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

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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.

47        Two test problems dealing with flow and mass transport in saturated and unsaturated fractured  
48        porous media are simulated to show the validity of the new model by comparison against (i) a  
49        1D-2D Comsol finite element model and (ii) a 2D-2D Discontinuous Galerkin (DG) model  
50        where both fractures and matrix continua are discretized with small 2D mesh elements. The  
51        robustness and efficiency of the developed 1D-2D MFE model are then investigated for a  
52        challenging problem dealing with infiltration of contaminated water into an initially dry soil  
53        involving a fracture network.

54        The new model yields stable results for advection-dominated and advection-dispersion  
55        transport configurations. Further, the results of the 1D-2D MFE model are in very good  
56        agreement with those of the 2D-2D DG model for both configurations. The simulation of  
57        infiltration of contaminated water into a dry fractured soil shows that the 1D-2D MFE model  
58        is within 15 times more efficient than the 2D-2D DG model, which confirms the high benefit  
59        of using robust and efficient DFM models for the simulation of flow and transport in fractured  
60        porous media.

61  
62        **Key words:**

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

## 65 **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  
79 equivalent permeability of the porous medium, which depends on the properties of the  
80 fractures and the fracture network (Durlafsky, 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

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

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

112 pressure at the gridcell interfaces as degrees of freedom (DOF), and hence, the cross-flow  
113 equilibrium can be directly assumed across the fractures (Hoteit and Firoozabadi, 2008). In  
114 this way, the matrix pressure at an element edge and the pressure at the fracture, which  
115 coincides with that edge, are assumed to be equal. As a consequence, no constraints are  
116 required for the mesh discretization near the fractures (Hoteit and Firoozabadi, 2008). This  
117 powerful feature is extended in this work by developing a fully MFE model for both  
118 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,  
121 with MFEs, the flux and the pressure unknowns are approximated simultaneously. The MFE  
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 (Durlafsky, 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.

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

## 168 2. Governing Equations

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

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

174 and the Darcy-Buckingham law:

$$175 \quad \mathbf{q} = -k_r \mathbf{K} \nabla H \quad (2)$$

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 [ $L^{-1}$ ],  $\theta$  is the current water content [ $L^3 L^{-3}$ ],  $\theta_s$  is the saturated water  
 178 content [ $L^3 L^{-3}$ ],  $H = h + y$  is the freshwater head [L],  $h$  is the pressure head [L],  $y$  is the  
 179 upward vertical coordinate [L],  $t$  is the time [T],  $\mathbf{q}$  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 [ $LT^{-1}$ ],  $\rho$  is the fluid



181 density  $[ML^{-3}]$ ,  $g$  is the gravity acceleration  $[LT^{-2}]$ ,  $\mu$  is the fluid dynamic viscosity  $[ML^{-1}T^{-1}]$  and  $\mathbf{k}$  is the permeability of the rock matrix as a tensor, or that of the fracture, as a scalar  
 182  $[L^2]$ .

184 The transport of contaminants in the unsaturated porous matrix and through the unsaturated  
 185 fractures is ruled by the advection-dispersion equation:

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

187 where  $C$  [-] is the relative concentration [-] and  $\mathbf{D}$  is the dispersion tensor given by:

$$188 \quad \mathbf{D} = D_m \mathbf{I} + (\alpha_L - \alpha_T) \mathbf{q} \otimes \mathbf{q} / |\mathbf{q}| + \alpha_T |\mathbf{q}| \mathbf{I} \quad (4)$$

189 In which  $\alpha_L$  and  $\alpha_T$  are the longitudinal and transverse dispersivities [L],  $D_m$  is the pore  
 190 water diffusion coefficient  $[L^2T^{-1}]$  and  $\mathbf{I}$  is the unit tensor.

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

$$193 \quad S_e = \frac{\theta(h) - \theta_r}{\theta_s - \theta_r} = \begin{cases} \frac{1}{(1 + |\alpha h|^n)^m} & h < 0 \\ 1 & h \geq 0 \end{cases} \quad (5)$$

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

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

198

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

199

The nonlinear system (1)-(6) is solved numerically on (i) unstructured triangular 2D elements

200

for the porous matrix and (ii) linear 1D elements for fracture branches. All hydraulic and

201

transport parameters in the system (1)-(6) are defined elementwise, and therefore, they can be

202

different for each matrix or fracture element.

203

### 3. The fully MFE numerical model

204

In this session, we recall the main stages for developing a robust MFE formulation for the

205

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  $\mathbf{q}$  inside each triangular element  $E$  is approximated

208

using the linear Raviart-Thomas basis functions (see Figure 1):

209

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

210

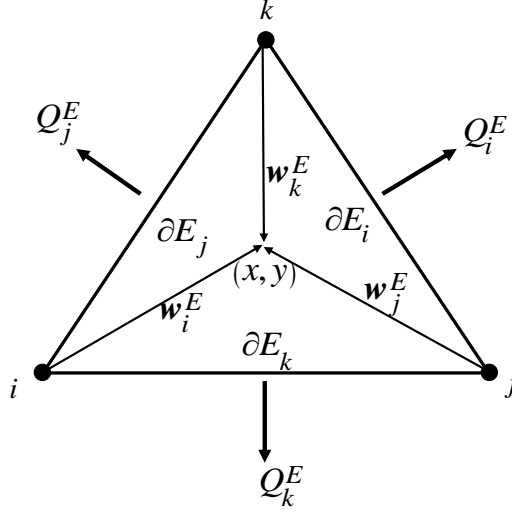
where  $Q_j^E$  is the flux across the edge  $\partial E_j$  of  $E$  and  $\mathbf{w}_j^E = \frac{1}{2|E|} \begin{pmatrix} x - x_j^E \\ y - y_j^E \end{pmatrix}$  is the Raviart-

211

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  $\partial E_j$  of  $E$  and  $|E|$  the area of  $E$ .



