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OM-MADE: an open-source program to simulate one-dimensional solute transport in multiple exchanging conduits and storage zones.

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Abstract

OM-MADE (One-dimensional Model for Multiple Advection, Dispersion, and storage in Exchanging zones) is an open-source python code for simulating one-dimensional solute transport in multiple exchanging conduits and storage zones in steady-state flow conditions. It aims at helping the interpretation of multi-peaked skewed breakthrough curves (BTCs) that can be observed in tracer tests conducted in karstic systems. OM-MADE is based on the resolution of classical mass conservation equations. In OM-MADE, all parallel and exchanging flow zones are divided along the direction of flow into reaches, in which all model parameters are kept constant. The total flowrate may be modified through lateral in and outflows. The solute may also be affected by decay processes either in mobile or immobile zones. Each reach is subdivided into discrete segments of equal length. The partial differential equations can be solved using two second order schemes, one based on an operator-split approach, the other on Crank-Nicholson pondered scheme. A verification is performed against analytical solutions, OTIS software (Runkel, 1998), and the Dual-Advection-Dispersion Equation (DADE) proposed by Field and Leij (2012). An application to a tracer test carried out in the karstic area of Furfooz (Belgium) is then performed to reproduce the double-peaked positively skewed BTC that has been observed. It constitutes a demonstration of the software capacities in the case of two reaches and three exchanging zones, among which two are mobile ones and one represents a storage zone. It thus permits to verify numerically the consistency of the conceptual interpretation of the observed BTC.

Keywords: Karsts; Tracer tests; Breakthrough curves; Software; One-dimensional solute transport

¹Author Contributions: AJT wrote the numerical code, with a small contribution of PC for the structure and interface. PC initiated the collaboration, made the application to Furfooz (with contribution of AJT) and wrote the paper (with contributions of AJT, LD and VH). A first code version was developed and tested during CP master's project, advised by AJT and PC. LD and VH initiated the Furfooz study and provided the field data.

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25 **Highlights:**

- 26 • An open-source python code to simulate one-dimensional solute transport in conduits.
- 27 • Simulate multiple exchanging flow and storage zones in steady-state flow conditions.
- 28 • Help the interpretation of multi-peaked breakthrough curves observed in karstic system tracer tests.

29 **1. Introduction**

30 The specific geometries of karstic systems have a huge impact on the underground fluid circulations. In
31 such media, hydraulic connections are difficult to predict with the classical laws describing porous media
32 transport: a more or less porous matrix co-exists with fractures and large open drains of various topologies
33 and sizes. Tracer tests are a common and powerful tool to assess groundwater transfers and get a first-
34 order understanding of a hydrogeological system (e.g., Goldscheider et al., 2003; Perrin and Luetscher, 2008;
35 Goldscheider et al., 2008; Field and Leij, 2012; Mudarra et al., 2014; Dewaide et al., 2016). Used in karstic
36 settings, they provide direct information on two major points: (i) the existence of a hydraulic connection
37 between two points - generally a sink or swallow hole and a spring - (e.g., Knöll and Scheytt, 2017), and (ii)
38 the time needed for the fluid to travel between these two points (e.g., Morales et al., 2007).

39 A careful analysis of breakthrough curves (BTCs) provides additional information on the major, and
40 potentially secondary, flows between inlets and outlets (e.g., Smart, 1988; Perrin and Luetscher, 2008).
41 In particular, asymmetric BTCs with long tails are commonly observed and are generally explained by
42 multiple conduit configurations, or interactions with pools or immobile water zones (e.g., Hubbard et al.,
43 1982; Bencala, 1983; Martin and McCutcheon, 1998; Goldscheider et al., 2003; Bonniver, 2011; Dewaide
44 et al., 2016). Multi-peaked BTC is a second specific feature that has been reported in some tracer tests
45 carried out in karstic systems (Goldscheider et al., 2008; Dewaide et al., 2018). Often interpreted as an effect
46 of auxiliary conduits (Smart, 1988; Goldscheider et al., 2008; Perrin and Luetscher, 2008), the presence of
47 large pools in the flow path is also proposed to explain this particular feature (Hauns et al., 1998). It has
48 been numerically and experimentally reproduced by Field and Leij (2012). Recently, Dewaide et al. (2018)
49 have provided field measurements in the Furfooz karstic system (Belgium) that show a double-peaked BTC.
50 The Furfooz system is characterized by the presence of a large underground lake, partly segmented into two
51 zones by a vertical wall. The authors have thus proposed a conceptual model of solute transport that would
52 imply a dual-advective transport within the lakes combined with a strong dispersive effect of this storage
53 zone.

54 If further field investigations should help to check these hypotheses, numerical tools could also be used
55 for that purpose. As dispersion is most significant in the flow direction, one-dimensional models have
56 been used to analyse and/or reproduce tracer tests (Goldscheider et al., 2008). They are generally based

57 on the resolution of the classical Advection-Dispersion Equation (ADE). They permit, through inversion
58 processes, to define average hydrodynamic parameters of underground paths (Hauns et al., 1998; Massei
59 et al., 2006; Goldscheider et al., 2008). Different software tools have been developed for that purpose.
60 The QTRACER2 program (Field, 2002) is a well-known example. However, such single-flow homogeneous
61 models could not easily assess the influence of immobile flow zones, like pools or eddies, commonly claimed
62 to explain long tail BTCs (e.g., Goldscheider et al., 2003; Birk et al., 2005; Bonniver, 2011). Different
63 approaches have thus emerged to handle the effect of immobile zones and generate more adaptable tails
64 (Field and Pinsky, 2000; Hauns et al., 2001; Massei et al., 2006; Geyer et al., 2007). Simulating retention
65 zones by stagnant cells, the approach recently proposed by Morales et al. (2010) provides the optimal
66 number of stagnant cells, and thus, of the retention zone volume to better fit the observed BTCs. In all
67 these approaches, each tracer test provides one BTC and the karstic system can not be discretized along
68 the flow when the tracer is observed at several successive locations. The OTIS program (One-dimensional
69 Transport with Inflow and Storage (Runkel, 1998)) also uses a two-region non equilibrium model allowing
70 to integrate immobile flow zones. Moreover, it permits to discretize the karstic system into several *reaches*
71 of homogeneous parameters, allowing to model tracer tests with multiple observation points. It has already
72 been used by Dewaide et al. (2016) to model tracer tests carried out in the Han-sur-Lesse karstic system
73 (Belgium) and help their interpretation in term of corresponding conduit geometries. OTIS supposes one
74 main flow zone. However, karstic systems can display particular configurations with auxiliary conduits that
75 divert the solute and then transport it back to the main one. To integrate the effect of auxiliary conduits
76 generating multi-peaked BTCs, multi-dispersion models (MDM: Goldscheider et al. (2008); Field and Leij
77 (2012)) have been soon proposed (Maloszewski et al., 1992; Käss, 1998). They consist of the superposition
78 of several independent advective-dispersive models, which supposes a complete independence of the flow
79 paths all along the modelled length. To better take into account the interactions that actually exist between
80 the different flow paths, Field and Leij (2012) have proposed a dual-advection dispersion equation (DADE)
81 that revealed to efficiently reproduce multi-peaked BTCs. This model does not allow to discretize the
82 conduits along the flow, nor to combine two exchanging advective-dispersive zones with a storage area,
83 but it is a relevant solution to model unknown parts of the network were the main flow can divide into
84 two conduits before merging back. To simulate more geometrically complex networks, several authors have
85 recently proposed to use pipe flow models (Campbell and Sullivan, 2002; Peterson and Wicks, 2006; Wu
86 et al., 2008; Chen and Goldscheider, 2014; Jeannin et al., 2015; Kaufmann et al., 2016; Vuilleumier, 2018).
87 Using Manning-Strickler formulae and resolving Saint-Venant equations, EPA's Stormwater Management
88 Model (SWMM, Rossman (2015)) has proved able to reproduce the turbulent flow often observed in high
89 flowrate conditions, and can deal with variably saturated pipes. It is thus used to reproduce and forecast
90 the flow discharge at springs (e.g., Kaufmann et al., 2016; Vuilleumier, 2018), as well as to assess the impact
91 of the conduit and network geometries on the flow response (Peterson and Wicks, 2006). In this approach,

92 the network has to be explicitly represented, as well as its dimensions.

93 In this paper, we present an open-source solution to help a first analysis and simulation of long tail multi-
94 peaked BTCs observed in karstic systems: OM-MADE (One-dimensional Model for Multiple Advection,
95 Dispersion, and storage in Exchanging zones). OM-MADE simulates one-dimensional solute transport along
96 a flow path: it does not require an explicit representation of the conduits, only the length and average cross-
97 sectional area are needed. OM-MADE is based on the resolution of classical mass conservation equations
98 (Section 2 and Appendix A). It combines the discretization of the flow path into several reaches and the
99 exchange with immobile flow zones proposed in OTIS (Runkel, 1998)) with the multiple flow zone approach
100 proposed by Field and Leij (2012). OM-MADE is written in Python, which is a commonly known and easily
101 accessible language. It uses the Numpy library, which permits to optimize the numerical equation resolution.
102 The design has been chosen to facilitate the use by non-expert developers (Appendix B). A verification has
103 been performed against analytical solutions, OTIS, and DADE models demonstrating the correct functioning
104 of the proposed solution and allowing to assess its performance (Section 3). The capacities of the software
105 to combine dual-advective-dispersive flow and interaction with immobile water along a flow path discretized
106 into several reaches is demonstrated on the Furfooz area (Section 4).

107 2. Methods

108 OM-MADE is an open-source software that simulates one-dimensional solute transport. Its specificity is
109 to allow multiple advective-dispersive parallel flow zones, or channels, that can exchange with each others,
110 as well as storage, or immobile, zones (Fig. 1). All zones are identically described, the difference between
111 mobile and immobile regions is done through the input flowrate Q , which is nil for immobile - storage -
112 zones. All parallel channels are divided along the direction of flow into *reaches*, in which all physical model
113 parameters are kept constant.

