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**A fully implicit edge/face centered Discontinuous Galerkin / Mixed
Finite Element scheme for the Advection-Dispersion Equation**

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26 **Abstract**

27 Mixed Finite Element (MFE) method is a robust numerical technique for solving elliptic and
28 parabolic partial differential equations (PDEs). However, MFE can generate solutions with
29 strong unphysical oscillations and/or large numerical diffusion for hyperbolic type PDEs. For
30 its part, Discontinuous Galerkin (DG) finite element method is well adapted to solve hyperbolic
31 systems and can accurately reproduce solutions involving sharp fronts. Therefore, the
32 combination of DG and MFE is a good strategy for solving hyperbolic/parabolic problems such
33 as advection – diffusion/dispersion equations. The classical formulation of the two methods is
34 based on operator and time splitting allowing for separate solutions to advection with an explicit
35 scheme and to dispersion with an implicit scheme. However, this kind of approach has the
36 following drawbacks: (i) it lacks efficiency, as two systems with different unknowns are solved
37 at each time step, (ii) it induces errors generated by the splitting, (iii) it can be CPU wise-
38 expensive because of the CFL constraint, and (iv) it cannot be employed for steady-state
39 transport simulations.

40 To overcome these difficulties, we develop in this work a fully implicit edge/face centered DG-
41 MFE formulation where the two methods share the same unknowns. In this formulation, the
42 DG method is developed on lumping regions associated with the mesh edges/faces instead of
43 mesh elements. Thus, the traces of concentration at mesh edges/faces, which are the Degrees
44 Of Freedom (DOF) of the hybrid-MFE, are also part of the DOFs of the DG. The temporal
45 discretization is based on the Crank–Nicolson method for both advection and dispersion.
46 Numerical tests are performed to validate the new scheme by comparison against an analytical
47 solution and to show its ability to handle steady-state transport simulations.

48 The procedure is developed for 2D triangular meshes but can easily be extended to other 2D
49 and 3D shape elements.

50

51 **Keywords:**

52 Advection dispersion, transport, Mixed Finite Element, Discontinuous Galerkin, numerical
53 oscillations.

54

55 **Highlights**

56 – Advection-dispersion solved at once by mixed and discontinuous finite elements.

57 – Comparisons with analytical solutions show the accuracy of the new scheme.

58 – Numerical tests show its ability to use large time steps and to achieve steady-state
59 simulations.

60

61

62 **1. Introduction**

63 Numerous physical processes are described by mathematical models using partial differential
64 equations (PDEs) of elliptic or parabolic types (as for instance, steady-state diffusion or
65 transient energy conduction) or of hyperbolic type (advection, shock propagation). Nowadays,
66 many numerical methods exist to solve these PDEs, mainly based on finite volume or finite
67 element approaches. We will focus here on the solution of the advection-dispersion equation
68 (ADE) governing solute transport in porous media. Compared to diffusion, dispersion is an
69 anisotropic process, described by a full tensor which depends on the fluid velocity, contrarily
70 to diffusion, described by a scalar coefficient independent of the velocity. Therefore, according
71 to the velocity distribution and magnitude, the transport process can locally be either advection
72 or dispersion dominated. Moreover, the dispersion tensor is a full tensor which is discontinuous
73 over space. To address these challenges, mixed and discontinuous finite element methods have
74 become more and more popular over the last decades.

75 Mixed Finite Element (MFE) ([1], [2], [3]) is a robust numerical method, well adapted to
76 solving elliptic and parabolic diffusion problems such as fluid flow or diffusion transport
77 equations in porous media. The MFE method is locally conservative; it rigorously treats highly
78 heterogeneous domains with full permeability and dispersion tensors and can easily handle
79 unstructured meshes ([4]). MFE provides more accurate fluxes than conventional numerical
80 methods ([5], [6]) and is more accurate than Local Discontinuous Galerkin (LDG) method for
81 non-smooth grids ([7]). The hybridization technique, initially proposed by [8], allows for
82 reducing the number of unknowns of the original MFE and results in a final system with a
83 symmetric positive-definite matrix ([9], [10]). The unknowns with the hybrid-MFE method are
84 the traces (also seen as average values) of the scalar variable at mesh edges (2D) or faces (3D)
85 ([2]). A lumped formulation of the MFE method has been developed in [11] to improve its
86 monotonicity and reduce the unphysical over- and under-shoots observed when simulations of

87 diffusion with small time steps are performed ([12], [13]). When the classical MFE method is
88 employed for advection diffusion transport, it returns solution with spurious oscillations
89 because of the hyperbolic nature of the advection equation ([14], [15]). The combination of
90 MFE with an upwind scheme renders a stable solution but with excessive numerical diffusion
91 smearing the sharp concentration front in the case of advection dominated transport ([15]).
92 Discontinuous Galerkin finite element (DG) method is well adapted to hyperbolic problems
93 ([14]). The method has been developed for hyperbolic ([16], [17], [18]) and elliptic equations
94 ([19], [20], [21]). However, contrarily to DG applied to elliptic equations, the DG applied to
95 hyperbolic systems is clearly more accurate than other existing finite element methods ([22]).
96 The DG method yields a high-resolution scheme which is strictly conservative at the element
97 level and can accurately solve problems involving sharp front propagations ([14]). When used
98 with an explicit scheme, the time-step size has to fulfil the Courant–Friedrichs–Levy (CFL)
99 condition and a slope-limiting procedure is necessary to ensure the stability of the solution
100 ([23], [24], [25]). The DG method can also be used with an implicit time discretization which
101 avoids both the CFL constraint and the slope limiting procedure ([26]). In the literature, DG is
102 often used with piecewise linear approximation and with degrees of freedom (DOF)
103 corresponding to the discontinuous interior concentrations at the nodes of each element (see,
104 for example, [2], [14], [27], [28]).

105 Both mixed and discontinuous finite element methods have the interesting property of
106 preserving mass locally, and as such, they can be linked to the finite volume method. For
107 instance, the MFE method was shown to be equivalent to some finite volume methods in ([29],
108 [30],[31]). For its part, the DG method is a high-resolution scheme for advection that maintains
109 the local conservation of finite volume methods but also allows for high-order approximations
110 through a variational formulation instead of a functional reconstruction [32].

111 Thus, an efficient way to solve the ADE is to rely upon the most appropriate method for each
112 operator, that is, MFE for the diffusion operator and DG for advection. However, because MFE
113 and DG methods use different DOFs, their combination requires additional approximations. In
114 the literature, the combination has been ensured by operator and time splitting ([14], [27], [28],
115 [33], [34]), a procedure which is based on the following two steps (see [14] for details):

- 116 1. the advection equation is solved with the DG method to obtain the concentrations at the
117 new time level.
- 118 2. these concentrations are used as initial concentrations to solve the dispersion equation
119 with the MFE method.

120 The time splitting procedure has been employed in [35], [36] and [37] by coupling the implicit
121 MFE method in its hybrid form for dispersion with high resolution explicit finite volumes for
122 advection. In [38], it is suggested to use the linear Galerkin method instead of the MFE method
123 for the dispersion operator in the case of strong anisotropic dispersion tensor coefficients.

124 Note that one of the major drawbacks of the explicit time discretization of advection is a time
125 step selection based on the CFL condition which requires the time step to be less than the time
126 for flow to pass through one mesh element. The impact of this condition can be highly severe
127 in the case of local mesh refinement and/or locally high velocity magnitude such as around
128 injection or pumping wells. To alleviate this drawback, spatially variable time stepping
129 procedures have been developed to improve computational efficiency (e.g., [39, 40]), but their
130 usage remains scarce due to the difficulty of their implementation when the velocity field
131 changes at each time step.

132 To sum up, the classical MFE-DG combination based on operator and time splitting procedure
133 is convenient but has the following drawbacks: *(i)* the procedure is not very efficient since two
134 linear systems with different unknowns are solved at each time step, *(ii)* the procedure generates
135 splitting errors which can be important for large time steps, *(iii)* it can be CPU-wise expensive

136 in the case of explicit time discretization of advection, and (iv) steady-state transport
137 simulations cannot be performed.

138 The main objective of this work is to develop a new and alternative coupling of the MFE and
139 DG methods that avoids these drawbacks. The basic idea in this formulation is to develop the
140 DG method on the lumping regions associated with the mesh edges/faces, instead of mesh
141 elements. In this way, the traces of concentration at mesh edges/faces, which are the DOFs of
142 the hybrid-MFE, are also part of the DOFs of the DG. This yields a unique system where
143 advection and dispersion are assembled and solved simultaneously. In this way, the proposed
144 scheme uses different numerical techniques that are specifically suited to achieve high accuracy
145 for each type of equation while avoiding the splitting procedure. Both advection and dispersion
146 are discretized with the Crank-Nicolson implicit time discretization which allows for both large
147 time steps and steady-state transport simulation in a single step.

148 The outline of the paper is as follows. Section 2, reminds us on the classical approach combining
149 MFE and DGs based on operator and time splitting. In Section 3, we present the lumped-MFE
150 for the discretization of the dispersive transport equation. In Section 4, we introduce the
151 edge/face centred DG method for advection and its combination with the lumped-MFE for
152 dispersion. Numerical experiments are reported in the last Section to investigate on the
153 efficiency and accuracy of the new approach for advection-dispersion problems.

154

155 **2. The classical MFE-DG formulation for the advection-dispersion equation**

156 In this section, we recall the main steps of the classical MFE-DG formulation to solve the
157 advection-dispersion equation, based on the operator and time splitting procedure.