213

214 **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

$$216 \quad \int_E (k_r^{-1} \mathbf{K}^{-1} \mathbf{q}) \cdot \mathbf{w}_i^E = - \int_E \nabla H \cdot \mathbf{w}_i^E = \int_E H \nabla \cdot \mathbf{w}_i^E - \sum_j \int_{\partial E_j} H \mathbf{w}_i^E \cdot \boldsymbol{\eta}_j^E \quad (8)$$

217 where  $\boldsymbol{\eta}_j^E$  is the outward unit normal vector to the edge  $E_j$ .

218 Defining  $\mathbf{B}^E$  the elemental matrix of terms  $B_{i,j}^E = \int_E (k_r^{-1,E} \mathbf{K}^{-1,E} \mathbf{w}_j^E) \cdot \mathbf{w}_i^E$ , we obtain (see

219 Younes *et al.*, 2004 for details)

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

221 with  $\ell_{ij} = \mathbf{r}_{ij}^T (k_r^{-1,E} \mathbf{K}^{-1,E})^{-1} \mathbf{r}_{ij}$  and  $\mathbf{r}_{ij}$  is the edge vector from the node  $i$  to the node  $j$ .

222 Using Eq. (7) and properties of  $\mathbf{w}_i^E$ , the Darcy Eq. (8) becomes

223 
$$\sum_j B_{i,j}^E Q_j^E = \frac{1}{|E|} \int_E H - \frac{1}{|\partial E_i|} \int_{\partial E_i} H$$
 (10)

224 
$$= H_E - TH_i^E$$

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

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

226 
$$Q_i^E = \delta_i^E H_E - \sum_j B_{i,j}^{-1,E} TH_j^E$$
 (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

- 229 • 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

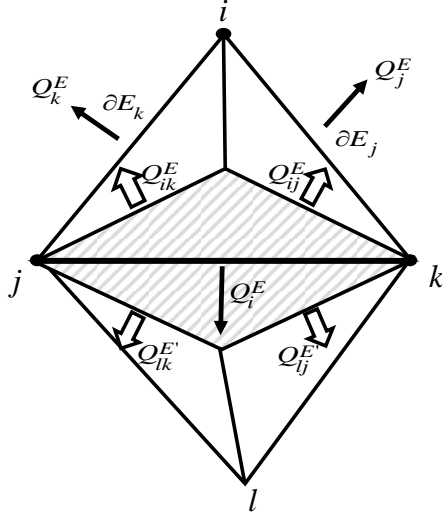
231 
$$H_E = \sum_i \frac{\delta_i^E}{\delta^E} TH_i^E$$
 (12)

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

233 Hence, the steady-state flux  $\underline{Q}_i^E$  across the edge  $\partial E_i$  writes

234 
$$\underline{Q}_i^E = \sum_j \left( \frac{\delta_i^E \delta_j^E}{\delta^E} - B_{i,j}^{-1,E} \right) TH_j^E$$
 (13)

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



238

239 **Figure 2:** The lumping region  $R_i$  associated to the edge  $i$  sharing the elements  $E$  and  $E'$

240 and formed by the two simplex regions  $S_i^E$  and  $S_i^{E'}$ .

241 The domain is now partitioned into lumping regions  $R_i$  (hatched area in Figure 2)

242 assigned to the edge  $i$  formed by the two simplex regions  $S_i^E$  and  $S_i^{E'}$  for an inner

243 edge  $i$  and by the sole simplex region  $S_i^E$  for a boundary edge. The simplex region  $S_i^E$

244 is defined by joining the centre of  $E$  with the nodes  $j$  and  $k$  forming the edge  $i$ . The

245 area of  $S_i^E$  is  $\frac{|E|}{3}$ .

246 • 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 
$$\frac{|E|}{3} r_E \frac{dTH_i^E}{dt} + \frac{|E'|}{3} r_{E'} \frac{dTH_l^E}{dt} + \underline{Q}_{ij}^E + \underline{Q}_{ik}^E + \underline{Q}_{lj}^{E'} + \underline{Q}_{lk}^{E'} = 0 \quad (14)$$

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

$$252 \quad \underline{Q}_{ij}^E = \frac{1}{3} (\underline{Q}_j^E - \underline{Q}_i^E) \quad (15)$$