114 Linear lateral in/outflow is allowed in the mobile zones following the description by Runkel (1998).
115 Lateral inflow is described by the inflow linear rate q_{in} and concentration C_{in} and may lead to a dilution
116 ($C_{in} < C$) or a concentration ($C_{in} > C$) of the solute. Lateral outflow (q_{out}), however, does not impact on
117 the concentration since the outflow concentration is the one of the channel. Lateral in/outflow modifies the
118 flowrate in the channel following equation 1.

$$\frac{dQ}{dx} = q_{in} - q_{out} \quad (1)$$

119 The temporal variation of the flowrate is neglected (steady state). The solute may also be affected by
120 adsorption / decay processes either in mobile or immobile zones.

121 Considering mass conservation, the general equation of a solute transport in a one-dimensional uniform
122 flow in a zone p that can exchange with other zones q can be written:

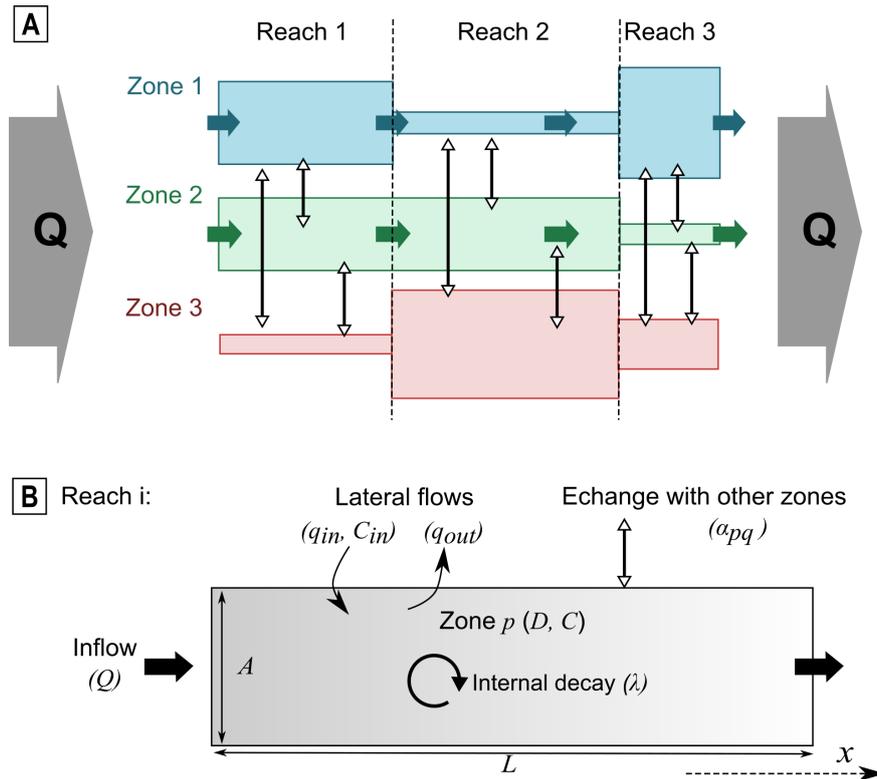


Fig. 1. Schematic representation of an OM-MADE model: (A) In this example, two mobile zones (zone 1 and 2) are interconnected with one storage zone (zone 3). The total flowrate Q is preserved all along the flow (steady flow regime). Three reaches are defined to allow longitudinal variations of the system geometrical characteristics. (B) Detailed representation of one reach of a zone p : a reach is defined by a given length L , a cross-sectional area A , a dispersion coefficient D , a solute concentration C , linear lateral flows (in/out flowrates and concentration q_{in} , q_{out} , C_{in}), internal decay (coefficient λ) and exchange(s) with other(s) zone(s) (coefficient(s) α_{pq}).

$$A \frac{\partial C}{\partial t} = -Q \frac{\partial C}{\partial x} + \frac{\partial}{\partial x} \left(AD \frac{\partial C}{\partial x} \right) + q_{in} (C_{in} - C) + \sum_{q \neq p} \alpha_{qp} (C_q - C) - \lambda AC \quad (2)$$

123 where t (T) designates the time and x (L) the distance, A (L²) is the stream channel cross-sectional area
 124 of the zone p , C (CU) is the solute concentration in zone p , Q (L³/T) is the volumetric flowrate across p , D
 125 (L²/T) is the hydrodynamic dispersion coefficient (which combines diffusion and mechanical dispersion), q_{in}
 126 (L²/T) is the lateral inflow rate per unit of distance, C_{in} (CU) is the solute concentration in lateral inflow,
 127 α_{qp} (L²/T) is the exchange coefficient between the zones p and q multiplied by the exchange surface area,
 128 λ (T⁻¹) is the first order decay coefficient in p .

129 In an immobile - storage - zone, the inflow rate Q is nil. Physically, mechanical dispersion is also nil but
 130 molecular diffusion can be considered by setting an adapted value of the hydrodynamic dispersion coefficient
 131 D , for example in the case of fluoresceine tracing tests: $D \approx 0.64 \times 10^{-9} m^2/s$ (Galambos and Forster, 1998).

132 This global formulation can also be adapted to describe sedimentation zones ($Q = q_{in} = 0$) with the
 133 following relations:

$$C = \frac{C_{sed}}{K_d} \quad (3)$$

$$\alpha_{qp} = \frac{M_{sed}}{L} \hat{\lambda} K_d \quad (4)$$

135 where K_d (volume/mass unit) is the coefficient of partition, $\hat{\lambda}$ the decay coefficient, M_{sed} the mass of
 136 available sediments, C_{sed} the adsorbed concentration on sediments and L the total length of the zone.

137 To solve the partial differential equation 2, two discretization schemes have been implemented in the OM-
 138 MADE software. The first one is based on an operator-split approach (sequential split) for the temporal
 139 discretization (Geiser, 2010; Khan and Liu, 1998). The second one is similar to the one used in OTIS. Both
 140 discretization schemes are detailed in Appendix A.

141 OM-MADE is written in Python v3. The software architecture is described in Appendix B. The
 142 OM-MADE package is freely available on GitHub as a Python project ([https://github.com/OM-MADE/](https://github.com/OM-MADE/OM-MADE)
 143 [OM-MADE](https://github.com/OM-MADE/OM-MADE)). It is provided with examples of applications on the following verification case studies (Section 3),
 144 as well as an application on the Furfooz karstic area (Section 4).

145 3. Verification against analytical solutions and alternative models

146 When developing a numerical solution, its correct functioning should be assessed. This verification of
 147 the software also allows understanding the software performance, both regarding computing performance
 148 and accuracy. The verification finally showcases the weak points of the numerical solution so as to provide
 149 the end-user indicators to use the software in the best conditions. The first set of verifications concerns
 150 analytical solutions. Pure diffusion and pure advection allow testing the extreme values of the Peclet
 151 number ($Pe = |Qdx/AD|$) which characterizes the transport phenomena in steady-state flow conditions.

152 The analytical Advection-Dispersion Equation (ADE) allows the verification at an intermediate Peclet and
 153 corresponds to the most common application. The second set of verifications concerns numerical comparison
 154 to other software. Such verifications allow to check the capability of the software's added functionalities
 155 compared to the ADE: multiple flow zones with and without an exchange term (section 3.4), multi-reach,
 156 lateral flow, and degradation/adsorption (section 3.5). To compare objectively the OM-MADE results with
 157 the reference cases, the Normalized Root Mean Square Error (NRMSE) is computed. All values can be
 158 found in the online examples, and main results are given here.

159 3.1. Pure diffusion

160 A pure diffusive flow, no flowrate (it is an immobile flow zone) is simulated in a single conduit of 1500 m
 161 length, 1 m² cross-sectional area. The hydrodynamic dispersion coefficient is set to 0.05 m²/s. Initial
 162 concentration is nil, and a constant concentration of 350 mg/l is injected continuously. The total simulation
 163 time is 40 h, space step is 1 m and time step is 9000 s. Fig. 2 plots the concentration profiles observed along
 164 the conduit each 150 h. It is compared to the analytical solution in case of a semi-infinite wall:

$$C(t) = C_0 \operatorname{erf} \left(\frac{x}{2\sqrt{Dt}} \right) \quad (5)$$

165 with C_0 the injected concentration and D the hydrodynamic dispersion. Considering that the outlet bound-
 166 ary conditions of the numerical model and of the analytical solution are different, a comparison between the
 167 two is only valid when the outlet boundary impact on the solution is negligible, i.e. at short-times. This
 168 explains the small differences observed at $x = 1500$ m, when the tracer arrives at the output location at
 169 $t = 1200$ h. But still for $t = 1200$ h, the Normalised Root Mean Square Error (NRMSE) remains inferior to
 170 0.05% for both schemes.

171 3.2. Pure advection

172 A pure advective flow is simulated in a single conduit of 1500 m length, 1 m² cross-sectional area, with
 173 a flowrate of 0.01 m³/s. Initial concentration is nil, and a concentration of 350 mg/l is injected during 3 h.
 174 The total simulation is 40 h. The simulation time step of 300 s leads to a Courant number of 3. As a
 175 consequence, the operator-split scheme requires 3 sub-loops of advection, each with a Courant number of 1,
 176 compared to the Crank-Nicholson scheme. A second simulation time step of 250 s is used to demonstrate the
 177 impact of a Courant number strictly below 1 (0.5 for the last sub-loop in the present case) on the behavior
 178 of the operator-split scheme. Figure 3 plots the concentration profiles observed along the conduit each 5 h,
 179 using operator-split scheme for both time steps, and the Crank-Nicholson scheme for a time step of 300 s.

