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

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ABSTRACT

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

Software availability

Name of software: EPANET
Programming language: C/C++
Operating system: Windows
Availability: http://www.epa.gov/water-research/epanet
Documentation: http://www.epa.gov/water-research/epanet
User interface: Graphical user interface or Programmer's toolkit
License: Public domain software that may be freely copied and distributed

1. Introduction

In drinking water networks, the chlorine concentration field is one of the main indicators of the water quality. Legislation dictates that a minimum level of chlorine at each point in the network has to be ensured. To overcome the lack of measurements in drinking water networks, hydraulic and water quality models are considered. In water network applications, the hydraulic state is generally computed using algebraic equations, *i.e.,* flow continuity at the nodes and headloss in the pipes. Regarding the water quality models, one-dimensional (1D) advection-reaction equations are considered in pipes, and perfect and instantaneous mixing is assumed in pipe junctions. The decrease of the chlorine concentration due to bulk flow reactions and pipe wall reactions, *e.g.,* reaction with the biofilm at the pipe wall, is modeled using a reaction term (Powell et al., 2000). This term is characterized by the reaction order and the reaction coefficient. The software EPANET (Rossman and Boulos, 1996; Rossman, 2000) is commonly used to simulate the hydraulics and the water quality states.

French water companies can observe a gap higher than 30% between the chlorine sensor outputs and the chlorine concentration obtained from a direct simulation of the water quality model. This gap may be due to uncertainties in the hydraulic state, particularly the water demands, and to the model parameters associated with the chlorine reactions. To represent the variability in water demands, stochastic models are typically considered. The calibration of these models can be achieved using direct measurements (Buchberger and Wells, 1996; Bakker et al., 2013; Cominola et al., 2015), *i.e.,* monitoring of the user water

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consumption in residences, or indirect measurements (Kang and Lansey, 2009; Alcocer-Yamanaka et al., 2012), *i.e.,* pressure and/or flow rate outputs into the drinking water network. To locate and quantify abnormal water demands due to leaks, inverse techniques based on pressure sensor outputs have been proposed in Liggett and Chen (1994) and Meseguer et al. (2014). In this inverse problem, the goal is to determine the unknown model parameters by minimizing the gap between the sensor outputs and the simulation. Finally, flow sensor outputs may also be used in inverse techniques. Indeed, an inverse computational fluid dynamics technique has been developed in Waeytens et al. (2015) to identify the unknown boundary conditions of 2D incompressible Navier-Stokes equations and thus to obtain a high description in 2D of the flow profile in water networks. A detailed description of the flow in 2D or 3D can provide more representative chlorine simulations than using the mean flow velocity, particularly in the distribution mains of the drinking water networks where the flow can be laminar, thus inducing different chlorine propagation velocities. 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 non-coverage area, the number of sensors, the time to detection, and so forth.

In the present article, we propose a numerical strategy based on the adjoint framework to determine and quantify the non-coverage area for a given set of sensor placements. This practical information can be useful for water companies to determine the optimal placement of chlorine sensors for maximizing the coverage area for a given number of sensors. The method requires the resolution and the post-treatment of the solution of the adjoint problem, *i.e.,* advection-reaction equations backward in time with virtual chlorine injection at the position of the sensors and a dynamic back flow. The adjoint framework is used in various applications. First, it provides at a low computational cost the functional gradient involved in inverse calculations to update the model parameters of the water flow (Liggett and Chen, 1994; Waeytens et al., 2015) and to reconstruct the concentration fields (Elbern et al., 2000; Waeytens et al., 2013, 2017). Then, it is used in sensitivity analyses to study the influence of the physical model parameters on a quantity of interest (Andrews, 2013; Kauker et al., 2016). The adjoint framework is also considered for estimating the modeling or the discretization error on a quantity of interest (Becker and Rannacher, 2001; Waeytens et al., 2012; Oden and Prudhomme, 2002). Note that the determination and quantification of the coverage area can also be obtained from Xu et al. (2008), which is based on the knowledge of the flow and graph theory. The main advantage of the proposed adjoint approach is that it uses standard hydraulic software such as EPANET. Moreover, the adjoint solution can also be used in an inverse advection-reaction procedure to identify the reaction coefficient.

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 $\mathbb{C}$.

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 $\mathbb{k} = \{k_1, \ldots, k_N\}$ 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 $\mathbb{C}$ of the water quality model mentioned in the previous section. One seeks the vector $\mathbb{k}$ of reaction coefficients by solving the following optimization problem: