid unphysical oscillations in the case 45 of advection dominant transport. The temporal discretization is performed using high-order 46 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.

61

62 Key words:

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

65 **1. Introduction**

Flow and transport in fractured porous media are important in many applications such as
water resource management (Wireman 2003, Kavouri *et al.*, 2017), contaminant transport
(Berkowitz, 2002; Brutz and Rajaram 2017, Klammler *et al.* 2016), nuclear waste
management (Follin and Stigsson 2014, Mattila and Tammisto 2012) and oil and gas
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.*,
2004).

89 The second approach uses on an explicit representation of the fractures. Among this approach, 90 the discrete fracture network (DFN) model. With DFN, the geometry and properties of 91 discrete fractures are explicitly incorporated as a central component controlling flow and 92 transport. Discrete fracture matrix (DFM) models consider that flow and transport processes 93 occur through both, the porous matrix and the explicitly represented fractures. As a 94 consequence, the DFM model is more appropriate for handling fractures in a permeable 95 porous medium (Berre *et al.*, 2019). Considering that the aperture of the fractures is small as 96 compared to the matrix scale, the main idea of DFM is to use the cross-flow equilibrium 97 concept across the fractures (Noorishad and Mehran, 1982; Baca et al., 1984; Granet et al., 98 1998; Hoteit *et al.*,2008). As a consequence, the fractures can be discretized with elements of 99 co-dimension one with respect to the dimension of the surrounding matrix (Flemish et al., 100 2018; Martin et al., 2005), such as 1D fracture elements with 2D matrix elements. This 101 simplification makes DFM models much more efficient than the single porosity 2D-2D 102 model, where 2D elements are used for both matrix and fracture continua. Note that the 103 applicability of the 2D-2D models is often hampered by their expansive computational cost 104 since they require very fine mesh elements to correctly discretize the fractures with small 105 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

4

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.

119 The MFE (Raviart and Thomas, 1977; Chavent and Jaffré, 1986) is a robust numerical method 120 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 121 122 method ensures local mass balance and can easily handle general unstructured meshes 123 (Younes et al., 2010). Further, it yields an accurate velocity field in highly heterogeneous and 124 anisotropic media (Durlofsky, 1994). The hybridization procedure of the MFE method allows 125 improving its efficiency by reducing the total number of unknowns and producing a final 126 system with a positive symmetric definite matrix (Chavent and Jaffré, 1986). The unknowns, 127 in this case, are the traces of the variable at the edges.

128 A lumped formulation of the MFE method has been developed by Younes et al. (2006) to 129 improve the monotonicity of the solution and reduce the unphysical oscillations observed with 130 transient problems. Belfort et al. (2009) showed that the lumped formulation is more efficient 131 and more robust than the standard one for the simulation of water infiltration into initially dry 132 soils. Further, contrarily to the standard MFE method, the lumped formulation maintains the 133 time derivative continuous and thus, allows employment of high-order time integration 134 methods via the method of lines (MOL), which can be very efficient for solving nonlinear 135 problems (Fahs et al., 2009 and Younes et al., 2009).

136 Although the MFE method is well adapted for diffusion type equations, when applied for the 137 advection-dispersion transport equation, the solution can exhibit strong unphysical 138 oscillations because of the hyperbolic nature of the advection operator. Therefore, the main 139 objective of this work is to develop a stable MFE model for unsaturated flow and mass 140 transport through both the 2D-matrix and the 1D-fracture elements. Both fluid and 141 contaminant matrix-fracture and fracture-fracture exchanges are implicitly taken into account, 142 without using any transfer functions, even for the case of several intersecting fractures. To 143 avoid instabilities caused by the hyperbolic advection term, we use a robust monotonic 144 upwind MFE scheme where the traces of concentration at edges are upwinded depending on 145 the direction of the local velocity. An implicit scheme is used for the time discretization of the 146 flow and transport equations. This alleviates restriction on the size of the time step from the 147 CFL condition of explicit schemes. For the sake of brevity, the lumped hybrid MFE method 148 employed in this work will also be denoted MFE.

149 Modeling flow and transport in unsaturated fractured porous media is likely to be highly CPU 150 consuming due to (i) the strongly nonlinear Richards flow equation (RE), (ii) the high contrast 151 of permeability between the conductive fractures and the low permeable matrix and (iii) the 152 presence of sharp wetting and/or contaminant fronts. These difficulties make the commonly 153 used, first-order backward Euler scheme combined with the heuristic time step management, 154 inappropriate to obtain accurate solutions in a reasonable CPU time. To overcome these 155 difficulties, time integration is performed using high-order time integration methods via the 156 Method of Lines (MOL). The MOL allows versatile time step length and order of the 157 temporal discretization to reduce the computational time while maintaining accuracy. The 158 MOL was shown to be effective for the solution of the RE in the unsaturated zone (Fahs et al, 159 2009; Khoobor et al., 2020) and is used hereafter for the first time for coupled flow and 160 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.

168 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:

173
$$\frac{\partial \theta}{\partial t} = \left(c\left(h\right) + S_s \frac{\theta}{\theta_s}\right) \frac{\partial H}{\partial t} = -\nabla \cdot \boldsymbol{q} = 0 \tag{1}$$

and the Darcy-Buckingham law:

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

176 where $c(h) = \partial \theta / \partial h$ is the specific moisture capacity $[L^{-1}]$, S_s is the specific mass storativity 177 related to head changes $[L^{-1}]$, θ is the current water content $[L^3L^{-3}]$, θ_s is the saturated water 178 content $[L^3L^{-3}]$, H = h + y is the freshwater head [L], h is the pressure head [L], y is the 179 upward vertical coordinate [L], t is the time [T], q is the Darcy velocity $[LT^{-1}]$, k_r is the 180 relative conductivity [-], $\mathbf{K} = \frac{\rho g}{\mu} \mathbf{k}$ is the hydraulic conductivity tensor $[LT^{-1}]$, ρ is the fluid 181 density [ML⁻³], g is the gravity acceleration [LT⁻²], μ is the fluid dynamic viscosity [ML⁻¹T⁻ 182 ¹] and k is the permeability of the rock matrix as a tensor, or that of the fracture, as a scalar 183 [L²].