180 In all cases, the model reproduces correctly the arrival time of the pollutant step. The computing time in
 181 the present cases is around 1 minute on a regular hardware with the operator-split being roughly 1.7 times
 182 faster. For the explicit Lax-Wendroff scheme (Figure 3A), the model demonstrates a satisfying behaviour

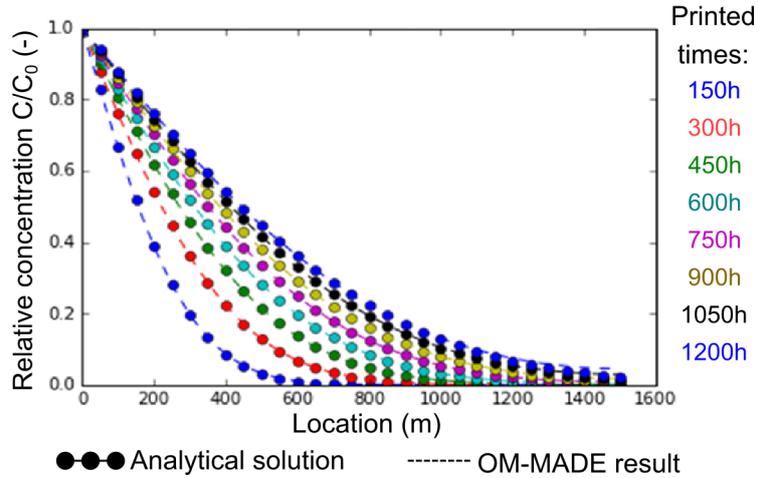


Fig. 2. Comparison of OM-MADE result with an analytical solution in the case of a pure diffusive flow. At $t = 1200h$, the tracer arrives at the output location, thus the semi-infinite wall condition is no more valuable and explains the small differences that can be observed with the analytical solution.

183 with a NRMSE of the size of rounding error (0.6%). This error is generated by the interpolation of the
 184 solution between two actual solution points and the beginning and ending of the concentration step rather
 185 than by the numerical solution itself. However, when the Courant number is below 1, which is partly the case
 186 when the time step equals 250 s, notable spurious oscillations occur and increase with time (NRMSE going
 187 from 1% at 5 h to 1.6% at 40 h). Regarding the Crank-Nicholson model, spurious oscillations also occurs and
 188 lead to a significant error (NRMSE = 3.6% at 40 h). These oscillations are attenuated through numerical
 189 dispersion which also adds to the error. It should be noted that the spurious oscillations are characteristic
 190 of second order spatial schemes such as Lax-Wendroff and centred approaches (Lax and Wendroff, 1960;
 191 Zheng and Wang, 1999). Therefore, OM-MADE may not be used in pure advection conditions ($Pe = \infty$).

192 3.3. Advection - Dispersion

193 A solute transport by advection-dispersion is simulated in the same conduit of 1500 m length and 1 m²
 194 cross-sectional area, with a flowrate $Q = 0.01 \text{ m}^3/\text{s}$ and a hydrodynamic dispersion coefficient $D = 0.05 \text{ m}^2/\text{s}$
 195 (leading to $Pe = 0.2$) or $D = 0.0025 \text{ m}^2/\text{s}$ (leading to $Pe = 4$). A value of Peclet number of 4 is often
 196 considered as the usability limit of second order schemes (Zheng and Wang, 1999). Initial concentration is
 197 nil, and we consider an instantaneous solute pike corresponding to the injection of $M = 900 \text{ g}$ of tracer. The
 198 total simulation time is 40 h, space step is 1 m and time step is 360 s. For the simulation, instantaneous
 199 injection is not possible to model: the tracer is injected during one time step $dt = 360 \text{ s}$. Thus, it corresponds
 200 to a concentration $C_0 = M/(Q * dt) = 250 \text{ mg/l}$. Fig. 4 plots the concentration profiles observed along the
 201 conduit each 5 h using the operator-split approach, and compared to its corresponding analytical solution

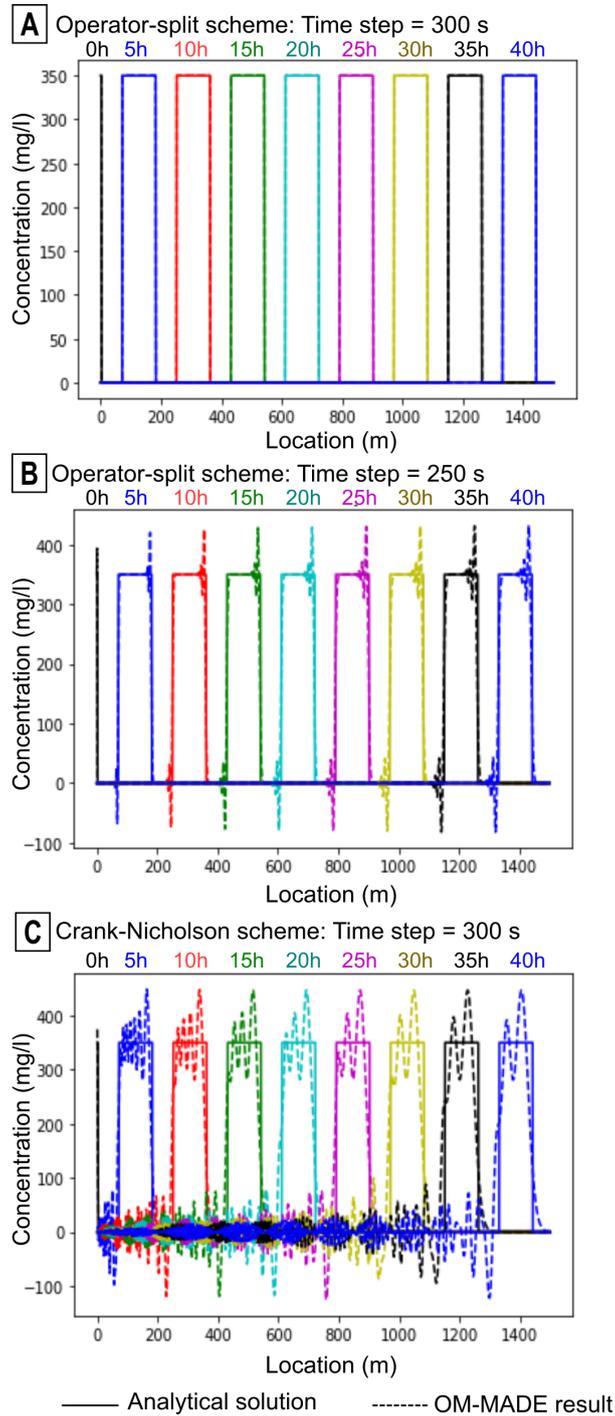


Fig. 3. Comparison of OM-MADE results with an analytical solution in the case of a pure advective flow: the concentration profiles are plotted each 5 h along the conduit. In (A) and (B), OM-MADE uses the operator-split scheme (Lax-Wendroff scheme for advection resolution) with a time step of 300 s in (A) and 250 s in (B). In (C) OM-MADE is run using a Crank-Nicholson scheme and a time step of 300 s.

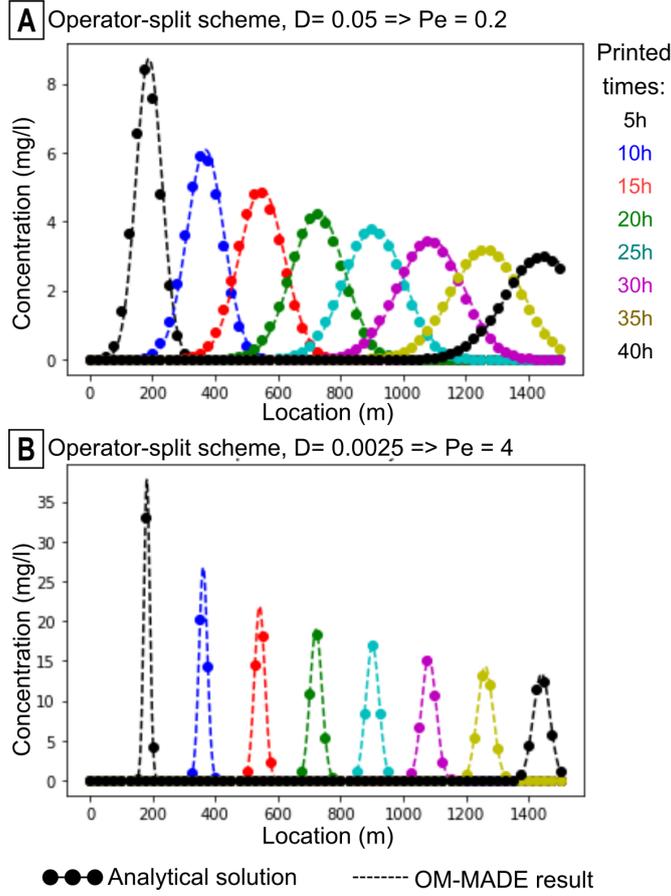


Fig. 4. Comparison of OM-MADE results (operator-split scheme) with an analytical solution in the case of advective-dispersive flow. In (A) the hydrodynamic dispersion coefficient $D = 0.05 \text{ m}^2/\text{s}$ which leads to $Pe = 0.2$. In (B) $D = 0.0025 \text{ m}^2/\text{s}$ which leads to $Pe = 4$, a value often considered as the usability limit of second order schemes.

202 in a semi-infinite media:

$$C(t) = \frac{M}{A\sqrt{4\pi Dt}} \exp\left(-\frac{(x - Ut)^2}{4Dt}\right) \quad (6)$$

203 with U the velocity of the fluids, and A the cross-sectional area.

204 As shown in Fig. 4, the model behaves adequately with a NRMSE of 0.32% and 0.55% for the operator-
 205 split scheme at time = 40 h and, respectively, $Pe = 0.2$ and $Pe = 4$. The Crank-Nicholson solution generates
 206 a similar error (0.34%) at $Pe = 0.2$ but retains a slight oscillatory behavior at $Pe = 4$ (NRMSE = 0.94%).
 207 Therefore for advective-dominant flows, the operator-split approach is more advisable. Besides, the limit of
 208 $Pe = 4$ is acceptable to use the OM-MADE software.

209 3.4. Dual advection and dispersion: verification against WSADE and DADE solutions

210 To validate the model for multiple mobile flow zones we used two examples published in Field and Leij
 211 (2012).

212 The first one considers two mobile flow zones with no exchange. The channels are 200 cm long, and
 213 the concentrations are observed at 10 cm, 25 cm and 40 cm. In the reference paper q_i is referred to as
 214 “volumetric flow rate in conduit i per total cross-sectional area” (in cm/d) and set as $q_i = \theta_i v_i$. In the
 215 application $\theta_1 = \theta_2 = 0.5$. With both cross-sectional areas equal to 1 cm^2 , flowrates in conduits are
 216 so $Q_1 = 10\text{ cm}^3/d$ and $Q_2 = 5\text{ cm}^3/d$. As the dispersivity $\kappa = 0.25\text{ cm}$, the respective hydrodynamic
 217 dispersion coefficients are $D_1 = 2.5\text{ cm}^2/d$ and $D_2 = 1.25\text{ cm}^2/d$. The total simulation time is 10 s, space
 218 step is 0.2 cm and time step is 0.01 s. An instantaneous solute pike of 12 mg is injected in each channel. In
 219 the simulation, we inject during one time step $dt = 0.01\text{ s}$. The corresponding input concentration $C_{0,i}$ for
 220 each zone i , is deduced by the following relation: $C_{0,i} = m_i/(q_i * dt)$ with $m_1 = m_2 = 6\text{ mg/cm}^3$ the mass
 221 injected in each zone. For each zone, it corresponds to $C_{0,1} = 120\text{ mg/cm}^3$ and $C_{0,2} = 240\text{ mg/cm}^3$.