158 ***2.1 The advection-dispersion transport equation***

159 The transport of a non-reactive solute in a saturated porous medium is governed by the
 160 following advection-dispersion equation:

$$161 \quad \varepsilon \frac{\partial C}{\partial t} + \nabla \cdot (\mathbf{q}_a + \mathbf{q}_d) = 0 \quad (1)$$

162 where C is the concentration [ML^{-3}], ε is the porosity [L^3L^{-3}], t is the time [T], $\mathbf{q}_a = \mathbf{q}C$ is
 163 the advective flux with \mathbf{q} the Darcy velocity [LT^{-1}], and \mathbf{q}_d is the dispersive flux given by:

$$164 \quad \mathbf{q}_d = -\mathbf{D}\nabla C \quad (2)$$

165 with \mathbf{D} , the dispersion tensor, expressed by:

$$166 \quad \mathbf{D} = D_m \mathbf{I} + (\alpha_L - \alpha_T) \mathbf{q} \otimes \mathbf{q} / |\mathbf{q}| + \alpha_T |\mathbf{q}| \mathbf{I} \quad (3)$$

167 in which α_L and α_T are the longitudinal and transverse dispersivities [L]. D_m is the pore water
 168 diffusion coefficient [L^2T^{-1}] and \mathbf{I} is the unit (diagonal) tensor.

169 Equation (1) is subject to the following initial and boundary conditions:

$$170 \quad \begin{aligned} C(\mathbf{x}, 0) &= C_0(\mathbf{x}) & \mathbf{x} \in \Omega \\ C(\mathbf{x}, t) &= g_1(\mathbf{x}, t) & (\mathbf{x} \in \partial\Omega^1, t > 0) \\ (\mathbf{q}C - \mathbf{D}\nabla C) \cdot \boldsymbol{\eta}_{\partial\Omega} &= g_2(\mathbf{x}, t) & (\mathbf{x} \in \partial\Omega^2, t > 0) \\ (-\mathbf{D}\nabla C) \cdot \boldsymbol{\eta}_{\partial\Omega} &= 0 & (\mathbf{x} \in \partial\Omega^3, t > 0) \end{aligned} \quad (4)$$

171 where Ω is a bounded, polygonal open set of R^2 , $\partial\Omega^1$, $\partial\Omega^2$ and $\partial\Omega^3$ are partitions of the
 172 boundary $\partial\Omega$ of Ω corresponding to Dirichlet, total flux, and outflow boundary conditions,
 173 respectively and $\boldsymbol{\eta}_{\partial\Omega}$ is the unit outward normal to the boundary $\partial\Omega$. The outflow boundary
 174 condition considered in this work corresponds to a null dispersive flux (*i.e.*, the solute exits only
 175 by advection).

176 **2.2 The operator and time splitting procedure**

177 Operator and time splitting (e.g., [33]) offers the possibility to adapt the numerical technique to
 178 each type of PDE. To this aim, the advection equation is solved first by writing:

179
$$\varepsilon \frac{C^{n+1,ad} - C^n}{\Delta t} + \nabla \cdot (\mathbf{q}_a) = 0 \quad (5)$$

180 where C^n is the known concentration at the previous time level (n) and $C^{n+1,ad}$ is the
 181 concentration at the new time level ($n+1$) due to the advection process only.

182 In a second step, the dispersion equation is solved using $C^{n+1,ad}$ as the initial concentration:

183
$$\varepsilon \frac{C^{n+1} - C^{n+1,ad}}{\Delta t} + \nabla \cdot (\mathbf{q}_d) = 0 \quad (6)$$

184 where C^{n+1} is the final concentration at the new time level ($n+1$) resulting from both advection
 185 and dispersion.

186

187 **2.3 The DG discretization of the advection part of the transport equation**

188 The advection equation (5) solved by DG is usually approximated by linear functions (P1-DG)
 189 on triangles:

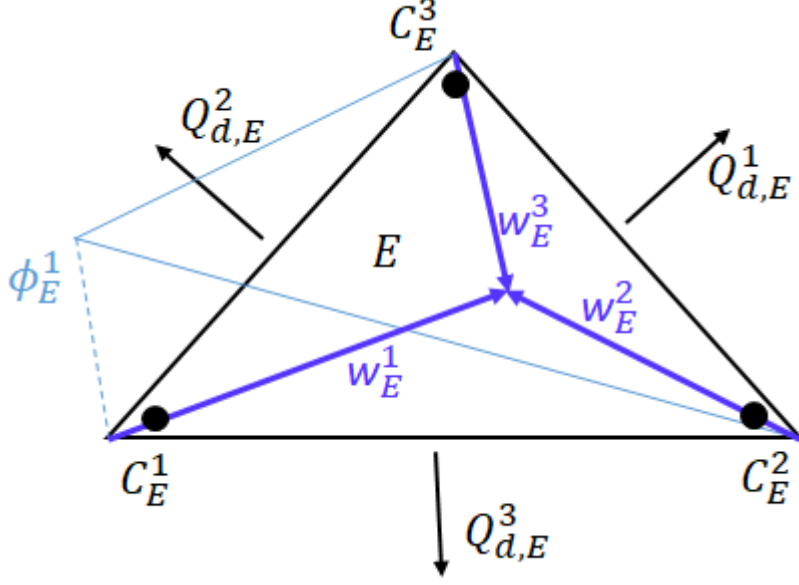
190
$$C_E(x, y) = \sum_{i=1}^3 \phi_E^i C_E^i \quad (7)$$

191 where C_E^i ($i = 1, \dots, 3$) are the three DOFs for the approximated concentration.

192 The DOFs of the P1-DG generally correspond to the discontinuous concentrations at the nodes
 193 ([2], [7], [27], [28]). Thus, C_E^i is the concentration at the node i of element E and ϕ_E^i is the
 194 classical linear chapeau interpolation function (see Fig. 1).

195

196



197

198 **Fig. 1.** DOFs (C_E^i) for the classical P1-DG, linear chapeau interpolation function (ϕ_E^i),

199 Raviart-Thomas vector basis functions (w_E^j), and diffusive fluxes ($Q_{d,E}^i$) through the edges of
 200 an element E .

201 Assuming a constant porosity over the element, the variational formulation of Eq. (5) on the
 202 element E using the test function ϕ_E^i writes:

$$203 \quad \varepsilon_E \sum_j \frac{dC_E^j}{dt} \int_E \phi_E^j \phi_E^i dx + \int_E \nabla \cdot (\mathbf{q} C \phi_E^i) dx - \sum_j \int_E C_E^j \phi_E^j \mathbf{q} \cdot \nabla \phi_E^i dx = 0 \quad (8)$$

204 By approximating the Darcy velocity \mathbf{q} inside each triangular element E with the lowest order
 205 Raviart-Thomas (RT0) basis functions, the second term of Eq. (8) can be transformed into a
 206 boundary element integral and evaluated using upstream concentrations as:

$$207 \quad \int_E \nabla \cdot (\mathbf{q} C \phi_E^i) dx = \sum_{j=1}^3 \frac{Q_E^j}{|\partial E_j|} \int_{\partial E_j} \bar{C}_{E^*}^j \phi_E^i d\gamma \quad (9)$$

208 where $\bar{C}_{E^*}^j$ is the upstream concentration at the edge ∂E_j of element E . It is either calculated
 209 as the approximation of the concentration in the element E in the case of outflow

210 ($\bar{C}_{E^*}^j = \bar{C}_E^j$ if $Q_E^j > 0$), or the approximated concentration of its adjacent element E' in the case

211 of inflow ($\bar{C}_{E^*}^j = \bar{C}_{E'}^j$ if $Q_E^j < 0$). $Q_E^j = \int_{\partial E_j} \mathbf{q} \cdot \boldsymbol{\eta}_{\partial E_j} d\gamma$ is the water flux (counted positive for
 212 outflow) across the edge ∂E_j of unit outward normal vector $\boldsymbol{\eta}_{\partial E_j}$ and shared by the two adjacent
 213 elements E and E' .

214 Substituting Eq. (9) into Eq. (8) and using the three test functions ϕ_E^i leads to a local system of
 215 ordinary differential equations for the DOFs of element E and eventually for the DOFs of its
 216 three adjacent elements. In the case of an explicit time discretization, this local system is
 217 independently solved for each element E to obtain $C_E^{i,adv}$, the concentrations at the node
 218 $i = 1, \dots, 3$ of the element E at the new time level. In the case of an implicit or a θ -scheme
 219 temporal discretization, all local systems are assembled into a global system, then solved to
 220 obtain all the $C_E^{i,adv}$ of all elements. Then, the mean concentration at each element E due to

221 advection is calculated as the average of the three nodal concentrations $\left(C_E^{adv} = \frac{1}{3} \sum_{i=1}^3 C_E^{i,adv} \right)$ and

222 used as a starting concentration for the solution of the dispersion equation.

223

224 **2.4 The MFE discretization of the dispersion equation**

225 The dispersive flux \mathbf{q}_d is approximated using the Raviart-Thomas (RT0) vectorial basis
 226 functions \mathbf{w}_E^j :

$$227 \quad \mathbf{q}_d = \sum_{j=1}^3 Q_{d,E}^j \mathbf{w}_E^j \quad (10)$$

228 where $Q_{d,E}^j = \int_j \mathbf{q}_d \cdot \boldsymbol{\eta}_j^E d\gamma$ is the dispersive flux across the edge ∂E_j of element E and

229 $\mathbf{w}_E^j = \frac{1}{2|E|} \begin{pmatrix} x - x_E^j \\ y - y_E^j \end{pmatrix}$ is the RT0 basis function ([4]), with (x_E^j, y_E^j) the coordinates of the node

230 j opposite to the edge ∂E_j of E and $|E|$ the area of E (see Fig. 1).

231 The variational formulation of Eq. (2) (rewritten as $\nabla C = -\mathbf{D}^{-1} \mathbf{q}$) over the element E using

232 the test function \mathbf{w}_E^i yields:

$$233 \quad \int_E \mathbf{D}_E^{-1} \mathbf{q}_d \cdot \mathbf{w}_E^i dx = \int_E C \nabla \cdot \mathbf{w}_E^i dx - \sum_j \int_{\partial E_j} C \mathbf{w}_E^i \cdot \boldsymbol{\eta}_E^j d\gamma \quad (11)$$

234 where \mathbf{D}_E is the local dispersion tensor at the element E and $\boldsymbol{\eta}_E^j$ the unit outward normal vector

235 to the edge ∂E_j .

