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1 Adjoint-based numerical method using standard  
2 engineering software for the optimal placement of chlorine  
3 sensors in drinking water networks

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8 **Abstract**

9 To obtain representative water quality simulations, unknown model param-  
10 eters have to be updated by combining information from the water quality  
11 model and the sensor outputs. An adjoint-based numerical method has  
12 been developed to determine the optimal placement of chlorine sensors in  
13 drinking water networks at a low computational cost. From a practical en-  
14 gineering perspective, the proposed optimal placement corresponds to the  
15 set of sensors that minimizes the area in which the unknown model param-  
16 eters cannot be identified. The numerical strategy is implemented in the  
17 hydraulic software EPANET. Using the adjoint framework, we develop and  
18 apply an adaptive strategy in a French drinking water network that provides  
19 the optimal placement from 1 sensor to 6 sensors. We show that the highest  
20 reduction of the non-identifiable area is obtained at the first stages of the  
21 adaptive strategy. After 4 sensors, a plateau is reached.

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22 *Keywords:* sensor placement, water quality simulations, drinking water  
23 network, adjoint method

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## 24 **Software availability**

25 Name of software: EPANET

26 Programming language: C/C++

27 Operating system: Windows

28 Availability: <http://www.epa.gov/water-research/epanet>

29 Documentation: <http://www.epa.gov/water-research/epanet>

30 User interface: Graphical user interface or Programmer's toolkit

31 License: Public domain software that may be freely copied and distributed

## 32 **1. Introduction**

33 In drinking water networks, the chlorine concentration field is one of the  
34 main indicators of the water quality. Legislation dictates that a minimum  
35 level of chlorine at each point in the network has to be ensured. To overcome  
36 the lack of measurements in drinking water networks, hydraulic and water  
37 quality models are considered. In water network applications, the hydraulic  
38 state is generally computed using algebraic equations, *i.e.*, flow continuity  
39 at the nodes and headloss in the pipes. Regarding the water quality models,  
40 one-dimensional (1D) advection-reaction equations are considered in pipes,  
41 and perfect and instantaneous mixing is assumed in pipe junctions. The de-  
42 crease of the chlorine concentration due to bulk flow reactions and pipe wall  
43 reactions, *e.g.*, reaction with the biofilm at the pipe wall, is modeled using  
44 a reaction term (Powell et al. (2000)). This term is characterized by the

45 reaction order and the reaction coefficient. The software EPANET (Ross-  
46 man and Boulos (1996); Rossman (2000)) is commonly used to simulate the  
47 hydraulics and the water quality states.

48 French water companies can observe a gap higher than 30% between the  
49 chlorine sensor outputs and the chlorine concentration obtained from a di-  
50 rect simulation of the water quality model. This gap may be due to un-  
51 certainties in the hydraulic state, particularly the water demands, and to  
52 the model parameters associated with the chlorine reactions. To represent  
53 the variability in water demands, stochastic models are typically considered.  
54 The calibration of these models can be achieved using direct measurements  
55 (Buchberger and Wells (1996); Bakker et al. (2013); Cominola et al. (2015)),  
56 *i.e.*, monitoring of the user water consumption in residences, or indirect mea-  
57 surements (Kang and Lansey (2009); Alcocer-Yamanaka et al. (2012)), *i.e.*,  
58 pressure and/or flow rate outputs into the drinking water network. To lo-  
59 cate and quantify abnormal water demands due to leaks, inverse techniques  
60 based on pressure sensor outputs have been proposed in (Liggett and Chen  
61 (1994); Meseguer et al. (2014)). In this inverse problem, the goal is to  
62 determine the unknown model parameters by minimizing the gap between  
63 the sensor outputs and the simulation. Finally, flow sensor outputs may  
64 also be used in inverse techniques. Indeed, an inverse computational fluid  
65 dynamics technique has been developed in (Waeytens et al. (2015)) to iden-  
66 tify the unknown boundary conditions of 2D incompressible Navier-Stokes  
67 equations and thus to obtain a high description in 2D of the flow profile in  
68 water networks. A detailed description of the flow in 2D or 3D can provide  
69 more representative chlorine simulations than using the mean flow velocity,  
70 particularly in the distribution mains of the drinking water networks where  
71 the flow can be laminar, thus inducing different chlorine propagation veloc-

ities. Note that the measurement of chlorine or tracer concentrations can also provide information on the water demands (Jonkergouw et al. (2008); Al-Omari and Abdulla (2009)).

Regarding the water quality models, first-order reaction kinetics is commonly assumed for the free chlorine decay. Many articles address the identification of the reaction coefficient (Sharp et al. (1991); Rodriguez et al. (1997); Munavalli and Kumar (2005); Pasha and Lansey (2012)), but few aim to determine the reaction order and the reaction coefficient (Vasconcelos et al. (1997); Gancel (2006)). Because the reaction coefficient is associated with bulk flow reactions and pipe wall reactions, it is not uniform in the entire network. Nevertheless, to limit the number of unknowns to be determined, the reaction coefficient is considered to be piecewise constant on subsections of the water network. The choice of the domain decomposition is based on the age, the roughness, the pipe material, the pipe diameter and the flow rate.

Because drinking water networks are sparsely instrumented, the use of numerical tools can indicate to the water companies the coverage area ensured by the existing chlorine sensors and the optimal deployment of new chlorine sensors. A considerable amount of literature addresses the optimal sensor position for detecting a contaminant intrusion in drinking water networks. Three categories can be distinguished: the non-model-based methods using the topology of the water network, the methods based solely on hydraulic simulations (Lee and Deininger (1992); Kessler et al. (1998); Berry et al. (2005); Xu et al. (2008)) and the methods based on hydraulic and water quality simulations (Berry et al. (2006); Preis and Ostfeld (2008); Krause et al. (2008)). The majority of the methods formulate the optimal sensor placement as a multiobjective optimization. The goal is to minimize the

99 non-coverage area, the number of sensors, the time to detection, and so  
100 forth.

101 In the present article, we propose a numerical strategy based on the adjoint  
102 framework to determine and quantify the non-coverage area for a given set  
103 of sensor placements. This practical information can be useful for water  
104 companies to determine the optimal placement of chlorine sensors for maxi-  
105 mizing the coverage area for a given number of sensors. The method requires  
106 the resolution and the post-treatment of the solution of the adjoint problem,  
107 *i.e.*, advection-reaction equations backward in time with virtual chlorine in-  
108 jection at the position of the sensors and a dynamic back flow. The adjoint  
109 framework is used in various applications. First, it provides at a low com-  
110 putational cost the functional gradient involved in inverse calculations to  
111 update the model parameters of the water flow (Liggett and Chen (1994);  
112 Waeytens et al. (2015)) and to reconstruct the concentration fields (Elbern  
113 et al. (2000); Waeytens et al. (2013, 2017)). Then, it is used in sensitiv-  
114 ity analyses to study the influence of the physical model parameters on a  
115 quantity of interest (Andrews (2013); Kauker et al. (2016)). The adjoint  
116 framework is also considered for estimating the modeling or the discretiza-  
117 tion error on a quantity of interest (Becker and Rannacher (2001); Waeytens  
118 et al. (2012); Oden and Prudhomme (2002)). Note that the determination  
119 and quantification of the coverage area can also be obtained from (Xu et al.  
120 (2008)), which is based on the knowledge of the flow and graph theory. The  
121 main advantage of the proposed adjoint approach is that it uses standard  
122 hydraulic software such as EPANET. Moreover, the adjoint solution can also  
123 be used in an inverse advection-reaction procedure to identify the reaction  
124 coefficient.