222 As shown in Fig. 5A, OM-MADE gives similar results than the Weighted-Sum Advection Dispersion
 223 Equation (WSADE) solution given by Field and Leij (2012) from the subsolution by Leij and Toride (1995)
 224 with NRMSE values at 40 cm equal to 0.32% and 0.30% respectively for the flow zones 1 and 2 using the
 225 operator-split approach, and 0.30% and 0.28% using Crank-Nicholson.

226 The second example is the same than the first one, except that an exchange is effective between both mo-
 227 bile zones. The exchange coefficient applied in Field and Leij (2012) is equal to 0.05 d^{-1} , which corresponds
 228 in OM-MADE to $\alpha_{1-2} = 0.1\text{ cm}^2/d$.

229 Fig. 5B shows that OM-MADE gives similar results than the DADE approach for two exchanging mobile
 230 zones with NRMSE at 40 cm of 0.13% (0.12%) using the operator-split (Crank-Nicholson) approach.

231 3.5. Multi-reaches single flow with storage zone or degradation rate: verification against OTIS

232 To test the capacity of our software to model single mobile zones discretized into several reaches and
 233 exchanging with storage zones, we compare it to the results obtained with OTIS to simulate a conservative
 234 transport in a stream with immobile zones (Application 1 in Runkel (1998)). This simulation has been itself
 235 validated against field measurements of a chloride tracer test in Uvas Creek, a small pool-and-riffle stream
 236 in northern California (US) (Bencala and Walters, 1983). The main stream is represented by a mobile zone
 237 with a constant flowrate of $Q = 0.0125\text{ m}^3/s$. Pools are modelled by exchanging mobile zones. The stream
 238 is characterized by an initial concentration equals to 3.7 mg/l. The experiment consisted in the injection
 239 during 3 h of chloride at a constant rate of 11.4 mg/l starting from 8.25 h for the reference experiment. In
 240 our simulation, this initial period is skipped, and the injection is started at 540 s, and thus ends at 11340 s.
 241 The total simulation time is 24 h, which corresponds in our simulation to 56700 s. The time step is 180 s
 242 (= 0.05 h), the space step is 1 m, and the concentrations are printed at 5 locations: 38, 105, 281, 433, and
 243 619 m from the injection point, corresponding to the five sampling points and the exact limit of the reaches.
 244 The domain is divided into 5 reaches whose characteristics are given in Table 1. The reaches 3, 4, and 5
 245 are characterized by the presence of pools. To reproduce the increasing flow in the downstream direction,

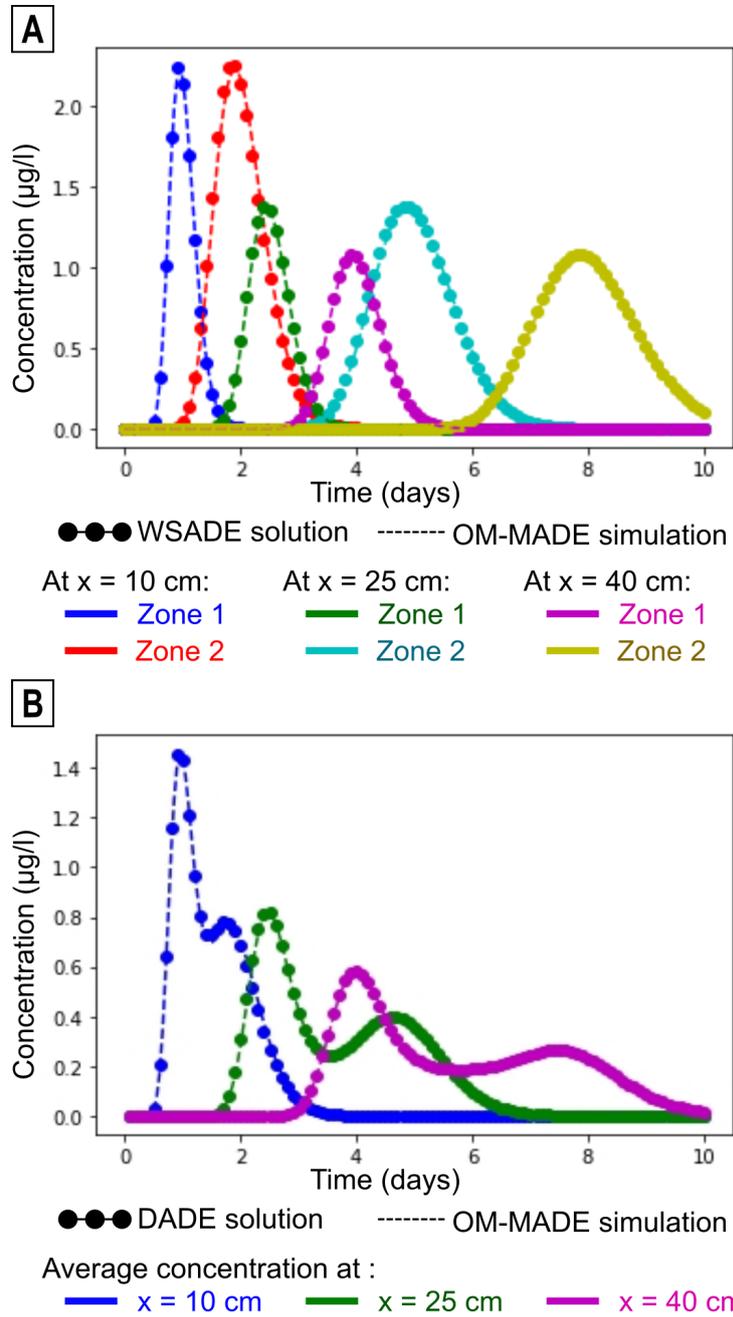


Fig. 5. Simulation of two mobile zones and comparison with solutions of Field and Leij (2012) at three positions: (A) in the case where no exchange are allowed between the two zones (WSADE solution); (B) in the case where exchanges are taken into account between both zones (DADE solution)

Table 1

Parameters of the OM-MADE simulation for multi-reach single flow with storage. These are based on the ones realized with OTIS by Runkel (1998) for the tracer tests by Bencala and Walters (1983) in Uvas Creek.

	Exchange	Mobile zone (Main Stream)					Storage Zone (Pools)				
	$\alpha_{1,2}$ (m^2/s)	A (m^2)	D (m^2/s)	q_{in} (m^2/s)	q_{out} (m^2/s)	C_{in} (mg/l)	A (m^2)	D (m^2/s)	q_{in} (m^2/s)	q_{out} (m^2/s)	C_{in} (mg/l)
Reach 1	0	0.30	0.12	0	0	3.7	0.05	0	0	0	0
Reach 2	0	0.42	0.15	0	0	3.7	0.05	0	0	0	0
Reach 3	1.08e-5	0.36	0.24	4.545e-6	0	3.7	0.36	0	0	0	0
Reach 4	4.10e-6	0.41	0.31	1.974e-6	0	3.7	0.41	0	0	0	0
Reach 5	2.34e-5	0.52	0.40	2.151e-6	0	3.7	1.56	0	0	0	0

246 lateral inflows are introduced in reaches 3, 4, and 5. For the sake of comparison and unlike in Runkel (1998),
 247 interpolation of the results in between calculated points is allowed in the OTIS solution. All parameters are
 248 the same in OM-MADE and OTIS, except for the exchange coefficients which are not defined the same way
 249 (Table 1). For homogeneity purposes (Eq. A.5), we defined indeed the exchange coefficient between two
 250 zones as a value expressed in [m^2/d]. In OTIS, the exchange coefficient is expressed in d^{-1} and defined as:
 251 $\alpha_{OTIS} = \alpha_{OM-MADE}/A$, where A is the cross-sectional area of the mobile zone. Results show a very good
 252 fitting with observation at the five observation locations (Fig. 6) with NRMSE in the flow zone of around
 253 0.13% for the operator-split approach and 0.17% for Crank-Nicholson as well as in the storage zone with
 254 NRMSE of 0.02% for both schemes.

255 A second comparison with OTIS was performed to validate the simulation of transport with first-order
 256 degradation rate (Application 3 in Runkel (1998)). It illustrates a hypothetical problem of a single reach
 257 - single flow zone transport of a decaying substance, which has been analytically solved in Runkel (1996).
 258 The simulation is thus characterized by one mobile zone of 2200 m long and 1 m^2 cross-sectional area, with
 259 an initial null concentration and a constant flowrate $Q = 0.1 m^3/s$. Its hydrodynamic dispersion coefficient
 260 is $D = 5 m^2/s$. The unique reach is discretized in 10 m cells, and the concentrations are observed at 100 m
 261 and 2000 m. The simulation lasts 12 h (= 43200 s) with a time step $dt = 144 s$. The decaying substance
 262 is injected during 2 hours starting at $t = 3600 s$ with a constant input concentration $C_0 = 100 mg/l$. The
 263 degradation rate is $\lambda = 1.10 \cdot 10^{-4} s^{-1}$. The results obtained with OM-MADE are, again, similar to those
 264 obtained with OTIS and validated against analytical solution by Runkel (1998) (Fig. 7), with a NRMSE of
 265 0.46% for the operator-split approach at 2000 m, and 0.31% for the Crank-Nicholson approach. It should also
 266 be noted that this is the only verification case, among those presented, when the Crank-Nicholson approach
 267 is more efficient than the operator-split approach. But it should also be noted that we are comparing with
 268 the data from OTIS which uses a Crank-Nicholson scheme.

