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Quality Modeling of Water Distribution Systems using Sensitivity Equations

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Abstract:

In this paper, unsteady water quality modeling and the associated sensitivity equations are solved for Water Distribution Systems (WDS). A new solution algorithm is proposed, designed for slow varying velocity and based on a time splitting method to separate and solve efficiently each phenomenon such as advection and chemical reaction. This numerical approach allows simultaneous solution of both the direct problem and the sensitivity equations. Special attention is given to the treatment of advection, which is handled with a Total Variation Diminishing (TVD) scheme. The general model presented in this study permits global sensitivity analysis of the system to be performed and its efficiency is illustrated on two pipe networks. The importance of the sensitivity analysis is shown as part of the calibration process on a real network.

CE Database subject headings: Water distribution systems; Water quality; Models; Sensitivity analysis; Algorithm.

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Introduction

The quality of water supplied by a distribution network is usually assessed by various indicators, such as residence times, source tracing and disinfectant concentration. These indicators can be obtained by solving mathematical models that depend on estimates of physical parameters. Kinetic parameters characterizing disinfection (bulk and wall) reactions are rarely known with any precision because of uncertainties. To overcome this problem, parameter calibration is required and the sensitivity of the solution to parameter variations in the model should be analyzed. Studies have been carried out for hydraulic sensitivity purposes (Bargiela and Hainsworth, 1989; Kapelan, 2002), for hydraulic calibration (Piller, 1995) and for hydraulic and water quality sampling design/meter placement (Bush and Uber, 1998; Chesneau et al., 2003; Piller et al., 1999).

Sensitivity analysis and calibration are important needs in water network engineering. In most previous research, finite difference methods were used to compute sensitivity gradients. These methods are only approximate and quite costly in computer processing time. The sensitivity analysis is then less accurate compared to the approach to be proposed, namely, *the direct solution of sensitivity equations.* The structure of the latter is very close to the original problem, facilitating their simultaneous solution.

The vast majority of practitioners performing water quality studies have used either *EPANET* or an *EPANET*-like approach. Thus, these users will be employing the advection-reaction equation with assumed hydraulic conditions to predict concentrations, source tracings and water ages in the network. However, velocity is a step and piecewise function with regards to time in *EPANET*, using an extended period simulation approach: only the equilibrium solution is sought for each step, not the whole trajectory. The *EPANET* software is an efficient Lagrangian event-driven code: nevertheless, accounting for continuously time-varying velocity in quality calculations is inefficient. In *EPANET* only one variable is calculated for each simulation (e.g. concentration and residence time).

In this work sensitivity equations are directly derived from the transport-reaction for-

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mulations. Then, a solving algorithm for the advection-reaction is specially designed and adapted for a smooth and slowly varying input time-dependent velocity variable. The velocities are computed using a rigid column technique that takes into account the inertial and mass oscillatory characteristics. The new technique also allows simultaneous calculation of several quality indicators and derivatives.

A new time-splitting approach to solve the coupled hydraulic-quality problem is presented. This is a non-linear problem that is impossible to solve exactly, so the technique proposed in the paper is designed to reduce substantially the approximation errors. The advantage of time-splitting is the use of a specific numerical solver for each physical phenomenon (Sportisse, 2000). Each operator (advection, chemical reaction) is considered separately, with special attention to the advection modeling. Because the physical phenomenon is dominated by the advection and the chemistry, the diffusive term is not considered in this work. Nevertheless, the technique easily allows including diffusion for more complex case studies. This behavior was already studied by (Islam and Chaudhry, 1998) who used a splitting method to compute the constituent transport in unsteady flows, including diffusion, in pipes. They observed that the differences in concentration profiles were insignificant between computations with and without diffusion. Recently, many authors have used different techniques like Eulerian (fixed grid), Lagrangian (deforming grid), or methods of characteristics (MOC) to solve such problems. Rossman and Boulos (1996) concluded that Eulerian methods are as accurate as Lagrangian ones except for sharp concentration fronts. Based on this conclusion, we have developed an Eulerian Total Variation Diminishing (TVD) scheme for water quality transport and sensitivity analysis (Gancel et al., 2006). This approach is appropriate to take into account variations of concentration fronts (smooth or sharp). The TVD techniques should also overcome the oscillations of classical Eulerian schemes.

An important point that needed to be improved in WDS modeling, is the calibration of the parameters for the quality assessment in the transport-reaction level described by three categories: the lack of measurements, the difficulty to estimate accurately the velocities (and therefore the transport) and the complexity of the reaction pro-

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cedure. In this study, using an efficient sensitivity analysis we are able to fit the optimal locations for the measurement devices. The new model also takes into account the inertial terms and it is more efficient in considering the unsteady behavior of the system. Finally, the derivatives for calibration are directly computed for the reaction term, more accurately and faster than previous existing techniques that use finite differences or simply don't compute the derivatives (e.g. genetic algorithms). All these three developments together contribute to improve the goodness-of-fit of the direct model and facilitate the calibration process.

The paper is organized as follows: The physical transport-reaction problem in WDS is first described. The proposed time splitting method, is then validated by a numerical comparison with other approaches. Next, sensitivity equations are derived from the original problem and the computational algorithms to solve the global model are described. Finally, the model is applied to three illustrative network examples: a simple network that allows the results to be easily checked, a benchmark example from the *EPANET* 2 distribution (U.S. Environmental Protection Agency, 2002) and at last a real network, showing the importance of sensitivity analysis for parameter calibrations.

Water quality in WDS

Water quality modeling consists primarily of predicting disinfectant (chlorine) concentration, residence times and source tracing at network nodes. The propagation of these constituents (quality indicators) in a WDS relies on solving an advection equation in each pipe with a kinetic reaction mechanism and mixing at nodes.

Direct Problem

Assuming that the effect of longitudinal diffusion is negligible (Rossman and Boulos, 1996), the change in *quality indicator* constituent, C, due to transport through a pipe can be described by a one-dimensional hyperbolic Partial Differential Equation (PDE) of the form:

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$$\begin{cases} \partial_t C(t,x) + u(t)\partial_x C(t,x) + f(C) = 0, \\ C(0,x) = C_0(x), \quad \forall x \in \mathbb{R}^+, \\ C(t,0) = \Phi(t), \quad \forall t \geq 0. \end{cases} \tag{1}$$

A boundary condition at $x = 0$ is needed to solve Eq. (1) for a non-negative time-varying, but spatially uniform, velocity field, determined from the network hydraulic solution. This velocity is obtained using the rigid column equation for slowly varying flows in pipe networks. $f(C)$ is a reaction function describing the transformation of each indicator. If C stands for a concentration, the reaction term is given by the following:

$$f(C) = kC^{\alpha}(t,x) \quad \text{with} \quad \alpha \geq 1, \tag{2}$$

where α is the order of reaction and k is the overall decay constant (Powell and West 2000). Then, the residence time and the water source can be tracked by specifying:

$$\begin{cases} f(C) = -1, & \text{(3a)} \\ f(C) = 0. & \text{(3b)} \end{cases}$$

Residence time is obtained with Eq. (3a), while Eq. (3b) can be used for source identification which is very useful for tracing bacteria.

Junction and tank mixing

A WDS is mainly composed of pipes, tanks, reservoirs and junction nodes. Water arriving at a junction in different pipes is commonly assumed to be mixed perfectly and instantaneously. At each junction node n, the resulting water indicator constituent, $C_n(t)$, is therefore the flow-weighted average of the individual constituents of the incoming flows:

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$$\begin{cases} C_n(t) = \dfrac{\sum_{i \in N_{in}} q_i C_i(t)}{\sum_{i \in N_{in}} q_i}, \\ C_n(0) = C_{n_{t_0}}. \end{cases} \tag{4}$$

where $C_i(t)$ is the considered quantity input at node n at time t from pipe i; N_{in} is the set of pipes that are incident to node n and q_i is the flow rate entering the junction node from pipe i.

Again, a mass balance of water indicator constituent entering or leaving a variable-level tank can be performed:

$$\begin{cases} \dfrac{dC_T}{dt} = \dfrac{\sum_{i \in N_{in}} q_i (C_i - C_T)}{V_T} + f(C_T) \\ C_T(t=0) = C_{T_{t_0}} \\ V_T(t=0) = V_{T_{t_0}} \end{cases} \tag{5}$$

where $C_T(t)$ is the water indicator constituent within tank T; q_i is the flow rate entering the tank from pipe i; $f(C_T)$ is the reaction term given by Eq. (2) for concentration and Eq. (3) for residence time and source tracing; finally V_T is the water volume in tank T.

To indicate a range for residence time we calculate not only the flow-weighted average but also the minimal and maximum values with time.

To summarize, water quality modeling for a network consists of solving for each time step Eq. (1) with the mixing relations: Equations (4) and (5), for each water quality indicator using the appropriate f function. The minimal and maximum values at mixing nodes are also worked out.

Numerical scheme

Various numerical methods for the water quality models have already been proposed and their comparison has been performed by Rossman and Boulos (1996). Their main

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conclusion was that the Lagrangian methods are more efficient for simulating chemical transport. *EPANET* which is the most widely used water quality simulator uses such a Lagrangian time-based approach to track the fate of discrete parcels of water as they move along pipes and mix together at junctions, between fixed-length time steps (Rossman, 2000). It is difficult to extend the *EPANET*'s model to variable-length time steps to account for slow varying velocities in pipes. So, a new method using a time splitting approach has been developed for this purpose and to solve sensitivity equation with coupling approach.