184 The transport of contaminants in the unsaturated porous matrix and through the unsaturated 185 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)

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

188
$$\boldsymbol{D} = D_m \boldsymbol{I} + (\boldsymbol{\alpha}_L - \boldsymbol{\alpha}_T) \boldsymbol{q} \otimes \boldsymbol{q} / |\boldsymbol{q}| + \boldsymbol{\alpha}_T |\boldsymbol{q}| \boldsymbol{I}$$
(4)

189 In which α_L and α_T are the longitudinal and transverse dispersivities [L], D_m is the pore 190 water diffusion coefficient [L²T⁻¹] and *I* is the unit tensor.

191 The standard van Genuchten (van Genuchten, 1980) model is used for the relationship192 between water content and pressure head:

193
$$S_{e} = \frac{\theta(h) - \theta_{r}}{\theta_{s} - \theta_{r}} = \begin{cases} \frac{1}{\left(1 + |\alpha h|^{n}\right)^{m}} & h < 0\\ 1 & h \ge 0 \end{cases}$$
(5)

194 where α [L^{-1}] and n [-] are the van Genuchten parameters, m = 1 - 1/n, S_e is the effective 195 saturation [-], and θ_r is the residual water content [L^3L^{-3}].

196 The conductivity-saturation relationship is analytically expressed from the Mualem (Mualem,197 1976) model,

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

203 **3. The fully MFE numerical model**

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):

209
$$\boldsymbol{q} = \sum_{j=1}^{3} \boldsymbol{Q}_{j}^{E} \boldsymbol{w}_{j}^{E}$$
(7)

210 where Q_j^E is the flux across the edge ∂E_j of E and $w_j^E = \frac{1}{2|E|} \begin{pmatrix} x - x_j^E \\ y - y_j^E \end{pmatrix}$ is the Raviart-

Thomas basis functions (Raviart and Thomas, 1977) with (x_j^E, y_j^E) the coordinates of the node *j* faced to the edge ∂E_j of *E* and |E| the area of *E*.





Figure 1: RT0 vectorial basis functions and orientation of fluxes for a 2D triangular element.

215 Using w_i^E as a test function, the variational formulation of the Darcy law Eq. (2) writes

216
$$\int_{E} \left(k_{r}^{-1} \boldsymbol{K}^{-1} \boldsymbol{q} \right) \boldsymbol{w}_{i}^{E} = -\int_{E} \nabla H \boldsymbol{w}_{i}^{E} = \int_{E} H \nabla \boldsymbol{w}_{i}^{E} - \sum_{j} \int_{\partial E_{j}} H \boldsymbol{w}_{i}^{E} \boldsymbol{\eta}_{j}^{E}$$
(8)

217 where $\boldsymbol{\eta}_{j}^{E}$ is the outward unit normal vector to the edge E_{j} .

218 Defining \boldsymbol{B}^{E} the elemental matrix of terms $B_{i,j}^{E} = \int_{E} \left(k_{r}^{-1,E}\boldsymbol{K}^{-1,E}\boldsymbol{w}_{j}^{E}\right) \cdot \boldsymbol{w}_{i}^{E}$, we obtain (see

219 Younes et al., 2004 for details)

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

221 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*.

222 Using Eq. (7) and properties of w_i^E , the Darcy Eq. (8) becomes

223
$$\sum_{j} B_{i,j}^{E} Q_{j}^{E} = \frac{1}{|E|} \int_{E} H - \frac{1}{|\partial E_{i}|} \int_{\partial E_{i}} H$$
$$= H_{E} - TH_{i}^{E}$$
(10)

224 where H_E is the mean head at the element E and TH_i^E is the mean head at the edge ∂E_i .

225 Inverting Eq. (10) provides the water flux Q_i^E across the edge ∂E_i as

226
$$Q_i^E = \delta_i^E H_E - \sum_j B_{i,j}^{-1,E} T H_j^E$$
(11)

227 where
$$\delta_i^E = \sum_j B_{i,j}^{-1,E}$$
.

228 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*, 230 assuming a steady-state flow $(\partial \theta / \partial t = 0)$ and substituting Eq. (11), yields

231
$$H_E = \sum_i \frac{\delta_i^E}{\delta^E} T H_i^E$$
(12)

232 where
$$\delta^E = \sum_i \delta^E_i$$

233 Hence, the steady-state flux \underline{Q}_{i}^{E} across the edge ∂E_{i} writes

234
$$\underline{Q}_{i}^{E} = \sum_{j} \left(\frac{\delta_{i}^{E} \delta_{j}^{E}}{\delta^{E}} - B_{i,j}^{-1,E} \right) T H_{j}^{E}$$
(13)

• In a second step, a lumped region R_i is constructed around each edge ∂E_i by joining the two nodes of ∂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 *j* and *k* forming the edge *i*. The area of S_i^E is $\frac{|E|}{3}$.