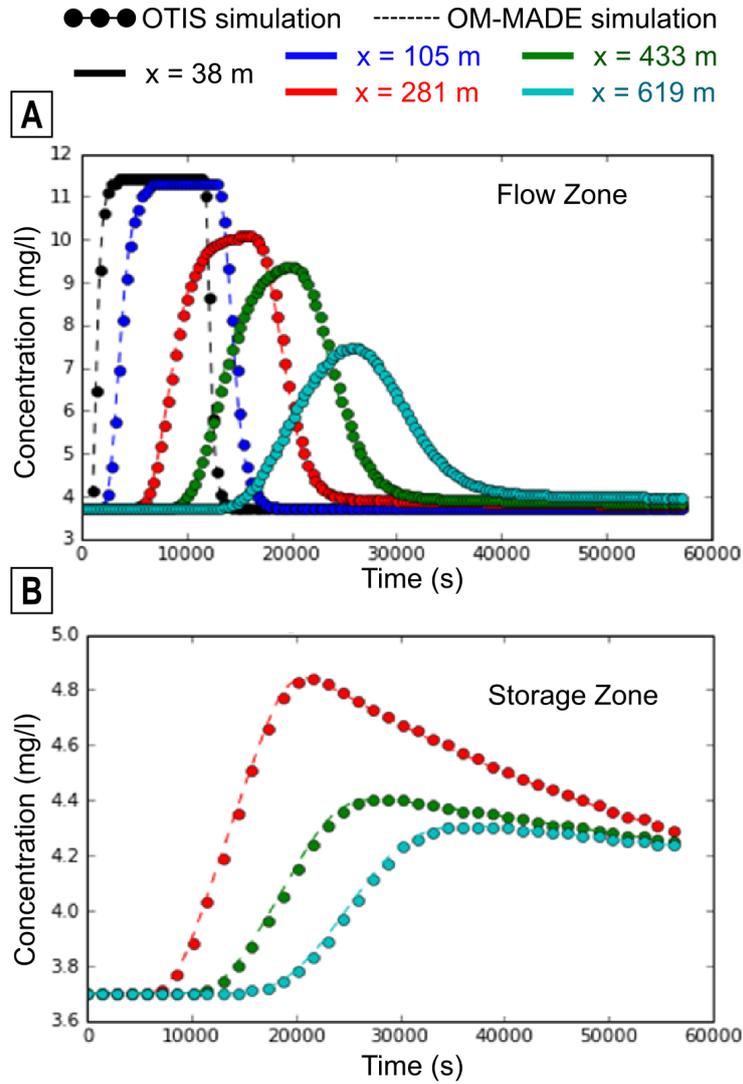


Fig. 6. Simulation of BTCs in the case of multi-reach single flow with storage: the domain is divided in 5 reaches, one mobile zone exchanges with storage zones in the reaches 3, 4, and 5. Simulated concentrations with OTIS and OM-MADE: (A) in the flow zone and (B) in the storage zones.

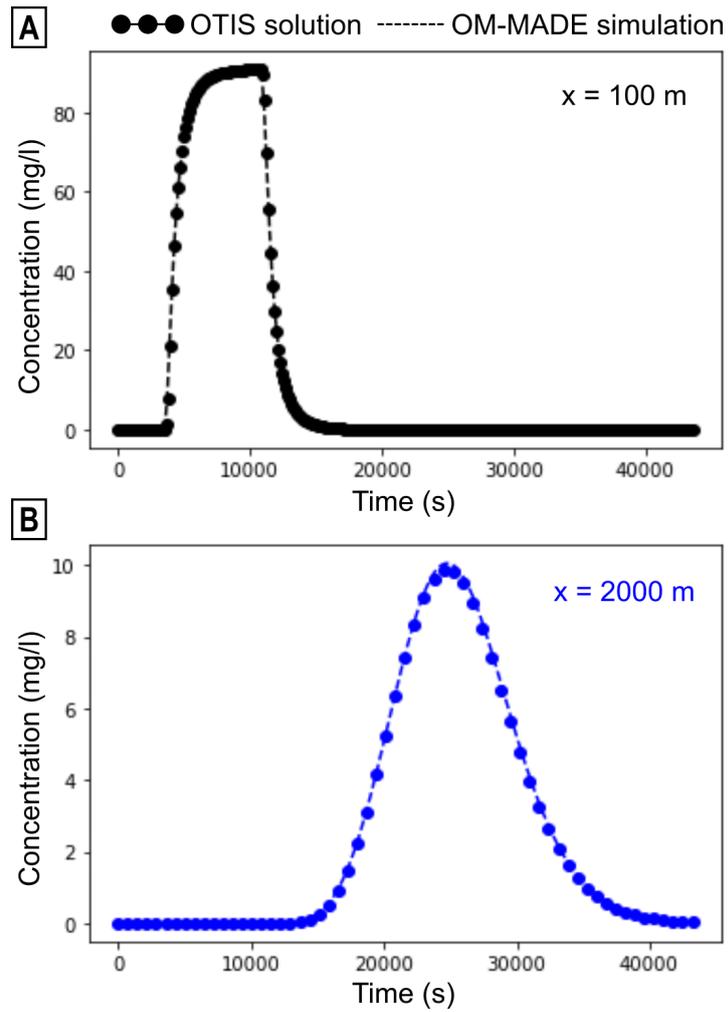


Fig. 7. OM-MADE results compared to OTIS solution in the case of transport with first-order decay.

269 4. Application on the Furfooz karstic system

270 The karstic system of Furfooz is located in the South of Belgium, near Dinant. The Furfooz karst has
271 developed in the limestones of Carboniferous Dinantian, more specially in the Waulsortian mudmounds
272 (Dewaide et al., 2014). The network mainly consists in conduits with flooded cross-sections of 1-2 m² in
273 moderate flow conditions, and has the specificity to cross two successive underground lakes (Fig. 8). It
274 constitutes an underground system of approximately 1.2 km length which catches partially the Lesse River
275 and returns the water back to surface through a diffusive resurgence. While a large part of the system has
276 been explored, the downstream part of the lakes remains unknown, as well as the first 70 m downstream
277 the swallow hole.

278 A tracer test has been performed, consisting in the injection of 200 g of sulforhodamine B at the swallow
279 hole, located 210 m upstream the lakes, during stable low flow conditions. Several flow measurements were
280 performed during the tracer test at several locations and times, and provide integrated values that vary in
281 the underground network between 5.5 l/s to 5.97 l/s from the *Trou qui fume* to the *Galerie des Sources*
282 (Dewaide, 2018). At the swallow hole, the flowrate was, however, estimated around 3.5-3.8 l/s, suggesting
283 that around 2 l/s are penetrating the karstic system through diffuse entries before the main karstic conduit
284 of the *Trou qui fume*. Water samples were analysed on site using field fluorometers at two locations: in
285 the *Trou qui fume*, and in the *Galerie des Sources* (Fig. 8). The *Trou qui fume* is the first explorable
286 part of the Furfooz karstic system. It is preceded by an impenetrable zone, probably tortuous and highly
287 fractured, right after the swallow hole, that hydrogeologists and speleologists consider to represent a flow
288 path of approximately 70 m long. Then, in the *Trou qui fume*, the water is mainly confined in a single
289 conduit of approximately 140 m long, only partly flooded and easy of access, that ends in the first lake.
290 These two zones represent a first section of approximately 210 m that links the swallow hole to the lake.
291 Located in the middle of this single conduit, the first sampling point is estimated to be 150 m downstream
292 the swallow hole.

293 The water flows a minimum distance of 150 m through the lakes before penetrating an unexplored conduit
294 part to the *Galerie des Sources*. Inside the *Galerie des Sources*, the second sampling point is considered by
295 hydrogeologists and speleologists to be located approximately 410 m downstream the lakes (and so, 770 m
296 downstream the swallow hole). It should be noted that these lengths are approximative lengths based on
297 map study. They could potentially be under-estimated.

298 At the first sampling point, the tracer recovery results in a classical single peaked BTC with a slight
299 asymmetry. Downstream the lakes at the *Galerie des Sources*, tracer recovery results in a skewed dual-
300 peaked BTC. Further investigations have conducted Dewaide (2018) to propose a conceptual model of the
301 system that explains this BTC by a combination of a storage zone effect and a dual-advective flow zone
302 within the lake area. Thus, analysing this BTC with OM-MADE seems appropriate.