236 Using Eq. (10) and properties of \mathbf{w}_E^i (see [4] for details) results in:

$$237 \quad \sum_j Q_{d,E}^j \int_E (\mathbf{D}_E^{-1} \mathbf{w}_E^j) \cdot \mathbf{w}_E^i dx = C_E - TC_E^i \quad (12)$$

238 where C_E is the mean concentration at element E and TC_E^i is the mean concentration at the

239 edge ∂E_i . Inverting Eq. (12) yields the following expression for the dispersive flux $Q_{d,E}^i$:

$$240 \quad Q_{d,E}^i = \sum_j B_{i,j}^{E,-1} (C_E - TC_E^j) \quad (13)$$

241 where $B_{i,j}^E = \int_E (\mathbf{D}_E^{-1} \mathbf{w}_E^j) \cdot \mathbf{w}_E^i dx$ are the terms of a local matrix \mathbf{B}^E , assuming that the tensor \mathbf{D}_E

242 is constant over the element E .

243 The MFE solution of the dispersion Eq. (6) is then calculated in two steps as follows:

244 *Step1*: A finite volume (FV) discretization of the dispersion equation over the element E is

245 written using an implicit scheme and starting with C_E^{adv} :

$$246 \quad \varepsilon_E \frac{|E|}{\Delta t} (C_E^{n+1} - C_E^{adv}) + \sum_i Q_{d,E}^{i,n+1} = 0 \quad (14)$$

247 Substituting Eq. (13) into Eq. (14) gives C_E^{n+1} as:

$$248 \quad C_E^{n+1} = \frac{1}{\beta_E} \sum_i \alpha_E^i TC_E^{i,n+1} + \frac{\lambda_E}{\beta_E} C_E^{adv} \quad (15)$$

249 in which $\alpha_E^i = \sum_j B_{i,j}^{E,-1}$, $\alpha_E = \sum_i \alpha_E^i$, $\lambda_E = \varepsilon_E \frac{|E|}{\Delta t}$ and $\beta_E = \lambda_E + \alpha_E$.

250 Finally, plugging Eq. (15) with the dispersive flux Eq. (13) yields:

$$251 \quad Q_{d,E}^{i,n+1} = \sum_j \left(\frac{\alpha_E^i \alpha_E^j}{\beta_E} - B_{i,j}^{E,-1} \right) TC_E^{j,n+1} + \frac{\lambda_E}{\beta_E} \alpha_E^i C_E^{adv} \quad (16)$$

252

253 *Step2:* At each interior edge ∂E_i , shared by the two adjacent elements E and E' , the continuity
254 of the dispersive flux is written as:

$$255 \quad Q_{d,E}^{i,n+1} + Q_{d,E'}^{i,n+1} = 0 \quad (17)$$

256 Thus, substituting Eq. (16) into Eq. (17) renders the final system solved to obtain the traces of
257 concentration at edges $TC_E^{i,n+1}$ at the new time level.

258 Knowing the values $TC_E^{i,n+1}$, the average concentration at the new time level C_E^{n+1} can be
259 calculated using Eq. (15) and the nodal concentrations (the DOFs of DG) are updated by equally
260 distributing the change of mass due to dispersion in the element E :

$$261 \quad C_E^{i,n+1} = C_E^{i,n} + \left(C_E^{n+1} - C_E^{adv} \right) \quad (18)$$

262 These nodal concentrations are then used as initial DG concentrations for the new time step
263 calculation solving Eq. (8).

264

265 **3. The new edge-centered MFE-DG formulation**

266 The previous classical MFE-DG formulation suffers from loss of efficiency. In the case of
267 implicit time discretization, two different systems must be solved at each time step, generating

268 significant splitting errors in the case of large time steps ([30]). In addition, the scheme cannot
 269 treat steady-state transport simulations. To overcome these difficulties, we present in this
 270 section a new MFE-DG formulation where the two methods are developed with the same DOFs
 271 on mesh edges. We rely upon the lumped formulation developed by [11] for the MFE method,
 272 to which we combine the DG method developed on the lumping regions associated with the
 273 mesh edges.

274

275 3.1 The lumped hybrid-MFE method for dispersion transport

276 We consider a simplex region S_E^i , associated with each edge ∂E_i of an element E by joining
 277 the centre of E with the nodes j and k forming the edge i (Fig. 2). A lumping region R_i (the
 278 grey area in Fig. 2), is then associated with the edge i . It is formed by the two simplex regions
 279 S_E^i and $S_{E'}^i$ for an interior edge i , shared by two adjacent elements E and E' . For a boundary
 280 edge i , the lumping region R_i is only formed by the single simplex region S_E^i .

281 The lumped MFE formulation is developed in two steps as follows ([15]):

282 *Step1:* The transient term is not considered, resulting in a dispersive transport over the element
 283 E written as:

$$284 \quad \sum_i \underline{Q}_{d,E}^{i,n+1} = 0 \quad (19)$$

285 with $\underline{Q}_{d,E}^{i,n+1}$ the steady-state dispersive fluxes across the edges i .

286 Using Eq. (13), we obtain:

$$287 \quad C_E^{n+1} = \sum_i \frac{\alpha_E^i}{\alpha_E} TC_E^{i,n+1} \quad (20)$$

288 and Eq. (16) reduces to:

$$289 \quad \underline{Q}_{d,E}^{i,n+1} = \sum_j \left(\frac{\alpha_E^i \alpha_E^j}{\alpha_E} - B_{i,j}^{E,-1} \right) TC_E^{j,n+1} \quad (21)$$

290 *Step2*: The transient term is allocated to the mesh edges and not to the element by simply writing
 291 the FV dispersion equation over the lumping region R_i :

$$292 \quad \int_{R_i} \varepsilon \frac{\partial C}{\partial t} dx + \int_{R_i} \nabla \cdot \mathbf{q}_d dx = 0 \quad (22)$$

293 where R_i is associated with the edge i corresponding to ∂E_i of concentration TC_E^i . This leads
 294 to (see notations in Fig. 2):

$$295 \quad \left(\varepsilon_E \frac{|E|}{3} + \varepsilon_{E'} \frac{|E'|}{3} \right) \frac{\partial TC_E^i}{\partial t} + \underline{Q}_{d,E}^{ij,n+1} + \underline{Q}_{d,E}^{ik,n+1} + \underline{Q}_{d,E'}^{ij,n+1} + \underline{Q}_{d,E'}^{ik,n+1} = 0 \quad (23)$$

296 where $\underline{Q}_{d,E}^{i\alpha,n+1}$ are the (interior) dispersive fluxes through the edges of R_i . Using Eq. (10), an
 297 interior dispersive flux between the lumping regions R_i and R_j writes:

$$298 \quad \underline{Q}_{d,E}^{ij,n+1} = \frac{1}{3} \left(\underline{Q}_{d,E}^{j,n+1} - \underline{Q}_{d,E}^{i,n+1} \right) \quad (24)$$

299 Hence, Eq.(23) becomes:

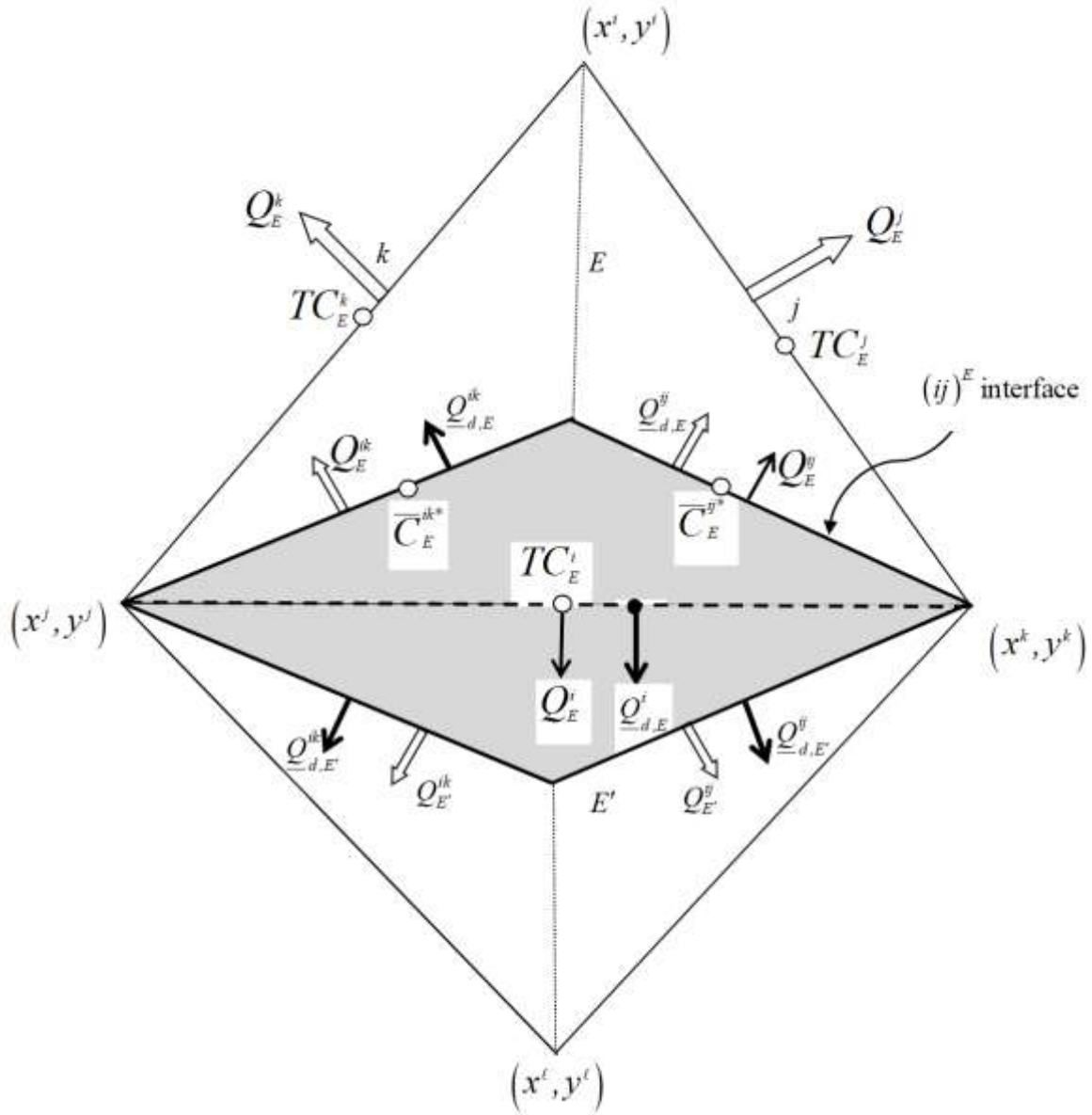
$$300 \quad \left(\varepsilon_E \frac{|E|}{3} + \varepsilon_{E'} \frac{|E'|}{3} \right) \frac{\partial TC_E^i}{\partial t} - \underline{Q}_{d,E}^{i,n+1} - \underline{Q}_{d,E'}^{i,n+1} = 0 \quad (25)$$