• In a third step, the integration of the transient mass conservation Eq. (1) over the 247 lumped region R_i yields (see Figure 2 for notations):

248
$$\frac{|E|}{3}r_{E}\frac{dTH_{i}^{E}}{dt} + \frac{|E'|}{3}r_{E'}\frac{dTH_{l}^{E}}{dt} + \underline{Q}_{ij}^{E} + \underline{Q}_{li}^{E} + \underline{Q}_{lj}^{E'} + \underline{Q}_{lk}^{E'} = 0$$
(14)

249 where
$$r_E = c(h_E) + S_S \theta(h_E)/\theta_S$$
 is the accumulation coefficient in Richards'
250 equation and \underline{Q}_{ij}^E the interior flux, evaluated using the RT0 approximation of the

251 velocity inside the element E given by Eq. (7), which yields

252
$$\underline{Q}_{ij}^{E} = \frac{1}{3} \left(\underline{Q}_{j}^{E} - \underline{Q}_{i}^{E} \right)$$
(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

257
$$\begin{cases} Q_i^E + Q_i^{E'} = 0\\ Q_i^E = \sum_j \left(\frac{\delta_i^E \delta_j^E}{\delta^E} - B_{i,j}^{-1,E}\right) T H_j^E - \frac{|E|}{3} r_E \frac{dT H_i^E}{dt} \end{cases}$$
(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 $(TH_i = TH_i^E = TH_i^{E'})$. The obtained system is highly nonlinear since the local matrix **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.

267 *3.2 Spatial discretization of the flow in the presence of a fracture*

Let's consider a fracture k of length ℓ_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.



273

Figure 3: Schematic representation of the one-dimensional fracture k, which coincides with

275 the edge *i* shared by the matrix elements *E* and *E'*. The flux Q_i^E (respectively $Q_i^{E'}$)

276 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,

279
$$q^{k} = q_{1}^{k} w_{1}^{k} + q_{2}^{k} w_{2}^{k}$$
(17)

280 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 $w_2^k = \frac{x}{e_k\ell_k}$

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

282 The mass conservation Eq. (1) integrated over the fracture k of length ℓ_k and aperture e_k 283 yields

284
$$e_k \ell_k r_k \frac{dTH^k}{dt} + q_1^k + q_2^k - Q_i^E - Q_i^{E'} = 0$$
(18)

285 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 matrixfracture exchange.

288 The variational formulation of the Darcy law Eq. (2) on the fracture k writes

289
$$\sum_{j} q_{j}^{k} \int_{0}^{\ell_{k}} w_{i}^{k} w_{j}^{k} = -k_{r}^{k} \mathbf{K}_{f}^{k} \int_{0}^{\ell_{k}} (\nabla H) w_{i}^{k}$$
(19)

290 Integration by part leads to

291
$$\sum_{j} q_{j}^{k} \int_{0}^{\ell_{k}} w_{i}^{k} w_{j}^{k} = \frac{k_{r}^{k} \mathbf{K}_{f}^{k}}{e_{k}} \left(TH^{k} - NH_{i}^{k} \right)$$
(20)

292 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
(see Koohbor *et al.*, 2020) yields

295
$$q_i^k = e_k k_r^k \frac{2K_f^k}{\ell_k} \left(TH^k - NH_i^k \right)$$
(21)

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

299
$$\sum_{j} \left(\frac{\delta_{i}^{E} \delta_{j}^{E}}{\delta^{E}} - B_{i,j}^{-1,E} \right) TH_{j}^{E} + \sum_{j} \left(\frac{\delta_{i}^{E'} \delta_{j}^{E'}}{\delta^{E'}} - B_{i,j}^{-1,E'} \right) TH_{j}^{E'} - e_{k} k_{r}^{k} \frac{2K_{f}^{k}}{\ell_{k}} \left(2TH_{i}^{E} - NH_{1}^{k} - NH_{2}^{k} \right) \\ - \left(\frac{|E|}{3} r_{E} + \frac{|E'|}{3} r_{E'} + e_{k} \ell_{k} r_{k} \right) \frac{dTH_{i}^{E}}{dt} = 0$$
(22)

300 To close the system of Eq. (22), the mass conservation is written at each intersection of 301 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

304
$$\sum_{k} e_{k} k_{r}^{k} \frac{2K_{f}^{k}}{\ell_{k}} \left(TH^{k} - NH_{i}^{k} \right) = 0$$
(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 $(NH_i = NH_i^k)$ 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.

310 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:

312
$$C\left(\frac{\partial\theta}{\partial t} + \nabla \boldsymbol{.}\boldsymbol{q}\right) + \theta \frac{\partial C}{\partial t} + \boldsymbol{q}\nabla C - \nabla \boldsymbol{.}\left(\boldsymbol{D}\nabla C\right) = 0$$
(25)

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

315
$$\begin{cases} \theta \frac{\partial C}{\partial t} + q \nabla C + \nabla . \tilde{q} = 0\\ \tilde{q} = -D \nabla C \end{cases}$$
(26)

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

319
$$\tilde{\boldsymbol{q}} = \sum_{j} \tilde{\boldsymbol{Q}}_{j}^{E} \boldsymbol{w}_{j}^{E}$$
(27)

320 where $\tilde{Q}_{j}^{E} = \int_{\partial E_{j}} \tilde{q}_{d} \cdot \eta_{j}^{E}$ is the dispersive flux across the edge ∂E_{j} of the element E.