125 The remainder of this article is organized as follows. Section 2 introduces the

126 model updating technique for identifying the reaction coefficient of the water  
127 quality model and the definition of the adjoint problem. The adjoint-based  
128 numerical strategy for the optimal chlorine sensor placement is developed  
129 in Section 3. This strategy is applied to a French drinking water network in  
130 Section 4 before drawing concluding remarks and prospects in Section 5.

## 131 **2. Modeling the water quality in drinking water networks and** 132 **updating the kinetic reaction coefficient**

### 133 *2.1. Simulating the water quality in drinking water networks*

134 In drinking water networks, the chlorine concentration is the primary  
135 indicator of the water quality. The chlorine propagates in the network  
136 according to the flow induced by water demands, and the chlorine con-  
137 centration decreases due to reactions occurring in the bulk or at the wall.  
138 Physical models can be employed to predict the propagation and the re-  
139 action of chlorine in drinking water networks. Generally, one-dimensional  
140 (1D) advection-reaction partial differential equations are considered in the  
141 pipes, and the mixing in the junctions is modeled using algebraic equations.  
142 The set of equations, detailed in (Rossman (2000)), for modeling the water  
143 quality in the drinking water network is called a “direct problem”. It can  
144 be solved using standard engineering software such as EPANET (Rossman  
145 and Boulos (1996)). Let us define the simulated chlorine concentration in  
146 the water network as  $\mathbf{C}$ .

147 In practice, water companies may observe a gap higher than 30% between  
148 the simulated and measured chlorine concentrations. Hence, to obtain a  
149 representative simulation of the water quality, the model parameters, such  
150 as the kinetic reaction coefficient, have to be updated. The model updating

151 strategy is described in the following sections.

## 152 2.2. Cost functional used in model updating

153 To obtain representative water quality simulations, one needs to update  
154 the unknown parameters of the model. Herein, we focus on determining the  
155 vector  $\mathbf{k} = \{k_1, \dots, k_N\}$  of reaction coefficients, where  $N$  corresponds to the  
156 number of water pipes in the drinking water network. For this purpose, an  
157 inverse modeling technique can be employed. Let us choose a quadratic cost  
158 functional that quantifies the difference between the sensor outputs  $C_m^{mes}$   
159 and the numerical solution  $\mathbf{C}$  of the water quality model mentioned in the  
160 previous section. One seeks the vector  $\mathbf{k}$  of reaction coefficients by solving  
161 the following optimization problem:

$$\min_{\mathbf{k}} J(\mathbf{C}, \mathbf{k}) = \frac{1}{2} \sum_{m=1}^N a_m \int_0^T \left( C_m(\mathbf{k}; x = x_m, t) - C_m^{mes}(t) \right)^2 dt + \beta b \sum_{m=1}^N (k_m - k_m^0)^2 \quad (1)$$

162 where  $\mathbf{C} = \{C_1(x, t), \dots, C_N(x, t)\}$  is the vector of chlorine concentrations.  
163 The Boolean parameter  $a_m$  is set to 1 (resp. 0) if the  $m^{th}$  water pipe is  
164 equipped (resp. is not equipped) with a chlorine sensor recording the con-  
165 centration level on the observation time interval  $[0, T]$ . The position of the  
166  $m^{th}$  sensor is denoted as  $x_m$ . Note that Eq. (1) is a constrained optimization  
167 problem. Indeed, the chlorine concentration field  $\mathbf{C}$  has to satisfy the set of  
168 water quality equations mentioned in Section 2.1.

169

170 In general, the inverse problem is not well posed. First, in practice, to  
171 reduce the number of model parameters to be updated, the reaction coef-  
172 ficient is assumed to be the same on a group of water pipes that have the  
173 same characteristics, *e.g.*, age, diameter and material (Fabrie et al. (2010)).  
174 Second, a Tikhonov regularization term such as the second term in Eq. (1)  
175 can be introduced in the cost functional. This term aims at improving the



176 convexity of the functional. The parameter  $b$  ensures the physical homo-  
177 geneity of both terms, and  $k_m^0$  corresponds to the initial guess of the  $m^{th}$   
178 reaction coefficient.  $\beta$  corresponds to a normalized weighting coefficient.

179

180 The minimization of the cost functional (1) can be performed using a  
181 gradient-like approach. In the present article, note that the functional gra-  
182 dient is obtained at a low computational cost using the adjoint framework.  
183 The methodology to derive the adjoint equation and the gradient formula  
184 are presented in the next section.

### 185 *2.3. Derivation and physical meaning of adjoint equations*

186 The constrained minimization problem (1) can be rewritten as an un-  
187 constrained minimization problem by introducing the Lagrangian  $\mathcal{L}(\mathbf{k}, \mathbf{C}, \mathbf{P})$   
188 and the Lagrange multiplier  $\mathbf{P}$ . The stationarity of the Lagrangian according  
189 to the Lagrange multiplier  $\mathbf{P}$  provides the equations of the direct problem  
190 mentioned in Section 2.1, whereas the equations of the adjoint problem are  
191 obtained from the stationarity of the Lagrangian according to  $\mathbf{C}$ .

192

193 Herein, the adjoint problem is quite similar to the direct problem. It  
194 is still an advection problem with a reaction term. In the adjoint problem,  
195 chlorine is virtually injected at the sensor location  $x_m$ . The temporal evo-  
196 lution of the chlorine injection is provided by the data misfit. In contrast  
197 to the direct problem, the adjoint problem has a final condition in time.  
198 Moreover, the flow is reversed in the adjoint problem, *i.e.*, the velocity  $\mathbf{v}$  is  
199 replaced by  $(-\mathbf{v})$ .

200 Physically, the adjoint state corresponds to a “sensitivity concentration”.

201 Considering a sensor at a given location in the drinking water network, the

202 “sensitivity concentration” propagates from the sensor location toward the  
203 upstream flow direction with increasing reversed time. Hence, it shows that  
204 all of the sensitivity of the sensor measurement is located upstream of the  
205 sensor location. In other words, the sensor is not sensitive to locations down-  
206 stream of the sensor, nor is it sensitive to chlorine concentrations that were  
207 present prior to the initial observation time.

208

209 The adjoint state can provide sensitivity information, but it can also be  
210 used to compute the functional gradient  $\nabla \mathbf{J}$ , which is involved in model  
211 updating techniques, at a low computation cost. Indeed,  $n + 1$  transport  
212 reaction problems have to be solved in standard finite-difference techniques,  
213 whereas only two transport reaction problems are needed when using the  
214 adjoint framework to compute the  $n$  components of the functional gradi-  
215 ent. The functional gradient  $\nabla \mathbf{J}$  is obtained from the derivative of the  
216 Lagrangian according to the reaction coefficient  $k_m$ .

217

218 To provide a better understanding, the derivation of the adjoint equa-  
219 tions and the functional gradient are illustrated on a divergent node of a  
220 water network in Appendix B.

#### 221 *2.4. Practical technique to update the reaction coefficient of the water quality* 222 *model*

223 Drinking water networks are not massively instrumented with chlorine  
224 sensors. As mentioned in Section 2.2, to limit the number of model pa-  
225 rameters to be updated, the reaction coefficient is assumed to be uniform  
226 on subdomains of the water network that have the same characteristics.  
227 To update the vector  $\mathbf{k}$  of reaction coefficients, one can follow the iterative

228 strategy detailed below.