301 Substituting Eq. (21) in Eq. (25), we obtain the final system to solve for dispersive transport in
 302 the form:

$$303 \quad \left(\varepsilon_E \frac{|E|}{3} + \varepsilon_{E'} \frac{|E'|}{3} \right) \frac{\partial TC_E^i}{\partial t} + \sum_j \left(B_{i,j}^{E,-1} - \frac{\alpha_E^i \alpha_E^j}{\alpha_E} \right) TC_E^{j,n+1} + \sum_j \left(B_{i,j}^{E',-1} - \frac{\alpha_{E'}^i \alpha_{E'}^j}{\alpha_{E'}} \right) TC_{E'}^{j,n+1} = 0 \quad (26)$$

304 It is worth noting that the solution of this system has an improved monotonicity compared to
 305 the standard hybrid MFE formulation (see [11]). Indeed, with the lumped formulation, the
 306 maximum principle is respected for parabolic diffusion equations on acute triangulations, which
 307 is not the case of the standard mixed hybrid finite element method. For more general shapes of
 308 2D and 3D elements, numerical experiments showed that the lumping procedure significantly
 309 improved the monotonous character of the hybrid-MFE solution [11]. The lumped formulation

310 was applied to unsaturated flow and revealed more efficient and more robust than the standard
 311 hybrid formulation for both unfractured ([41]) and fractured ([42]) aquifers.
 312



313
 314 **Fig. 2:** The lumping region R_i associated with the edge ∂E_i , sharing the elements E and
 315 E' and formed by the two simplex regions S_E^i and $S_{E'}^i$.

316

317 *3.2 The edge/face centred DG-MFE scheme for advection dispersion transport*

318 The main idea of the new scheme is to combine an edge-based upwind DG method for advection
 319 with the previously discussed lumped hybrid-MFE for dispersion. The DG method is developed
 320 on the dual mesh formed by the lumping regions R_i instead of the original mesh formed by the
 321 elements E .

322 The concentration over each lumping region R_i is approximated via linear basis
 323 functions ϕ_i^m as:

$$324 \quad C_i(\mathbf{x}, t) = \sum_{m=1}^3 \tilde{C}_i^m(\mathbf{x}) \quad (27)$$

325 where \tilde{C}_i^m are the new DOFs for the P1-DG concentration approximation.

326 For each lumping region R_i centred at (\bar{x}_i, \bar{y}_i) , the new DOFs correspond to the edge
 327 concentration TC^i considered as the mean concentration at R_i , associated with a deviation of
 328 the concentration in each space direction ([18]) evaluated by the three following interpolation
 329 functions:

$$330 \quad \begin{aligned} \tilde{C}_i^1 &= TC^i, & \phi_i^1(x, y) &= 1 \\ \tilde{C}_i^2 &= \frac{\partial C_i}{\partial x}, & \phi_i^2(x, y) &= x - \bar{x}_i, \\ \tilde{C}_i^3 &= \frac{\partial C_i}{\partial y}, & \phi_i^3(x, y) &= y - \bar{y}_i. \end{aligned} \quad (28)$$

331 The variational formulation of the whole transport equation (1) over the lumping area R_i using
 332 ϕ_i^m as test functions writes:

$$333 \quad \int_{R_i} \varepsilon \frac{\partial C_i}{\partial t} \phi_i^m dx + \int_{R_i} \nabla \cdot (\mathbf{q} C_i) \phi_i^m dx + \int_{R_i} (\nabla \cdot \mathbf{q}_d) \phi_i^m dx = 0 \quad (29)$$

334 The first integral corresponds to the (mass) accumulation term:

$$335 \quad \int_{R_i} \varepsilon \frac{\partial C_i}{\partial t} \phi_i^m dx = \sum_{l=1}^3 \frac{\partial \tilde{C}_i^l}{\partial t} \int_{R_i} \varepsilon \psi_l \phi_i^m dx \quad (30)$$

336 Using Green's formula, the second integral in Eq. (29) is decomposed into:

$$337 \quad \int_{R_i} \nabla \cdot (\mathbf{q} C_i) \phi_i^m dx = \int_{\partial R_i} C^* \phi_i^m \mathbf{q} \cdot \boldsymbol{\eta}_{\partial R_i} d\gamma - \sum_{l=1}^3 \tilde{C}_{R_i} \phi_i^m dx \quad (31)$$

338 in which, the boundary integral is developed as (see notations in Fig. 2):

$$339 \quad \int_{\partial R_i} C^* \phi_i^m \mathbf{q} \cdot \boldsymbol{\eta}_{\partial R_i} d\gamma = \frac{Q_E^{ij}}{|E_{ij}|} \int_{E_{ij}} \bar{C}_E^{ij*} \phi_i^m d\gamma + \frac{Q_E^{ik}}{|E_{ik}|} \int_{E_{ik}} \bar{C}_E^{ik*} \phi_i^m d\gamma + \frac{Q_{E'}^{ik}}{|E'_{ik}|} \int_{E'_{ik}} \bar{C}_{E'}^{ik*} \phi_i^m d\gamma + \frac{Q_{E'}^{ij}}{|E'_{ij}|} \int_{E'_{ij}} \bar{C}_{E'}^{ij*} \phi_i^m d\gamma$$

340 (32)

341 where Q_E^{ij} is the water flux across the interior interface E_{ij} (between R_i and R_j) of length $|E_{ij}|$

342 . \bar{C}_E^{ij*} is the upstream concentration at E_{ij} , defined as:

$$343 \quad \bar{C}_E^{ij*} = \lambda_i^{E,ij} \bar{C}_i^{ij} + (1 - \lambda_i^{E,ij}) \bar{C}_j^{ij} \quad (33)$$

344 where \bar{C}_i^{ij} (respectively \bar{C}_j^{ij}) is the concentration at the interface E_{ij} calculated by the

345 approximation (Eq. (27)) of the concentration in R_i (respectively R_j) and $\lambda_i^{E,ij}$ is defined at E_{ij}

346 by:

$$347 \quad \lambda_i^{E,ij} = \begin{cases} 1 & \text{if } Q_E^{ij} \geq 0 \\ 0 & \text{if } Q_E^{ij} < 0 \end{cases} \quad (34)$$

348 The third term in Eq. (29) corresponds to the dispersion integral, which is approximated by:

$$349 \quad \int_{R_i} (\nabla \cdot \mathbf{q}_d) \phi_i^m dx = \frac{1}{|R_i|} \left(\underline{Q}_{d,E}^{ij,n+1} + \underline{Q}_{d,E}^{ik,n+1} + \underline{Q}_{d,E'}^{ij,n+1} + \underline{Q}_{d,E'}^{ik,n+1} \right) \int_{R_i} \phi_i^m dx \quad (35)$$

350 Using Eq. (24) in Eq. (35) renders:

$$351 \quad \int_{R_i} (\nabla \cdot \mathbf{q}_d) \phi_i^m dx = -\frac{1}{|R_i|} \left(\underline{Q}_{d,E}^{i,n+1} + \underline{Q}_{d,E'}^{i,n+1} \right) \int_{R_i} \phi_i^m dx \quad (36)$$

352 Substituting Eq. (21) in Eq. (36) results in:

$$353 \quad \int_{R_i} (\nabla \cdot \mathbf{q}_d) \phi_i^m dx = -\frac{1}{|R_i|} \left(\sum_l \left(\frac{\alpha_E^i \alpha_E^l}{\alpha_E} - B_{i,l}^{E,-1} \right) T C_E^{l,n+1} + \sum_l \left(\frac{\alpha_{E'}^i \alpha_{E'}^l}{\alpha_{E'}} - B_{i,l}^{E',-1} \right) T C_{E'}^{l,n+1} \right) \int_{R_i} \phi_i^m dx \quad (37)$$

354 Hence, using the three test functions ϕ_i^m in Eq. (29) leads to the following local system:

$$\begin{aligned}
 355 \quad [A] \begin{bmatrix} \frac{\partial \tilde{c}}{\partial t} \\ \frac{\partial \tilde{c}}{\partial t} \\ \frac{\partial \tilde{c}}{\partial t} \end{bmatrix} &= [D] \begin{bmatrix} \tilde{c} & & & & \\ & \tilde{c} & & & \\ & & \tilde{c} & & \\ & & & \tilde{c} & \\ & & & & \tilde{c} \end{bmatrix} \begin{bmatrix} \tilde{c} \\ \tilde{c} \\ \tilde{c} \end{bmatrix} - [M^3 + N^3] \begin{bmatrix} \tilde{c} \\ \tilde{c} \\ \tilde{c} \end{bmatrix} - [M^4 + N^4] \begin{bmatrix} \tilde{c} \\ \tilde{c} \\ \tilde{c} \end{bmatrix} \quad (38)
 \end{aligned}$$