321 The variational formulation of Eq. (26) is written as

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

323 which can take the following form

324
$$\sum_{j} \tilde{B}_{i,j}^{E} \tilde{Q}_{j}^{E} = C_{E} - TC_{i}^{E}$$
(29)

325 where C_E is the mean concentration at the element E and TC_i^E is the trace of concentration 326 at the edge ∂E_i of the element E and \tilde{B} is the elemental matrix of terms 327 $\tilde{B}_{i,j}^E = \int_E (D_E^{-1} w_j^E) w_i^E$ 328 Inverting Eq. (29) yields the dispersive flux across ∂E_i as

329
$$\tilde{Q}_{i}^{E} = \sum_{j} \tilde{\boldsymbol{B}}_{i,j}^{-1,E} \left(C_{E} - TC_{j}^{E} \right)$$
(30)

An upwind lumped MFE scheme is used to avoid unphysical oscillations caused by the
hyperbolic advection part of the transport equation. The main steps of this scheme are as
follows:

• In a first step, both advective and transient terms are removed from the first equation in the system of Eq. (26), yielding a steady-state dispersive flux \tilde{Q}_i^E expressed by (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)

337 with
$$\tilde{\delta}_i^E = \sum_j \tilde{B}_{i,j}^{-1,E}$$
 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):

$$340 \qquad \left\{\frac{|E|}{3}\theta_E\frac{\partial TC_i^E}{\partial t} + Q_{ij}^ETC_{ij}^E + Q_{ik}^ETC_{ik}^E - \left(Q_{ij}^E + Q_{ik}^E\right)TC_i^E - \underline{\tilde{Q}}_i^E\right\} + \left\{\right\}' = 0 \qquad (32)$$

341 where
$$Q_{ij}^E = \frac{1}{3} \left(Q_j^E - Q_i^E \right)$$
 is the interior flux between edges *i* and *j* (see Eq. (15)).

342 The interior concentration TC_{ij}^{E} is calculated using the upstream edge concentration 343 as:

344
$$TC_{ij}^{E} = \tau_{ij}^{E}TC_{i}^{E} + \left(1 - \tau_{ij}^{E}\right)TC_{j}^{E}$$
(33)

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

$$\begin{cases}
Qt_{i}^{E} + Qt_{i}^{E'} = 0 \\
Qt_{i}^{E} = \sum_{j} \left(\frac{\tilde{\delta}_{i}^{E} \tilde{\delta}_{j}^{E}}{\tilde{\delta}^{E}} - \tilde{B}_{i,j}^{-1,E} \right) TC_{j}^{E} + Q_{ij}^{E} \left(1 - \tau_{ij}^{E} \right) \left(TC_{i}^{E} - TC_{j}^{E} \right) + Q_{ik}^{E} \left(1 - \tau_{ik}^{E} \right) \left(TC_{i}^{E} - TC_{k}^{E} \right) - \theta_{E} \frac{|E|}{3} \frac{\partial TC_{i}^{E}}{\partial t} \\
350 \qquad (34)
\end{cases}$$

351 3.4 Spatial discretization of the advection-dispersion transport equation through a fracture

352 Let's consider a fracture k of length ℓ_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

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

356 where α_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.

359 Similarly to Eq. (21), the dispersive flux \tilde{q}_i^k at the extremity i = 1, 2 of the fracture k writes

360
$$\tilde{q}_i^k = \frac{2e_k D_k}{\ell_k} \left(TC^k - N\tilde{C}_i \right)$$
(36)



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

373 $N\tilde{C}_{i} = \frac{\sum_{l} \frac{e_{l}}{\ell_{l}} D_{l} T C^{l}}{\sum_{l} \frac{e_{l}}{\ell_{l}} D_{l}}$

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

(38)

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)

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

378
$$\theta_k e_k \int_0^{\ell_k} \frac{\partial C}{\partial t} + e_k \int_0^{\ell_k} \nabla \cdot (\boldsymbol{q}C) - e_k \int_0^{\ell_k} C \nabla \cdot \boldsymbol{q} + e_k \int_0^{\ell_k} \nabla \cdot \tilde{\boldsymbol{q}} - Q t_i^E - Q t_i^{E'} = 0$$
(40)

379 The calculation of the different integrals yields

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

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

382
$$C_i^{k,*} = \lambda_i^k N C_{i,in}^k + \left(1 - \lambda_i^k\right) \overline{NC}_{i,out}$$
(42)

in which $NC_{i,in}^{k} = TC^{k}$ is the interior concentration and the parameter λ_{i}^{k} is used to select the upstream concentration, it depends on the sign of q_{i}^{k} as

385
$$\lambda_i^k = \begin{cases} 1 & \text{if} \quad q_i^k \ge 0\\ 0 & \text{if} \quad q_i^k < 0 \end{cases}$$
(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 $\overline{NC}_{i,out}$. 389 To calculate $\overline{NC}_{i,out}$, we use the contaminant conservation at the node *i*, shared by *l* fractures, 390 which writes

391
$$\sum_{k=1}^{l} q_i^k C_i^{k,*} = 0$$
 (44)

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

$$\overline{NC}_{i,out} = \frac{\sum_{k=1}^{l} q_i^k \lambda_i^k T C^k}{\sum_{k=1}^{l} q_i^k \left(\lambda_i^k - 1\right)}$$
(45)

394 Note that the number of unknowns for the transport system to be solved does not depend on 395 the number of fractures in the domain. Indeed, the final transport system has the concentration 396 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 the edge matrix and at the fracture equal at are $\left(TC_i = TC_i^E = TC_i^{E'} = TC^k\right).$ 404

405 3.5 The temporal discretization of the nonlinear flow-transport system

406 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

409
$$F(t, y, y') = 0$$
 (46)

410 Where
$$\mathbf{y} = \left[\left(TH_i \right)_{i=1,\dots,nb_edges}, \left(NH_i \right)_{i=1,\dots,nb_nodefractures}, \left(TC_i \right)_{i=1,\dots,nb_edges} \right]$$
 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.