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

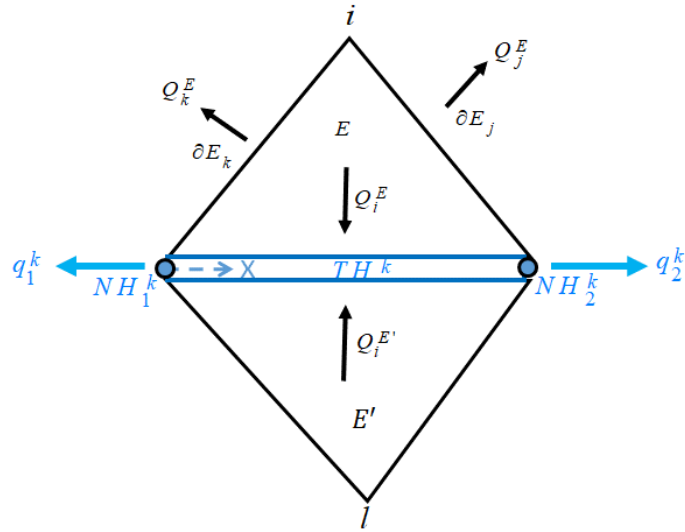
$$257 \quad \begin{cases} Q_i^E + Q_i^{E'} = 0 \\ Q_i^E = \sum_j \left( \frac{\delta_i^E \delta_j^E}{\delta^E} - B_{i,j}^{-1,E} \right) TH_j^E - \frac{|E|}{3} r_E \frac{dTH_i^E}{dt} \end{cases} \quad (16)$$

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

265 Note that, contrarily to the standard MFE method, the time derivative remains continuous in  
 266 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

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



273  
 274 **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  $k$ .

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

279 
$$q^k = q_1^k w_1^k + q_2^k w_2^k \quad (17)$$

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  $\ell_k$  and aperture  $e_k$   
 283 yields

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

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  
 286 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.

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

$$289 \quad \sum_j q_j^k \int_0^{\ell_k} w_i^k w_j^k = -k_r^k \mathbf{K}_f^k \int_0^{\ell_k} (\nabla H) w_i^k \quad (19)$$

290 Integration by part leads to

$$291 \quad \sum_j q_j^k \int_0^{\ell_k} w_i^k w_j^k = \frac{k_r^k \mathbf{K}_f^k}{e_k} (TH^k - NH_i^k) \quad (20)$$

292 where  $NH_i^k$  corresponds to the head at the node  $i$  located at the extremity of the fracture  $k$ .

293 Using numerical integration, based on the trapezoidal rule, for the calculation of the left term  
 294 (see Koohbor *et al.*, 2020) yields

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



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

$$\begin{aligned}
 299 \quad & \sum_j \left( \frac{\delta_i^E \delta_j^E}{\delta^E} - B_{i,j}^{-1,E} \right) TH_j^E + \sum_j \left( \frac{\delta_i^{E'} \delta_j^{E'}}{\delta^{E'}} - B_{i,j}^{-1,E'} \right) TH_j^{E'} - e_k k_r^k \frac{2K_f^k}{\ell_k} (2TH_i^E - NH_1^k - NH_2^k) \\
 & - \left( \frac{|E|}{3} r_E + \frac{|E'|}{3} r_{E'} + e_k \ell_k r_k \right) \frac{dTH_i^E}{dt} = 0
 \end{aligned} \tag{22}$$

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

$$302 \quad \sum_k q_i^k = 0 \tag{23}$$

303 Using Eq. (21), we obtain

$$304 \quad \sum_k e_k k_r^k \frac{2K_f^k}{\ell_k} (TH^k - NH_i^k) = 0 \tag{24}$$

305 Finally, the global flow system is formed by Eq. (16) for all the edges which do not coincide  
 306 with a fracture and by Eq. (22) else. This system is supplemented by Eq. (24) for all the nodes  
 307 of the fracture branches and assuming the continuity of the head ( $NH_i = NH_i^k$ ) at the node  $i$ ,  
 308 intersection of  $k$  fracture branches. Therefore, the final flow system has the heads at the edges  
 309 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 
$$C \left( \frac{\partial \theta}{\partial t} + \nabla \cdot \mathbf{q} \right) + \theta \frac{\partial C}{\partial t} + \mathbf{q} \cdot \nabla C - \nabla \cdot (\mathbf{D} \nabla C) = 0 \quad (25)$$

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

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

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

319 
$$\tilde{\mathbf{q}} = \sum_j \tilde{Q}_j^E \mathbf{w}_j^E \quad (27)$$

320 where  $\tilde{Q}_j^E = \int_{\partial E_j} \tilde{\mathbf{q}}_d \cdot \boldsymbol{\eta}_j^E$  is the dispersive flux across the edge  $\partial E_j$  of the element  $E$ .

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

322 
$$\int_E (\mathbf{D}_E^{-1} \tilde{\mathbf{q}}) \cdot \mathbf{w}_i^E = - \int_E \nabla C \cdot \mathbf{w}_i^E \quad (28)$$

323 which can take the following form

324 
$$\sum_j \tilde{B}_{i,j}^E \tilde{Q}_j^E = C_E - TC_i^E \quad (29)$$

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  $\partial E_i$  of the element  $E$  and  $\tilde{\mathbf{B}}$  is the elemental matrix of terms

327 
$$\tilde{B}_{i,j}^E = \int_E (\mathbf{D}_E^{-1} \mathbf{w}_j^E) \cdot \mathbf{w}_i^E$$

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

$$329 \quad \tilde{Q}_i^E = \sum_j \tilde{B}_{i,j}^{-1,E} (C_E - TC_j^E) \quad (30)$$

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:

- 333 • 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  $\underline{\tilde{Q}}_i^E$  expressed by  
 335 (similarly to Eq. (12)):

$$336 \quad \underline{\tilde{Q}}_i^E = \sum_j \frac{\tilde{\delta}_i^E \tilde{\delta}_j^E}{\tilde{\delta}^E} TC_j^E - \sum_j \tilde{B}_{i,j}^{-1,E} TC_j^E \quad (31)$$

$$337 \quad \text{with } \tilde{\delta}_i^E = \sum_j \tilde{B}_{i,j}^{-1,E} \text{ and } \tilde{\delta}^E = \sum_i \tilde{\delta}_i^E .$$

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

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

341 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)).