356 with

$$\begin{aligned}
 A_{l,m} &= \int_{R_i} \varepsilon \phi_i^l \phi_i^m dx, & B_{l,m} &= \int_{R_i} \phi_i^l \mathbf{q} \cdot \nabla \phi_i^m dx \\
 M_{l,m}^0 &= \lambda_i^{E,ij} \frac{Q_E^{ij}}{|E_{ij}|} \int \phi_i^l \phi_i^m d\gamma + \lambda_i^{E,ik} \frac{Q_E^{ik}}{|E_{ik}|} \int \phi_i^l \phi_i^m d\gamma + \lambda_i^{E',ij} \frac{Q_{E'}^{ij}}{|E'_{ij}|} \int \phi_i^l \phi_i^m d\gamma + \lambda_i^{E',ik} \frac{Q_{E'}^{ik}}{|E'_{ik}|} \int \phi_i^l \phi_i^m d\gamma \\
 N_{l,m}^0 &= \left(\frac{\alpha_E^i \alpha_E^i}{\alpha_E} - B_{i,i}^{E,-1} \right) \delta_{1,l} \delta_{1,m} + \left(\frac{\alpha_{E'}^i \alpha_{E'}^i}{\alpha_{E'}} - B_{i,i}^{E',-1} \right) \delta_{1,l} \delta_{1,m} \\
 M_{l,m}^1 &= (1 - \lambda_i^{E,ij}) \frac{Q_E^{ij}}{|E_{ij}|} \int \phi_j^l \phi_i^m d\gamma, & N_{l,m}^1 &= \left(\frac{\alpha_E^i \alpha_E^j}{\alpha_E} - B_{i,j}^{E,-1} \right) \delta_{1,l} \delta_{1,m} \\
 M_{l,m}^2 &= (1 - \lambda_i^{E,ik}) \frac{Q_E^{ik}}{|E_{ik}|} \int \phi_k^l \phi_i^m d\gamma, & N_{l,m}^2 &= \left(\frac{\alpha_E^i \alpha_E^k}{\alpha_E} - B_{i,k}^{E,-1} \right) \delta_{1,l} \delta_{1,m} \\
 M_{l,m}^3 &= (1 - \lambda_i^{E',ij}) \frac{Q_{E'}^{ij}}{|E'_{ij}|} \int \phi_j^l \phi_i^m d\gamma, & N_{l,m}^3 &= \left(\frac{\alpha_{E'}^i \alpha_{E'}^j}{\alpha_{E'}} - B_{i,j}^{E',-1} \right) \delta_{1,l} \delta_{1,m} \\
 357 \quad M_{l,m}^4 &= (1 - \lambda_i^{E',ik}) \frac{Q_{E'}^{ik}}{|E'_{ik}|} \int \phi_k^l \phi_i^m d\gamma, & N_{l,m}^4 &= \left(\frac{\alpha_{E'}^i \alpha_{E'}^k}{\alpha_{E'}} - B_{i,k}^{E',-1} \right) \delta_{1,l} \delta_{1,m}
 \end{aligned}$$

358 If the edge ∂E_j of element E is a boundary edge with a prescribed concentration

$$359 \quad \overline{TC_j} = g_1(\mathbf{x}, t), \quad \text{the term } [M^1 + N^1] \begin{bmatrix} \tilde{c} \\ \tilde{c} \\ \tilde{c} \end{bmatrix}, \quad \text{in Eq. (38) is replaced by}$$

360 $\left((1 - \lambda_i^{E,ij}) Q_E^{ij} + \left(\frac{\alpha_E^i \alpha_E^j}{\alpha_E} - B_{i,j}^{E,-1} \right) \right) \begin{pmatrix} g_1 \\ 0 \\ 0 \end{pmatrix}$ and placed in the right hand side of the system to solve.

361 If ∂E_i is a boundary edge with a total flux $Q_i^i = g_2(\mathbf{x}, t)$, all the contributions of the element

362 E' are removed from Eq. (38). Finally, if the edge ∂E_i is an outflow boundary with a null

363 diffusive flux, the total flux Q_i^i in the system (38) is replaced by the advective flux $Q_E^i \tilde{C}$.

364 The time discretization of the system (38) is performed using an implicit θ -scheme with for

365 both advection and dispersion, which leads to:

$$\begin{aligned}
 & \frac{1}{\Delta t} [A] \begin{bmatrix} \tilde{C} \\ \tilde{C} \\ \tilde{C} \end{bmatrix} + \theta [M^2 + N^2] \begin{bmatrix} \tilde{C} \\ \tilde{C} \\ \tilde{C} \end{bmatrix} + \theta [M^4 + N^4] \begin{bmatrix} \tilde{C} \\ \tilde{C} \\ \tilde{C} \end{bmatrix} \\
 & = \frac{1}{\Delta t} [A] \begin{bmatrix} \tilde{C} \\ \tilde{C} \\ \tilde{C} \end{bmatrix} - (1-\theta) [M^2 + N^2] \begin{bmatrix} \tilde{C} \\ \tilde{C} \\ \tilde{C} \end{bmatrix} + \theta [M^4 + N^4] \begin{bmatrix} \tilde{C} \\ \tilde{C} \\ \tilde{C} \end{bmatrix} \\
 & \hspace{10em} + \theta [M^4 + N^4] \begin{bmatrix} \tilde{C} \\ \tilde{C} \\ \tilde{C} \end{bmatrix}^{n+1}
 \end{aligned} \tag{39}$$

366

367

368 Notice that the developed DG method comes down to the upwind finite volume scheme on the

369 lumping regions if the second and the third equations of system (39) are removed. In all the

370 simulations reported hereafter, the value of θ is fixed to 1/2, which corresponds to the Crank-

371 Nicolson scheme.

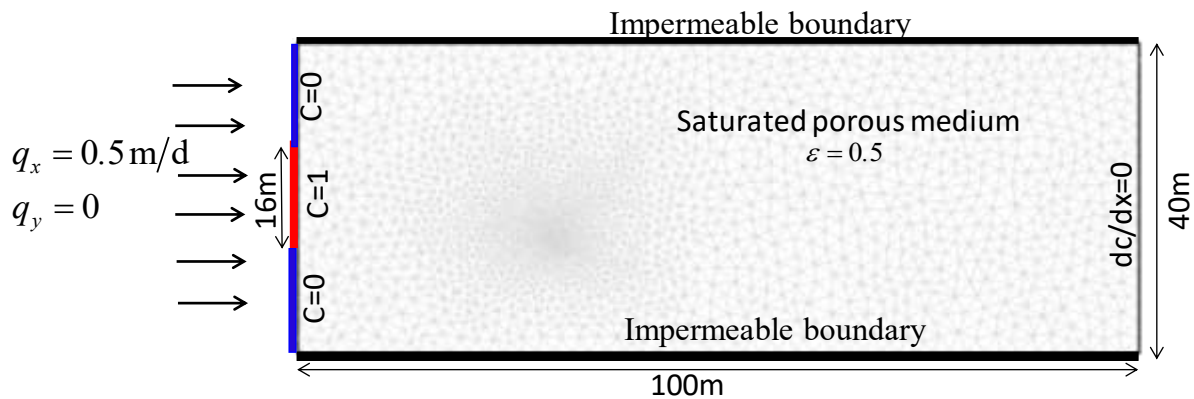
372 **4. Numerical Experiments**

373 The new DG-MFE formulation is first compared with an analytical solution. It is then used to
 374 simulate: (i) solute transport in the case of surface contamination with a total flux boundary
 375 condition, and (ii) in the case of a steady-state transport problem between an injection/extraction
 376 well pair.

377

378 *4.1 Comparison against the analytical solution*

379 The analytical solution was developed by [43] for a simplified 2D transport problem (Fig. 3)
 380 and was employed by [14] and [15] for the verification of numerical codes. The domain is a
 381 rectangle of dimension $(0-100m) \times (0-40m)$ with a uniform flow from left to right (Fig. 3).



382

383 **Fig.3.** Description of the problem of transport in a 2D domain with a uniform flow.

384 A Dirichlet boundary condition is prescribed for the concentration at the inflow boundary with:

385
$$C = \begin{cases} 0 & \text{for } 0 \leq y < 12 \\ 1 \text{ g/l} & \text{for } 12 \leq y \leq 28 \\ 0 & \text{for } 28 < y \leq 40 \end{cases} \quad (40)$$

386 The right side is an outflow boundary (null diffusive flux) and the lateral (no flow) boundaries
 387 are impermeable. The fluid flow is uniform over the domain with a constant horizontal velocity
 388 $q_x = 0.5$ m/day imposed at the left boundary and a uniform porosity $\varepsilon = 0.5$. The simulation

389 is performed for a final simulation time $T = 30$ days.

390 The analytical solution to this test case for an infinite domain is given by [43]:

$$391 \quad C_{analy}(x, y, t) = \frac{x}{(16\pi\alpha_L)^{1/2}} \int_0^T \tau^{-3/2} \left\{ erf \left[\frac{y-12}{(4\alpha_T\tau)^{1/2}} \right] + erf \left[\frac{28-y}{(4\alpha_T\tau)^{1/2}} \right] \right\} exp \left[-\frac{(x-\tau)^2}{4\alpha_L\tau} \right] d\tau$$

392 (41)

393 with $erf(x) = \frac{2}{\sqrt{\pi}} \int_0^x exp(-\tau^2) d\tau$.

394 The domain is discretized with an unstructured triangular mesh formed by 4000 elements.

395 Although, the test case involves a uniform velocity field, a local refinement is performed around

396 the point (30m, 15m) to obtain a highly unstructured mesh with significant differences in the

397 distribution of the Courant and grid Peclet numbers inside the domain. Furthermore, we located

398 the refinement in the expected transition zone, where the gradient of the concentration is high,

399 in order to detect the eventual impact of the mesh on the solution.

400 The comparison between the analytical and numerical solutions is performed for three test

401 cases, from highly convective to highly dispersive scenarios (Table 1), characterized by their

402 Peclet number defined for the investigated horizontal flow as:

$$403 \quad Pe_{L,T} = \frac{\sum_j |Q_j^E|}{2\alpha_{L,T} \|q\|} \quad (42)$$

404 where $Pe_{L,T}$ is the grid Peclet number in either the longitudinal (L) or the transverse (T) direction

405 and $\|q\|$ is the velocity norm. The different values of dispersivities (α) are given in Table 1

406 with the range of Peclet numbers (irregular grid).