229 *Direct problem:*. First, considering an initial guess  $\mathbf{k}^0$  or the kinematic  
230 parameters obtained at the end of the previous iteration, the advection-  
231 reaction direct problem is solved, thereby providing the concentration field  
232  $\mathbf{C}$  in the water network.

233 *Comparison of simulated chlorine and sensor outputs:*. Knowing the sim-  
234 ulated concentration field  $\mathbf{C}$  in the entire water network, we compute the  
235 data misfit at each sensor location.

236 *Adjoint problem:*. In a water network, the adjoint problem is defined as an  
237 advection-reaction problem backward in time considering a reversed flow.  
238 It corresponds to the retropropagation of chlorine virtually injected at the  
239 sensor location. The higher is the data misfit, the higher is the chlorine to  
240 be injected.

241 After changing the time variable  $t$  to  $\tau = T - t$ , the final time condition  
242 begins as an initial condition. Hence, standard hydraulic and water quality  
243 software can be employed to solve the adjoint problem. By solving this  
244 problem, we obtain the adjoint state  $\mathbf{P}$ .

245 *Functional gradient:*. Let us consider the reaction coefficient  $k_p$  modeling the  
246 chlorine reaction in a subdomain  $\Omega_p$  of the water network. This subdomain  
247 is composed of  $n_p$  water pipes. Thus, the formula of the derivative of the  
248 functional according to  $k_p$  can be expressed as

$$\frac{\partial J}{\partial k_p} = - \sum_{i=1}^{n_p} S_i \int_0^T \int_0^{L_i} C_i P_i dx dt + \beta b(k_p - k_p^0) \quad (2)$$

249 In Eq. (2), the first term is associated with the sensitivity of the data  
250 misfit to the reaction coefficient  $k_p$ , and the second term is dedicated to the

251 functional regularization.

252 All the components of the functional gradient  $\nabla J$  are computed from Eq.  
253 (2).

254 *Updating of the reaction coefficients:*. Using the functional gradient  $\nabla J$   
255 as the descent direction, we obtain the updated vector  $\mathbf{k}_{\text{new}}$  of reaction  
256 coefficients by

$$\mathbf{k}_{\text{new}} = \mathbf{k}_{\text{old}} - \alpha \nabla J \quad (3)$$

257 where  $\alpha$  is the descent step. Several solutions are required to determine the  
258 descent step minimizing the cost functional  $J$ .

259 If the data misfit functional reaches the measurement error, the model up-  
260 dating process is stopped. Otherwise, the iterative process continues.

### 261 **3. Optimal chlorine sensor placement using the adjoint framework**

#### 262 *3.1. Theoretical foundations of the optimal chlorine sensor placement method*

263 **Proposition 3.1.** *Let us denote  $\phi^*(x, t)$  as the modified adjoint solution.*

264 *If  $\phi^*(x, t) = 0$  in  $\Omega_p \times [0, T]$ , then the reaction coefficient  $k(x)$  is not iden-*  
265 *tifiable on the subdomain  $\Omega_p$ .*

266 *The modified adjoint solution  $\phi^*(x, t)$  verifies the following transport equa-*  
267 *tions in the pipes of the water networks*

$$-\frac{\partial \phi_m^*}{\partial t} - v_m \frac{\partial \phi_m^*}{\partial x} = a_m H(t) \delta(x - x_m), \quad \text{in } [0, L_m] \times [0, T], \quad m \in \{1, \dots, N\} \quad (4)$$

268 *The boolean  $a_m$  is equal to 1 (resp. 0) if the  $m^{\text{th}}$  water pipe is equipped*  
269 *with a chlorine sensor (resp. is not equipped with a chlorine sensor). As with*  
270 *the adjoint problem, the pipe junctions are governed by the standard equa-*  
271 *tions of convergent or divergent nodes depending on the direction of the flow*

272  $(-v_m)$ . The flow  $(-v_m)$  is considered stationary. Finally, in the modified  
273 adjoint problem, the final condition and the Dirichlet boundary conditions  
274 vanish.

275 Note that the modified adjoint problem resembles the adjoint problem.  
276 The two differences are as follows. First, no reaction term is involved in the  
277 modified adjoint problem. Second, in the adjoint problem, the amplitude  
278 of the injected chlorine at the sensor location is given by the data misfit,  
279 whereas a constant amplitude in time is considered in the modified adjoint  
280 problem.

281

282 The proof of Proposition 3.1 is given for a reduced water network in  
283 Appendix B. Although a reduced water network is considered to facilitate  
284 the notations, it includes key elements of a real water network, *i.e.*, divergent  
285 and convergent nodes.

### 286 3.2. Numerical method for optimal chlorine sensor placement

287 For a given number  $n_s$  of chlorine sensors, we seek the placement of  
288 chlorine sensors that minimizes the non-identifiable area associated with  
289 the reaction coefficient  $k(x)$ . For this purpose, we propose an adjoint-based  
290 numerical method, which is detailed below.

291 First, the hydraulic  $v(x, t)$  has to be simulated in the drinking water network.  
292 From the hydraulic, we deduce the reversed velocity field, *i.e.*,  $(-1) \times v(x, t)$ .  
293 In agreement with the deployment constraints in the water network, a pos-  
294 sible placement of  $n_s$  chlorine sensor is considered. Then, the reversed ve-  
295 locity field is used to obtain the modified adjoint concentration  $\phi^*(x, t)$ .  
296 The modified adjoint problem, introduced in Proposition 3.1, corresponds  
297 to the retropropagation of chlorine virtually injected at the sensor locations

298 with a constant unitary amplitude in time. In practice, after making the  
 299 change of variable  $\tau = T - t$ , this problem can be solved using standard  
 300 engineering software, *e.g.*, EPANET. In Proposition 3.1, we show that in-  
 301 formation concerning the non-identifiable area associated with the reaction  
 302 coefficient  $k(x)$  can be provided by the modified adjoint concentration field  
 303  $\phi^*(x, t)$ . The subdomain  $\Omega_p$  having a null modified adjoint concentration on  
 304 the entire time interval  $[0, T]$  corresponds to the non-identifiable area. To  
 305 quantify and compare different sensor locations in view of minimizing the  
 306 non-identifiable area, we introduce the dimensionless non-coverage indicator  
 307  $\eta$ , which is defined as

$$\eta = \frac{\text{Total length of water pipes in the non-identifiable area}}{\text{Total length of water pipes in the drinking water network}} \quad (5)$$

308 The proposed indicator is rapidly computable and readily usable. Thus, it  
 309 meets the expectations of hydraulic engineers.

#### 310 4. Numerical results using the software EPANET

311 Let us consider a part of the French drinking water network presented in  
 312 Figure 1. The water network is composed of two tanks, 298 junctions and 318  
 313 pipes. The total water pipe length is approximately 15 km. Due to technical  
 314 and deployment constrains, chlorine sensors cannot be installed anywhere in  
 315 the drinking water network. Hence, the water company Suez-Environnement  
 316 has pre-selected 6 potential chlorine sensor positions, as presented in Figure  
 317 1. The chlorine sensors are useful for comparing the measurements and the  
 318 water quality simulations. As we previously mentioned, more representative  
 319 water quality simulations can be achieved by updating the unknown reac-  
 320 tion coefficient  $k(x)$ .