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

344 
$$TC_{ij}^E = \tau_{ij}^E TC_i^E + (1 - \tau_{ij}^E) TC_j^E \quad (33)$$

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

346 Thus, if we note  $Qt_i^E$  the total (advection + dispersion) flux leaving the element  $E$   
 347 from the edge  $i$ , Eq. (32) can be rewritten as the continuity of the total flux between  
 348 two adjacent elements  $E$  and  $E'$  sharing the edge  $i$  as

349 
$$\begin{cases} Qt_i^E + Qt_i^{E'} = 0 \\ Qt_i^E = \sum_j \left( \frac{\tilde{\delta}_i^E \tilde{\delta}_j^E}{\tilde{\delta}^E} - \tilde{B}_{i,j}^{-1,E} \right) TC_j^E + Q_{ij}^E (1 - \tau_{ij}^E) (TC_i^E - TC_j^E) + Q_{ik}^E (1 - \tau_{ik}^E) (TC_i^E - TC_k^E) - \theta_E \frac{|E|}{3} \frac{\partial TC_i^E}{\partial t} \end{cases}$$

350 (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

355 
$$D_k = \alpha_L^k |\bar{q}_k| + D_m^k \quad (35)$$

356 where  $\alpha_L^k$  is the longitudinal dispersivity through the fracture  $k$ ,  $D_m^k$  is the molecular diffusion

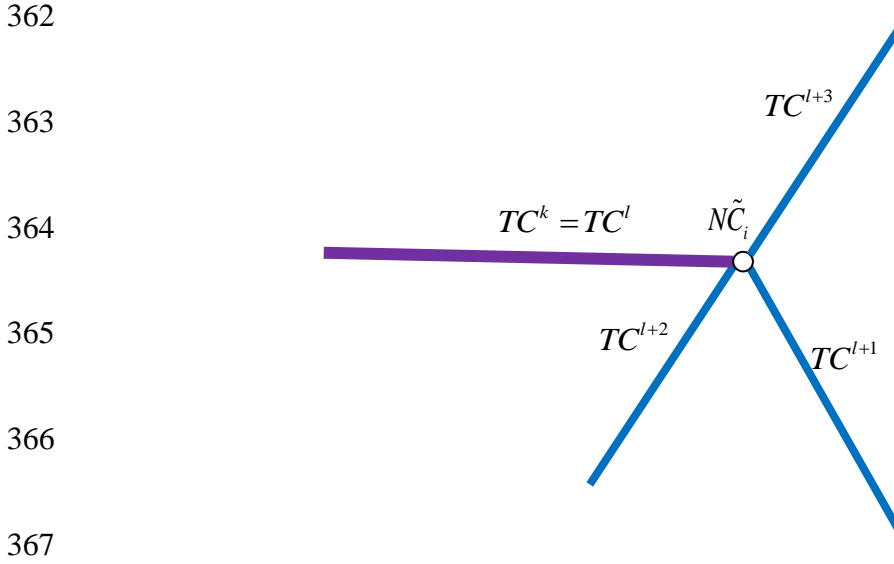
357 through  $k$ , and  $\bar{q}_k = \frac{(q_2^k - q_1^k)}{2e_k}$  is the mean velocity in the fracture  $k$ .

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

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



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

369 Imposing the continuity of the dispersive fluxes arriving from all fracture branches sharing the  
 370 node  $i$  (see Figure 4) writes

371 
$$\sum_l \frac{2e_l D_l}{\ell_l} (TC^l - N\tilde{C}_i) = 0 \quad (37)$$

372 Which yields

373 
$$N\tilde{C}_i = \frac{\sum_l \frac{e_l}{\ell_l} D_l TC^l}{\sum_l \frac{e_l}{\ell_l} D_l} \quad (38)$$

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

375 
$$\tilde{q}_i^k = \frac{2e_k D_k}{\ell_k} \left( TC^k - \frac{\sum_l \frac{e_l}{\ell_l} D_l TC^l}{\sum_l \frac{e_l}{\ell_l} D_l} \right) \quad (39)$$

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 
$$\theta_k e_k \int_0^{\ell_k} \frac{\partial C}{\partial t} + e_k \int_0^{\ell_k} \nabla \cdot (\mathbf{q}C) - e_k \int_0^{\ell_k} C \nabla \cdot \mathbf{q} + e_k \int_0^{\ell_k} \nabla \cdot \tilde{\mathbf{q}} - Qt_i^E - Qt_i^{E'} = 0 \quad (40)$$

379 The calculation of the different integrals yields

380 
$$\theta_k e_k \ell_k \frac{\partial TC^k}{\partial t} + q_1^k C_1^{k,*} + q_2^k C_2^{k,*} - (q_1^k + q_2^k) TC^k + \tilde{q}_1^k + \tilde{q}_2^k = Qt_i^E + Qt_i^{E'} \quad (41)$$

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

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

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

386 Hence, in the case of an outflow at the node  $i$  of  $k$ , the nodal concentration is  $C_i^{k,*} = TC^k$ ,

387 whereas, in the case of an inflow at the node  $i$  of the fracture  $k$ , the nodal concentration is

388  $\overline{NC}_{i,out}$ .