416 For the time discretization, we use high-order methods, which are known to be more efficient 417 and require less effort in the nonlinear solver compared to the lowest order methods (Farthing 418 et al., 2002). An efficient automatic time-stepping scheme is employed to improve the 419 computational efficiency while maintaining accuracy (Tocci et al., 1997; Kavetski et al., 420 2001). The time integration is performed with the DASPK time solver, which uses the 421 preconditioned Krylov iterative method to solve the linear systems arising at each time step. 422 DASPK is based on the Fixed Leading Coefficient Backward Difference Formulas 423 (FLCBDF), which has good stability properties and is well adapted for time integration of 424 stiff problems (Kees and Miller, 2002). The nonlinear problem is linearized using the Newton 425 method with a numerical approximation of the Jacobian matrix. To improve efficiency, the 426 Jacobian is reused for several time steps and is calculated by the solver only when necessary. 427 Furthermore, the column grouping technique (Hindmarsh, 1982) is employed to reduce the 428 computational time for the evaluation of the Jacobian matrix by perturbing variables by 429 group, knowing the structure and sparsity of the Jacobian.

430 During calculation, the order (up to fifth order) of the time discretization and the time step 431 size are adapted to improve efficiency while the relative and absolute convergence criteria are 432 maintained under a fixed tolerance (10^{-6} in this work).

433 **4. Numerical experiments**

434 In this section, three test problems dealing with flow and mass transport in saturated and 435 unsaturated fractured porous media are simulated to investigate the robustness of the new 436 MFE code. The first test case deals with flow and transport in a saturated porous medium 437 involving a single fracture. This test case is used to validate the developed 1D-2D MFE code 438 against the solution obtained with Comsol multiphysics 1D-2D model. Comosl uses the 439 standard finite element (FE) method and an adaptive time stepping scheme. The test problem 440 is also simulated with a 2D-2D model where 2D triangular elements are employed for the 441 spatial discretization of both the matrix and the fractures continua using a very fine mesh in 442 order to correctly discretize the fracture branches with a small aperture. We use the advanced 443 2D-2D DG model developed by Younes et al. (2021), based on the discontinuous Galerkin 444 (DG) finite element and the multipoint flux approximation methods and high-order time 445 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.

453

454

455 4.1 Fractured saturated quarter-five-spot problem

We consider a quadratic 2D domain (quarter-five-spot configuration) of size $[0,1m] \times [0,1m]$ 456 457 with impermeable walls except at the lower-left and the upper-right corners. The source at the 458 lower-left corner is represented by a boundary flux $q_{ini} = 10^{-3} \,\mathrm{m/s}$ at $(0 \le x \le 0.03m) \cap (y=0) \cup (x=0) \cap (0 \le y \le 0.03m)$. The sink at the right-upper corner is 459 460 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 461 homogeneous material with a diagonal fracture of 1mm aperture, located between 462 (0.2m, 0.2m) and (0.8m, 0.8m). The hydraulic and transport properties of the porous matrix 463 464 and the fracture continuum are depicted in Table 1. The initial conditions correspond to a 465 domain free from pollutants. The simulation is performed for a time of 3456s.

466

	<i>K</i> _s (m/s)	<i>S_s</i> (1/ <i>m</i>)	$ heta_{s}$	$\alpha_L(m)$	$\alpha_{T}(\mathrm{m})$	$D_m (m^2/s)$
Matrix	10-6	10-10	0.4	0.0	0.0	10-6
Fracture	10-3	10-10	0.4	0.0	0.0	10-6

467

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



470

471 Figure 5: Concentration distribution for the fractured saturated quarter-five-spot problem.
472 Results of the new 1D-2D MFE model (dashed lines), the 1D-2D Comsol FE model (purple
473 lines), and 2D-2D DG model (color map).

474 The problem is simulated with the new 1D-2D MFE model as well as with the 1D-2D Comsol 475 FE model and the 2D-2D DG model of Younes et al. (2021). In the latter, the hydraulic and 476 transport parameters used for the fractures in the 1D-2D approach are attributed to the 2D 477 triangular elements located inside the fractures. The 2D-2D DG model is used with a fine 478 mesh with local mesh refinement around fractures. The three models were used with the MOL 479 and a variable high-order (up to 5) time integration BDF method. Figure 5 shows that the 480 three models yield almost similar concentration distributions, which demonstrates the validity 481 of the developed 1D-2D MFE model for simulating flow and transport in fractured saturated 482 porous media.

483

484 *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 489 300cm×200 cm with a water table located at 65cm from the bottom. Initial conditions 490 correspond to a hydrostatic pressure distribution and a zero concentration in the domain. 491 Boundary conditions are as follows: contaminated water is infiltrated under a constant flux of 492 335cm/day over the first 50cm of the soil surface. The lower 65cm of the right side of the 493 domain has a Dirichlet boundary condition with a fixed head of 65cm. A no-flow boundary is 494 prescribed for the rest of the boundaries. The homogeneous porous medium includes an 495 inclined fracture of 1cm aperture and 2m length, located near the infiltration zone. The 496 hydraulic and transport parameters are depicted in Table 2.

497

	<i>K</i> _s (m/s)	<i>S</i> _s (1/m)	$ heta_{s}$	$ heta_r$	α (1/m)	п	α_L (m)	α_T (m)	D_m (m ² /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

498 Table 2: Hydraulic and transport parameters for the problem of infiltration of contaminated
499 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).



508 Figure 6: Water content (a) and concentration (b) distributions for the problem of infiltration 509 of contaminated water in a fractured unsaturated-saturated porous medium. Results of the new 510 1D-2D MFE model (dashed lines), 2D-2D DG model (purple lines), and 2D-2D FE Comsol 511 model (color map).

512

513 A more in-depth comparison is then performed between the new 1D-2D MFE model and the 514 2D-2D DG model. To this aim, the fluid and contaminant mass fluxes at the outlet are 515 calculated with both models over the simulation time of 55 hours. The results of the Figure 7 516 show that the outlet fluid flux is almost constant after around 15 hours which indicates that an 517 almost steady state water content distribution is reached at this time. A first contaminant front, 518 caused by the fast mobility of the contaminated water through the fractures, is observed in the 519 Figure 7 after around 10 hours. A second slower and more dispersed contaminant front was 520 occurred, which was caused by the transport of the contaminant through the rock matrix. The

521 results of Fgure 7 show a very good agreement between the 1D-2D MFE and the 2D-2D DG 522 models for both fluid and contaminant outlet mass fluxes. These results demonstrate the 523 validity of the new 1D-2D MFE model for the simulation of flow and transport in fractured 524 unsaturated porous media.