321

322 Our goal is to determine the best set of chlorine sensors that maximize  
 323 the coverage area, *i.e.*, minimizing the non-identifiable area associated with  
 324 the reaction coefficient  $k(x)$ . In this section, we apply the proposed adjoint-  
 325 based numerical method. It has been implemented in the software EPANET.  
 326

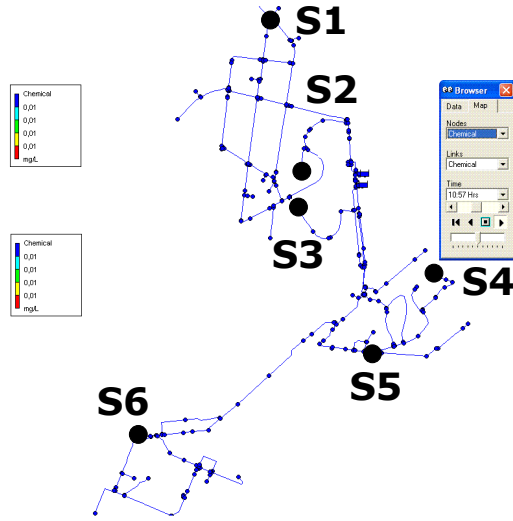


Figure 1: Geometry of a French drinking water network with 2 water towers - 6 possible locations of chlorine sensors

327 Following the methodology presented in the previous section, the first  
 328 step consists of the hydraulic simulation in the water network using EPANET.  
 329 As input for the hydraulic simulation, we use estimated varying consumer  
 330 demands and the initial water level in water towers. The information as-  
 331 sociated with one day in August 2011 was provided by the water company  
 332 Suez-Environnement. Then, we reverse the simulated flow, *i.e.*,  $-v(x, t)$ , for  
 333 simulating the modified adjoint problem  $\phi^*(x, t)$ . We recall that the modi-  
 334 fied adjoint problem is defined as the retropropagation of chlorine virtually

335 injected at the sensor locations with a constant unitary amplitude in time.

336

337 As a first step, we consider the deployment of only one chlorine sensor in  
338 the water network. We test several locations of the sensor, and for each po-  
339 sition from  $S_1$  to  $S_6$  (see Figure 1), we solve the associated modified adjoint  
340 problem. In Figure 2, we show the non-identifiable area when considering a  
341 sensor placed at  $S_1$  or at  $S_6$ . The blue color (resp. the red color) denotes  
342 the area where the modified adjoint solution vanishes (resp. is not null) on  
343 the entire daily time interval. According to the theoretical results of the  
344 previous section, the blue color area is associated with the non-identifiable  
345 area. To quantify this area, the indicator  $\eta$  defined in Eq. (5) is computed.  
346 The results are summarized in Table 1. The non-identifiable area represents  
347 87.5% of the water network for a sensor placed at  $S_1$ , whereas it represents  
348 73.4% of the water network for  $S_6$ . Moreover, in Figure 2, we observe that  
349 a sensor placed at  $S_1$  (resp. at  $S_6$ ) is not able to provide information on  
350 chlorine reactions in the lower part of the network (resp. in the upper part  
351 of the network). When considering a unique sensor, note that the optimal  
352 sensor placement for minimizing the non-identifiable area corresponds to  $S_6$ .

353 To reduce the non-identifiable area, more chlorine sensors should be de-  
354 ployed in the water network. In the following, combinations of chlorine  
355 sensors are studied. In Figure 3, we can observe that when using the com-  
356 bination of the three chlorine sensors  $S_1 - S_3 - S_6$ , the non-identifiable area  
357 represents 54.4% of the drinking water network. Considering these 3 sensors  
358 rather than only sensor  $S_1$  provides a 3 km reduction in the non-identifiable  
359 area. Nevertheless, increasing the number of sensors does not strongly re-  
360 duce the non-identifiable area. Indeed, in Figures 3 and 4, we observe that  
361 from 3 to 5 chlorine sensors, the non-identifiable area indicator changes from



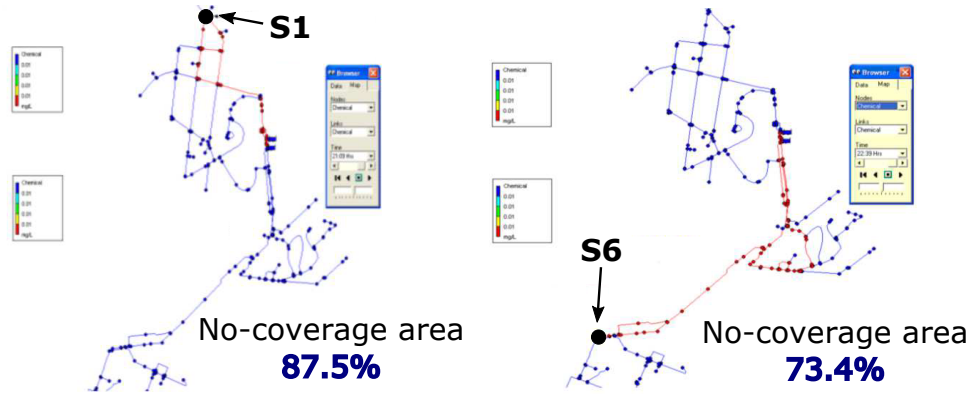


Figure 2: Sensor position  $S_1$ :  $\eta = 87.5\%$  (left), Sensor position  $S_6$ :  $\eta = 73.4\%$  (right)

Sensor	Non-coverage indicator $\eta$
$S_1$	87.5 %
$S_2$	97.5 %
$S_3$	88.5 %
$S_4$	81.9 %
$S_5$	86.3 %
$S_6$	73.4 %

Table 1: Non-coverage area of the drinking water network when considering a unique chlorine sensor

362 54.4% to 48.1%. No improvements are observed when adding a sixth sensor.

363 An adaptive strategy can be applied to obtain a desired threshold of  
 364 non-identifiable area. The adaptive process starts by considering a unique  
 365 chlorine sensor. Using the proposed adjoint-based technique, we retain the  
 366 sensor placement  $S_I^{opt}$  that has the lowest non-identifiable area indicator  
 367  $\eta$ . Then, to continue decreasing the non-identifiable area, an additional  
 368 chlorine sensor is considered in the drinking water network. The indicator