407

Test case	α_L (m)	α_T (m)	$\langle Pe_L \rangle$ (-)	σ_{Pe_L} (-)	$\langle Pe_T \rangle$ (-)	σ_{Pe_T} (-)
TC1_A	0.05	0.01	27.3	13.3	136.3	66.7
TC1_AD	0.5	0.2	2.73	1.33	6.81	3.33
TC1_D	5.0	1.0	0.273	0.133	1.36	0.66

408 Table 1. Dispersivities and Peclet numbers (average and standard deviation) for the different
 409 test cases (_A stands for advective dominant, _AD for advective-dispersive, and _D for
 410 dispersive dominant transport).

411 The three test cases are simulated using a large time step of $\Delta t = 1$ d. It is worth noting that the
 412 new developed scheme is not constrained by the CFL condition since we use an implicit
 413 scheme. This feature departs from the classical approach, based on operator and time splitting
 414 (Eqs (5)-(6)) with an explicit time discretization for the advection operator and an implicit
 415 discretization for dispersion [14, 27, 35, 36 and 37]. For stability reasons, the explicit time
 416 discretization requires the strict respect of the CFL condition ($CFL \leq 0.5$), with a CFL defined
 417 by [44]):

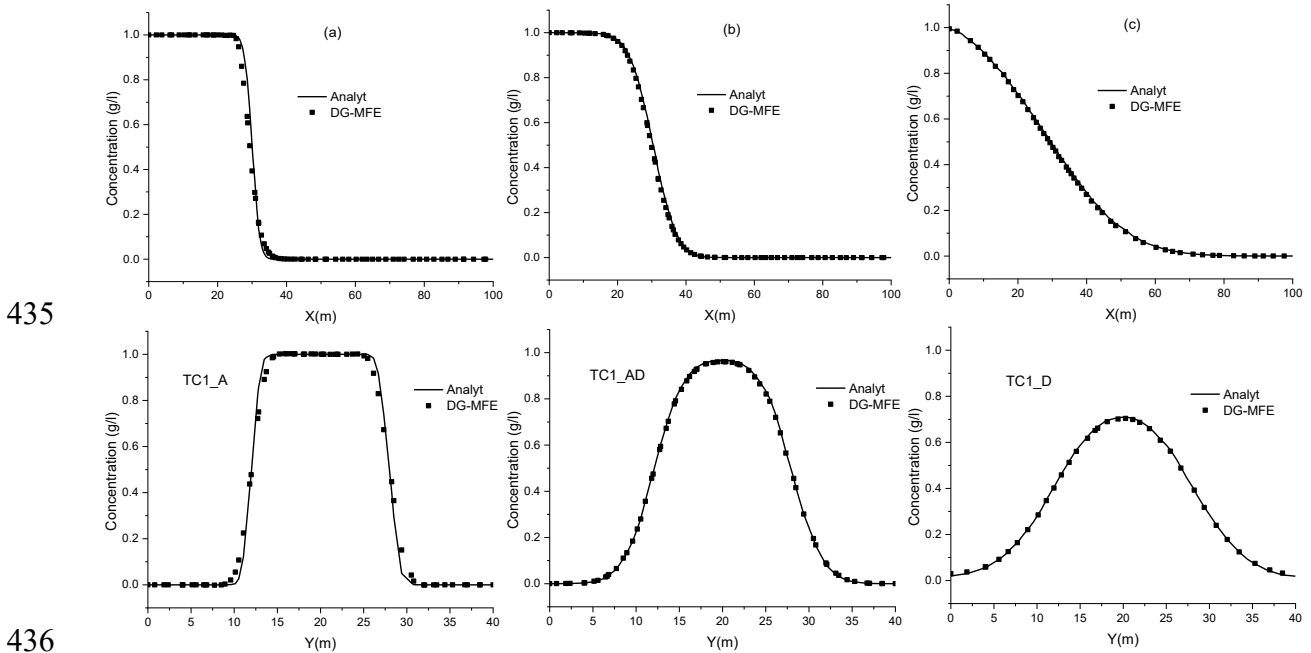
$$418 \quad CFL = \frac{\sum_j |Q_j^E|}{2|E|} \Delta t \quad (43)$$

419 where $|E|$ is the area of element E .

420 Thus, for the classical approach with an explicit time discretization, the time step should be less
 421 than a critical value $\Delta t_c = 0.04$ d corresponding to ($CFL = 0.5$). This critical time step
 422 corresponds to the smallest element in the domain since the velocity field is uniform. The time
 423 step with the new model is therefore 25 times greater than that allowed by the explicit scheme.
 424 This gain can be much more important if the CFL constraint is more severe, as for instance, in
 425 the presence of an injection or a pumping well, where the region around the well is usually
 426 characterized by mesh refinement and high velocities.

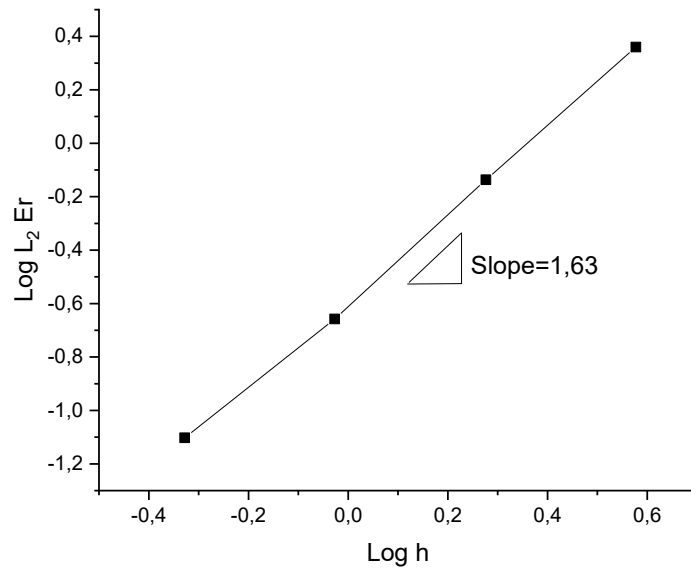
427 Fig. 4 depicts the numerical and analytical concentration profiles at $x = 20$ m and $y = 20$ m for
 428 the three test cases. Sharp longitudinal and transverse concentration profiles are observed for
 429 the advection dominated scenario (TC1_A) whereas, widely spread concentration fronts are
 430 obtained in the dispersion dominated test scenario (TC1_D).

431 The results of the three test cases show a very good agreement between the analytical and the
 432 numerical solutions. These results validate the new edge-centered DG-MFE model as able to
 433 accurately simulate solute transport in a wide panel of settings from advection dominated to
 434 dispersion dominated transport.



438 **Fig. 4:** Analytical and numerical concentrations for longitudinal profiles at $x = 20\text{m}$ and
 439 transversal profiles at $y = 20\text{m}$ for the three test cases.

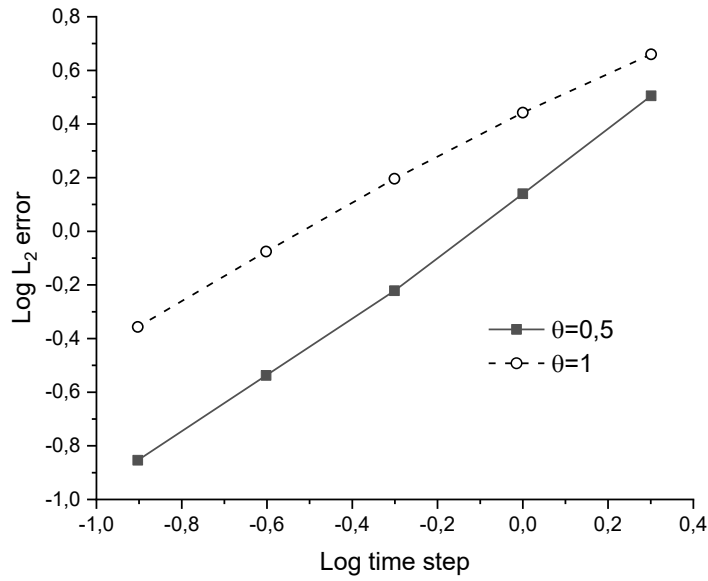
440 To investigate the order of convergence of the edge-centered DG-MFE formulation, the
 441 advective-dispersive test problem **TC1_AD** is simulated using different mesh sizes. We start
 442 with a uniform unstructured mesh formed by 1004 triangles and fix the time step to a small
 443 value of $\Delta t = 0.01d$ for all simulations. In each level of refinement, each triangle is subdivided
 444 into four similar triangles, by joining its three mid-edges of the initial triangle. The L_2 error
 445 (L_2Er) is then calculated at the simulation time $T_f = 20d$ for the different meshes. The runs
 446 are performed on a single computer with an Intel Xeon E-2246G processor and 32 GB memory.
 447 The results of the simulations, plotted in Fig. 5, show an average order of convergence in space
 448 of 1.63 for the investigated **TC1_AD** test problem.



449
450

451 **Fig. 5:** Convergence in space of the edge-centered DG-MFE formulation for the **TC1_AD** test
452 problem.

453 To investigate the convergence in time, the **TC1_AD** test problem is simulated using a fine
454 spatial discretization formed by 16064 elements and different time steps for $\theta = 1$ (full-implicit)
455 and $\theta = 0.5$ (Crank-Nicolson) schemes. Results in Fig. 6 show that both schemes yield an order
456 of convergence around 1. Nevertheless, the Crank-Nicolson scheme is much more accurate than
457 the implicit scheme. For a given space and time discretization, the L_2 error with the Crank-
458 Nicolson scheme is on average 2.3 lower than that of the implicit scheme (Table2).



459

460 **Fig. 6:** Convergence in time of the edge-centered DG-MFE formulation with $\theta = 1$ (implicit)
 461 and $\theta = 0.5$ (Crank-Nicolson) schemes for **TC1_AD** test problem.