525

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.

529

530 *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 4×10^{-4} cm/s. The simulation is performed for a period of 2×10^5 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.



544

545

546

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

548 (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).

550

549

	K _s (cm/s)	<i>S</i> _s (1/cm)	$ heta_{s}$	$ heta_r$	α (1/cm)	п
Matrix	5.25 10-6	10 ⁻⁸	0.34	0.01	0.0139	1.6
Fracture	1.16 10 ⁻²	10-8	0.8	0.001	0.0139	1.6

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

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

554 The simulation of this last test case with the 2D-2D FE Comsol model encountered several 555 convergence issues because of the initial high dry conditions. Indeed, the initial dry conditions 556 are responsible of the appearance of several unphysical oscillations leading to the non-557 convergence of the nonlinear flow-transport model. These difficulties are avoided with the 558 2D-2D DG model thanks to the incorporated advanced numerical methods (see Younes et al. 559 (2021) for more details). As a consequence, the results of the new 1D-2D MFE model are 560 only compared to those of the 2D-2D DG model. The final water content distribution obtained 561 with the two models is depicted in Figure 8. Similar distributions are obtained with the two 562 models. As expected, the infiltrated water invades the fracture network, and high water 563 saturation is observed in almost all fracture branches (Figure 8) because of their high 564 saturated hydraulic conductivity, which is around 2200 times higher than that of the matrix 565 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 566 fractures are zero $(\alpha_L^m = \alpha_T^m = \alpha_L^f = 0)$, and a small molecular diffusion occurs in both 567 continua $(D_m^m = D_m^f = 10^{-6} cm^2/s)$. In the second configuration, a more significant dispersion 568 569 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 570 $\alpha_L^f = 5m$. The molecular diffusion in both continua is $10^{-5} cm^2/s$. For the 1D-2D model, the 571 domain is discretized using 15400 triangles for the matrix continuum and 853 lines for the 572 573 fracture branches without any constraint on the size of mesh elements next to the fractures 574 (Figure 9a). The 2D-2D model is used on a fine mesh of 76000 elements with local mesh 575 refinement in the fractures in order to correctly discretize the flow and transport through the 576 fracture branches with a small aperture of 1cm (Figure 9b).



577

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

582 Two versions of the 1D-2D MFE model are employed for the simulations: (i) the upwind 583 scheme described above and (ii) a centered scheme where no upwinding is used for the 584 advection operator in the matrix nor in the fractures. The results of Figure 10 show that the 585 centered scheme provides similar results to the upwind scheme in the case of high dispersion 586 (Figures 10d and 10e). However, in the case of advection-dominated transport, the centered 587 scheme fails to provide accurate results and generates strong unphysical concentrations both 588 in the matrix and in the fracture continuum (Figure 10b). The results of the upwind 1D-2D 589 MFE model are exempted from unphysical oscillations (negative concentration are 590 completely avoided) for both advection dominated and advection-dispersion configurations 591 which demonstrates the robustness of the developed upwind 1D-2D MFE scheme. 592 Furthermore, the solution of the upwind 1D-2D MFE model is in good agreement with the 593 solution of the 2D-2D DG model both in the case of advection-dominated transport (Figure 594 10a vs 10c) and in the case of advection-dispersion transport (Figure 10d vs. 10f).

595 The advantage of using a high-order time discretization scheme is investgated by comparison 596 against the first-order (conventional) scheme. The simulation using the upwind 1D-2D MFE 597 model with a first-order time discretization scheme requires 20902 time steps and needs 598 6566s, whereas the high-order scheme requires only 3401 time steps and needs 375s. Thus, 599 the high-order method is around four times faster than the first order method. Concerning the 600 efficiency of the 1D-2D approach in comparison to the 2D-2D approach, the 2D-2D DG 601 model required 5259s for the whole simulation, whereas the new 1D-2D MFE model requires 602 only 375s. Thus, the new 1D-2D MFE model is around 15 times more efficient than the 2D-

- 603 2D DG model, which highlights the great benefit of robust and accurate 1D-2D models to
- 604 simulate flow and transport processes in unsaturated and saturated fractured porous media.

605



607 **Figure 10**: Infiltration of contaminated water in a fractured initially dry soil: Results of the upwind 1D-2D MFE model, the centered 1D-2D

608 MFE model and the 2D-2D DG model in the case of advection dominated transport $\left(\alpha_L^m = \alpha_T^m = \alpha_L^f = 0 \text{ and } D_m^m = D_m^f = 10^{-6} \text{ } cm^2/s\right)$ and in the 609 case of advection-dispersion transport $\left(\alpha_L^m = \alpha_L^f = 5m, \alpha_T^m = 2m, \text{ and } D_m^m = D_m^f = 10^{-5} \text{ } cm^2/s\right)$.

610

611 **5. Conclusion**

612 A new model has been developed for nonlinear flow and transport in unsaturated fractured 613 porous media with implicit matrix-fracture and fracture-fracture fluid and contaminant 614 exchanges. The model is based on the DFM approach, which describes fractures and matrix 615 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 616 617 both the matrix and the fracture continua. The MFE method avoids the constraints on the 618 mesh size next to the fractures and allows to approximate the matrix-fracture and fracture-619 fracture exchange without any transfer functions. An upwind scheme is employed to avoid 620 unphysical oscillations in the case of advection dominant transport. The time integration is 621 performed with variable high-order methods via the MOL. An efficient automatic time-622 stepping scheme is used to improve the computational efficiency while maintaining accuracy 623 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 1D2D 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.