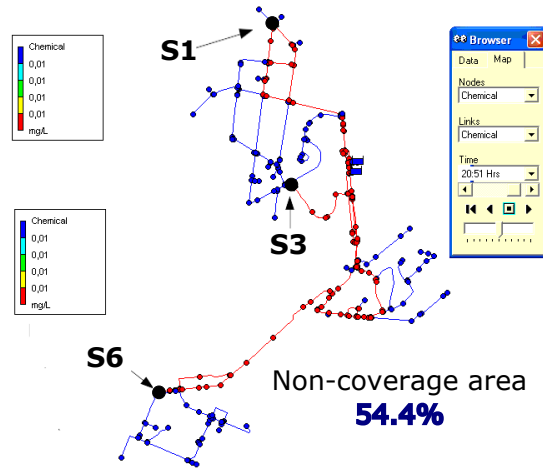


Figure 3: Combination of three sensors  $S_6 - S_1 - S_3$ :  $\eta = 54.4\%$

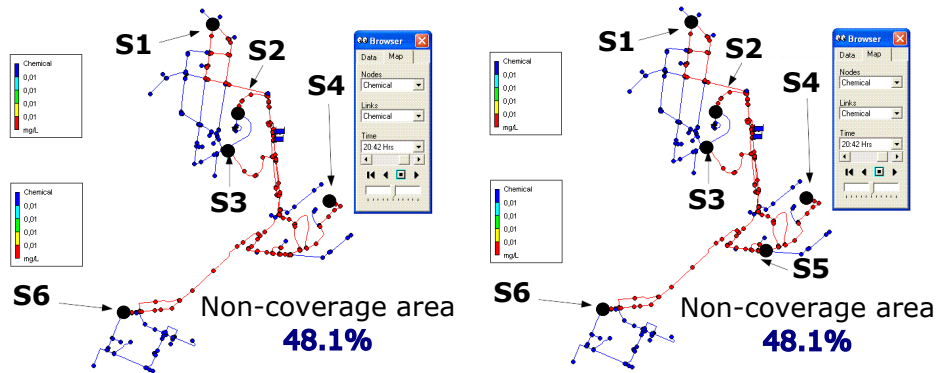


Figure 4: Combination of 5 sensors  $S_6 - S_1 - S_3 - S_4 - S_2$ :  $\eta = 48.1\%$  (right), Combination of 6 sensors  $S_1$  to  $S_6$ :  $\eta = 48.1\%$  (left)

369  $\eta$  is computed for all combinations of two sensors, including the sensor  $S_I^{opt}$   
 370 determined at the previous stage. Hence, we obtain the optimal combination  
 371 of two sensors  $(S_I^{opt}, S_{II}^{opt})$ . The adaptive procedure continues until we reach  
 372 the maximum number of chlorine sensors affordable for the water network.

373 This adaptive strategy has been applied to the investigated water network.  
374 The results are summarized in Tables 2 and 3. For a fixed number of sensors,  
375 the optimal placement is noted in bold in Tables 2 and 3. Figure 5 presents  
376 the evolution of the coverage area indicator  $1 - \eta$  for the optimal placement  
377 of chlorine sensors. The highest reduction in the non-identifiable area is  
378 obtained at the first stages of the adaptive strategy. After 4 sensors, a  
379 plateau is reached. The non-coverage indicator is approximately 50%.

1 Sensor	Non-coverage indicator $\eta$	2 Sensors	Non-coverage indicator $\eta$	3 Sensors	Non-coverage indicator $\eta$
$S_1$	87.5 %	<b><math>S_6, S_1</math></b>	<b>61.7 %</b>	$S_6, S_1, S_2$	59.2 %
$S_2$	97.5%	$S_6, S_2$	70.9 %	<b><math>S_6, S_1, S_3</math></b>	<b>54.4 %</b>
$S_3$	88.5%	$S_6, S_3$	63.5 %	$S_6, S_1, S_4$	56.1 %
$S_4$	81.9 %	$S_6, S_4$	67.8 %	$S_6, S_1, S_5$	61.8 %
$S_5$	86.3%	$S_6, S_5$	72.1 %		
<b><math>S_6</math></b>	<b>73.4%</b>				

Table 2: Non-coverage area of the drinking water network when considering 1, 2 or 3 chlorine sensors - optimal combinations of sensors are noted in bold

4 Sensors	Non-coverage indicator $\eta$	5 Sensors	Non-coverage indicator $\eta$	6 Sensors	Non-coverage indicator $\eta$
$S_6, S_1, S_3, S_2$	53.7 %	<b><math>S_6, S_1, S_3, S_4, S_2</math></b>	<b>48.1%</b>	<b><math>S_6, S_1, S_3, S_4, S_2, S_5</math></b>	<b>48.1 %</b>
<b><math>S_6, S_1, S_3, S_4</math></b>	<b>48.8 %</b>	$S_6, S_1, S_3, S_4, S_5$	48.8 %		
$S_6, S_1, S_3, S_5$	54.4 %				

Table 3: Non-coverage area of the drinking water network when considering 4, 5 or 6 chlorine sensors - optimal combinations of sensors are noted in bold

## 380 5. Conclusions

381 To obtain representative water quality simulations in drinking water net-  
382 works, the unknown model parameters, such as the reaction coefficient,

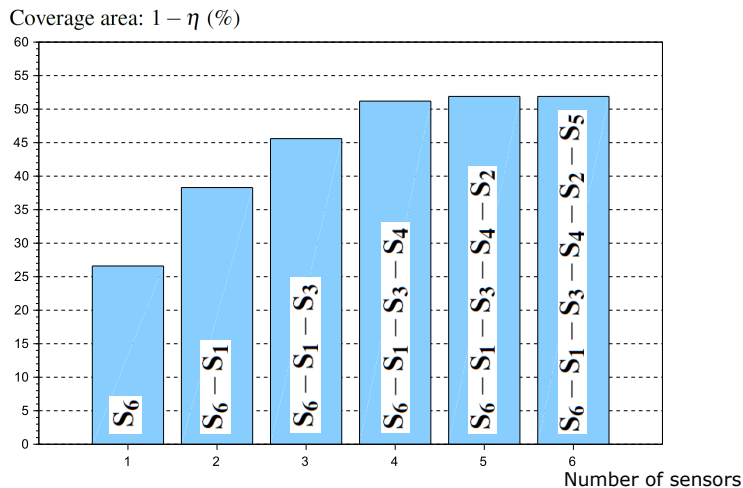


Figure 5: Synthesis of optimal sensor placement to maximize the coverage area

383 should be updated using chlorine sensor outputs. In the present article,  
 384 an adjoint-based numerical method dedicated to drinking water networks  
 385 has been developed to optimally deploy chlorine sensors in view of minimiz-  
 386 ing the non-identifiable area associated with the reaction coefficient. The  
 387 computation of the one-dimensional adjoint advection solution using the  
 388 standard engineering software EPANET allows us to localize and quantify  
 389 the non-coverage area for a given set of sensors. On a French drinking water  
 390 network, we applied an adaptive strategy starting from the optimal place-  
 391 ment of 1 sensor to 6 sensors. We showed that the highest reduction in the  
 392 non-identifiable area is obtained at the first stages of the adaptive strategy.  
 393 After 4 sensors, a plateau is reached. In the model updating process of the  
 394 reaction coefficient, the computed adjoint solution can also be used to obtain  
 395 the functional gradient at a lower computational cost than straightforward  
 396 difference techniques. Herein, we focus on the optimal sensor placement that

397 minimizes the non-coverage area. The non-coverage area indicator computed  
 398 from the modified adjoint solution can be used in a more general optimal  
 399 sensor placement strategy considering the minimization of a multiobjective  
 400 function. Finally, the proposed method can be extended for the detection of  
 401 species intrusion in drinking water networks. The modified adjoint solution  
 402 can highlight the area where species intrusion may not be detected.

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 408 Advitam, Ondeo Systems (Suez Environnement), EFS, A3IP, ESIEE Paris,  
 409 and IFSTTAR.