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

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

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

$$393 \quad \overline{NC}_{i,out} = \frac{\sum_{k=1}^l q_i^k \lambda_i^k TC^k}{\sum_{k=1}^l q_i^k (\lambda_i^k - 1)} \quad (45)$$

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

397 • For all edges  $i$  sharing two matrix elements  $E$  and  $E'$  such that  $i$  does not coincide with  
 398 a fracture  $k$ , Eq. (34) is solved for the unknown edge concentration  $TC_i$  assuming  
 399 continuity of edge concentration ( $TC_i = TC_i^E = TC_i^{E'}$ ).

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  
 402 Eq. (45), is solved for the unknown edge concentration  $TC_i$  assuming that the  
 403 concentration at the edge matrix and at the fracture are equal  
 404 ( $TC_i = TC_i^E = TC_i^{E'} = TC^k$ ).

### 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

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

$$409 \quad F(t, \mathbf{y}, \mathbf{y}') = 0 \quad (46)$$

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

446 The second test case deals with flow and transport in a fractured unsaturated-saturated porous  
447 medium. The porous medium has initially wet conditions and involves a single fracture. This  
448 test case is used to validate the developed 1D-2D MFE model against the solution obtained  
449 with the 2D-2D DG model in the case of unsaturated flow.

450 The last test case is a challenging problem dealing with flow and transport into an initially dry  
451 soil containing a fracture network. This last problem is simulated to highlight the efficiency  
452 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*

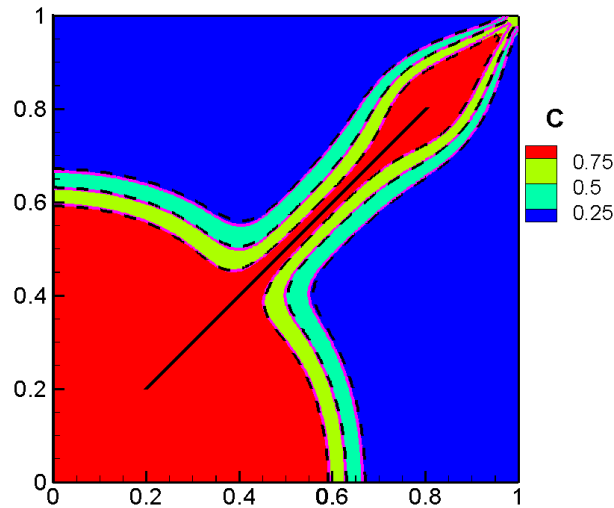
456 We consider a quadratic 2D domain (quarter-five-spot configuration) of size  $[0,1\text{m}] \times [0,1\text{m}]$   
 457 with impermeable walls except at the lower-left and the upper-right corners. The source at the  
 458 lower-left corner is represented by a boundary flux  $q_{inj} = 10^{-3} \text{ m/s}$  at  
 459  $(0 \leq x \leq 0.03\text{m}) \cap (y = 0) \cup (x = 0) \cap (0 \leq y \leq 0.03\text{m})$ . The sink at the right-upper corner is  
 460 represented by a Dirichlet boundary condition with a zero head at  
 461  $(0.97\text{m} \leq x \leq 1\text{m}) \cap (y = 1) \cup (x = 1) \cap (0.97\text{m} \leq y \leq 1\text{m})$ . The porous medium is formed by a  
 462 homogeneous material with a diagonal fracture of 1mm aperture, located between  
 463  $(0.2\text{m}, 0.2\text{m})$  and  $(0.8\text{m}, 0.8\text{m})$ . The hydraulic and transport properties of the porous matrix  
 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

	$K_s$ (m/s)	$S_s$ (1/m)	$\theta_s$	$\alpha_L$ (m)	$\alpha_T$ (m)	$D_m$ (m <sup>2</sup> /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.

485 This test case, inspired by the laboratory experiments of Vauclin *et al.*, (1979), was proposed

486 by Koohbor *et al.* (2020) to investigate unsaturated flow in fractured porous media. The

487 problem is extended hereafter to tackle both flow and transport in the case of a homogeneous

488 porous medium, including a single inclined fracture. The domain has a rectangular shape of