638 The last test case is a challenging problem dealing with flow and transport in an initially dry 639 soil containing a fracture network. For this problem, the 2D-2D FE Comsol model 640 encountered several convergence issues because of the initial high dry soil conditions. The 641 problem has been simulated using the 1D-2D MFE model using upwind and centered 642 schemes. The results show that both schemes yield accurate results in the case of high 643 dispersion. However, in the case of advection-dominated transport, only the upwind scheme 644 provides stable results. The solution of the upwind 1D-2D MFE model is in good agreement 645 with the solution of the 2D-2D DG model both in the case of advection-dominated transport 646 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.

- 651
- 652
- 653
- 654

REFERENCES

- Wireman, M., 2003. EPA update: Characterization and management of ground water
 resources in fractured-rock hydrogeologic settings. Ground Water Monitoring &
 Remediation, 23(3), 34-40. doi:10.1111/j.1745-6592.2003.tb00681.x.
- Kavouri, K.P., Karatzas, G.P., Plagnes, V., 2017. A coupled groundwater-flow-modelling and
 vulnerability-mapping methodology for karstic terrain management. Hydrogeol J 25,
 1301–1317. https://doi.org/10.1007/s10040-017-1548-6
- Berkowitz, B. 2002. Characterizing flow and transport in fractured geological media: a
 review. Advances in Water Resources, 25(8), 861–884. doi:10.1016/S03091708(02)00042-8.
- Brutz, M., and Rajaram, H., 2017. Coarse-scale particle tracking approaches for contaminant
 transport in fractured rock. Applied Mathematical Modelling, 41, 549-561. doi:
 10.1016/j.apm.2016.09.023.
- Klammler, H., Hatfield, K., Newman, M. A., Cho, J., Annable, M. D., Parker, B. L., Cherry,
 J. A., and Perminova, I., 2016. A new device for characterizing fracture networks and
 measuring groundwater and contaminant fluxes in fractured rock aquifers. Water
 Resources Research, 52(7), 5400-5420. doi: 10.1002/2015WR018389.
- Follin, S., and Stigsson, M., 2014. A transmissivity model for deformation zones in fracture
 crystalline rock and its possible correlation to in situ stress at the proposed high-level
 nuclear waste repository site at Forsmark, Sweden. Hydrogeology Journal, 22(2), 299311. doi:10.1007/s10040-013-1078-9.
- Mattila, J., and Tammisto, E., 2012. Stress-controlled fluid flow in fractures at the site of a
 potential nuclear waste repository, Finland. Geology, 40(4), 299-302. doi:
 10.1130/G32832.1.
- Li, X., Zhang, D., Li, S., 2015. A multi-continuum multiple flow mechanism simulator for
 unconventional oil and gas recovery. Journal of Natural Gas Science and Engineering
 26, 652–669. <u>https://doi.org/10.1016/j.jngse.2015.07.005</u>
- Shen, W., Xu, Y., Li, X., Huang, W., Gu, J., 2016. Numerical simulation of gas and water
 flow mechanism in hydraulically fractured shale gas reservoirs. Journal of Natural Gas
 Science and Engineering 35, 726–735. <u>https://doi.org/10.1016/j.jngse.2016.08.078</u>
- Berre, I., Doster, F. & Keilegavlen, E. Flow in Fractured Porous Media: A Review of
 Conceptual Models and Discretization Approaches. Transp Porous Med 130, 215–236
 (2019). <u>https://doi.org/10.1007/s11242-018-1171-6</u>
- Koohbor, B.; Fahs, M.; Hoteit, H.; Doummar, J.; Younes, A.; Belfort, B. An Advanced
 Discrete Fracture Model for Variably Saturated Flow in Fractured Porous Media. Adv.
 Water Resour. 2020, 140, 103602
- Durlofsky, L.: Numerical calculation of equivalent grid block permeability tensors for
 heterogenous porous media. Water Resour. Res. 27(5), 699–708 (1991)
- Liu, R., Li, B., Jiang, Y., Huang, N.: Review:Mathematical expressions for estimating
 equivalent permeability of rock fracture networks. Hydrogeol. J. 24(7), 1623–1649
 (2016)
- Jourde, H., Cornaton, F., Pistre, S., Bidaux, P., 2002. Flow behavior in a dual fracture
 network. Journal of Hydrology 266, 99–119. <u>https://doi.org/10.1016/S0022-</u>
 <u>1694(02)00120-8</u>
- Kordilla, J., Sauter, M., Reimann, T., Geyer, T., 2012. Simulation of saturated and
 unsaturated flow in karst systems at catchment scale using a double continuum
 approach. Hydrol. Earth Syst. Sci. 16, 3909–3923. <u>https://doi.org/10.5194/hess-16-3909-2012</u>
- 703 Kuhlman, K.L., Malama, B., Heath, J.E., 2015. Multiporosity flow in fractured low-

