Computational study and sensitivity analysis for quality modeling in Water Distribution Systems.

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Abstract:

In this paper, direct water quality modelling and the associated unsteady sensitivity equations, are solved in Water Distribution Systems (WDS). A new solution algorithm is proposed, based on a time splitting method to separate and solve efficiently each phenomenon such as advection and chemical reaction. This numerical approach allows a 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 a global sensitivity analysis of the system and its efficiency is illustrated on two pipe networks. The importance of the sensitivity analysis is shown as part of a fitting process on a real network.

CE Database subject headings: Sensitivity Equations, Water Quality, TVD

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scheme, Water Distribution Network, Splitting Method.

Introduction

The quality of water supplied by a distribution network is assessed by means of various indicators. In particular, residence times, source tracking and disinfectant concentration are among the most significant ones.

These indicators can be obtained by solving mathematical models that depend on estimates of physical parameters. For example, kinetic parameters characterizing disinfection (bulk and wall) reactions are rarely known with any pressure because of these uncertainties, and to have a better calibration, it is important to analyse how the solution derived from the model would change if the values assigned to the parameters are varied. This process is referred to the sensitivity analysis. It was successfully applied for hydraulic sensitivity purpose (Bargiela and Hainsworth, 1989; Kapelan, 2002), for hydraulic calibration (Piller, 1995) and for hydraulic and water quality sampling design (Bush and Uber, 1998; Chesneau et al., 2003; Piller et al., 1999).

In most previous works, finite difference methods were used to compute sensitivity gradients. 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 of the direct problem, facilitating their simultaneous solution with the water quality problem.

In this paper we present an new approach to solve this coupled problem. This is a no-linear problem impossible to solve exactly, because the velocities may vary with time, needing an approximation approach. The technique proposed here is designed to reduce sensibly the approximation errors.

The method is "time splitting". The advantage of this approach is the use of specific numerical solver for each physical phenomenon (Sportisse, 2000). Each operator: advection, chemical reaction, is considered separately, with a special attention to the advection modelling. Because the physical phenomenon is dominated by the advec-

tion and the chemistry, the diffusive term is not considered in this work. Nevertheless, the technique easily allows to include the diffusion for more complex case studies. This behaviour was already studied by (Islam and Chaudhry, 1998) who used a splitting method to compute the constituent transport in unsteady flows, including the 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 smooth variation of concentration fronts. Moreover, using the TVD techniques, should overcome the classical Eulerian schemes oscillations.

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. Sensitivity equations are then derived from the direct problem and the computational algorithms to solve the global model is described. 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 finally a real network, showing the importance of a sensitivity analysis for parameter calibrations.

Water quality in WDS

Water quality modelling consists primarily of predicting disinfectant (chlorine) concentration, residence times and source location. The propagation of these constituents (quality indicators) in a WDS relies on solving in each pipe an advection equation 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 constituent due to transport through a pipe can be described by a one dimensional hyperbolic Partial Differential Equation (PDE) of the form:

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

The boundary condition at $x = 0$ is needed to solve equation 1 for a non-negative velocity field. C denotes the constituent concentration within the pipe and u the cross-sectional averaged pipe flow velocity, only time variable and given by the network hydraulic solution. This velocity is obtained formally using the rigid column equation for slowly varying flows in pipe networks. $f(C)$ is a reaction function describing the transformation of each indicator:

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

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

$$\begin{cases} f(C) = -1, \\ f(C) = 0. \end{cases} \tag{3}$$

Residence time is obtained with the first equation. The second one, can be used for source identification which is very useful for the trace of 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 assumed to be mixed perfectly and instantaneously. At each node, the resulting concentration is therefore the flow-weighted average of the individual concentration of the incoming flows. This average is based

on conservation of mass and has many properties in common with the first Kirchoff law.

At each node, the water mixing involves then a new concentration, age, or source tracking value. For the simple nodes the mass conservation relationship yields:

Ω: a fixed control volume.

ν: outlet unit normal.

Γ: boundary volume Ω.

$\vec{U} : \mathbb{R}^3 \longrightarrow \mathbb{R}^3$: velocity vector.

$q(t)$: The flow in the pipe.

We assume a tank with instantaneous, homogenous and perfect mixing. Taking $C_T(t)$ as the constituent concentration at time t and $f_T(t) = kC_T^{\alpha}$ as the reaction function within the tank, we can write:

$$\frac{d}{dt}\int_{\Omega} C d\Omega + \int_{\partial\Gamma} C\vec{U}.\nu d\Gamma + \int_{\Omega} f(C)_T d\Omega = 0$$

Then, we get :

$$\frac{d(C_T V_T)}{dt} - \sum_{i\in N_{in}} q_i C_i + \sum_{j\in N_{out}} q_j C_T + f(C)_T V_T = 0 \quad \text{with} \int_{\Omega} d\Omega = V_T \quad \text{tank volume}$$

Where, N_{in} and N_{out} correspond to the number of inlet and outlet pipes into and from the tank.