462

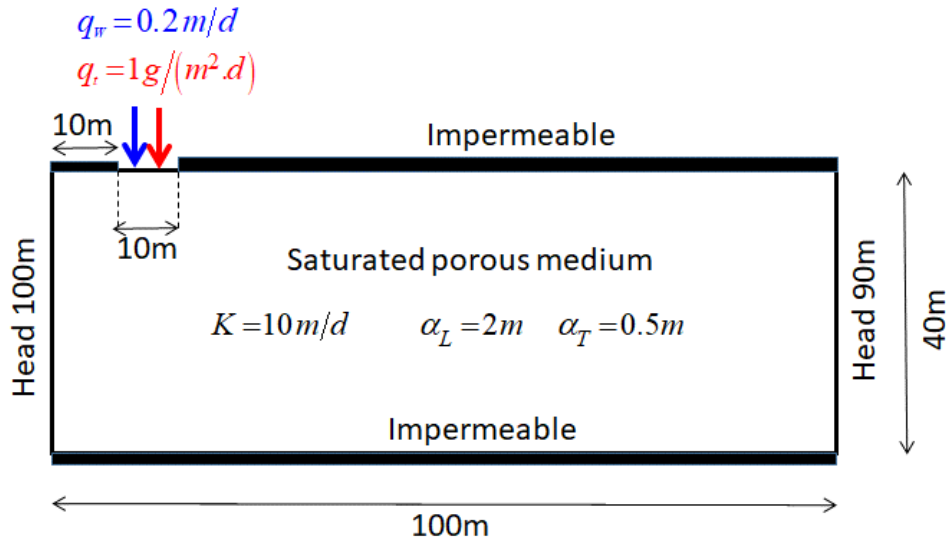
Δt	$L_2^{\theta=0.5} Er$	$L_2^{\theta=1} Er$	$L_2^{\theta=1} Er / L_2^{\theta=0.5} Er$	CPU time (s)
2	3.2	4.57	1.43	0.7
1	1.38	2.77	2.0	1.0
0.5	0.6	1.57	2.6	1.65
0.25	0.29	0.84	2.9	3.0
0.125	0.14	0.44	2.6	5.62

463 Table 2: Convergence in time of the edge-centered DG-MFE formulation for **TC1_AD** test
 464 problem.

465 *4.2 Transport simulation with total flux boundary condition*

466 The proposed edge-centered DG-MFE formulation is well adapted to simulate transport
 467 problems involving total flux boundary conditions since advection and dispersion are treated in
 468 a single system. A 2D transport problem is simulated with a total flux boundary condition over

469 the same domain as that of the previous test case TC1.
 470 The boundary conditions for flow and transport are described in Fig. 7. The hydraulic
 471 conductivity of the porous material is $K=10m/d$. The prescribed total (advection and
 472 dispersion) lateral solute flux is $q_t = 1g/(m^2.d)$ and the injected water flux is $q_w = 0.2m/d$.



473
 474 **Fig. 7:** Description of the 2D transport problem with lateral injection as a total flux boundary
 475 condition.

476 To obtain the velocity field, we first solve the following steady-state Darcy's flow:

$$477 \quad \begin{cases} \nabla \cdot \mathbf{q} = q_s \\ \mathbf{q} = -\mathbf{K} \nabla H \end{cases} \quad (44)$$

478 where \mathbf{q} is the Darcy velocity [LT^{-1}], q_s the source/sink term [T^{-1}], H the water head [L], and
 479 \mathbf{K} the hydraulic conductivity tensor [LT^{-1}].

480 The flow system is solved with the mixed finite element method ([4]) under the corresponding
 481 Dirichlet (prescribed head) and Neumann (prescribed flux) boundary conditions reported in Fig.
 482 7.

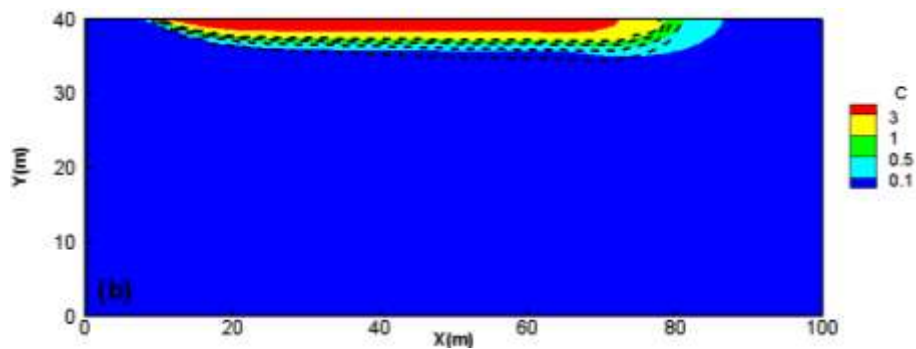
483 Since there is no analytical solution for the investigated problem, the transport solution of the
 484 new DG-MFE scheme is compared to the solution obtained with COMSOL multiphysics

485 software v. 6.1. (www.comsol.com) which is based on the standard Galerkin Finite Element
486 (GFE) method. Two test cases are investigated: TC2_A (advection dominated) with
487 $\alpha_L = 0.02m$ and $\alpha_T = 0.005m$, and TC2_D (dispersion dominated) with $\alpha_L = 2m$ and
488 $\alpha_T = 0.5m$.

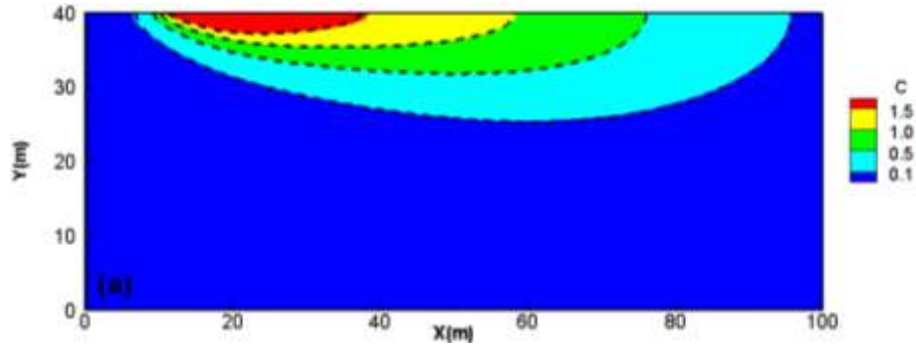
489 The concentration distributions at $t = 60$ days for both cases are plotted in Fig. 8. For the case
490 TC2_A, the solute remains near the injected lateral boundary of the domain, whereas, for
491 TC2_D, solute is more spread over the domain because of large transverse dispersion. Results
492 in Fig. 6 show a very good agreement between DG-MFE and GFE solutions in the case of high
493 dispersion. When advection is dominant, a less satisfactory agreement is observed between the
494 two solutions. The DG-MFE solution shows a sharp solute interface (see the tight iso-
495 concentration lines in Fig. 8), while the interface is smoother with the GFE scheme due to
496 numerical diffusion. Notice that in both test cases and for both DG-MFE and FE models, the
497 concentration at the injection region is not fixed but calculated during the simulation to fulfill
498 the total (advection + dispersion) flux conditions. For TC2_A, the concentration at the injection
499 region reaches 4.96 g/l. For TC2_D, it is lower, due to dispersion ($C = 2.8$ g/l).

500

501



502



503

504

505 **Fig. 8.** Concentration distributions for transport with a prescribed total flux boundary
 506 condition. Results of FE (color map) and DG-MFE (dashed lines) models for TC2_A (top)
 507 and TC2_D (bottom).

508

509 For a deeper comparison between the two models, we plot in Fig. 9 the evolution of

510 concentrations near the injection region, at the observation point located in $(x = 20m, y = 40m)$

511 . There is a very good agreement between the GFE and DG-MFE breakthrough curves for the

512 case TC2_D with high dispersion. For TC2_A, the breakthrough curve from the GFE model

513 shows unphysical oscillations near the sharp concentration front, those being absent from the

514 DG-MFE results. Notably, by neglecting dispersion and assuming a total flux as that of

515 advection only, the concentration at the injection region should be $\bar{C} = \frac{q_t}{q_w} = 5 \text{ g/l}$. When

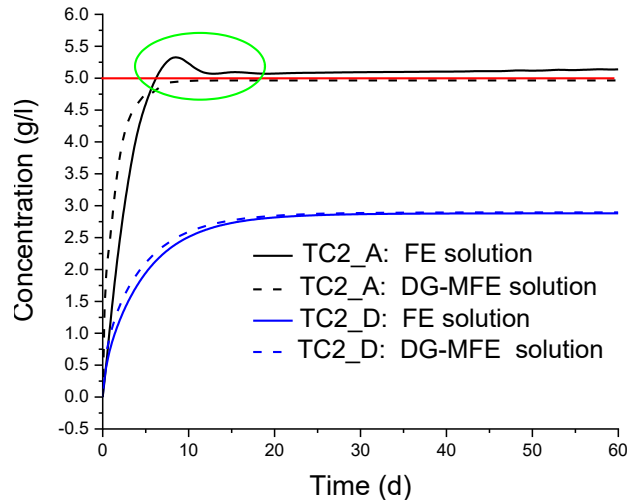
516 dispersion is present, the concentration C should always be smaller than \bar{C} (red line in Fig. 9).

517 The asymptotic value reached by the DG-MFE model at the observation point is 4.96 g/l (Fig.

518 9), whereas the GFE model shows an asymptotic concentration value of 5.12 g/l which is

519 unphysical since it exceeds \bar{C} . These results highlight the very good accuracy of the DG-MFE

520 model for advection-dominated transport problems with total flux boundary conditions.



521

522 **Fig. 9.** Concentration evolution at $(20m, 40m)$ with the GFE and DG-MFE schemes.