- 704 permeability rocks. Water Resources Research 51, 848–860.
- 705 <u>https://doi.org/10.1002/2014WR016502</u>
- Wu, Y.-S., Liu, H.H., Bodvarsson, G.S., 2004. A triple-continuum approach for modeling
 flow and transport processes in fractured rock. Journal of Contaminant Hydrology 73,
 145–179. <u>https://doi.org/10.1016/j.jconhyd.2004.01.002</u>
- Noorishad, J., and M. Mehran (1982), An upstream finite element method for solution of
 transient transport equation in fractured porous media, Water Resour. Res., 18(3), 588 –
 596.
- Baca, R., R. Arnett, and D. Langford (1984), Modeling fluid flow in frac tured porous rock
 masses by finite element techniques, Int. J. Numer. Methods Fluids, 4, 337 348.
- Granet S, Fabrie P, Lemmonier P, Quitard M. A single phase flow simulation of fractured
 reservoir using a discrete representation of fractures. In: Proceedings of the 6th
 European conference on the mathematics of oil recovery (ECMOR VI), September 8–
 11, Peebles, Scotland, UK; 1998.
- Hoteit H., Firoozabadi A. (2008) An efficient numerical model for incompressible two-phase
 flow in fractured media, Adv. Water Resour. 31, 891–905.
- Flemisch B, Inga Berre, Wietse Boon, Alessio Fumagalli, Nicolas Schwenck, Anna Scotti,
 Ivar Stefansson, Alexandru Tatomir, Benchmarks for single-phase flow in fractured
 porous media, Advances in Water Resources, Volume 111, 2018, Pages 239-258, ISSN
 0309-1708, <u>https://doi.org/10.1016/j.advwatres.2017.10.036</u>.
- Martin, V., Jaffré, J., Roberts, J.E., 2005. Modeling fractures and barriers as interfaces for
 flow in porous media. SIAM J. Sci. Comput. 26 (5), 1667–1691.
- Hoteit H, Firoozabadi A. Multicomponent fluid flow by discontinuous Galerkin and mixed
 methods in unfractured and fractured media. Water Resour Res 2005;41(11):W11412.
- Hoteit H, Firoozabadi A. Compositional modeling of discrete-fractured media without
 transfer functions by the discontinuous Galerkin and mixed methods. SPE J
 2006;11(3):341–52.
- Raviart PA, Thomas JM. A mixed finite element method for second order elliptic problems, in
 Mathematical Aspects of Finite Element Method, Lecture Notes in Mathematics, 1977;
 Vol. 606, Springer, New York, 292-315.
- Chavent G, J. Jaffré (1986), Mathematical models and finite elements for reservoir
 simulation, North-Holland, Amsterdam.
- Younes, A., Ackerer, P., Delay, F. 2010. Mixed finite element for solving 2D diffusion-type
 equations. Reviews of Geophysics, 48(1).
- Durlofsky, L. (1994), Accuracy of mixed and control volume finite element approximations to
 darcy velocity and related quantities, Water Resour. Res., 30(4), 965 974.
- Younes, A., Ackerer, P., Lehmann, F., 2006. A new mass lumping scheme for the mixed
 hybrid finite element method. International Journal for Numerical Methods in
 Engineering 67(1), 89-107.
- Belfort, B., Ramasomanan, F., Younes, A., Lehmann, F., 2009. An efficient Lumped Mixed
 Hybrid Finite Element Formulation for variably saturated groundwater flow. Vadose
 Zone Journal. 8, 352-362.
- Fahs, M., Younes, A., Lehmann, F., 2009. An easy and efficient combination of the Mixed
 Finite Element Method and the Method of Lines for the resolution of Richards'
 Equation. Environmental Modelling & Software 24(9), 1122-1126.
- Younes, A., Fahs, M., Ahmed, S., 2009. Solving density driven flow problems with efficient
 spatial discretizations and higher-order time integration methods. Advances in Water
 Resources 32(3), 340-352.

- Fahs, M., Younes, A., Lehmann, F., 2009. An easy and efficient combination of the Mixed
 Finite Element Method and the Method of Lines for the resolution of Richards'
 Equation. Environmental Modelling & Software 24(9), 1122-1126.
- van Genuchten, M.Th., 1980. A Closed-form Equation for Predicting the Hydraulic
 Conductivity of Unsaturated Soils. Soil Science Society of America Journal 44(5), 892898.
- Mualem, Y., 1976. A new model for predicting the hydraulic conductivity of unsaturated
 porous media. Water Resources Research 12, 513–522.
- Younes, A., Ackerer, P., Chavent, G., 2004. From mixed finite elements to finite volumes for
 elliptic PDE in 2 and 3 dimensions. International Journal for Numerical Methods in
 Engineering, 59, 365–388.
- Farthing, M.W., Kees, C.E., Miller, C.T., 2002. Mixed finite element methods and higher order temporal approximations. Advances in Water Resources 25, 85-101.
- Tocci, M.D., Kelly, C.T., Miller, C.T., 1997. Accurate and economical solution of the
 pressure-head form of Richards' equation by the method of lines. Advances in Water
 Resources 20, 1–14.
- Kavetski, D., Binning, P., Sloan, S.W., 2001. Adaptative backward Euler time stepping with
 truncation error control for numerical modelling of unsaturated fluid flow. International
 Journal for Numerical Methods in Engineering 53,1301–1322.
- Kees, C.E., Miller, C.T., 2002. Higher order time integration methods for two-phase flow.
 Advances in Water Resources 25(2), 159-177.
- Hindmarsh, A.C., 1982. Large ordinary differential equation systems and software. IEEE
 Control System Magazine 2, 24-30.
- Younes, A., Koohbor, B., Belfort, B., Ackerer, P., Doummar, J., Fahs, M., 2021. Modeling
 variable-density flow in saturated-unsaturated porous media: An advanced numerical
 model. Advances in Water Resources, Volume 159, January 2022, 104077.
 10.1016/j.advwatres.2021.104077
- Vauclin, M., Khanji, D., Vachaud, G., 1979. Experimental and numerical study of a transient,
 two-dimensional unsaturated-saturated water table recharge problem. Water Resour.
 Res. 15, 1089–1101. https://doi.org/10.1029/WR015i005p01089
- Zha, Y., Yang, J., Yin, L., Zhang, Y., Zeng, W., Shi, L., 2017. A modified Picard iteration
 scheme for overcoming numerical difficulties of simulating infiltration into dry soil.
 Journal of Hydrology 551, 56–69.
- 785