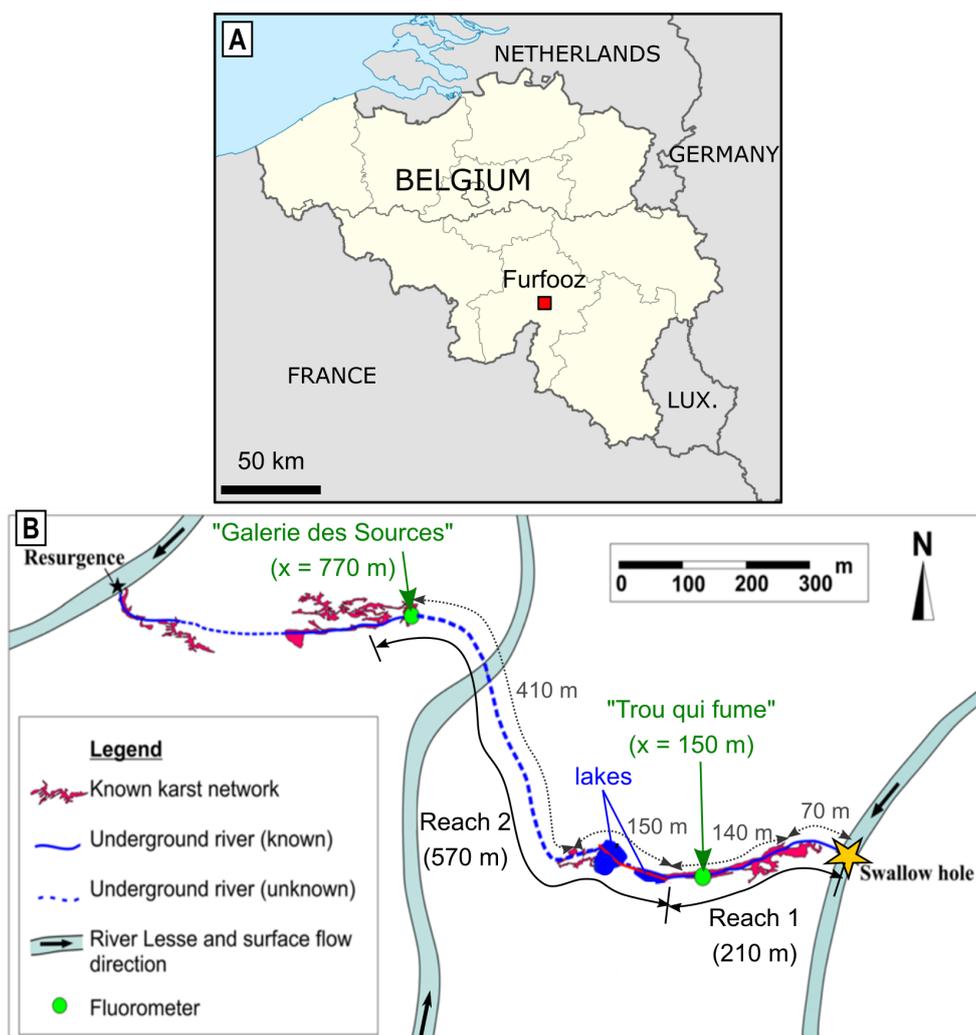


Fig. 8. The Furfooz karstic system and its numerical representation. Two sampling locations are considered : the *Trou qui fume* and the *Galerie des Sources*. The system is approximated by two reaches: (i) the first one represents a first mainly advective part ; (ii) the second reach represents the ensemble made by the lakes and their unexplored downstream part.

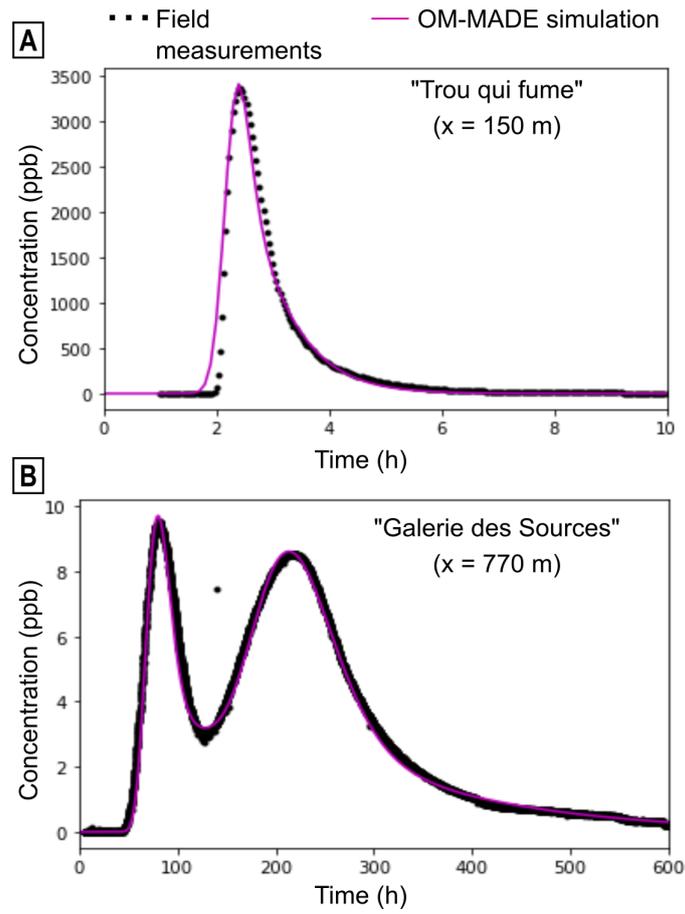


Fig. 9. OM-MADE simulated BTC fit to a tracer test conducted in Furfooz. The first site, named "Trou qui fume" is located 150 m downstream the swallow hole while the second site, the "Galerie des Sources" is located 770 m downstream the injection point.

303 Fig. 9 depicts the OM-MADE fit to the BTC observed at the *Trou qui fume* and the *Galerie des Sources*.
 304 The system is represented by a succession of 2 reaches, corresponding to both monitored zones: (i) the first
 305 one represents the first part of 210 m long, which is observed at the *Trou qui fume*, 150 m downstream the
 306 injection point; (ii) the second reach corresponds to a transport distance of 570 m downstream the lakes
 307 and illustrates the combined effect of the lakes and of their downstream part until the *Galerie des sources*,
 308 located at a supposed distance of 770 m downstream the injection point. Note that to avoid eventual
 309 boundary effects, the reach terminates further than the observation point location. In this application, the
 310 intermediary sampling sites (sites 2 and 3 in Dewaide et al. (2018)) are not considered. Indeed, the probes
 311 were located at the surface of the lakes, and do not account for an average behaviour of the water lake
 312 volume: later field experiments (Dewaide, 2018) have demonstrated that these probes were only registering
 313 dispersion inside the lake while an advective quicker transport occurred deeper in it.

314 The first BTC expresses a quick (in less than 3 hours) and mainly advective transport of the tracer.
 315 Thus, to avoid numerical dispersion while keeping reasonable computational times to simulate a tracer test
 316 of 600 h (= 2160000 s), we use a space step of 2.5 m and a time step of 360 s. With those numerical
 317 parameters, the simulation takes 4 min 30s on a standard laptop with 8 Go RAM and a 2.60 GHz Intel(R)
 318 Core(TM) Processor. In this model, which largely approximates the natural behaviour and uses a steady
 319 flow regime, we consider a total mean discharge of $Q = 5.7 \text{ l/s}$. Given the observations at the swallow hole,
 320 we decided to distribute this discharge between the two mobile zones as followed: 3.7 l/s is considered to
 321 penetrate in the first mobile zone, while zone 2 is characterized by an input discharge of 2 l/s. The initial
 322 concentration of the water is nil, and at $t = 0$ an injection of 200 g of the tracer is performed in zone 1 only,
 323 which, applied to our time step and with an input flowrate of 3.7 l/s, corresponds to an input concentration
 324 of $C_1 = 150.15 \text{ mg/l} = 150150 \text{ ppb}$ during the first 360 s. The input concentration is nil in zone 2.

325 To illustrate the fact that all water is drained by a single conduit in the main part of the first reach, and
 326 especially where the sampling is performed, we have decided to impose almost the same flowrate v_i in both
 327 mobile zones by an adapted choice of the corresponding cross-sectional areas A_i ($A_2 \simeq Q_2/Q_1 \times A_1$). We
 328 chose to distribute the coefficient effects by using equal values in both zones. The first order decay coefficients
 329 λ express the probable sorption of the sulfhorhodamine, even if it is not rigorously a sorption effect that
 330 is numerically reproduced (no consideration of exchange surface or relative concentration). Sabatini (2000)
 331 demonstrated, indeed, that sulforhodamine B tends to sorb on positively charged limestone surfaces, more
 332 than uranine. This has also been observed during a multi-tracer test by Geyer et al. (2007). In Furfooz,
 333 the first part of the underground network is characterized by an important amount of muddy material and
 334 a limited tracer recovery has been observed at both sites: a quick integration of the BTCs indicates, when
 335 considering a mean discharge of 5.7 l/s, a restitution of around 35% at the *Trou qui fume* and 19% at the
 336 *Galerie des sources* (Dewaide, 2018).

337 Introducing a small storage zone is necessary to reproduce the BTC asymmetry. This could be related to

Table 2

Parameters of the OM-MADE simulation for modelling one tracing test carried out in the Furfooz karstic system : the system is described by a model with multi-reaches dual-mobile zones with storage. Lateral flows (q_{lat} and C_{lat}) are nil. The simulation is performed with a spatial step $dx = 2.5m$ and a time step $dt = 360s$. A total mass of 200 g of sulforhodamine B is injected at $t = 0$ in zone 1.

Reach 1: 0 - 210 m						
	A	D	λ	Exchange coefficients α_{ij} (m^2/s)		
	(m^2)	(m^2/s)	($1/s$)	zone 1	zone 2	zone 3
Zone 1 ($Q = 3.7L/s$)	0.217	0.014	1.25e-4	0	1e-2	2.2e-5
Zone 2 ($Q = 2L/s$)	0.116	0.009	1.25e-4	1e-2	0	2.2e-5
Zone 3 (Storage)	0.063	0.6e-9	0	2.2e-5	2.2e-5	0
Reach 2: 210 - 780 m						
	A	D	λ	Exchange coefficients α_{ij} (m^2/s)		
	(m^2)	(m^2/s)	($1/s$)	zone 1	zone 2	zone 3
Zone 1 ($Q = 3.7L/s$)	1.90	0.015	9.4e-7	0	1e-7	9.8e-6
Zone 2 ($Q = 2L/s$)	2.88	0.007	4e-8	1e-7	0	8.5e-7
Zone 3 (Storage)	4	0.6e-9	2e-7	9.8e-6	8.5e-7	0

338 the unknown part, in the first 70 m of the system, probably combined with an effect of the small pools and of
 339 the variations of the underground stream geometry all along the karstic system, as it has been demonstrated
 340 on other karstic sites (Hauns et al., 2001). In the second reach, a partial independence of both mobile zones
 341 is set thanks to a lowest exchange coefficient, and the cross-sectional areas of both mobile zones are not
 342 linked any more.

343 With these input constraints, the different parameter values were manually tuned to fit the two measured
 344 BTCs. The resulting set of parameters, presented in Table 2, represent an average behaviour of the two
 345 parts of the system, with a given conceptual scenario. They demonstrate the capacity of OM-MADE to
 346 model one-dimensional solute transport in mutiple exchanging flow and storage zones with a multi-reach
 347 discretization.

348 5. Discussion and conclusion

349 OM-MADE has been created as an answer to field hydrologists who could not represent their observed
 350 breakthrough curves using easily available and usable software (in this case OTIS and DADE) and needed to
 351 model more complex interactions. OM-MADE combines advantages of the OTIS software - a discretization
 352 of the flow path into several homogeneous reaches and exchanges with immobile flow zones - and the DADE
 353 solution - multiple exchanging mobile zones. It provides so a flexible solution to simulate one-dimensional
 354 transport in the case of multiple exchanging mobile and immobile flow zones. Such configurations are, indeed,
 355 often suggested to explain multi-peaked BTCs observed when performing tracer tests in karstic systems. It

356 also allows to segment the domain of interest into several reaches of constant model parameters, which is
357 useful to represent the different parts of a karst network that field investigation can reveal, especially when
358 multi-sampling sites are used.