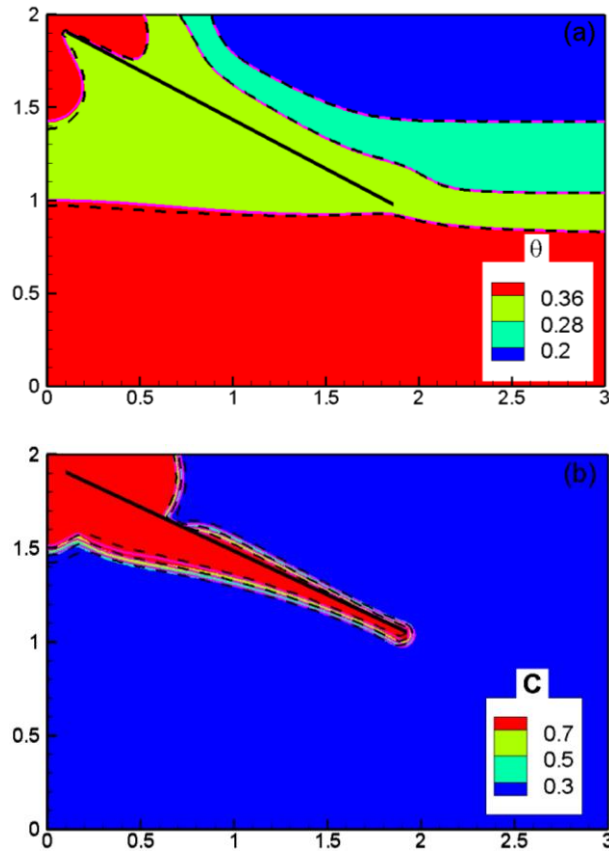
489 300cm×200 cm with a water table located at 65cm from the bottom. Initial conditions  
 490 correspond to a hydrostatic pressure distribution and a zero concentration in the domain.  
 491 Boundary conditions are as follows: contaminated water is infiltrated under a constant flux of  
 492 335cm/day 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

	$K_s$ (m/s)	$S_s$ (1/m)	$\theta_s$	$\theta_r$	$\alpha$ (1/m)	$n$	$\alpha_L$ (m)	$\alpha_T$ (m)	$D_m$ (m <sup>2</sup> /s)
Matrix	$5 \cdot 10^{-5}$	$10^{-10}$	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.

500 The simulation of this problem cannot be performed with the 1D-2D Comsol FE model since  
 501 Comsol cannot treat unsaturated flow in the fractures. The problem is simulated with the 1D-  
 502 2D MFE model as well as with the 2D-2D DG model and the 2D-2D FE model of Comsol.  
 503 Figure 6 depicts the water content and the concentration distributions at  $t = 1000s$  obtained  
 504 with the three models. A good agreement is observed between the results of the three models  
 505 for the volumetric water content as well as for the concentration contours (Figure 6).

506



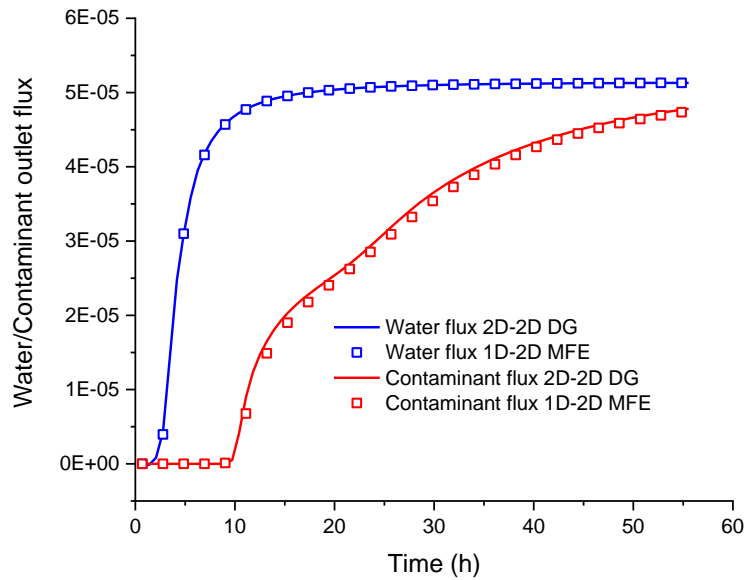
507

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 Figure 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.

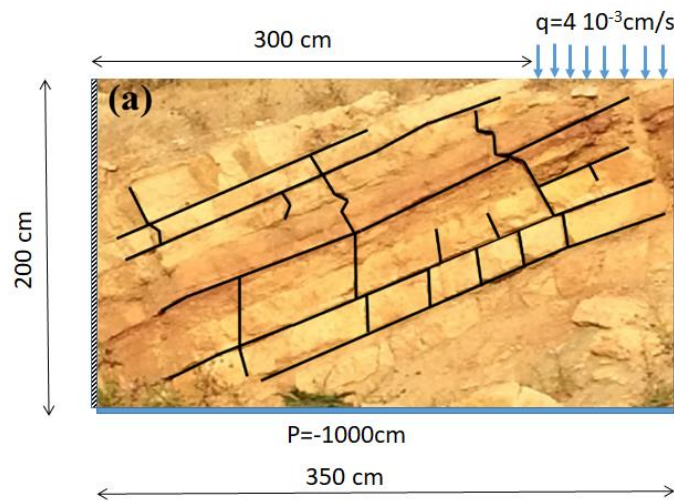


525  
 526 **Figure 7:** Outlet fluid and contaminant mass fluxes obtained with the 1D-2D MFE and the  
 527 2D-2D DG models for the problem of infiltration of contaminated water in a fractured  
 528 unsaturated-saturated porous medium.