Time splitting method

The advantage of this approach is the use of a specific numerical solver for each physical phenomenon, here the advection and chemical reaction. This method is particularly recommended in the case where evolution equations to be simulated are stiff (Yee, 1988; Sportisse, 2000; Islam and Chaudhry, 1998) which is the case here mainly due to chemical terms with several scales. It results in a better accuracy and stability. Islam and Chaudhry who solved the waterborne substance transport-reaction problem using a two step splitting method mentioned this technique is useful to reduce the numerical diffusion. It can been demonstrated, thought, that two-step (A-B) splitting introduces an error that can be limitative (of first-order) for two linear operators that do not commute (see e.g.: Sportisse, 2000). This is confirmed for advection (A) and pipe-dependent reaction (B) operators. In order to improve the accuracy, the following second-order Strang's (B-A-B) splitting scheme is applied to Eq. (1):

$$\begin{cases} \partial_t C^* + f\left(C^*\right) = 0, \quad C^*(0) = C_0, \qquad \text{on} \left[0, \dfrac{\delta t}{2}\right], & \text{(6a)} \\ \partial_t C^{**} + u(t)\partial_x C^{**} = 0, \quad C^{**}(0) = C^*\left(\dfrac{\delta t}{2}\right), \quad \text{on}\left[0, \delta t\right], & \text{(6b)} \\ \partial_t C^{***} + f\left(C^{***}\right) = 0, \quad C^{***}(0) = C^{**}(\delta t), \quad \text{on} \left[0, \dfrac{\delta t}{2}\right]. & \text{(6c)} \end{cases}$$

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where in sub-step 1, reaction terms are integrated over $\delta t/2$ by solving Eq. (6a); the initial condition C_0 is the final state C from the previous time step, and the solution to Eq. (6a) is $C^*(\delta t/2)$.

Next in sub-step 2, pure advection is integrated over δt by solving Eq. (6b); the initial condition $C^{**}(0)$ corresponds to the final state from the previous sub-step, $C^*(\delta t/2)$, and the solution to Eq. (6b) is $C^{**}(\delta t)$.

Finally in sub-step 3, again reaction terms are integrated over $\delta t/2$; the initial condition $C^{***}(0)$ is the final state from the previous sub-step, $C^{**}(\delta t)$, and the solution to Eq. (6c) is $C^{***}(\delta t/2)$, which in turn is the new final state $C(\delta t)$.

If each of the three sub-steps in the above splitting procedure is solved accurately (with at least second-order accuracy in time), the Strang splitting scheme is second-order accurate in time (Ren, 2008). To benefit from the latter, the reaction parts Eq. (6a) and Eq. (6c) are solved using a standard explicit fourth-order Runge Kutta method and a novel TVD scheme is chosen for the advection sub-problem solving Eq. (6b).

TVD Scheme

A new version of the TVD scheme that is well adapted to the present unsteady advection problem is proposed. This four-point scheme which is similar to that of Rasetarinera (1995), is L^∞-stable and belongs to the family of Takacs schemes. The main difference from the scheme of Rasetarinera arises from the presence of an unsteady velocity, $u(t)$, that depends only on time.

Let δx and δt be the space and time step respectively and C_i^n the approximate value at the point $(n\delta t, i\delta x)$. For time-independent velocities, the second or third order Takacs upwind schemes are written as follows:

$$C_i^{n+1} = \gamma_1 C_{i+1}^n + \gamma_0 C_i^n + \gamma_{-1} C_{i-1}^n + \gamma_{-2} C_{i-2}^n, \tag{7}$$

where the γ_k are chosen to obtain 2nd order formal accuracy.

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For an unsteady velocity:

$$\begin{aligned} C_i^{n+1} = C(t+\delta t, x) &= C(t,x) - \delta t \frac{\partial C}{\partial x}(t,x)\big[u(t) + \frac{\delta t}{2}\frac{\partial u}{\partial t}(t)\big] \\ &\quad + u^2(t)\frac{\delta t^2}{2}\frac{\partial^2 C}{\partial x^2}(t,x) + \mathcal{O}(\delta t^3). \end{aligned} \tag{8}$$

The velocity derivative $\dfrac{\partial u}{\partial t}$ in equation (8) is approximated to first order by:

$$\frac{\partial u}{\partial t} = (u(t+\delta t) - u(t))/\delta t + \mathcal{O}(\delta t^2) \quad \text{and we denote} \quad u^{(t+\delta t/2)} = \frac{u(t+\delta t) + u(t)}{2}.$$

such that:

$$C_i^{n+1} = C(t,x) - \delta t \frac{\partial C(t,x)}{\partial x} u^{(t+\delta t/2)} + u^2(t)\frac{\delta t^2}{2}\frac{\partial^2 C(t,x)}{\partial x^2} + \mathcal{O}(\delta t^3). \tag{9}$$

In the same way, the equations are also developed for C_{i+1}^n, C_{i-1}^n and C_{i-2}^n.
Noting $u^n \approx u(t,x)$ and $u^{n+\frac{1}{2}} \approx u(t+\delta t/2, x)$, the coefficients γ_i are determined as

$$\gamma_1 = \frac{\lambda(\lambda u^n u^n - u^{n+1/2})}{2} - \gamma_{-2}, \quad \gamma_{-1} = \frac{\lambda(\lambda u^n u^n + u^{n+1/2})}{2} - 3\gamma_{-2}, \quad \gamma_0 = 1 - \lambda^2 u^n u^n + 3\gamma_{-2},$$

where $\lambda = \dfrac{\delta t}{\delta x}$ and γ_{-2} is determined in order to get the exact solution for $u^{n+1} = 0, u^n = 0$ and $\lambda u^{n+1} = 1, \lambda u^n = 1$, that is:

$$\gamma_{-2} = \gamma\lambda(\lambda u^n u^n - u^{n+1/2}) \quad \text{with } \gamma \text{ a non negative constant,}$$

Now, Eq. (7) can be turned in a TVD and L^∞-stable scheme (Rasetarinera, 1995) by first re-ordering:

$$\begin{aligned} C_i^{n+1} &= C_i^n - \lambda u^{n+1/2}(C_i^n - C_{i-1}^n) - \frac{\lambda(u^{n+1/2} - \lambda u^n u^n)}{2}(C_{i+1}^n - 2C_i^n + C_{i-1}^n) \\ &\quad - \gamma\lambda(\lambda u^n u^n - u^{n+1/2})(C_{i+1}^n - 3C_i^n + 3C_{i-1}^n - C_{i-2}^n) \end{aligned} \tag{10}$$

and with $\Delta C_{i+1/2}^n = C_{i+1}^n - C_i^n$ and $r_{i+1/2}^n = \Delta C_{i-1/2}^n / \Delta C_{i+1/2}^n$,

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$$\begin{aligned} C_i^{n+1} &= C_i^n - \lambda u^{n+1/2}\Delta C_{i-1/2}^n - \frac{\lambda(u^{n+1/2} - \lambda u^n u^n)}{2}(\Delta C_{i+1/2}^n - \Delta C_{i-1/2}^n) \\ &\quad - \gamma\lambda(\lambda u^n u^n - u^{n+1/2})\big((1 - r_{i+1/2}^n)\Delta C_{i+1/2}^n - (1 - r_{i-1/2}^n)\Delta C_{i-1/2}^n\big) \quad (11) \end{aligned}$$

A TVD scheme is obtained by limiting the numerical flux of the initial Takacs scheme, as with the Lax-Wendroff scheme (Sweby, 1984; Rasetarinera, 1995):

$$\begin{aligned} C_i^{n+1} = C_i^n &- \lambda u^{n+1/2}\Delta C_{i-1/2}^n \\ &- \frac{\lambda}{2}(u^{n+1/2} - \lambda u^n u^n)(\phi(r_{i+1/2}^n)\Delta C_{i+1/2}^n - \phi(r_{i-1/2}^n)\Delta C_{i-1/2}^n), \quad (12) \end{aligned}$$

where $\phi(r) = 1 - 2\gamma(r)(1 - r)$. To have $\phi(r)$ in Sweby region we put: $\gamma_{i\pm1/2}^n = min\big(\frac{|1-r_{i\pm1/2}^n|}{2}, \frac{1}{2|1-r_{i\pm1/2}^n|}\big)$.
The final TVD scheme can be given as:

$$\begin{aligned} C_i^{n+1} &= C_i^n - \lambda u^{n+1/2}\Delta C_{i-1/2}^n - \frac{\lambda}{2}(u^{n+1/2} - \lambda u^n u^n)(\Delta C_{i+1/2}^n - \Delta C_{i-1/2}^n) \quad (13) \\ &- \lambda(\lambda u^n u^n - u^{n+1/2})\big(\gamma_{i+1/2}^n(1 - r_{i+1/2}^n)\Delta C_{i+1/2}^n - \gamma_{i-1/2}^n(1 - r_{i-1/2}^n)\Delta C_{i-1/2}^n\big). \end{aligned}$$

The scheme (13) is TVD and L^∞-stable under the following CFL condition: $\lambda \parallel u \parallel_\infty \leq 1$. It is formally second-order, where the solution is smooth enough, except in a neighborhood of critical points. The main advantage of using a TVD scheme is its capability to deal gracefully with shocks or large spatial gradients.

Validation for advection reaction problem

The proposed numerical method is first compared to other Eulerian techniques for a benchmark case. The compared methods are the Lax-Wendroff scheme, the θ-scheme, the Holly-Preissman method, the Van Leer scheme and the hybrid method used in the *Porteau* Software (Porteau, 2009). The *Porteau* Software, designed and

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commercialized in France by the *Cemagref* (Piller, 1996; Piller, 1997), combines the method of characteristics and a θ-scheme in a two-step process hereafter referred to as a hybrid scheme. First, the method of characteristics is applied on step $\Delta t \leq \delta t$ such as $u^{n+1/2}\Delta t = \delta x$. In the linear case ($\alpha = 1$),

$$C_i^{n+1/2} = C(n\delta t + \Delta t, i\delta x) = C(n\delta t, (i-1)\delta x)e^{-k\Delta t} \tag{14}$$

the upstream θ-scheme is then applied for $\tau = \delta t - \Delta t$:

$$\frac{C_i^{n+1} - C_i^{n+1/2}}{\tau} + \theta u^{n+1}\frac{C_i^{n+1} - C_{i-1}^{n+1}}{\delta x} + (1-\theta)u^{n+1/2}\frac{C_i^{n+1/2} - C_{i-1}^{n+1/2}}{\delta x} + k\theta C_i^{n+1} + k(1-\theta)C_i^{n+1/2} = 0 \tag{15}$$

where $\theta = 1/2$. The nonlinear case is more complex due to the approximation of the non linearity; the following change of variable is used:

$$\lambda(t,x) = C^{1-\alpha}(t,x) + (1-\alpha)kt \quad \Leftrightarrow \quad C(t,x) = \Big(\lambda(t,x) - (1-\alpha)kt\Big)^{\frac{1}{1-\alpha}} \quad \alpha \neq 1 \tag{16}$$

(16) is also useful to take into account the nonlinear term for the classical numerical methods like Lax-Wendroff and θ-scheme.

The benchmark problem is a single pipe of $500m$ length with a constant pipe velocity of $u = 0.5\ m/s$ and a steady chlorine injection at the pipe inlet beginning at time t_1 during a period T and then stopping, i.e.:

$$\begin{cases} C(t,0) = 1 & \text{if } t \in]t_1, t_1 + T] \\ C(t,0) = 0 & \text{otherwise} \end{cases} \tag{17}$$

A comparison for the advection reaction solution in the linear case is given in Fig. 1, where dimensionless $\delta x = 0.01$ (100 discretization points).

The Holly-Preissmann technique (Holly and Preissmann, 1977) that is often used in WDS, uses an Hermite interpolation formula of the third-order, to interpolate

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the "characteristic foot". This method is efficient but has two main drawbacks: its CPU time and the use of a solution derivative which creates oscillations with a non smooth solution (Fig. 1a). The Lax-Wendroff scheme Fig. 1b (second-order in time and space, L^2 stable) is efficient for continuous solutions but generates "overshooting" and "undershooting" near singularities. The θ-scheme (Fig. 1c) suffers from substantial numerical diffusion and a positivity condition which may be overly restrictive for our problem. Fig. 1d shows the solution with the hybrid method which is very accurate but can lead to high CPU time if used with an unsteady velocity that becomes close to zero, because of its variable space discretization effort (see Fig. 2). Finally, the Van Leer scheme (Van Leer, 1974) using the MUSCL approach with a Min-Mod limiter leads to a second-order accuracy (Fig. 1e), but less accurate than the splitting method (Fig. 1f), because it is more diffusive.

The two most accurate approximations are given by the proposed model (Fig. 1f) and the hybrid method (Fig. 1d). Nevertheless, the hybrid method is designed for piecewise constant velocity function (extended period simulation) and Δt must divide the pipe transit time to benefit from the characteristic ascent step the best. This method is cumbersome with continuously varying velocity close to zero as demonstrated with the same boundary condition in a single pipe but with $u(t) = cos(t)$ in Figure 2. The substantially better performance of the Splitting-TVD method is evident especially for small dimensionless δx.

Sensitivity and Uncertainty

Sensitivity analysis permits the identification of physical properties that can not be precisely estimated. It gives the most sensitive nodes where it would be most profitable to perform the necessary measures for calibration.

Three main approaches have been used for sensitivity analysis: finite differences, automatic differentiation and sensitivity equations. The finite difference techniques

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that can be used with a large number of commercial software to approximate the sensitivity are easy to implement but they suffer from a lack of accuracy. Automatic differentiation (AD) is a family of techniques for computing the derivatives of a function defined by a computer program. Even though this method is accurate and fast, it produces lengthy and complex computer codes. In this paper, sensitivity equations are considered because they give the most accurate results (Kapelan, 2002).

They are derived from the direct problem. Let N_a be the number of parameters and a_j the jth model parameter, the main problem is to find C_{a_j} for each pipe such as:

$$\begin{cases} \partial_t C_{a_j} + u(t)\partial_x C_{a_j} + \partial_{a_j}(kC^\alpha) = 0, \\ C_{a_j}(0,x) = 0, \quad \forall x \in \mathbb{R}^+ \\ C_{a_j}(t,0) = 0, \quad \forall t \geq 0, \end{cases} \tag{18}$$

where $C_{a_j} = \dfrac{\partial C}{\partial a_j}$ is the derivative of C with respect to a_j, C being the solution of the original problem (Eq. (1)). The parameters considered in this paper are: the overall decay coefficient k and the reaction order α.

Usually a constant k is assigned to the pipes made of the same material with the same age and diameter. So, to decrease the dimension of the problem relative to k, we group the decay coefficients, $\mathbf{K} = (\mathbf{K}_1, .., \mathbf{K}_{n_c})$ with n_c the number of class. To simplify the presentation of the problem, the same order of reaction term is assumed for all the pipes.

Thus, $n_c + 1$ Eq. (18), one for each parameter, can be written as follows for pipe i:

$$\begin{cases} \partial_t C_{\mathbf{K}_j} + u(t)\partial_x C_{\mathbf{K}_j} + \mathbf{K}_i \alpha C^{\alpha-1} C_{\mathbf{K}_j} + C^\alpha \delta_{ij} = 0, \quad j \leq n_c, \\ \partial_t C_\alpha + u(t)\partial_x C_\alpha + \mathbf{K}_i \alpha C^{\alpha-1} C_\alpha + \mathbf{K}_i C^\alpha \ln C = 0, \\ C_{\mathbf{K}_j}(0,x) = 0, \quad C_\alpha(0,x) = 0, \quad \forall x \in \mathbb{R}^+, \\ C_{\mathbf{K}_j}(t,0) = 0, \quad C_\alpha(t,0) = 0, \quad \forall t \geq 0, \end{cases} \tag{19}$$

where $C_{\mathbf{K}_j} = \dfrac{\partial C}{\partial \mathbf{K}_j}$ and $C_\alpha = \dfrac{\partial C}{\partial \alpha}$ are the sensitivity of the concentration with respect to the class K_j and α respectively.

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The time splitting technique is applied to the sensitivity equations:

$$\begin{cases} \partial_t C_{a_j}(t,x) + \big[u(t)\partial_x + \mathrm{B}\big] C_{a_j}(t,x) + f(t,x) = 0, \\ C_{a_j}(t,0) = C_0(t), \end{cases} \tag{20}$$

where f is a source term and $\mathrm{B}(t,x)$ a linear operator. An inhomogeneous, non autonomous linear ODE with variable coefficients is to be solved. Let $\mathbf{R}$ denote the solution of the homogeneous equations. To preserve second-order accuracy in the general case, the Duhamel formula is written to provide the exact solution of (20):

$$C_{a_j}(t+\delta t,.) = \mathbf{R}(u(t)\partial_x + \mathrm{B}, t+\delta t, t) C_{a_j}(t,.) + \int_t^{t+\delta t} \mathbf{R}(u(t)\partial_x + \mathrm{B}, t+\delta t, s) f(s) ds.$$

Trapezoidal integration gives:

$$\begin{aligned} C_{a_j}(t+\delta t,.) &\approx \mathbf{R}(u(t)\partial_x + \mathrm{B}, t+\delta t, t) C_{a_j}(t,.) + \frac{1}{2}\delta t \Big[\mathbf{R}(u(t)\partial_x + \mathrm{B}, t+\delta t, t) f(t) + f(t+\delta t)\Big], \\ &\approx \mathbf{R}(u(t)\partial_x + \mathrm{B}, t+\delta t, t)\big[C_{a_j}(t,.) + \frac{1}{2}\delta t f(t)\big] + \frac{1}{2}\delta t f(t+\delta t), \end{aligned}$$

with a local error of $\mathcal{O}(\delta t^3)$.

Application of Strang's splitting formula (see Eq. 6) results in:

$$\mathbf{R}(u(t)\partial_x + \mathrm{B}, t+\delta t, t) = \mathbf{R}(\mathrm{B}, t+\frac{\delta t}{2}, t)\mathbf{R}(u(t)\partial_x, t+\delta t, t)\mathbf{R}(\mathrm{B}, t+\frac{\delta t}{2}, t) + \mathcal{O}(\delta t^3).$$

Finally the solution is written as:

$$C_{a_j}(t+\delta t,.) \approx \mathbf{R}(\mathrm{B}, t+\frac{\delta t}{2}, t)\mathbf{R}(u(t)\partial_x, t+\delta t, t)\mathbf{R}(\mathrm{B}, t+\frac{\delta t}{2}, t)\big[C_{a_j}(t,.) + \frac{1}{2}\delta t f(t)\big] + \frac{1}{2}\delta t f(t+\delta t). \tag{21}$$

where the second-order accuracy has been maintained.

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Global scheme

The problem allowing the simultaneous solution of the water quality and the sensitivity equations on a network may now be formulated. With the time splitting method, the solving over the interval of $[0, \delta t]$ is performed in three steps.

First reaction and source terms equations are solved for a half time step:

$$\begin{cases} \partial_t C^* + \mathbf{K}_i C^{*\alpha} = 0, & C^*(0) = C_0 \\ \partial_t C^*_{\mathbf{K}_j} + \mathbf{K}_i \alpha C^{*\alpha-1} C^*_{\mathbf{K}_j} + C^{*\alpha}\delta_{ij} = 0 \quad j \leq N_{cl}, & C^*_{\mathbf{K}_j}(0) = C_{\mathbf{K}_j}(0) + \frac{\delta t}{2} f_1(0,x) \\ \partial_t C^*_\alpha + \mathbf{K}_i \alpha C^{*\alpha-1} C^*_\alpha + \mathbf{K}_i C^{*\alpha} \ln C^* = 0, & C^*_\alpha(0) = C_\alpha(0) + \frac{\delta t}{2} f_2(0,x) \\ \partial_t A^* - 1 = 0, & A^*(0) = A_0 \end{cases} \tag{22}$$

Then, the second step is devoted to the advection for a time step:

$$\begin{cases} \partial_t C^\bullet + u(t)\partial_x C^\bullet = 0, & C^\bullet(0) = C^*(\frac{\delta t}{2}) \\ \partial_t C^\bullet_{\mathbf{K}_j} + u(t)\partial_x C^\bullet_{\mathbf{K}_j} = 0, & C^\bullet_{\mathbf{K}_j}(0) = C^*_{\mathbf{K}_j}(\frac{\delta t}{2}) \\ \partial_t C^\bullet_\alpha + u(t)\partial_x C^\bullet_\alpha = 0, & C^\bullet_\alpha(0) = C^*_\alpha(\frac{\delta t}{2}) \\ \partial_t A^\bullet + u(t)\partial_x A^\bullet = 0, & A^\bullet(0) = A^*(\frac{\delta t}{2}) \\ \partial_t S + u(t)\partial_x S = 0, & S(0) = S_0 \end{cases} \tag{23}$$

Taking part of the second step the improved reaction and source term equations are solved again for a half time step:

$$\begin{cases} \partial_t C^\diamond + \mathbf{K}_i C^{\diamond\alpha} = 0, & C^\diamond(0) = C^\bullet(\delta t) \\ \partial_t C^\diamond_{\mathbf{K}_j} + \mathbf{K}_i \alpha C^{\diamond\alpha-1} C^\diamond_{\mathbf{K}_j} + C^{\diamond\alpha}\delta_{ij} = 0 \quad j \leq N_{cl}, & C^\diamond_{\mathbf{K}_j}(0) = C^\bullet_k(\delta t) \\ \partial_t C^\diamond_\alpha + \mathbf{K}_i \alpha C^{\diamond\alpha-1} C^\diamond_\alpha + \mathbf{K}_i C^{\diamond\alpha} \ln C^\diamond = 0, & C^\diamond_\alpha(0) = C^\bullet_\alpha(\delta t) \\ \partial_t A^\diamond - 1 = 0, & A^\diamond(0) = A^\bullet(\delta t) \end{cases} \tag{24}$$

with $f_1(t,x) = C^\alpha \delta_{ij}$; $f_2(t,x) = \mathbf{K}_i C^\alpha \ln C$.

$C^\diamond(\delta t), {C_{\mathbf{K}_j}}^\diamond(\delta t) + \frac{\delta t}{2} f_1(\delta t, x), {C_\alpha}^\diamond(\delta t) + \frac{\delta t}{2} f_2(\delta t, x), S(\delta t)$, $A^\diamond(\delta t)$ are the final values for the disinfectant concentration (C), the sensitivity coefficients $(C_{\mathbf{K}_j}, C_\alpha)$ with respect

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to $\mathbf{K}_j$ and α, the source tracing (S) and the residence time (A) respectively. In order to take into account a network with several pipes, nodal mixing equations (Eq. 4 and 5) need to be solved for each variable of interest.

With this formulation the numerical implementation of the global scheme is simple. Only two main functions are needed, one to solve the reaction and source terms with an ODE solver and the other using the TDV scheme to handle the advection term.

Results and discussion

The applicability of the proposed time Splitting-TVD technique is tested in this section, using three different pipe networks. First, a simple case study is considered in which the sensitivity solutions are easily verifiable. Then, a comparison with a commercial software is performed using the benchmark network in the *EPANET 2* user's manual. Finally, a validation study for a network in France is performed, showing the impact and the benefit of sensitivity analysis.

A simple case study

The simple test network found in (Rossman and Boulos, 1996) and shown in figure 3 is first considered. It is possible to compute analytical solutions because of its simplicity and this is a good test to check the ability to track sharp concentration fronts accurately. It consists of six nodes (three reservoirs and three junction nodes) and six links. The linear problem with first-order reaction is considered ($\alpha = 1$) with a class of constant reaction coefficient: $k = \mathbf{K}_1 = 2.4d^{-1}$ (per day/unit). Reactive Chemical tracers as constituent concentrations of 200 mg/L, 300 mg/L and 100 mg/L are assigned to reservoirs R1, R2, R3 respectively and hydraulic data are given in table 1. The time step is $\delta t = 300s$ and δx, the space step is selected to meet the CFL conditions. This study was originally tested in (Rossman and Boulos, 1996) for a conservative tracer; in this work we assume a first-order reaction in order to calculate the sensitivity to the reaction coefficient.

The results for C, the tracer concentration, (see Eq. 22, 23, 24) are compared with

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those obtained with *Porteau* (Porteau, 2009). Figure 4 shows no difference in concentration calculated by the proposed model and by the *Porteau* software at Node 1. The results for the sensitivities with respect to the overall decay constant C_k and reaction order C_α (see Eq. 19) are shown in Fig. 5. Because of the large C concentration value in R2, node 3 is the most sensitive node with respect to k and α. The source concentration and transit time are very influential parameters in sensitivity calculations. If the concentration for all the sources is equal to 100 mg/L and the same k ($2.4d^{-1}$) is applied, node 1 will be the most sensitive with respect to k and α. To our knowledge the sensitivity is not calculated in any water modeling software. So, this test is important as an analytical solution is available for this problem.
In the linear case, the sensitivity with respect to k at node 3 ($C_k(node3)$), is:

$$C_k(t,x) = -(t-t_0)C(t_0,0)e^{-k(t-t_0)}, \tag{25}$$

where $(t-t_0) = \dfrac{L}{u}$ is the residence time (L and u the pipe length and velocity respectively). Thus,

$$C_k(node3) \approx -5482581 \tag{26}$$

In the non-linear case, straight forward computations lead to (Gancel, 2006):

$$C_\alpha(t,x) = C(t,x)\Big[\frac{\ln\left(C(t_0,0)^{1-\alpha} - (1-\alpha)\,k\,(t-t_0)\right)}{(1-\alpha)^2} + \frac{-C(t_0,0)^{1-\alpha}\ln\left(C(t_0,0)\right) + k\,(t-t_0)}{(1-\alpha)\left(C(t_0,0)^{1-\alpha} - (1-\alpha)\,k\,(t-t_0)\right)}\Big].$$

Thus,

$$\lim_{\alpha\to 1} C_\alpha(t,x) = (C(t_0,0)e^{-k(t-t_0)})\Big[\ln\left(C(t_0,0)\right)k\,(t_0-t) + 1/2\,k^2\,(t-t_0)^2\Big] \tag{27}$$

yields to

$$C_\alpha(node3) \approx -84.82.$$

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$C_k(node3)$ and $C_\alpha(node3)$ verify exactly the result of the sensitivity given by figure 5.

Brushy Plains Network

The next considered network, the Brushy plain network (Fig 6) taken from the EPANET2 manual, is more complex. In this section comparisons are made both with *Porteau* and with *EPANET 2*. The network is composed of 41 pipes, 35 junction nodes, one storage tank and one pumping station. Chlorine transport is modeled assuming a first-order decay ($\alpha = 1$) and a constant decay coefficient: $k = 2.4d^{-1}$. The time step is chosen equal to $\delta t = 1min$, that is small enough to obtain an accurate solution.

In figure 7, the concentration results obtained by the new Splitting-TVD solver are compared to the values obtained by *EPANET 2* and *Porteau*. Like the previous example, no significant difference appears. Figure 8 shows the sensitivity for each node. At each of them there is a sensitivity vector $C_k(t)$ and $C_\alpha(t)$. To compare them better, the relative L^1 norm of each vector is plotted as follows:

$$\begin{aligned} C^*_{k \text{ or } \alpha}(N) &= \delta t \sum_t \left| C_{k \text{ or } \alpha}(t) \right| \\ C_{k \text{ or } \alpha}(N) &= \frac{C^*_{k \text{ or } \alpha}(N)}{\max\limits_N C^*_{k \text{ or } \alpha}(N)} \end{aligned}$$

where N is the node number.

The two most sensitive nodes with respect to k are nodes 8 and 19 and with respect to α are nodes 8 and the tank. The greatest impact of a small change in α or k is located at these nodes. Thus, the important positions to measure concentrations, describing the network behavior are nodes 8, 19 and the tank.

In this example, *EPANET 2* requires 12s (for each parameter computation) with $\delta t = 30s$ compared to 1 min 27s for Splitting-TVD solver and 2 min 05s for *Porteau*. However, the proposed model provides seven results at the same time: disinfectant concentration (C), minimum, maximum and average residence time (A), the trace of bacteria introduced to a node or source tracing (S), and two sensitivity results(C_k

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& C_α) with respect to α and k (*Porteau* gives also five results at the same time), whereas *EPANET 2* provides only three results that are given separately: disinfectant concentration, average residence time, the trace of bacteria introduced to a node or source tracing. The program needs to be run again separately to get any of these results.

Sensitivity analysis impact on a real network

The main benefit of a sensitivity analysis lies in the parameter calibration. Our method is the only one among the compared techniques, to be able to perform such an analysis simultaneously. The knowledge of the sensitivity solution with respect to the parameters is useful to determine where future measurements should be made. The direct impact of the choice of measurements is emphasized; accurate data set increases the conditioning of our fitting methods.

Figure 9 shows a real network in France composed of a tank, 63 nodes and 68 pipes. A sensitivity analysis is performed and the three most sensitive nodes as well as the three least sensitive ones are selected (Fig. 9). These nodes are used for the calibration of kinetic parameters k and α.

The kinetic parameters are estimated from a least-squares fit to measurements.

Figure 10 shows the dimensionless objective function of this minimization problem: with $\hat{x} \in \mathbb{R}^p \ / \ \forall x \in \mathbb{R}^p, g(\hat{x}) \leq g(x)$ where

$$g(x) = \frac{1}{2}\left|\left|C(x) - C^{mes}\right|\right|_2^2, \quad x = (\mathbf{K}_1, ..., \mathbf{K}_{n_c}, \alpha), \tag{28}$$

where C^{mes} is the concentration measured in the network and $p = n_c + 1$ the number of unknown parameters.

The fitting of kinetic parameters with sensitive nodes converges to the solution with 12 iterations. For other nodes more than 100 iterations are necessary. The use of less sensitive nodes has a direct impact on the Levenberg-Marquardt technique. This descent method derives benefit from the Jacobian matrix (sensitivity matrix) or first-

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order information as derivatives. With insensitive nodes, the ill-conditioning of the matrix decreases the convergence rate of the solution. Figure 10 shows that when the convergence is more difficult, it needs many more iterations.

The impact is very important on this real simple network. On a more complex network composed of valves, pumps or other hydraulic components, accurate measurements are difficult, mainly due to the complex hydraulic flow. Large measurement errors appear, leading to non-realistic solutions. Then measurement error importance with exact sensitivity coefficients help to calculate confidence intervals to emphasize the calibrated parameter precision; see developments in (Piller, 1995).

Conclusion

Constituent concentration, residence time and source tracking at network nodes of a Water Distribution System are quality indicators that are usually predicted in academic and commercial hydraulic modeling software. The main challenge is to determine the model parameters that best match field data. In this paper, solutions for exact sensitivities or derivatives of quality indicators are proposed with regards to the reaction parameters in order to improve the inverse or calibration problem.

Sensitivity equations are derived from the direct transport-reaction problem. For each pipe, the formulation is a one-dimensional hyperbolic Partial Differential Equation with a similar advection and reaction structure to the original problem. Solving economies are therefore possible.

One extension of usual practice is to consider a pipe velocity that is continuously time-dependant. For example in *EPANET*, that is a Lagrangian hydraulic code, known and used worldwide, the velocity is a stepwise constant function. This novel extension is a strong constraint that requires a new specific solving algorithm. The method proposed here consists of separating the advection operator from the reaction part and source term. A three-step splitting method of second-order is then used. This method is more flexible with respect to the choice of the advection scheme and is applied to both the sensitivity equations and the direct problem as these equations

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have the same structure. A Eulerian scheme, using the TVD technique, is chosen to solve the advection process. Discontinuous solutions can be computed without oscillations. Validation of the scheme and the numerical accuracy analysis is performed and compared to several other standard techniques. An explicit fourth-order Runge-Kutta scheme is used to achieve a good approximation of the reaction and source terms.

Numerical results are presented on three networks. Firstly, for a simple case study, solution accuracy is proven and compared with an analytical solution. A reactive tracer is injected in three sources and both the constituent concentration and the associated sensitivities with regards to reaction constant and order coefficients are analyzed at two different nodal points. The predicted values perfectly match the exact solutions. Secondly, a small but more complex network taken from the *EPANET* manual is simulated. These tests show that *EPANET 2* Lagrangian code is the fastest compared to both Eulerian methods and the Splitting-TVD scheme has a higher speed than *Porteau* (Eulerian). Nevertheless, the proposed model provides seven results at the same time, compared to five with *Porteau* and only one with *EPANET 2*. So, relative CPU time for each quality indicator calculation is the same for *EPANET 2* and the new proposed method. Selection of potential chlorine concentration measurements is also illustrated from the importance of relative sensitivity coefficients. Finally, the actual importance and necessity of accurate sensitivity assessment are shown on a real WDS through a calibration process. Selecting meters that are more sensitive may drastically improve the conditioning of the calibration problem. If the solving algorithm is a gradient type and uses exact derivatives or sensitivities, the number of iterations is considerably reduced. Finally, confidence intervals for parameters may be deduced from error measurement distribution and sensitivity assessments.

Future research is recommended to assess the possibility of simultaneous calibration of hydraulic model parameters such as roughness and nodal demand.

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Notation

The following principal symbols are used in this paper:

C = constituent concentration in a pipe; $C = C(t, x)$;

u = velocity in pipe; $u = u(t)$;

f = reaction function; $f(C)$

k = overall coefficient of reaction;

α = order of reaction;

q = flow in the pipe; $q = q(t)$;

S_{c_i} = constant pipe area;

N_{in} = set of pipes that are incident to node n;

N_{out} = set of pipe taking water out of the tank;

C_T = constituent concentration in the tank;

V_T = water volume in the tank;

f_T = reaction function in the tank;

C_i^n = approximate value at the point $(n\delta t, i\delta x)$;

$\mathbf{K}_j$ = jth of class of decay coefficient;

$C_{\mathbf{K}_j}$ = sensitivity of the concentration with respect to the class $\mathbf{K}_j$;

C_α = sensitivity of the concentration with respect to α;

A = residence time; $A = A(t, x)$;

S = source tracing; $S = S(t, x)$;

g = objective function;

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Table. 1: Hydraulic data

Pipe	Diameter, mm	Length, m	Roughness(HW coefficient)	Velocity, m/s	Flow
tank R1 to node 1	203	3050	116	1.75	56.54
node 1 to node 3	152	1830	116	-0.24	-4.31
node 1 to node 2	152	3660	116	-0.12	-2.25
tank R2 to node 3	203	3355	116	1.74	56.18
node 3 to node 2	152	6100	116	0.08	1.37
node 2 to tank R3	203	1525	116	-2.37	-76.69

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List of figure captions

Figure 1. Solution at fixed t for different schemes : Holly-Preissmann scheme (a), Lax-Wendroff scheme (b), θ-scheme (c), hybrid scheme (d), Van Leer scheme (e), Splitting-TVD scheme (f).

Figure 2. Hybrid discretization effort with $u(t) = cos(t)$

Figure 3. Test network

Figure 4. Concentration at node 1

Figure 5. Result of sensitivity with respect to k and α in the network

Figure 6. Brushy Plains Network

Figure 7. Result of concentration in chlorine at the tank

Figure 8. Sensitivity with respect to k and α for each node

Figure 9. Real network (France)

Figure 10. Objective function result

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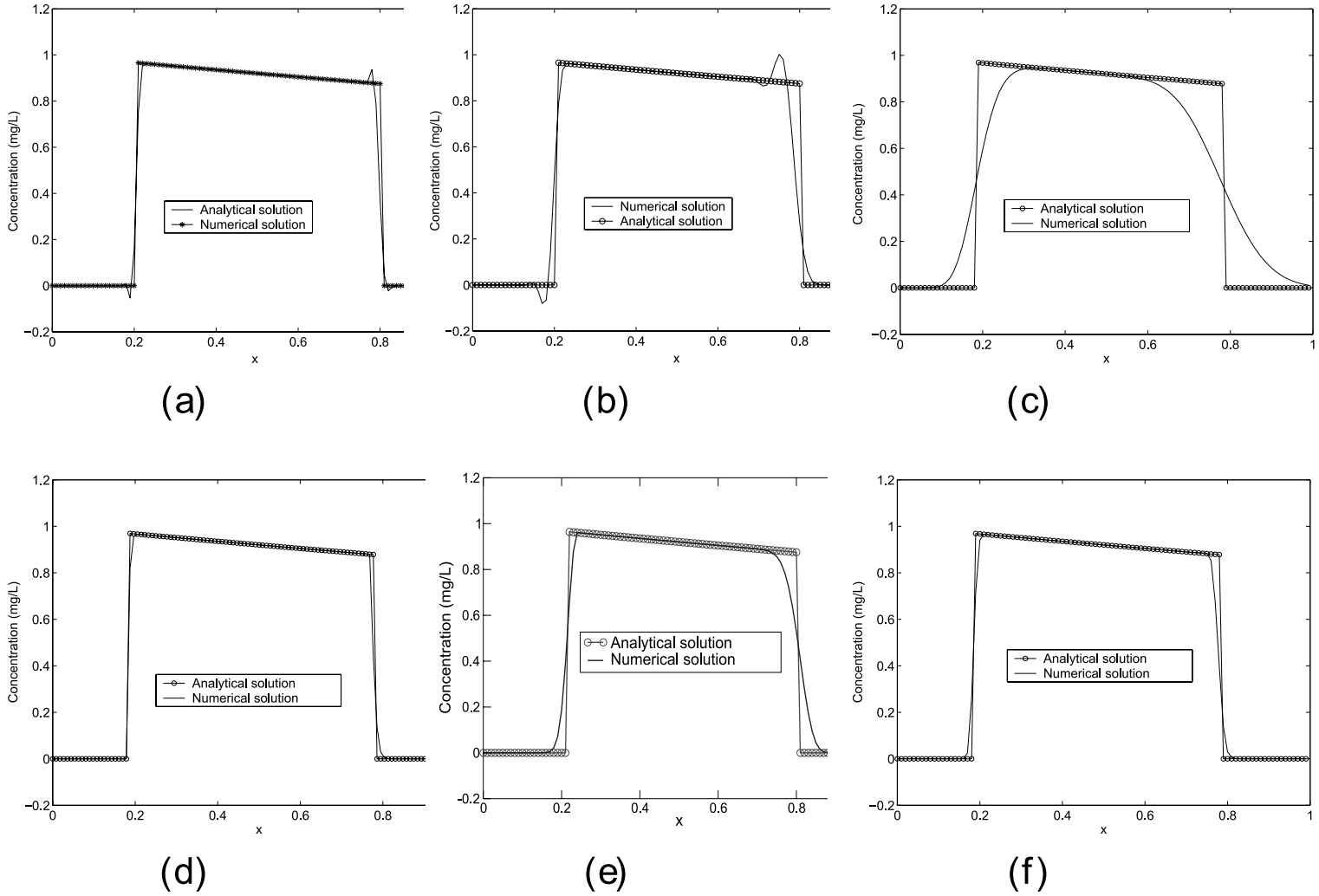

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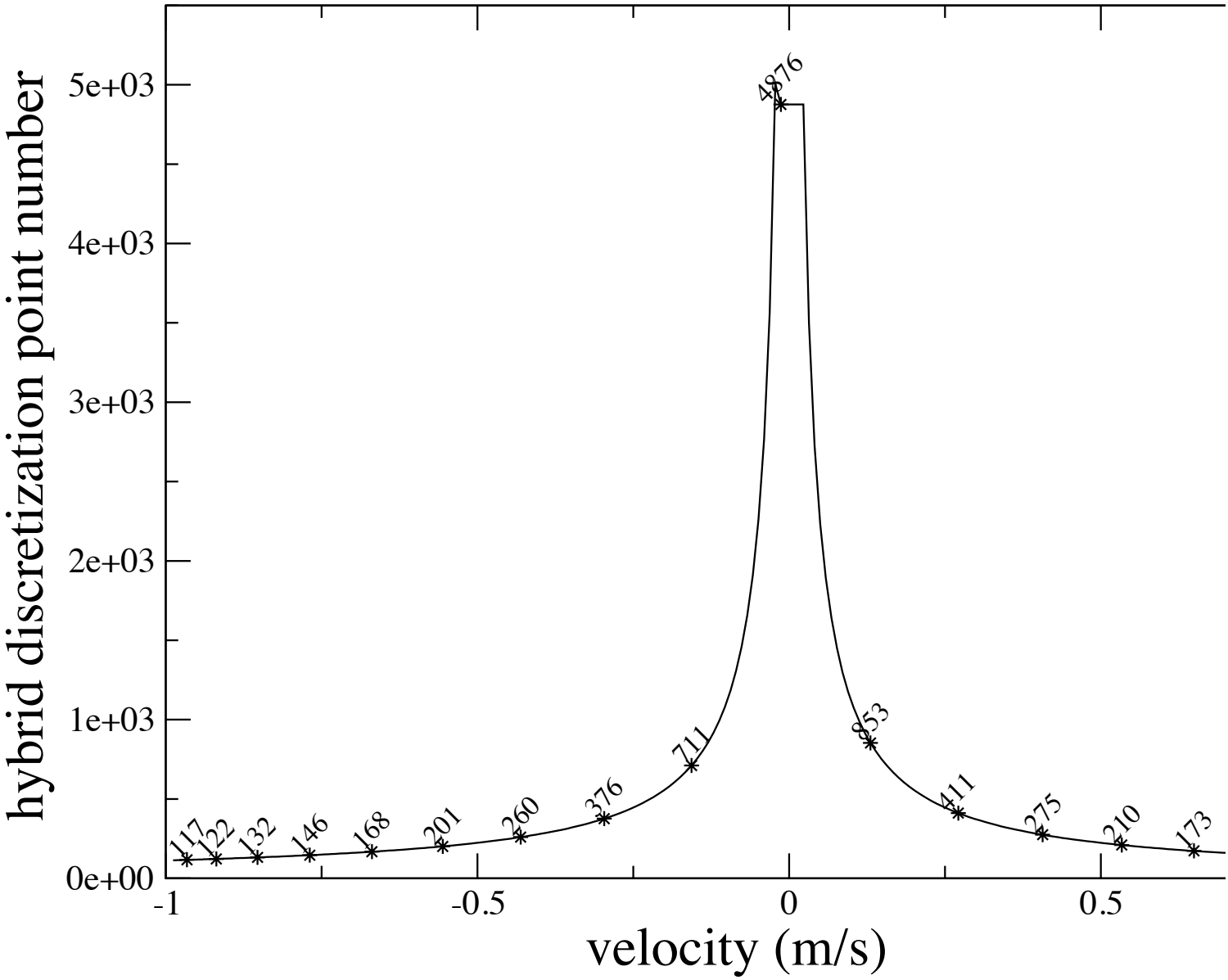