### 410 **Appendix A. Illustration of adjoint framework on a divergent node** 411 **of a water network and computation of the func-** 412 **tional gradient**

413 The advection reaction within a divergent node (see Figure A.6) is rep-  
 414 resented by the following equations:

$$\begin{aligned}
 \frac{\partial C_m}{\partial t} + v_m \frac{\partial C_m}{\partial x} + k_m C_m &= 0 && \text{in } [0, L_m] \times [0, T], m \in \{1, 2, 3\} \\
 C_1(x = 0, t) &= \chi_1(t) && \text{in } [0, T] \\
 C_2(x = 0, t) &= C_1(x = L_1, t) && \text{in } [0, T] \\
 C_3(x = 0, t) &= C_1(x = L_1, t) && \text{in } [0, T] \\
 C_m(x, t = 0) &= c_m^0(x) && \text{in } [0, L_m], m \in \{1, 2, 3\}
 \end{aligned}
 \tag{A.1}$$

415 where  $m$  denotes the pipe number,  $L_m$  is the length of pipe  $m$ ,  $C_m$  is  
 416 the chlorine concentration in water pipe  $m$  as a function of distance  $x$  and  
 417 time  $t$ ,  $v_m$  is the flow velocity, and  $k_m$  (resp.  $\alpha_m$ ) represents the reaction  
 418 coefficient (resp. the reaction order). As usual in drinking water networks,  
 419 a first-order reaction is considered to model the chlorine reaction. In the  
 420 following, we take  $\alpha_m = 1$ . The concentration boundary condition is  $\chi_1(t)$ ,  
 421 and  $c_m^0(x)$  denotes the initial chlorine concentration in water pipe  $m$ .  
 422

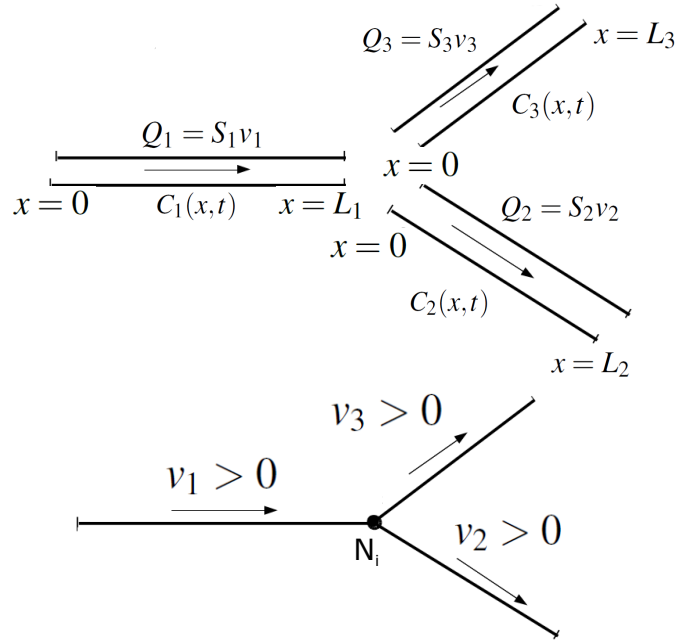


Figure A.6: Notations for advection reaction through divergent node - the flow velocity  $v_m$  in pipe  $m$  is considered positive when it passes from the starting node ( $x = 0$ ) to the ending node ( $x = L_m$ ) - herein,  $v_1 > 0$ ,  $v_2 > 0$  and  $v_3 > 0$

423 To derive the adjoint equations and the gradient formula, we introduce

424 the Lagrangian

$$\begin{aligned}
\mathcal{L}(\mathbf{k}, \mathbf{C}, \mathbf{P}, \boldsymbol{\lambda}, \boldsymbol{\mu}) = & J(\mathbf{C}, \mathbf{k}) - \sum_{m=1}^3 S_m \int_0^T \int_0^{L_m} \left( \frac{\partial C_m}{\partial t} + v_m \frac{\partial C_m}{\partial x} + k_m C_m \right) P_m(x, t) dx dt \\
& - S_1 \int_0^T (C_1(x=0, t) - \chi_1(t)) \lambda_1 dt - \sum_{m=2}^3 S_m \int_0^T (C_m(x=0, t) - C_1(x=L_1, t)) \lambda_m dt \\
& - \sum_{m=1}^3 S_m \int_0^{L_m} (C_m(x, t=0) - c_m^0(x)) \mu_m dx
\end{aligned} \tag{A.2}$$

425 and the cost functional is defined as

$$J(\mathbf{C}, \mathbf{k}) = \frac{1}{2} \sum_{m=1}^3 a_m \int_0^T (C_m(\mathbf{k}; x_m) - C_m^{mes})^2 dt + \beta b \sum_{m=1}^3 (k_m - k_m^0)^2 \tag{A.3}$$

426

427 where  $\mathbf{k} = \begin{pmatrix} k_1 \\ k_2 \\ k_3 \end{pmatrix}$ ,  $\mathbf{C} = \begin{pmatrix} C_1 \\ C_2 \\ C_3 \end{pmatrix}$ ,  $\mathbf{P} = \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix}$ ,  $\boldsymbol{\lambda} = \begin{pmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \end{pmatrix}$  and  $\boldsymbol{\mu} = \begin{pmatrix} \mu_1 \\ \mu_2 \\ \mu_3 \end{pmatrix}$

428 and  $S_m$  denotes the cross-sectional area of the  $m^{th}$  water pipe.

429

430 As mentioned in Section 2.3, by writing the stationarity of the La-  
431 grangian according to the Lagrange multipliers  $\mathbf{P}$ ,  $\boldsymbol{\lambda}$  and  $\boldsymbol{\mu}$ , we obtain the  
432 equations of the direct problem (A.1).

433

434 The equations of the adjoint problem are obtained from the stationarity

435 of the Lagrangian according to  $\mathbf{C}$ . Let us derive the adjoint equations.

$$\begin{aligned}
\frac{\partial \mathcal{L}}{\partial C_1} \delta C_1 = 0 \Rightarrow & a_1 \int_0^T \int_0^{L_1} (C_1(x_1) - C_1^{mes}) \delta(x - x_1) \delta C_1 dx dt \\
& - S_1 \int_0^T \int_0^{L_1} \left( \frac{\partial \delta C_1}{\partial t} + v_1 \frac{\partial \delta C_1}{\partial x} + k_1 \delta C_1 \right) P_1(x, t) dx dt - S_1 \int_0^T \delta C_1(x = 0, t) \lambda_1 dt \\
& + \sum_{m=2}^3 S_m \int_0^T \delta C_1(x = L_1, t) \lambda_m dt - S_1 \int_0^{L_1} \delta C_1(x, t = 0) \mu_1 dx = 0, \forall \delta C_1 \\
\frac{\partial \mathcal{L}}{\partial C_m} \delta C_m = 0 \Rightarrow & a_m \int_0^T \int_0^{L_m} (C_m(x_m) - C_m^{mes}) \delta(x - x_m) \delta C_m dx dt \\
& - S_m \int_0^T \int_0^{L_m} \left( \frac{\partial \delta C_m}{\partial t} + v_m \frac{\partial \delta C_m}{\partial x} + k_m \delta C_m \right) P_m(x, t) dx dt \\
& - S_m \int_0^T \delta C_m(x = 0, t) \lambda_m dt - S_m \int_0^{L_m} \delta C_m(x, t = 0) \mu_m dx = 0, \forall \delta C_m, m = 2, 3
\end{aligned} \tag{A.4}$$

436

437 After integrating by parts, one obtains

$$\begin{aligned}
S_m \int_0^T \int_0^{L_m} \frac{\partial \delta C_m}{\partial t} P_m(x, t) dx dt = & S_m \int_0^{L_m} P_m(x, t = T) \delta C_m(x, t = T) dx \\
& - S_m \int_0^{L_m} P_m(x, t = 0) \delta C_m(x, t = 0) dx \\
& - S_m \int_0^T \int_0^{L_m} \frac{\partial P_m}{\partial t} \delta C_m(x, t) dx dt \\
S_m \int_0^T \int_0^{L_m} v_m \frac{\partial \delta C_m}{\partial x} P_m(x, t) dx dt = & S_m v_m \int_0^T P_m(x = L_m, t) \delta C_m(x = L_m, t) dt \\
& - S_m v_m \int_0^T P_m(x = 0, t) \delta C_m(x = 0, t) dt \\
& - S_m \int_0^T \int_0^{L_m} v_m \frac{\partial P_m}{\partial x} \delta C_m(x, t) dx dt
\end{aligned} \tag{A.5}$$