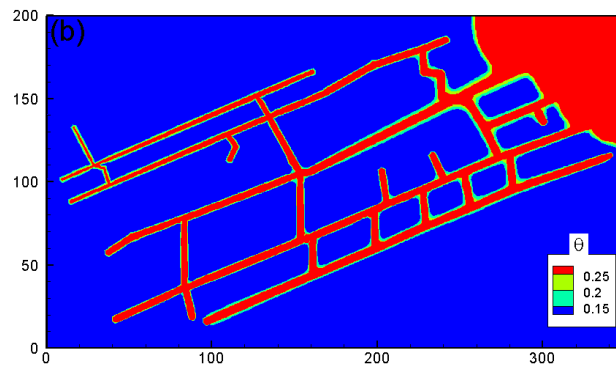
529  
 530 *4.3 Infiltration of contaminated water in a fractured dry soil.*

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

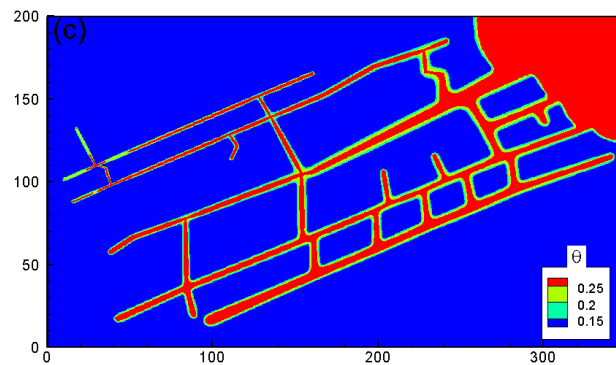
538 domain. Water is injected at the right part of the surface ( $300\text{cm} \leq x \leq 350\text{cm}$ ) with a constant  
 539 flow rate of  $4 \times 10^{-4}$  cm/s. The simulation is performed for a period of  $2 \times 10^5$  s. Clean water is  
 540 injected for the first half period ( $C = 0$  if  $t \leq 10^5$  s), and contaminated water is injected for  
 541 the second half period ( $C = 1$  if  $t > 10^5$  s). Initial conditions correspond to a highly dry soil  
 542 with a head of -1000cm in both matrix and fracture continua. All fractures have an aperture of  
 543 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-  
 549 2D MFE model and with the 2D-2D DG model (c).

550

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

	$K_s$ (cm/s)	$S_s$ (1/cm)	$\theta_s$	$\theta_r$	$\alpha$ (1/cm)	$n$
Matrix	$5.25 \cdot 10^{-6}$	$10^{-8}$	0.34	0.01	0.0139	1.6
Fracture	$1.16 \cdot 10^{-2}$	$10^{-8}$	0.8	0.001	0.0139	1.6

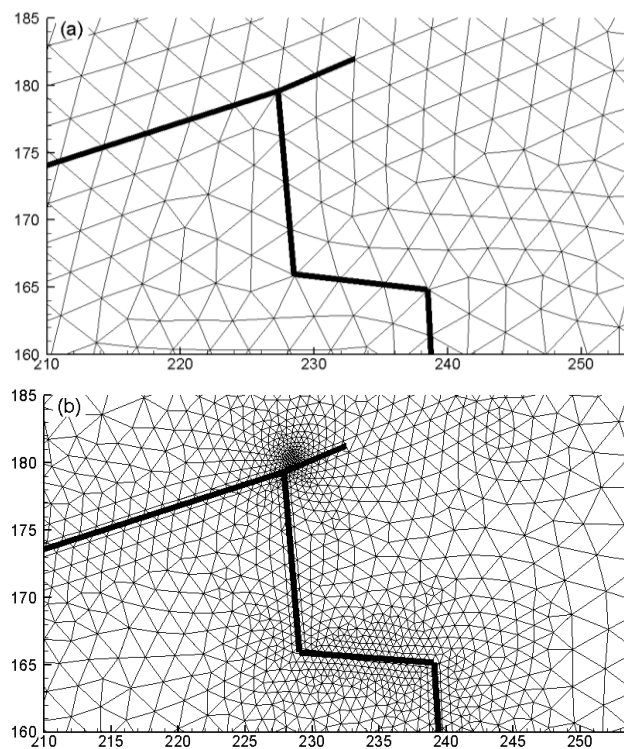
552 **Table 3:** Hydraulic parameters for the problem of infiltration of contaminated water in a  
 553 fracture initially dry soil.

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



566 highly advective transport problem. In this case, all dispersivities of the matrix and the  
567 fractures are zero ( $\alpha_L^m = \alpha_T^m = \alpha_L^f = 0$ ), and a small molecular diffusion occurs in both  
568 continua ( $D_m^m = D_m^f = 10^{-6} \text{ cm}^2/\text{s}$ ). In the second configuration, a more significant dispersion  
569 is considered for both continua with longitudinal and transverse dispersivities in the matrix,  
570 respectively  $\alpha_L^m = 5m$ , and  $\alpha_T^m = 2m$ . The longitudinal dispersivity in the fractures is  
571  $\alpha_L^f = 5m$ . The molecular diffusion in both continua is  $10^{-5} \text{ cm}^2/\text{s}$ . For the 1D-2D model, the  
572 domain is discretized using 15400 triangles for the matrix continuum and 853 lines for the  
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).