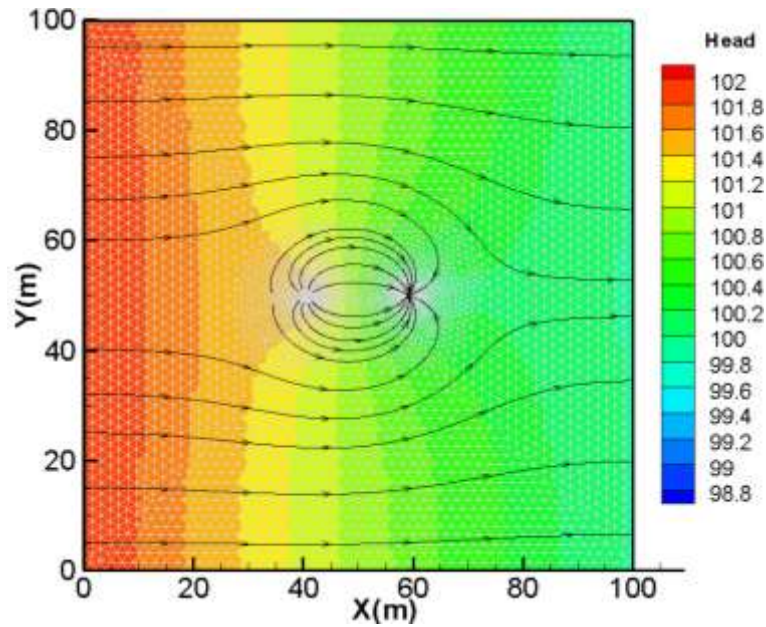
523

524 *4.3 Steady-state transport simulation of an injection/extraction well pair problem*

525 This test problem considers the contamination of a 2D confined homogeneous domain where
 526 the flow field is induced by a pair of extraction (sink) and injection (source) wells in an initially
 527 uniform sweeping flow over the whole modeled area. The domain has a square shape of
 528 $100m \times 100m$ (Fig. 10) with initial (before the wells are active) uniform flow, occurring from
 529 the left side, with head fixed to $H_L = 102m$ and inlet concentration fixed to $C_L = 0$, toward the
 530 right side, with head fixed to $H_R = 100m$ and a null diffusive flux for transport. The hydraulic
 531 conductivity is $2m/d$ and the longitudinal and transverse dispersivities are $\alpha_L = 2m$ and
 532 $\alpha_T = 0.5m$, respectively. The lag distance between the sink and source terms is 18 m. Solute is
 533 injected at a fixed rate of $3m^2/d$ at the location $(x = 41m, y = 50m)$ and extracted at $(x = 59m,$
 534 $y = 50m)$ where the hydraulic head is prescribed at $H_{extract} = 98m$. An unstructured triangular
 535 mesh with local mesh refinement in the vicinity of the injection and extraction wells (Fig. 10)
 536 is used for both flow and transport simulations.

537 The flow problem is solved by the MFE method ([4]). The hydraulic head distribution and path
 538 lines representing fluid particles trajectories are drawn in Fig. 11, showing that the extraction

539 well captures almost all the water from the injection and a fraction of water coming from the
 540 left boundary. Although the head at the sink ($H_{extract} = 98m$) is less than that of the right
 541 boundary ($H_R = 100m$), no flow occurs from the right boundary toward the extraction well.



542
 543 **Fig. 10.** Results of the flow simulation for the injection/extraction well pair problem.

544
 545 In this example, we are interested in the distribution of a solute invading the system from a
 546 continuous injection to a distant continuous extraction, the whole resulting in a steady-state
 547 solute plume. The direct steady-state simulation is not possible with the classical DG-MFE
 548 formulation based on operator and time splitting. In addition, the long-term transient simulation
 549 of transport until reaching the steady-state solution is hardly affordable with classical DG-MFE.
 550 Usually, the classical formulation is associated with an explicit time discretization of the
 551 advection operator which requires the strict respect of the CFL criterion. In the present test case,
 552 the high magnitude of velocities and the small element size in the vicinity of the injection and
 553 extraction wells, would imply a time step of $\Delta t \leq 1.310^{-3} d$ to respect the CFL criterion. Given
 554 that the steady-state regime (when the total mass in the system becomes constant) is reached at
 555 approximately $T = 5000d$, the classical approach with an explicit scheme would requires

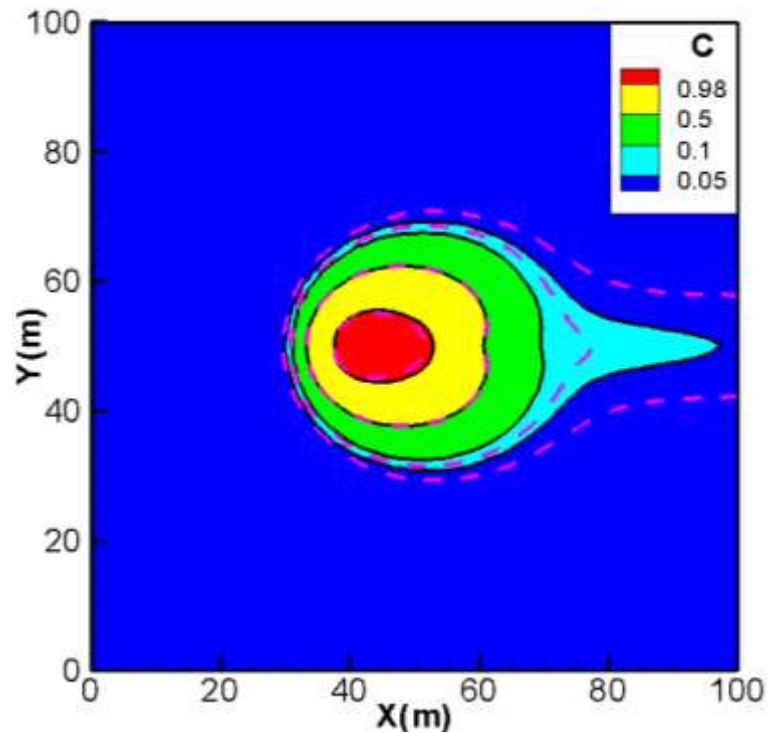
556 4×10^6 time steps to reach the steady-state regime.

557 The new DG-MFE numerical scheme can be employed to obtain the steady-state solution in a
558 single step only requiring 0.3s of CPU time. Fig. 11 compares the solution from the steady-state
559 calculation and that of a transient simulation (also performed by solving Eq. (39)) using 5000
560 time steps of $\Delta t = 1d$. In the latter, the whole simulation needs for approximately 87s of CPU
561 time.

562 A very good agreement is observed between the steady-state and the “transient” solutions (Fig.
563 11), while the steady-state calculation is approximately 300 times faster than the transient
564 calculation. Fig. 11 also reports on the steady-state solution obtained with a fully upwind MFE
565 method (described in [15]) in which the MFE is complemented by an upwind scheme for
566 advection to avoid unphysical oscillations due to the hyperbolic nature of the operator. As
567 expected, the steady-state solution from the fully upwind MFE scheme shows (dashed iso-
568 concentration lines in Fig. 11) large numerical diffusion, which renders it less accurate than the
569 DG-MFE solution.

570 These results point out the accuracy of the new DG-MFE scheme compared with the fully
571 upwind MFE solution; they also highlight how efficient the new scheme can be for single-step
572 steady-state simulations (and also here, accurate for implicit transient simulations even with
573 large time steps).

574



575

576 **Fig. 11:** Results of transport simulations for the injection/extraction pair problem. Steady-state

577 DG-MFE simulation (black lines), transient DG-MFE simulation using 5000 time steps of 1

578 day (color maps), and steady-state upwind-MFE simulation (purple dashed lines).

579

580 **5. Conclusions**

581

582 We propose in this work a new DG-MFE scheme to solve the advection-dispersion equation.

583 The DG method is developed over the lumping regions associated with the mesh edges and is

584 combined with the lumped MFE method. The DOFs of DG are the mean concentration on the

585 lumping region complemented by the deviation of the concentration in each space direction.

586 This allows for obtaining a single system of equations with common DOFs (edge concentration)

587 for both advection and dispersion discrete operators. The temporal discretization is based on

588 the Crank–Nicolson method for both advection and dispersion.

589 The accuracy of the new DG-MFE formulation was investigated using three types of problems

590 involving a full dispersion tensor. The first test problem highlights the accuracy of the DG-

591 MFE model by comparing the calculations with analytical solutions for highly advective
592 transport problems, moderately and highly dispersive problems. The results of the new DG-
593 MFE model showed very good agreements with the analytical solution for all the investigated
594 scenarios. The second test case handled a transport problem with a total flux boundary
595 condition. For this problem, the DG-MFE solution was compared to the GFE solution obtained
596 with Comsol software in the cases of both advection-dominated and dispersion-dominated
597 transports. The results showed a very good agreement between the GFE and DG-MFE
598 concentration curves in the case of high dispersion. In the case of high advection, the
599 concentration profile with GFE concealed unphysical oscillations and reached anomalous
600 asymptotic concentration values. These drawbacks are avoided with the new DG-MFE model.
601 Finally, the DG-MFE model was used for the steady-state transport simulation with sink and
602 source terms. A very good agreement was obtained between the steady-state and the long-term
603 transient simulation results, while, the steady-state calculation required approximately 300
604 times less CPU time than the transient calculation. The steady-state problem was also simulated
605 with the fully upwind MFE method which resulted in a solution with large numerical diffusion.
606 These results highlight the efficiency of the new DG-MFE model for steady-state transport
607 simulations that cannot be performed with the classical approach. They also point out the
608 accuracy of the obtained solution as compared to the fully upwind MFE solution.
609 The 2D formulation is quite generic and can be extended to 3D tetrahedral elements without
610 too much complicated numerical developments. These numerical investigations are under
611 progress.

612

613 **CRedit authorship contribution statement**

614 Anis Younes: Conceptualization, Methodology, Software, Supervision, Validation, Writing – original
615 draft, Writing – review & editing. Frederick Delay: Validation, Writing – original draft, Writing –
616 review & editing. Philippe Ackerer: Methodology, Validation, Writing – review & editing.

617

618 **Declaration of competing interest**

619 We declare that we have no known competing financial interests or personal relationships that could
620 have influenced the work reported in this paper.

621

622 **Data availability**

623 The FORTAN90 code is available on request.

624

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