359 OM-MADE has been tested to simulate a real tracer test performed in Furfooz (Belgium), allowing
360 to demonstrate its potential and also its limits. By modelling a one-dimensional transport, OM-MADE
361 simplifies a complex reality and, as other models, OM-MADE is parametrised by different variables that
362 can not all be measured on the field (e.g., the exchange coefficients, or even the average cross-sectional area
363 of each reach). To reproduce a double-peaked BTC, it was necessary to impose different relative cross-
364 sectional areas, and thus flow rates, in both mobile zones. In the Furfooz application, we have arbitrarily
365 decided to enlarge the second mobile zone, but it has to be reminded that at the end of the first reach,
366 the water has mixed between both conduits, and thus the tracer concentration is the same in both mobile
367 zones. As a consequence, another fit could probably be done by accelerating the flow in the second zone
368 rather than in the first one. Also, the flowrate could be divided differently between the two mobile zones of
369 this reach. Thus, the main interest of such approach, is to test numerically the consistency of a conceptual
370 representation of the natural system. In this simulation, the long tail observed at the *Galerie des Sources*
371 is the effect of a large storage zone that interacts with both mobile zones, which is consistent with field
372 observations and the existence of the lakes. It also shows that the observed dual-peaked skewed BTC could
373 be explained by two mobile zones exchanging with a storage zone in the part of the karst between the lakes
374 and the *Galerie des Sources*. This global behaviour does not imply a more precise interpretation : the
375 dual-advective exchanging zones could be an effect of the lakes or an expression of a local auxiliary conduit
376 that diverts the solute transport and then transports it back to the main conduit. More field investigations
377 should now be performed to precise the exact functioning of the Furfooz system. A recent discovery of a
378 conduit between the lakes and the *Galerie des Sources* will certainly help in that purpose.

379 Regarding the number of calibration parameters, the more complex the model is (i.e., the higher the
380 number of reaches and flow zones) the more parameters are required. For the end-users, it is advisable
381 to start from the simplest model and, if necessary, to increase complexity. For instance, in Furfooz, a
382 two zone approach (either mobile-immobile or mobile-mobile) was insufficient to correctly describe the
383 measured breakthrough curve. For this specific case, OM-MADE offers the solution to increase progressively
384 the complexity while remaining a very basic solution. However, especially considering increased model
385 complexity, it is to be expected that the calibration is non-unique. In OM-MADE, the values of the various
386 parameters have to be set by a try-and-error approach, which can become a long and difficult task as the
387 number of reaches increase. An obvious improvement should be to implement an automated parameter
388 estimation process, for example by minimizing the squared differences between the simulated and observed
389 concentrations. Nevertheless, such functionality should also allow to fix some of these parameters which,
390 depending on the field case that is studied, can be already known (e.g. cross-sectional areas of some

391 conduits, nil exchanging coefficients, ...), or stacked by the field knowledge, which should be appreciated in
392 such under-constrained problems.

393 OM-MADE only considers steady-state conditions for flow (no temporal variation of the flow rate). It
394 should be noted that, in the field, monitoring the flow rate along time can be very problematic in some hardly
395 accessible conduits. For instance, in Furfooz, only a time-averaged value could be measured. During short-
396 distance - and thus short-time - tracer-tests, steady state conditions can be an acceptable approach. But it
397 would be an obvious limitation as soon as precipitations, and thus, floods, occur. Adapting OM-MADE to
398 non-steady conditions is an interesting perspective. Another interesting avenue would be to use pipe-flow
399 models like SWMM, and adapt them to handle immobile flow zones and exchange between conduits.

400 OM-MADE uses an operator-split approach solving the advective part using a second order Lax-Wendroff
401 scheme with explicit temporal resolution. This choice has been made to limit the numerical dispersion.
402 Therefore, the issue of numerical dispersion is not occurring (or little) in our method. However, oscillatory
403 behaviour remains in specific conditions: oscillatory behaviour is a well-known drawback of second order
404 methods such as Lax-Wendroff or centred scheme in pure advection conditions. It should be noted that when
405 Courant number is strictly equal to one (or is an integer) there is almost no oscillation in the operator-split
406 solution. Following Zheng and Wang (1999), the limit of grid Peclet number of 4 is advised for good use of
407 the OM-MADE solution. In order to limit both numerical dispersion and oscillatory behaviour, it would be
408 necessary to use higher-order schemes such as the 3rd order TVD (Total-Variation-Diminishing method).
409 This was not implemented in the software, but could be an obvious perspective.

410 In order to provide a better flexibility to the end-user and easy comparison, OM-MADE allows the
411 end-user to choose between the operator-split Lax Wendroff explicit (advection) - implicit (dispersion and
412 exchange) or a centred Crank-Nicholson solution. The explicit solution is faster than implicit or Crank-
413 Nicholson solution for the same time step since it does not require the computationally expensive solving
414 of a linear system. However, the time step is limited to satisfy the CFL condition. Therefore, when the
415 simulation time step is much larger than the time step required for satisfying the CFL, the explicit solution
416 lacks computing performance. A larger simulation time step leads to a loss in accuracy, especially for the
417 advection. In multi-reach conditions, or when cross-sectional flow exists, the calculation of the CFL and
418 therefore the advection time step, is constrained by the maximum Courant number. However, the calculation
419 of the CFL is independent for each conduit since there is no coupling in the advection part.

420 OM-MADE is written in Python, which, compared to C/C++ for example, slows down the numerical
421 calculation. This choice was made, however, since Python is a commonly known, flexible, easy to pick up
422 by non-programmers, open-source and multi-platform language. It was also decided to limit the amount of
423 code optimization to maintain its easy reading. Thus, whilst the calculation speed remains reasonable (in
424 the order of minutes, depending on the discretization choices and the hardware used), it could be considered
425 lacking efficiency especially considered complex, highly discretized problems. In those cases, combining

426 python with another language (like C++) could be interesting to gain in simulation time.

427 Despite these limitations, OM-MADE proposes an open-source solution to help a first analysis and
428 simulation of multi-peaked BTCs observed in karstic systems, which can be now used in any institution and
429 location, and improved by everyone to fit their requirements.

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528 **Appendix A. Numerical resolution schemes**

529 The partial differential equation 2 that had to be solved for each zone p , requires temporal and spatial
 530 discretization schemes. Each reach is thus subdivided into discrete segments of length dx , referred to with
 531 the index i . In the OM-MADE software, two discretization schemes are made available to the end-user.

532 The first discretization scheme is based on an operator-split approach (sequential split) for the temporal
 533 discretization. The operator-split is a commonly used numerical method (Geiser, 2010; Khan and Liu, 1998)
 534 to allow the use of custom numerical solutions for distinct part of the equation. In our case, the equation is
 535 split sequentially between its hyperbolic part, the advection (represented by the operator A_{adv} in equations
 536 A.1-A.2), and its parabolic part, the dispersion-exchange-reaction (represented by the operator A_{der} in
 537 equations A.1-A.2). This means that equation 2, which could also be written as equation A.1 (with B being
 538 the part on equation 2 not dependent on the concentration), is replaced with the sub-problems shown in
 539 equation A.2.

$$A \frac{\partial C}{\partial t} = A_{adv}C + A_{der}C + B \quad (\text{A.1})$$

$$\begin{cases} \frac{\partial C^*}{\partial t} = A_{adv}C^* & \text{with } C^{*[t]} = C[t] \\ \frac{\partial C^{**}}{\partial t} = A_{der}C^{**} + B & \text{with } C^{**[t]} = C^{*[t+dt]} = C[t'] \end{cases} \quad (\text{A.2})$$

540 The approximated solution is then $C^{[t+dt]} = C^{**[t+dt]}$. The advective part is solved using the second
 541 order - in time and space - Lax-Wendroff scheme with explicit temporal resolution (equation A.3).

$$\frac{C^{[t',i]} - C^{[t,i]}}{dt} = -\frac{Q}{A_i} \left(\frac{C^{[t,i+1]} - C^{[t,i-1]}}{dx} \right) + \frac{dt}{2} \frac{Q}{A_i}^2 \left(\frac{C^{[t,i+1]} - 2C^{[t,i]} + C^{[t,i-1]}}{dx^2} \right) \quad (\text{A.3})$$

542 In such conditions, the Lax-Wendroff scheme is conditionally stable. A necessary condition is the
 543 Courant-Friedrichs-Lewy (CFL) that constrains the grid Courant number (equation A.4).

$$\left| \frac{Qdt}{Adx} \right| \leq 1 \quad (\text{A.4})$$

544 When the time step following the CFL condition (later named advection step) is lower than the desired
 545 time step dt , sub-looping of the advection solution is required until reaching the desired time step. In
 546 the OM-MADE software, the advection is independent for each channel, therefore the advection step may
 547 be computed independently. However, this value may be dependent on space when different reaches with
 548 different surfaces occur or when lateral flows are involved. In this case, the most constraining value for the
 549 advection step should be used for the whole channel.

