



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

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

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

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

2. Modeling the water quality in drinking water networks and updating the kinetic reaction coefficient

2.1. Simulating the water quality in drinking water networks

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

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

strategy is described in the following sections.

2.2. Cost functional used in model updating

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

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

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

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

convexity of the functional. The parameter b ensures the physical homogeneity of both terms, and k_m^0 corresponds to the initial guess of the m^{th} reaction coefficient. β corresponds to a normalized weighting coefficient.

179

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

2.3. Derivation and physical meaning of adjoint equations

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

192

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

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

functional regularization.

All the components of the functional gradient ∇J are computed from Eq. (2).

Updating of the reaction coefficients:. Using the functional gradient ∇J as the descent direction, we obtain the updated vector \mathbf{k}_{new} of reaction coefficients by

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

where α is the descent step. Several solutions are required to determine the descent step minimizing the cost functional J .

If the data misfit functional reaches the measurement error, the model updating process is stopped. Otherwise, the iterative process continues.

3. Optimal chlorine sensor placement using the adjoint framework

3.1. Theoretical foundations of the optimal chlorine sensor placement method

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

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

The modified adjoint solution $\phi^(x, t)$ verifies the following transport equations in the pipes of the water networks*

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

The boolean a_m is equal to 1 (resp. 0) if the m^{th} water pipe is equipped with a chlorine sensor (resp. is not equipped with a chlorine sensor). As with the adjoint problem, the pipe junctions are governed by the standard equations 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

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

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

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

4. Numerical results using the software EPANET

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

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

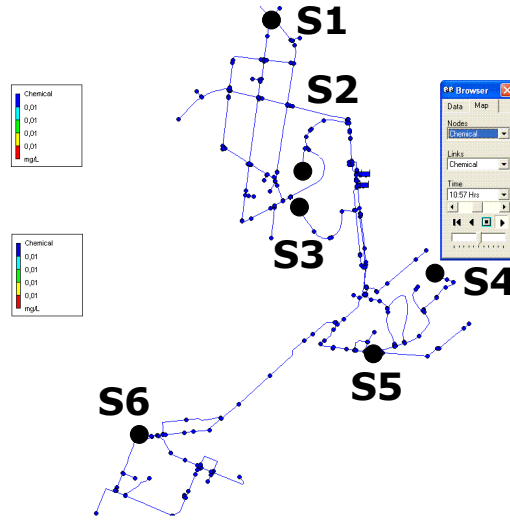


Figure 1: Geometry of a French drinking water network with 2 water towers - 6 possible locations of chlorine sensors

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 η 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

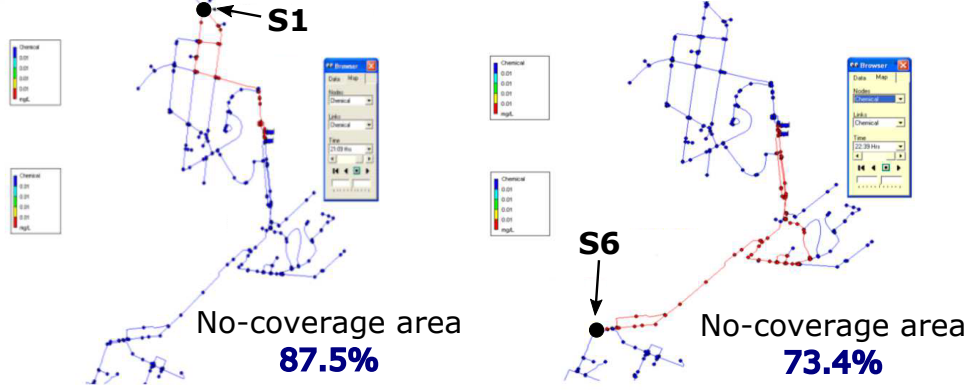


Figure 2: Sensor position S_1 : $\eta = 87.5\%$ (left), Sensor position S_6 : $\eta = 73.4\%$ (right)

Sensor	Non-coverage indicator η
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 η . Then, to continue decreasing the non-identifiable area, an additional
368 chlorine sensor is considered in the drinking water network. The indicator

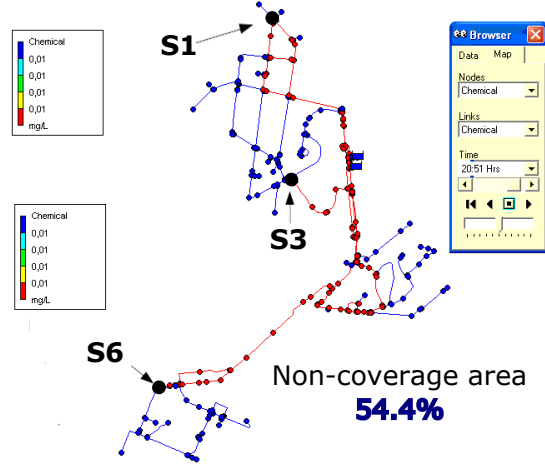


Figure 3: Combination of three sensors $S_6 - S_1 - S_3$: $\eta = 54.4\%$

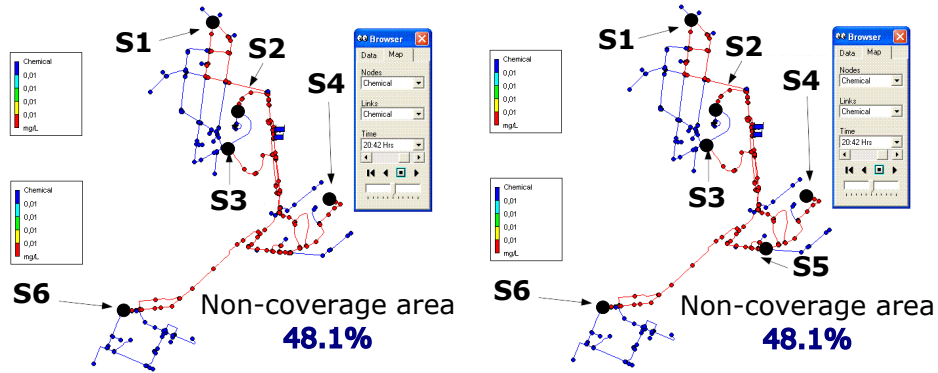


Figure 4: Combination of 5 sensors $S_6 - S_1 - S_3 - S_4 - S_2$: $\eta = 48.1\%$ (right), Combination of 6 sensors S_1 to S_6 : $\eta = 48.1\%$ (left)

369 η 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 η	2 Sensors	Non-coverage indicator η	3 Sensors	Non-coverage indicator η
S_1	87.5 %	S_6, S_1	61.7 %	S_6, S_1, S_2	59.2 %
S_2	97.5%	S_6, S_2	70.9 %	S_6, S_1, S_3	54.4 %
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 %		
S_6	73.4%				

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 η	5 Sensors	Non-coverage indicator η	6 Sensors	Non-coverage indicator η
S_6, S_1, S_3, S_2	53.7 %	S_6, S_1, S_3, S_4, S_2	48.1%	$S_6, S_1, S_3, S_4, S_2, S_5$	48.1 %
S_6, S_1, S_3, S_4	48.8 %	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,

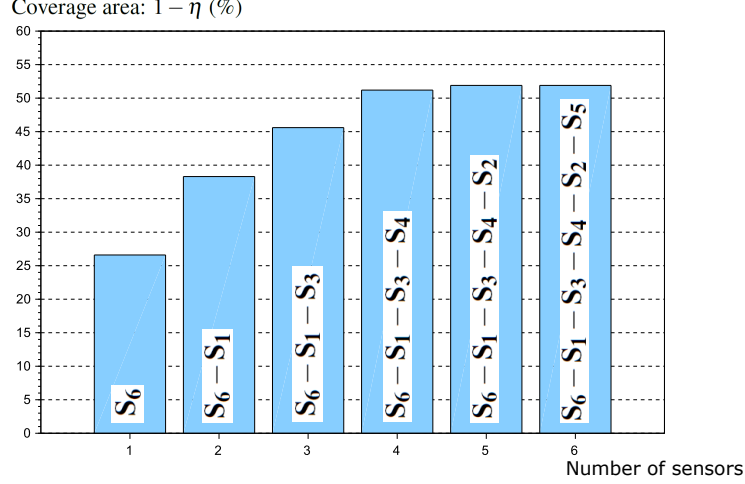


Figure 5: Synthesis of optimal sensor placement to maximize the coverage area

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.