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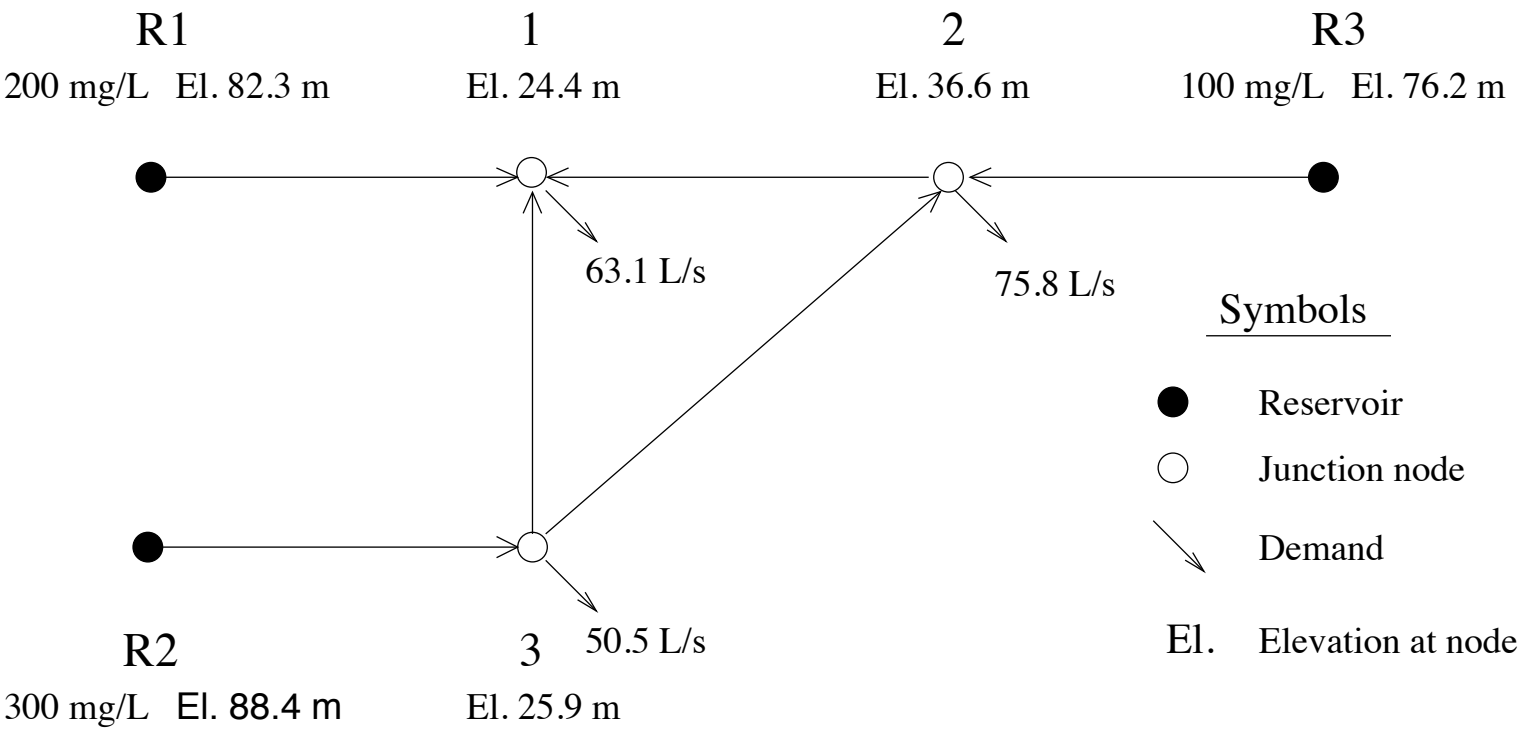

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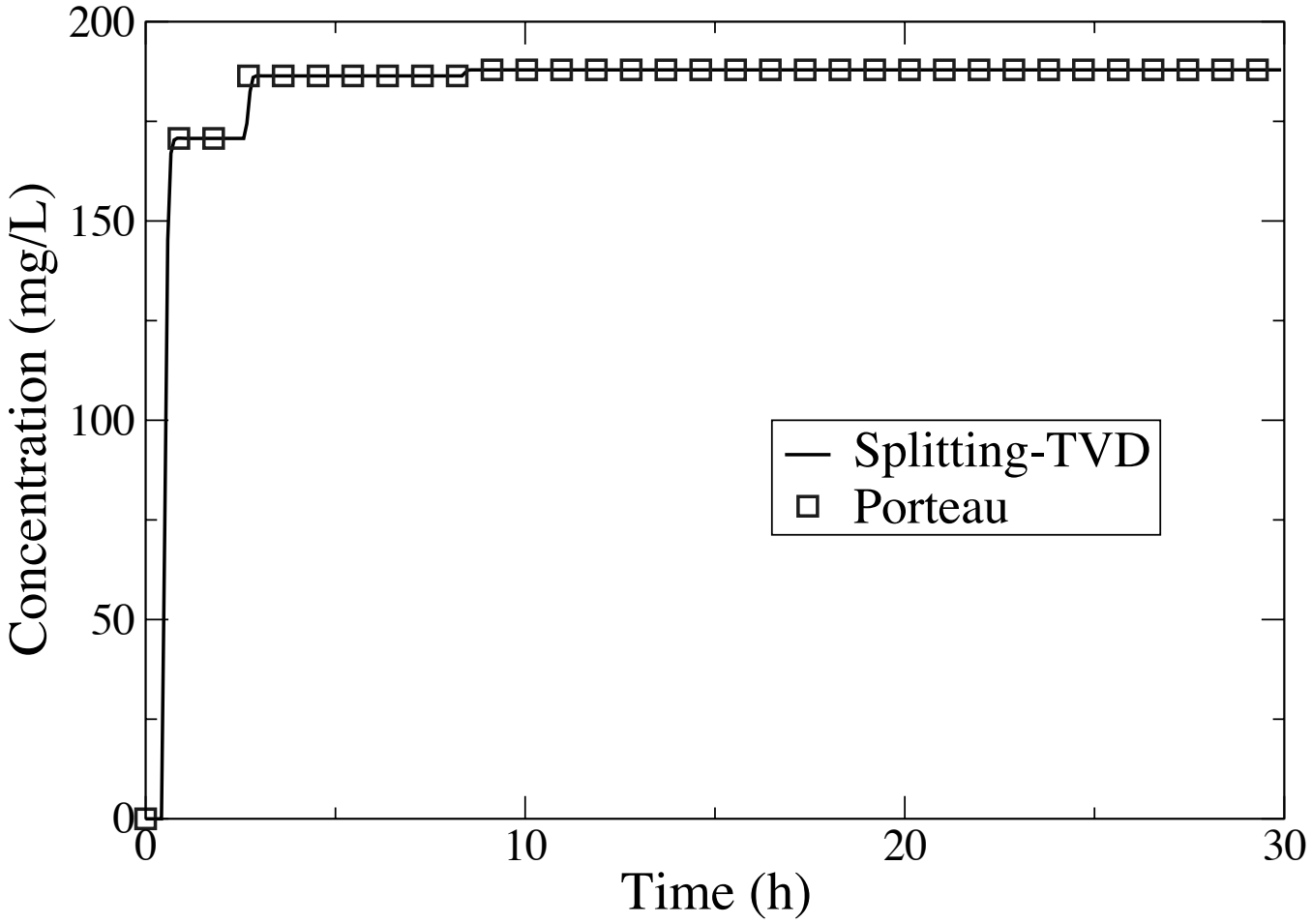

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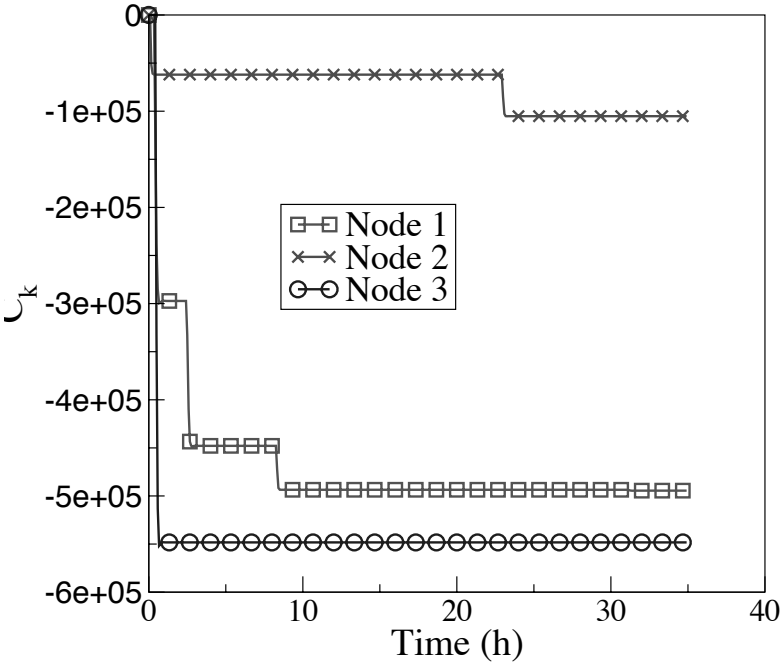