550 The dispersion-exchange-reaction part is solved using a second order - in space - scheme with implicit
 551 temporal solution (equation A.5). The implicit scheme is unconditionally stable, therefore does not require

552 sub-looping and may be used with large time steps. However, the implicit approach requires a linear system
 553 resolution, thus a higher numerical cost.

$$\begin{aligned} \frac{C^{[t+1,i]} - C^{[t',i]}}{dt} = & \frac{(AD)_{i+\frac{1}{2}} (C^{[t+1,i+1]} - C^{[t+1,i]}) - (AD)_{i-\frac{1}{2}} (C^{[t+1,i]} - C^{[t+1,i-1]})}{(A)_i dx^2} \\ & + \left(\frac{q_{in}}{A}\right)_i \left((C_{in})_i - C^{[t+1,i]}\right) + \sum_{q \neq p} \left(\frac{\alpha_{qp}}{A}\right)_i \left(C_q^{[t+1,i]} - C^{[t+1,i]}\right) - (\lambda)_i AC^{[t+1,i]} \end{aligned} \quad (\text{A.5})$$

554 The second discretization scheme is similar to the one used in OTIS. It is based on a second order - in
 555 time and space - resolution. The temporal scheme is the Crank-Nicholson pondered scheme and the spatial
 556 resolution for the advection part is the centered scheme as shown in equations (A.6-A.7).

$$\begin{aligned} f(t, i) = & -\left(\frac{Q}{A}\right)_i \frac{C^{[t,i+1]} - C^{[t,i-1]}}{2dx} + \frac{(AD)_{i+\frac{1}{2}} (C^{[t,i+1]} - C^{[t,i]}) - (AD)_{i-\frac{1}{2}} (C^{[t,i]} - C^{[t,i-1]})}{(A)_i dx^2} \\ & + \left(\frac{q_{in}}{A}\right)_i \left((C_{in})_i - C^{[t,i]}\right) + \sum_{q \neq p} \left(\frac{\alpha_{qp}}{A}\right)_i \left(C_q^{[t,i]} - C^{[t,i]}\right) - (\lambda)_i AC^{[t,i]} \end{aligned} \quad (\text{A.6})$$

$$\frac{C^{[t+1,i]} - C^{[t,i]}}{dt} = \frac{1}{2} (f(t+dt, i) + f(t, i)) \quad (\text{A.7})$$

557 It should be noted that the flowrate is calculated at each position using the analytical solution of equation
 558 1. These equations are solved for each time-step and each segment of each zone. An average concentration
 559 C_{av} can be computed, if wanted, for each location x and each time-step t as a weighted sum of each zone :

$$C_{av}(x, t) = \frac{\sum_p C_p Q_p}{\sum_p Q_p} \quad (\text{A.8})$$

560 But it is only meaningful in locations where all zones are considered to be mixed.

561 Solving the partial differential equations 2 describing the concentration evolution in each zone requires
 562 to specify initial and boundary conditions. At the inlet, a time-dependent imposed concentration conditions
 563 each zone. Therefore, both continuous and step-wise tracer injection can be simulated. A Dirac injection
 564 can be approximated by imposing concentration at one-time step only. When an inlet boundary condition
 565 is not explicitly given in the input data file, its value is computed by linear interpolation (Fig. A.10). The
 566 total mass M injected at the inlet along the simulation and for all zones may be calculated using equation
 567 A.9, given that the concentration C_p in unit of mass per unit of volume. Boundary condition at the outlet
 568 corresponds to a zero diffusive flux condition. At initial step, a constant concentration is imposed in all
 569 reaches for each zone.

$$M = \sum_{p=mobile} \int_{t_0}^{t_{max}} C_p(x=0, t) Q_p \delta t \quad (\text{A.9})$$

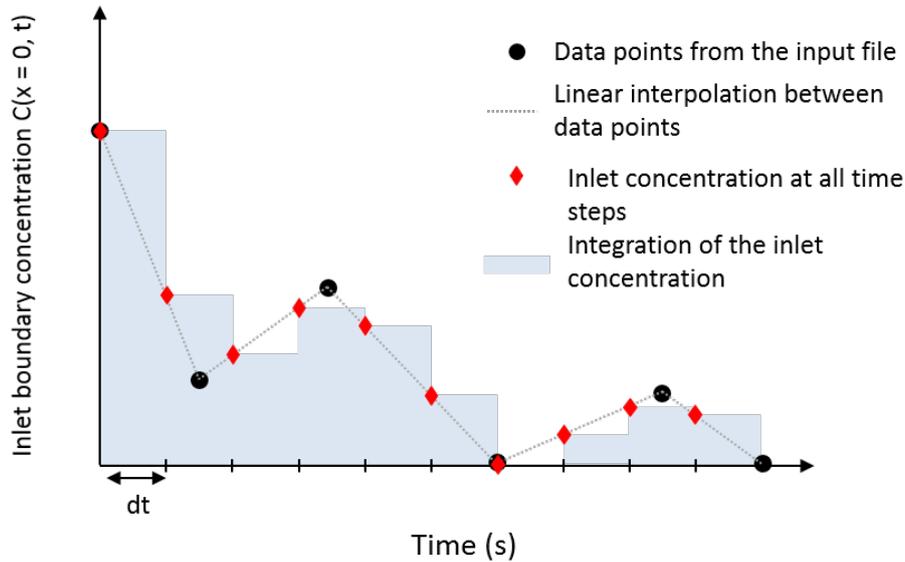


Fig. A.10. Boundary conditions: the input concentration is computed by a linear interpolation between the successive values provided by the user.

570 Appendix B. Description of the software architecture

571 OM-MADE is written in Python v3. We chose this high-level interpreted language because it allows
 572 rapid developments and is easy to pick up by non-programmers. Python is open-source, multi-platform and
 573 allows functional and object-oriented programming. Several powerful libraries have been developed that
 574 allow to directly use optimised and verified algorithms for matrix manipulations, scientific computation or
 575 result visualisation. In OM-MADE, we use *numpy* (<http://numpy.scipy.org>) to solve linear systems, and
 576 *matplotlib* (Hunter, 2007) is used in some examples of main programs to directly visualize the results of a
 577 simulation.

578 The program is divided into four modules - all reusable in any other Python program - that are called
 579 by an independent file containing the main program (Fig. B.11). In the package, different specific examples
 580 of main programs are given, which exploit directly the possibilities of a direct result visualization thanks
 581 to *matplotlib*, as well as a generic main program. The generic main program reads an *INPUTFILES.txt*
 582 text file, which should contain the path and names of the different input parameter files. Three input
 583 parameter files are required: (i) one describing the simulation parameters (chosen scheme, spatial step,
 584 time step, initial concentration, printing locations, and printing times), (ii) one for boundary conditions
 585 (input concentration through time for each zone), and (iii) one describing zone and reach characteristics
 586 (length, area, dispersion coefficient, degradation/adsorption rate, lateral in and outflow rates, lateral inflow
 587 concentration, and exchange coefficients). As output of the simulation, it produces one file per flow zone
 588 containing the concentration through time at the printing locations, and the corresponding time steps in the

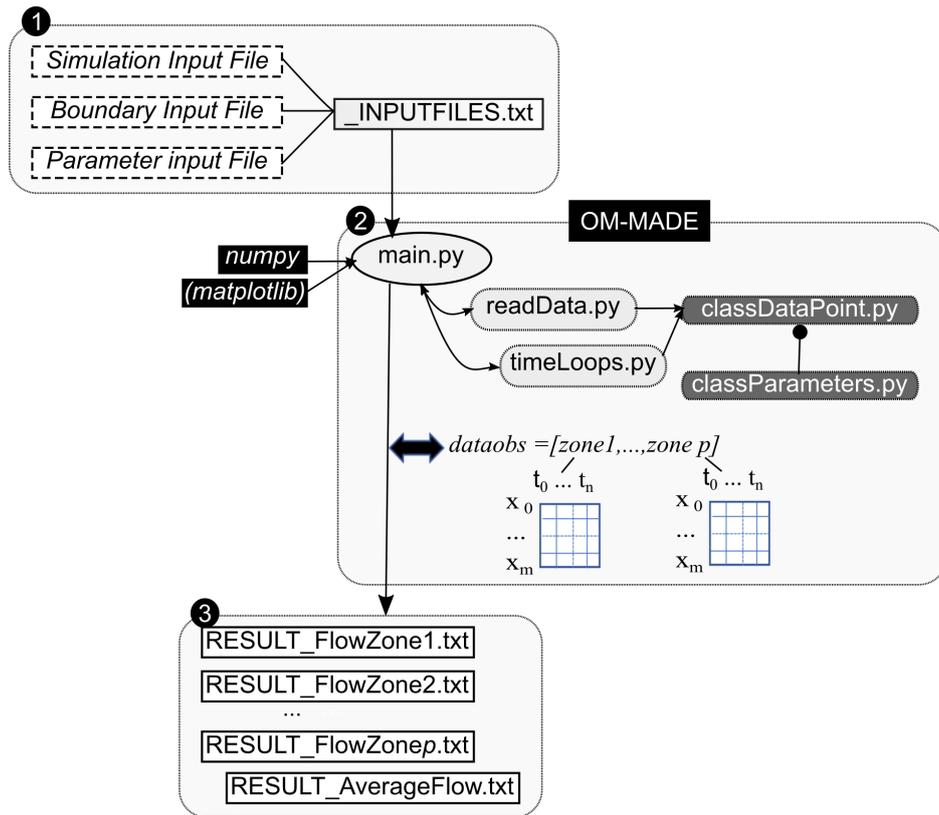


Fig. B.11. OM-MADE architecture: Three text input files are required by the `_INPUTFILES.txt` file (1). They contain all information to run a specific simulation. OM-MADE (2) should be launched by running the main program (several examples are provided), which calls four python modules. The result of a simulation is stored in the `dataobs` variable, which is a list of arrays containing, for each zone, the concentration for each printed time and distance. This variable can be used to generate several text files containing the result of the simulation (3)).

589 first column. An additional output file *RESULT_AverageFlow.txt* contains also the corresponding average
590 concentration for all mobile zones (Eq. A.8) at each printing location.

591 Two classes are defined in two modules : (i) the class *Parameters* defines all physical parameters for one
592 zone and reach of the domain; (ii) the class *DataPoint* contains the physical data required for computation
593 on one point (flow type and location) of the domain. It defines, punctually, the calculation of advection,
594 dispersion, mass exchange between two flow types co-located points and mass exchange through either
595 degradation/adsorption or lateral flow.

596 These classes are used by the functions implemented in the *readData* and *timeLoops* modules. The
597 first module gathers functions that permit the reading and storage of the simulation parameters from the
598 input text files. The second one initialises the concentration and does the overall loop (advection, and
599 then dispersion) for each time step, until reaching the total simulation time. It returns a matrix containing
600 the concentration for each printing location at each printing time step. In the operator-split scheme, the
601 sub-looping of the advection is performed in the function *advectionLoop*.

602 The OM-MADE package is freely available on GitHub as a Python project ([https://github.com/](https://github.com/OM-MADE/OM-MADE)
603 [OM-MADE/OM-MADE](https://github.com/OM-MADE/OM-MADE)). It is provided with examples of applications on the following verification case studies
604 (Section 3), as well as an application on the Furfooz karstic area (Section 4).