403 **Acknowledgments**

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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. α_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

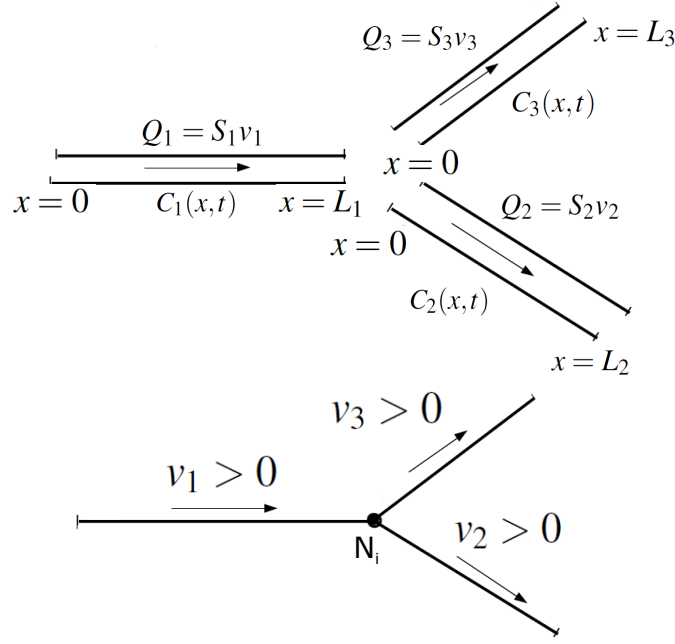


Figure A.6: Notations for advection reaction through divergent node - the flow velocity v_m in pipe m is considered positive when it passes from the starting node ($x = 0$) to the ending node ($x = L_m$) - herein, $v_1 > 0$, $v_2 > 0$ and $v_3 > 0$

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

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

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.**

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

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

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

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

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

458

The functional gradient can be expressed using the adjoint state. It allows computation of the functional gradient at a lower computational cost than standard finite difference schemes. The analytical formula of the functional gradient can be obtained from the derivative of the Lagrangian according to the reaction coefficient k_m .

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

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

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

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

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

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

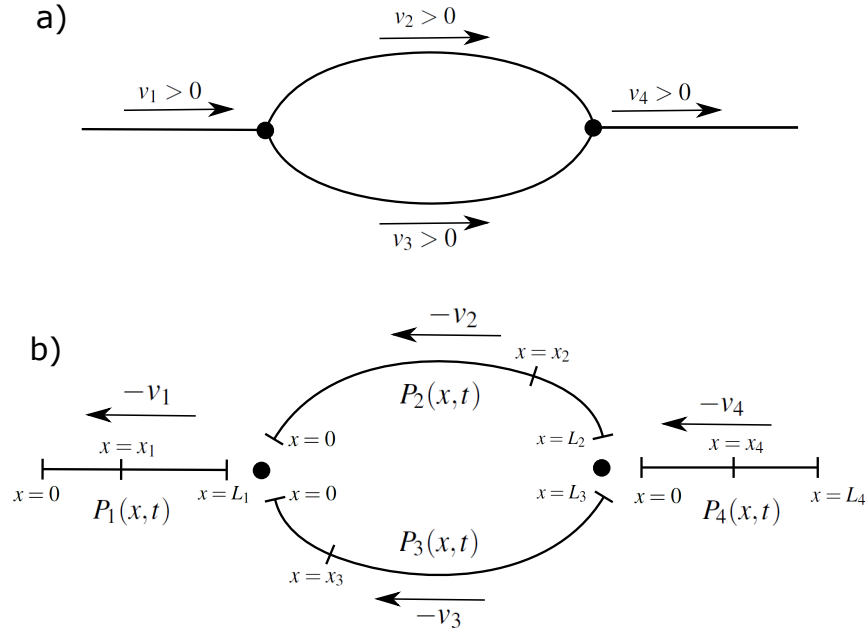


Figure B.7: Reduced water network: a) Flow direction b) Notations associated with the adjoint problem; in the advection-reaction adjoint problem, the flow is reversed; $\{x_1, x_2, x_3, x_4\}$ denote the potential locations of chlorine sensors

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

474 adjoint problem

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

475 Finally, if a unitary constant chlorine amplitude in time is injected at
476 the i^{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

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

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 ∇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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