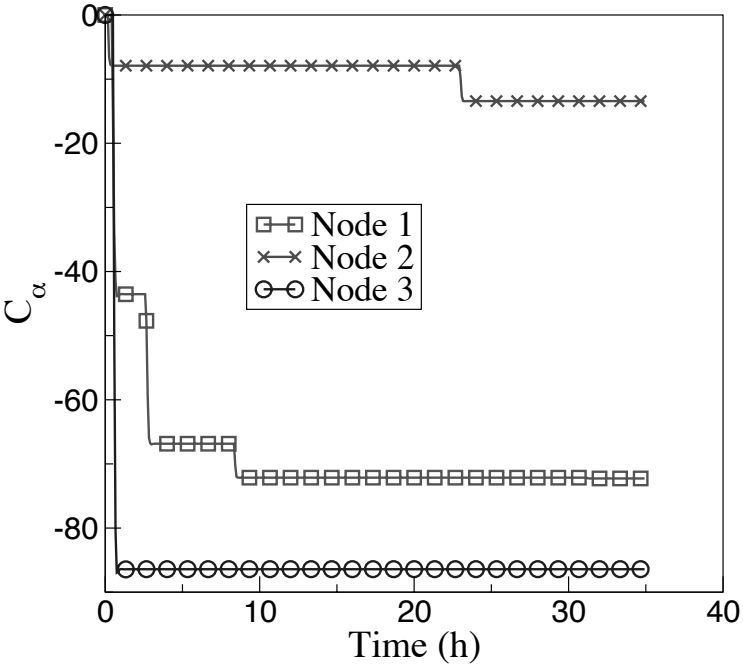

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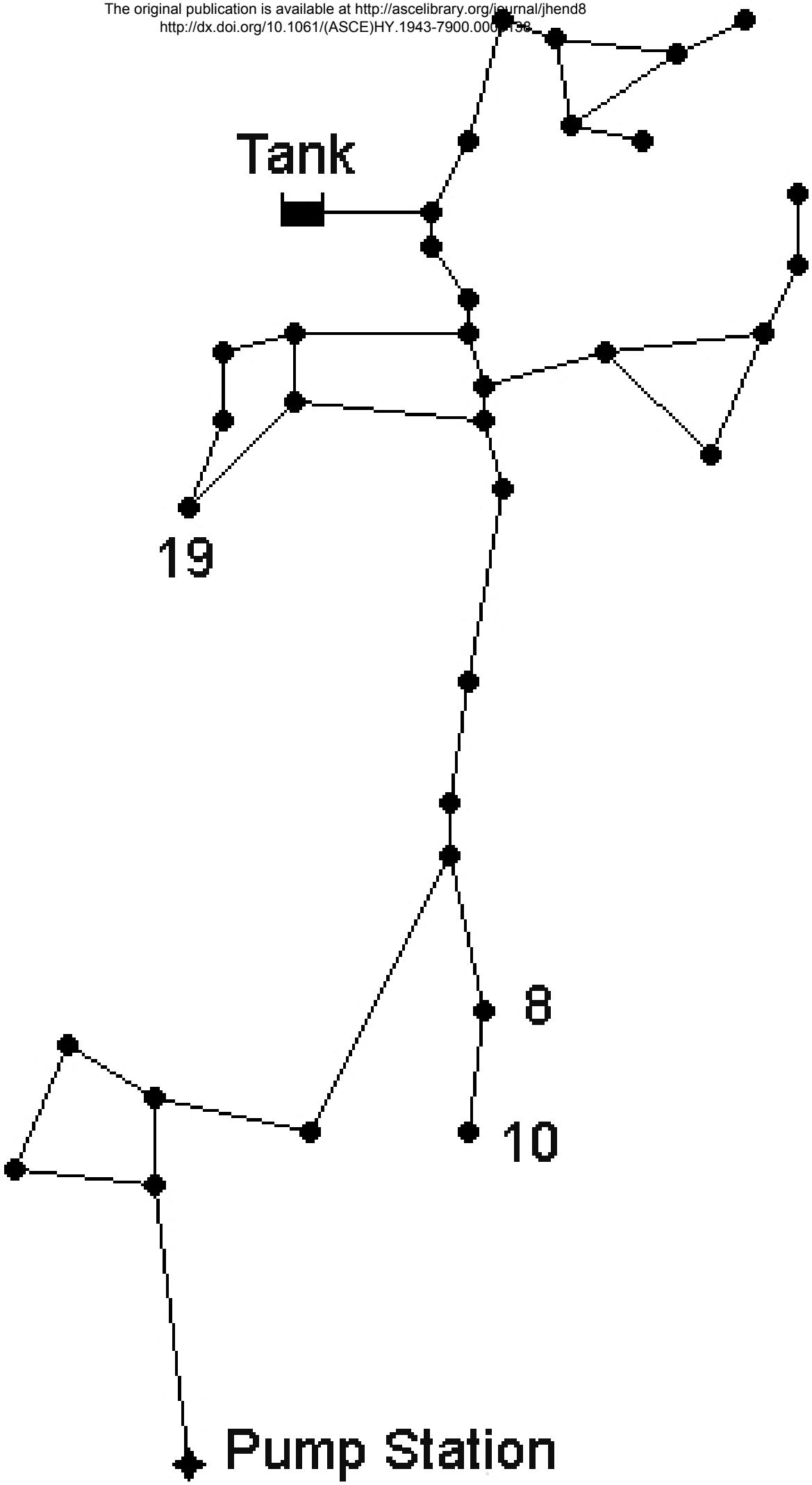

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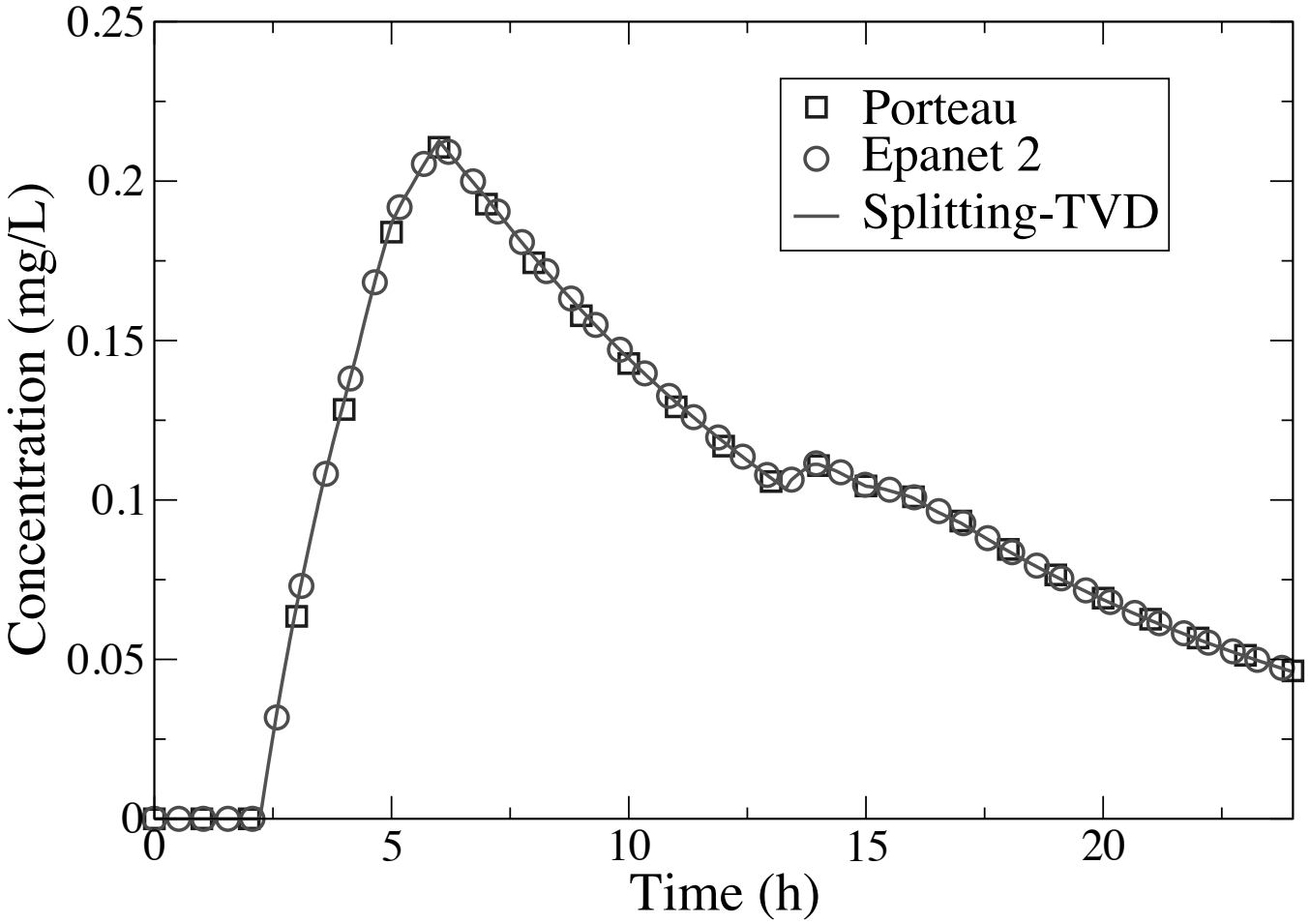