438 From Eqs. (A.4) and (A.5), we deduce the system of equations associated  
439 with the stationarity of the Lagrangian according to the concentration field



440 **C.**

$$\begin{aligned}
& -\frac{\partial P_m}{\partial t} - v_m \frac{\partial P_m}{\partial x} + k_m P_m = \frac{a_m}{S_m} (C(x_m, t) - C_m^{mes}(t)) \delta(x - x_m), \quad \text{in } [0, L_m] \times [0, T], \quad m \in \{1, 2, 3\} \\
& P_m(x, t = T) = 0, \quad \text{in } [0, L_m], \quad m \in \{1, 2, 3\} \\
& S_1 v_1 P_1(x = L, t) = S_2 \lambda_2 + S_3 \lambda_3, \quad \text{in } [0, T] \\
& P_m(x = L_m, t) = 0, \quad \text{in } [0, L_m], \quad m \in \{2, 3\} \\
& \mu_m = P_m(x, t = 0), \quad \text{in } [0, L_m], \quad m \in \{1, 2, 3\} \\
& \lambda_m = v_m P_m(x = 0, t), \quad \text{in } [0, T], \quad m \in \{1, 2, 3\}
\end{aligned} \tag{A.6}$$

441

442 In Eq. (A.6), note that the Lagrange multiplier  $P_m$  corresponds to the  
443 adjoint state. Thus, the equations of the adjoint are given by

$$\begin{aligned}
& -\frac{\partial P_m}{\partial t} - v_m \frac{\partial P_m}{\partial x} + k_m P_m = \frac{a_m}{S_m} (C(x_m, t) - C_m^{mes}(t)) \delta(x - x_m), \quad \text{in } [0, L_m] \times [0, T], \quad m \in \{1, 2, 3\} \\
& P_m(x, t = T) = 0, \quad \text{in } [0, L_m], \quad m \in \{1, 2, 3\} \\
& S_1 v_1 P_1(x = L_1, t) = S_2 v_2 P_2(x = 0, t) + S_3 v_3 P_3(x = 0, t), \quad \text{in } [0, T] \\
& P_m(x = L, t) = 0, \quad \text{in } [0, L_m], \quad m \in \{2, 3\}
\end{aligned} \tag{A.7}$$

444

445 From Eq. (A.7), we observe that the adjoint problem of an advection-  
446 reaction problem through a divergent node corresponds to an advection-  
447 reaction problem through a convergent node. In contrast to the direct prob-  
448 lem, the adjoint problem is backward in time, *i.e.*, it has a final condition,  
449 and the flow is reversed in the adjoint problem, *i.e.*, the velocity  $v_m$  is re-  
450 placed by  $(-v_m)$ . The source term at the first line in Eq. (A.7) indicates  
451 that chlorine is virtually injected at sensor location  $x_m$ , and its amplitude  
452 is given by the data misfit. Hence, the chlorine retropropagates from the  
453 sensor locations.

454 In the same way, when considering an advection-reaction direct problem  
455 through a convergent node, it can be shown that its adjoint problem begins

456 as an advection-reaction problem backward in time through a divergent  
 457 node.

458

459 The functional gradient can be expressed using the adjoint state. It al-  
 460 lows computation of the functional gradient at a lower computational cost  
 461 than standard finite difference schemes. The analytical formula of the func-  
 462 tional gradient can be obtained from the derivative of the Lagrangian ac-  
 463 cording to the reaction coefficient  $k_m$ .

$$\nabla \mathbf{J} = \begin{pmatrix} \frac{\partial J}{\partial k_1} \\ \frac{\partial J}{\partial k_2} \\ \frac{\partial J}{\partial k_3} \end{pmatrix} = \begin{pmatrix} \frac{\partial \mathcal{L}}{\partial k_1} \\ \frac{\partial \mathcal{L}}{\partial k_2} \\ \frac{\partial \mathcal{L}}{\partial k_3} \end{pmatrix} = \begin{pmatrix} -S_1 \int_0^T \int_0^{L_m} C_1 P_1 dx dt + \beta b(k_1 - k_1^0) \\ -S_2 \int_0^T \int_0^{L_m} C_2 P_2 dx dt + \beta b(k_2 - k_2^0) \\ -S_3 \int_0^T \int_0^{L_m} C_3 P_3 dx dt + \beta b(k_3 - k_3^0) \end{pmatrix} \quad (\text{A.8})$$

## 464 Appendix B. Proof of Proposition 4.1 on a reduced water network

465 In the interests of simplifying notations, let us consider the reduced wa-  
 466 ter network presented in Figure B.7. It is composed of the main elements of  
 467 a water network, *i.e.*, water pipes, convergent nodes and divergent nodes.  
 468 Following the methodology presented in Section 2.3 and illustrated in Ap-  
 469 pendix A, we can show that the adjoint problem associated with the reduced  
 470 water network corresponds to

$$\begin{aligned} -\frac{\partial P_m}{\partial t} - v_m \frac{\partial P_m}{\partial x} + k_m P_m &= a_m f_m(x, t), & \text{in } [0, L_m] \times [0, T], m \in \{1, 2, 3, 4\} \\ P_m(x, t = T) &= 0, & \text{in } [0, L_m], m \in \{1, 2, 3, 4\} \\ P_4(x = L_4, t) &= 0, & \text{in } [0, T] \\ P_m(x = L_m, t) &= P_4(x = 0, t), & \text{in } [0, T], m \in \{2, 3\} \\ S_1 v_1 P_1(x = L_1, t) &= S_2 v_2 P_2(x = 0, t) + S_3 v_3 P_3(x = 0, t), & \text{in } [0, T] \end{aligned} \quad (\text{B.1})$$

471 The function  $f_m(x, t)$  corresponds to the virtual injection of chlorine at the  
 472 sensor location. It is defined by

$$f_m(x, t) = (C(x_m, t) - C_m^{mes}(t))\delta(x - x_m)/S_m. \quad (\text{B.2})$$

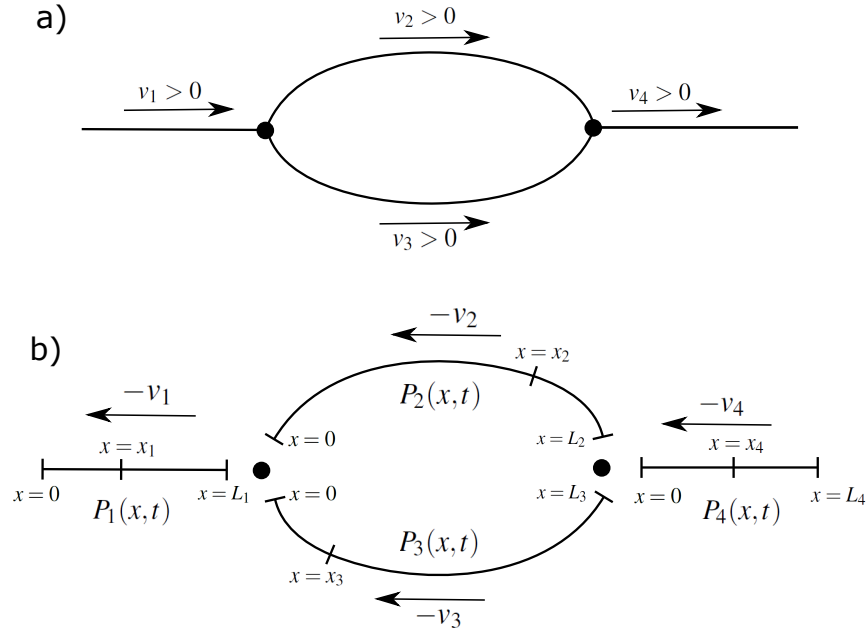


Figure B.7: Reduced water network: a) Flow direction b) Notations associated with the adjoint problem; in the advection-reaction adjoint problem, the flow is reversed;  $\{x_1, x_2, x_3, x_4\}$  denote the potential locations of chlorine sensors