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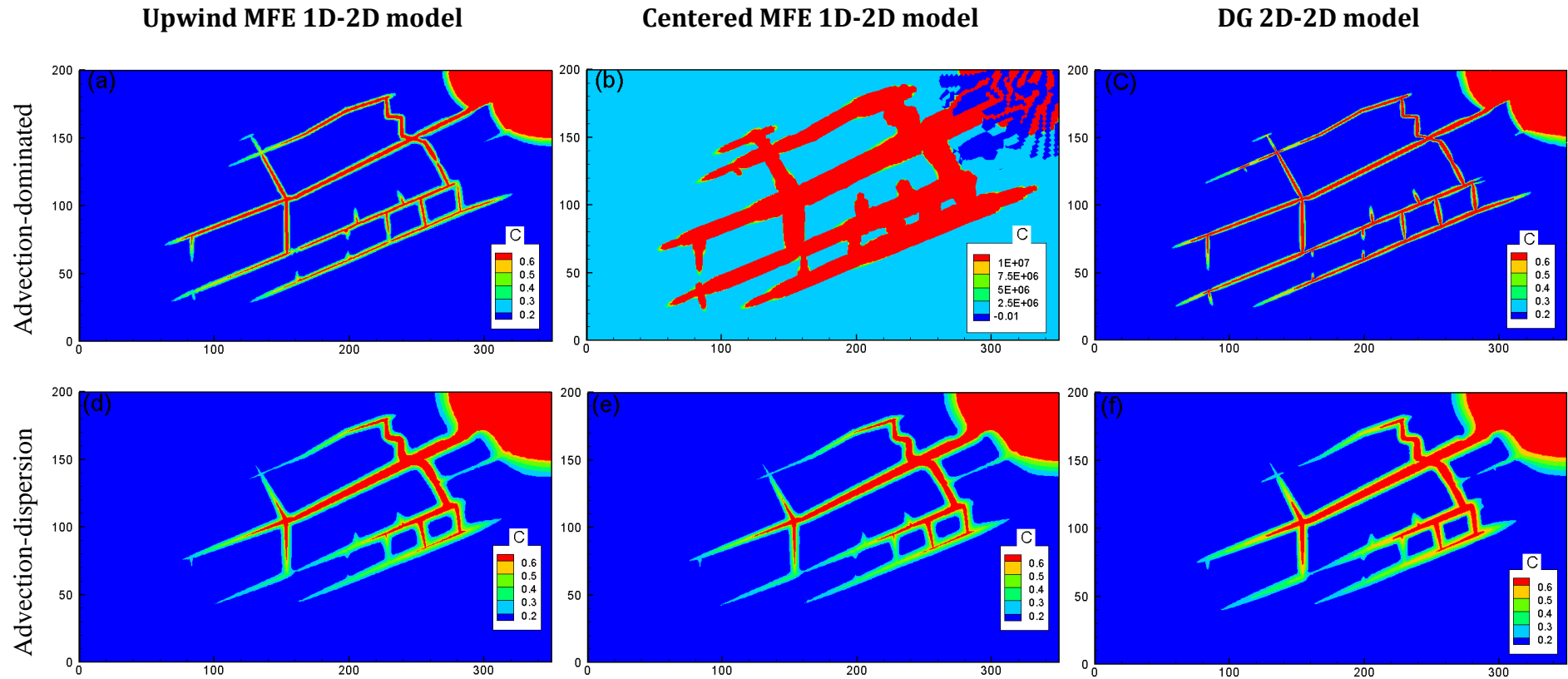
578

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 investigated 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 ( $\alpha_L^m = \alpha_T^m = \alpha_L^f = 0$  and  $D_m^m = D_m^f = 10^{-6} \text{ cm}^2/\text{s}$ ) and in the  
 609 case of advection-dispersion transport ( $\alpha_L^m = \alpha_L^f = 5m$ ,  $\alpha_T^m = 2m$ , and  $D_m^m = D_m^f = 10^{-5} \text{ cm}^2/\text{s}$ ).

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  
616 method which has been employed for the full spatial discretization of the flow and transport in  
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.

624 Three test problems dealing with flow and mass transport in saturated and unsaturated  
625 fractured porous media have been simulated to investigate the validity and robustness of the  
626 new 1D-2D MFE model. The first test case deals with the fractured quarter-five-spot problem  
627 and concerns flow and transport in a saturated porous medium involving a single fracture. The  
628 results of this test case with the 1D-2D MFE model were similar to those of the 1D-2D FE  
629 Comsol model and that of the 2D-2D DG model, which demonstrates the validity of the new  
630 model to simulate flow and transport in fractured saturated porous media.

631 The second test case deals with flow and transport in an unsaturated-saturated porous  
632 medium, including a single inclined fracture. This test case has been simulated with the 1D-  
633 2D MFE model as well as with the 2D-2D DG model and the 2D-2D FE model of Comsol

634 since the 1D-2D FE model of Comsol cannot treat unsaturated flow in fractures. A very good  
635 agreement is obtained between the three models for both the volumetric water content and the  
636 concentration contours, which demonstrates the validity of the new model for unsaturated  
637 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.

647 The new 1D-2D MFE model is much more efficient than the 2D-2D DG model. The new  
648 model allows a speedup of around 15, which confirms the usefulness of efficient and accurate  
649 models based on the DFM approach for the simulation of flow and transport in fractured  
650 porous media.

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