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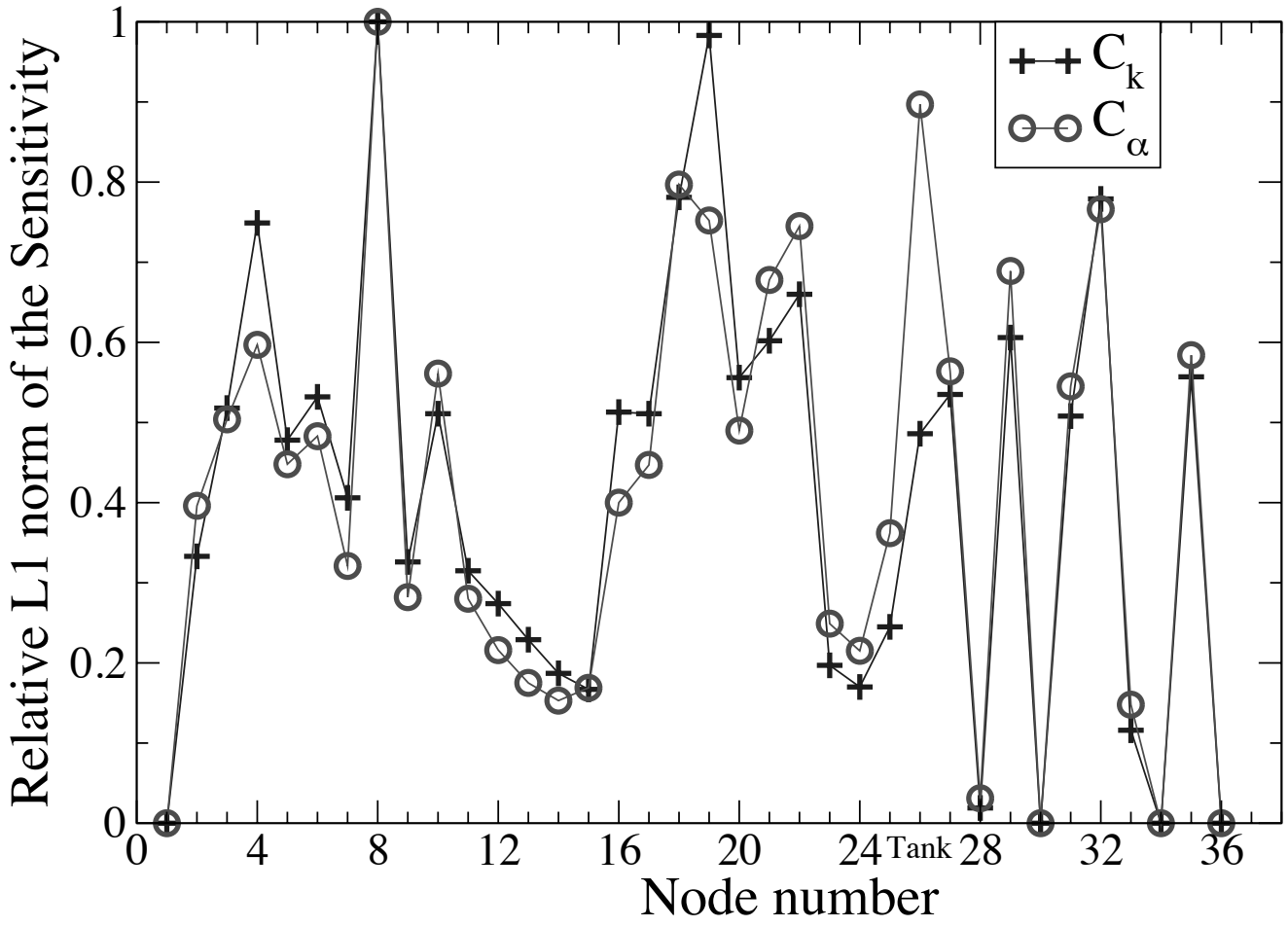

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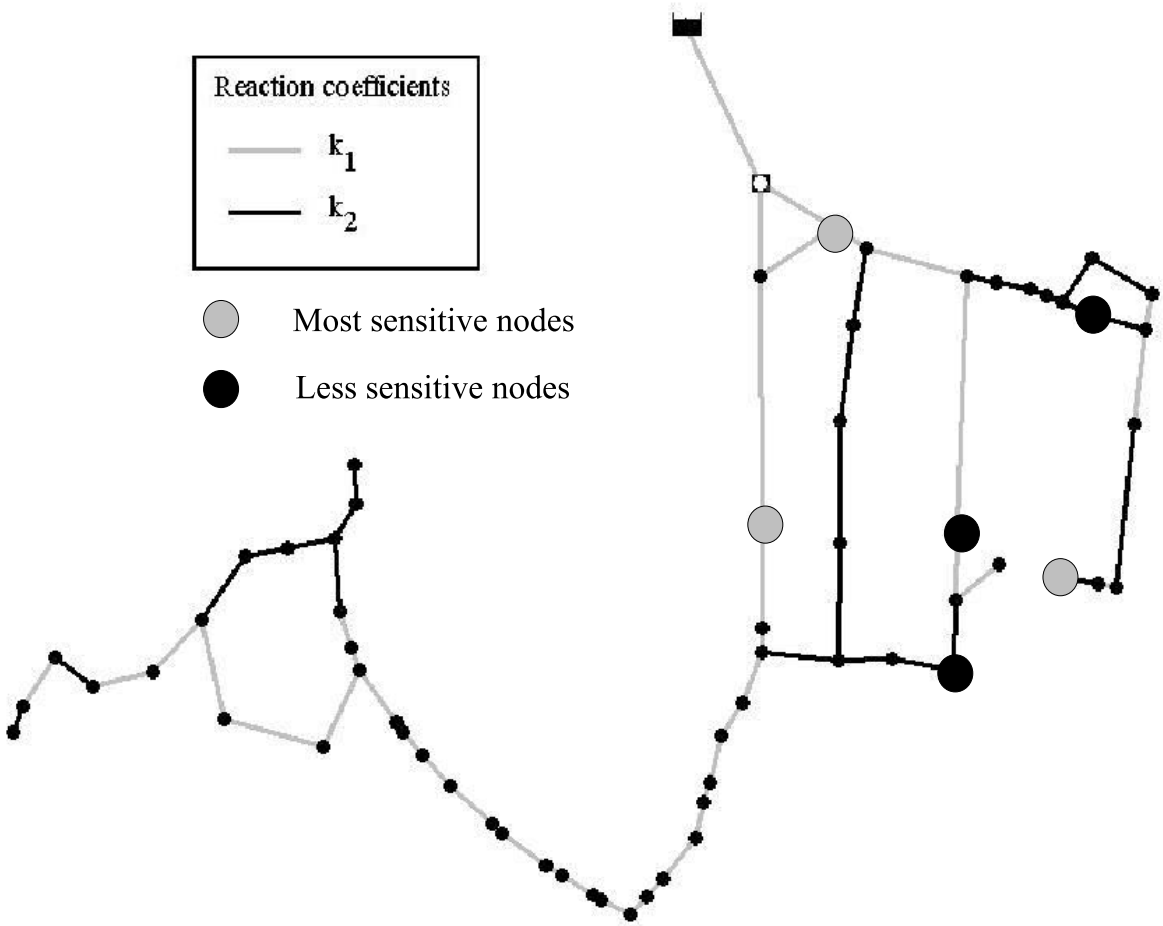
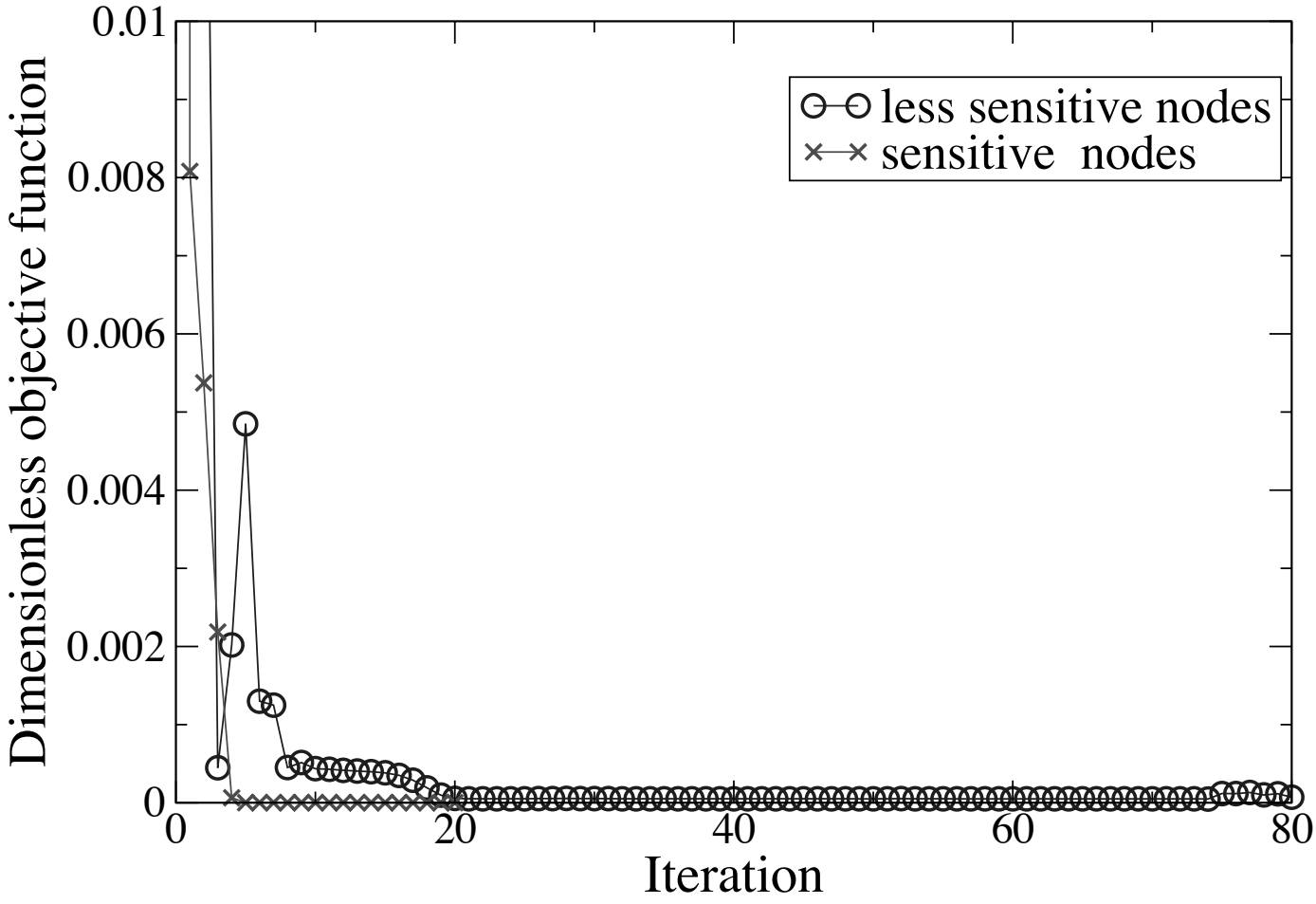
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