473 When considering no reaction term in (B.1), we obtain the no-reaction

474 adjoint problem

$$\begin{aligned}
-\frac{\partial \phi_m}{\partial t} - v_m \frac{\partial \phi_m}{\partial x} &= a_m f_m(x, t), & \text{in } [0, L_m] \times [0, T], \quad m \in \{1, 2, 3, 4\} \\
\phi_m(x, t = T) &= 0, & \text{in } [0, L_m], \quad m \in \{1, 2, 3, 4\} \\
\phi_4(x = L_4, t) &= 0, & \text{in } [0, T] \\
\phi_m(x = L_m, t) &= \phi_4(x = 0, t), & \text{in } [0, T], \quad m \in \{2, 3\} \\
S_1 v_1 \phi_1(x = L_1, t) &= S_2 v_2 \phi_2(x = 0, t) + S_3 v_3 \phi_3(x = 0, t), & \text{in } [0, T]
\end{aligned} \tag{B.3}$$

475 Finally, if a unitary constant chlorine amplitude in time is injected at  
476 the  $i^{\text{th}}$  sensor location rather than an amplitude given by the data misfit  
477 as in problems (B.1) and (B.3), one obtains the modified adjoint problem  
478 associated with sensor  $i$

$$\begin{aligned}
-\frac{\partial \phi_{m,i}^*}{\partial t} - v_m \frac{\partial \phi_{m,i}^*}{\partial x} &= H(t) \delta(x - x_i), & \text{in } [0, L_m] \times [0, T], \quad m = i \\
-\frac{\partial \phi_{m,i}^*}{\partial t} - v_m \frac{\partial \phi_{m,i}^*}{\partial x} &= 0, & \text{in } [0, L_m] \times [0, T], \quad m \neq i \\
\phi_{m,i}^*(x, t = T) &= 0, & \text{in } [0, L_m], \quad m \in \{1, 2, 3, 4\} \\
\phi_{4,i}^*(x = L_4, t) &= 0, & \text{in } [0, L_4] \\
\phi_{m,i}^*(x = L_m, t) &= \phi_{4,i}^*(x = 0, t), & \text{in } [0, L_m], \quad m \in \{2, 3\} \\
S_1 v_1 \phi_{1,i}^*(x = L_1, t) &= S_2 v_2 \phi_{2,i}^*(x = 0, t) + S_3 v_3 \phi_{3,i}^*(x = 0, t), & \text{in } [0, T]
\end{aligned} \tag{B.4}$$

479 This problem does not depend on reaction phenomena. Moreover, from the  
480 solution of Eq. (B.4), we can deduce the general solution of the modified  
481 adjoint problem (4) involved in Proposition 3.1

$$\phi_m^*(x, t) = \sum_{i=1}^N a_i \phi_{m,i}^*(x, t), \quad \text{in } [0, L_m] \times [0, T], \quad m \in \{1, 2, 3, 4\} \tag{B.5}$$

482 On the one hand, the solution  $\phi_m(x, t)$  of the no-reaction adjoint problem  
483 (B.3) can be obtained from the modified adjoint solution  $\phi_{m,i}^*$  (also called

484 “Green function”). Indeed, noting that

$$f_m(t) = [f_m * \delta](t) = [f'_m * H](t) \quad (\text{B.6})$$

485 where  $*$  denotes the convolution product in time and  $H$  is the Heaviside  
486 function, one has

$$\phi_m(x, t) = \sum_{i=1}^N a_i [f'_i * \phi_{m,i}^*](x, t), \quad m \in \{1, 2, 3, 4\} \quad (\text{B.7})$$

487 where  $f'_m$  is the derivative of the function  $f_m$  according to the time variable.

488 We recall that the flow  $(-v_m)$  is considered stationary in the present proof.

489 Consequently:

$$\phi_m^*(x, t) = 0 \text{ in } [0, L_m] \times [0, T] \Leftrightarrow \phi_{m,i}^*(x, t) = 0 \text{ in } [0, L_m] \times [0, T] \Rightarrow \phi_m(x, t) = 0 \text{ in } [0, L_m] \times [0, T] \quad (\text{B.8})$$

490

491 On the other hand, subtracting Eq. (B.1) from (B.3) and noting  $\delta P_m(x, t) =$

492  $P_m(x, t) - \phi_m(x, t)$ , one has

$$\begin{aligned} -\frac{\partial \delta P_m}{\partial t} - v_m \frac{\partial \delta P_m}{\partial x} + k_m \delta P_m &= -k_m \phi_m, & \text{in } [0, L_m] \times [0, T], \quad m \in \{1, 2, 3, 4\} \\ \delta P_m(x, t = T) &= 0, & \text{in } [0, L_m], \quad m \in \{1, 2, 3, 4\} \\ \delta P_4(x = L_4, t) &= 0, & \text{in } [0, T] \\ \delta P_m(x = L_m, t) &= \delta P_4(x = 0, t), & \text{in } [0, T], \quad m \in \{2, 3\} \\ S_1 v_1 \delta P_1(x = L_1, t) &= S_2 v_2 \delta P_2(x = 0, t) + S_3 v_3 \delta P_3(x = 0, t), & \text{in } [0, T] \end{aligned} \quad (\text{B.9})$$

493 From Eq. (B.9), we deduce that

$$\begin{cases} \phi_m(x, t) = 0, & \text{in } [0, L_m] \times [0, T] \\ \delta P_m(x = L_m, t) = 0, & \text{in } [0, T] \\ \delta P_m(x, t = T) = 0, & \text{in } [0, L_m] \end{cases} \quad (\text{B.10})$$

494 implies

$$\delta P_m(x, t) = 0, \text{ in } [0, L_m] \times [0, T] \Rightarrow P_m(x, t) = 0, \text{ in } [0, L_m] \times [0, T] \quad (\text{B.11})$$

495 As the gradient  $\nabla J$  can be expressed using the adjoint solution  $P_m$

$$\frac{\partial J}{\partial k_m} \delta k_m = -S_m \int_0^T \int_0^{L_m} C_m P_m \delta k_m dx dt + \beta b(k_m - k_m^0) \delta k_m \quad (\text{B.12})$$

496 it can be noted that a null adjoint solution  $P_m(x, t)$  in the pipe  $m$  on the  
497 entire time interval  $[0, T]$  implies that the first term of the gradient compo-  
498 nent according to the reaction coefficient  $k_m$  vanishes. Hence, the reaction  
499 coefficient in pipe  $m$  cannot be updated.

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