Assuming: $\frac{d(C_T V_T)}{dt} = V_T\frac{dC_T}{dt} + C_T\frac{dV_T}{dt}$ & $\frac{dV_T}{dt} = \sum_{i\in N_{in}} q_i - \sum_{j\in N_{out}} q_j$, we obtain the following system:

$$\begin{cases} \dfrac{dC_T}{dt} = \dfrac{\sum_{i\in N_{in}} q_i(C_{in} - C_T)}{V_T} + \sigma_T \\ C_T(t=0) = C_{T_{t_0}} \\ V_T(t=0) = V_{T_{t_0}} \end{cases} \tag{4}$$

with $V_T = V_{T_{t_0}} + \int_{t_0}^{t} (\sum_{i\in N_{in}} q_i - \sum_{j\in N_{out}} q_j)dt$.

Equation (4) describes the mixing of a constituent within a tank. where q_i is the flow-rate in pipe i and V_T is the water volume inside the tank. For a variable-level

tank, the change in concentration, residence time, source tracking value can also be determined from mass conservation. Equation (4) assumes that constituents within the tank are completely and instantaneously mixed.

It should be outlined that for a junction node n, the 1D resulting constituent is the flow-weighted average of the incoming ones

$$\begin{cases} C_n(t) = \dfrac{\sum_{i \in N_{in}} q_i C_i(t)}{\sum_{i \in N_{in}} q_i}, \quad q_i = u_i * S_{c_i}, \\ C_n(0) = C_{n_{t_0}}, \end{cases} \tag{5}$$

where $C_i(t)$ is the considered quantity input at node n at time t from pipe i and S_{c_i} the constant pipe area. N_{in} is the set of pipes that are incident to node n.

To summarize, Water quality modelling 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.

Numerical scheme

Various numerical methods for the water quality models have been proposed and a comparison of some of them has been performed in a previous study (Rossman and Boulos, 1996). A new efficient method using a time splitting approach that includes a TVD scheme for solving the advection problem is described in the following.

Time splitting method

The advantage of this approach is the use of a specific numerical solver for each physical phenomenon (e.g., advection and chemical reaction) (Yee, 1988) (Sportisse, 2000) (Islam and Chaudhry, 1998). Islam and Chaudhry, who solved the constituent transport problem using a two step splitting method mentioned that this technique is useful to reduce the numerical diffusion. This method interacts between solving the advection equation with no source terms and an ordinary differential equation (ODE) to model water chemistry. This splitting method allows to use the most

efficient approach for each stage of the procedure, taking advantage of their physical properties and resulting a better numerical accuracy and stability.

In this part we detail the Strang's splitting scheme. We can write equations (1) and (2) stated by:

$$\begin{cases} \partial_t C + u(t)\partial_x C + f(C) = 0 \qquad \text{where} \quad f(C) = kC^\alpha, \\ C(0,x) = C_0(x) \\ C(t,0) = \Psi(t). \end{cases} \tag{6}$$

We denote by $\mathcal{S}^t$ the operator solution of (6) and have: $C(t,.) = (S^t C_0)$.

We split the equation (6) into two ODEs, and get the two following subproblems:

$$\begin{cases} \partial_t w + u(t)\partial_x w = 0, \qquad \forall (t,x) \in \mathbb{R}^+ \times \mathbb{R}, \\ w(0,x) = w_0(x), \end{cases} \tag{7}$$

and we note $w(0,x) = \mathcal{F}^t(w_0)$. Then

$$\begin{cases} \partial_t v + f(v) = 0, \quad \forall (t,x) \in \mathbb{R}^+ \times \mathbb{R} \quad \text{where} \quad f(v) = kv^\alpha, \\ v(0,x) = v_0(x) \end{cases} \tag{8}$$

then we write $v(t,.) = \mathcal{X}^t(v_0)$.

This ODE is solved using an explicit fourth order Runge Kutta method. This scheme involves satisfactory stability and accuracy properties, necessary to take into account the reaction effects.

A Strang approximation formula (Strang, 1963; Strang, 1968), of the equation (6) allows to write for t small enough:

$$\mathcal{S}_1^t C_0 = \mathcal{F}^{t/2}(\mathcal{X}^t(\mathcal{F}^{t/2}(C_0))), \tag{9}$$

then, we denote

$$\mathcal{S}_1^t = \mathcal{F}^{t/2}\mathcal{X}^t\mathcal{F}^{t/2}. \tag{10}$$

We can change the sequence of successive integration for $\mathcal{F}^t$ and $\mathcal{X}^t$: $\mathcal{S}_2^t = \mathcal{X}^{t/2}\mathcal{F}^t\mathcal{X}^{t/2}$ using a Strang formula which starts and ends with reaction parts. It has been validated by numerical studies (Descombes and Massot, 2004). Also, in order to achieve

an efficient computational implementation, a sequential solution of the above equations is needed.

We can examine the error in this scheme by Taylor series, that results in the following error expression: ($||C(t,.)-S_1(t)||_{L^2} = \mathcal{O}(\delta t^3)$), giving the 2^{nd} order for the splitting, using the Strang Formula.
The two processes, advection and reaction being separated, different schemes exist to approximate each subproblem, as described in the following section.
The ODE's for the reaction subproblem are solved with an explicit fourth order Runge Kutta method. In this paper, a TVD scheme is chosen for the advection subproblem, because it preserves positivity (L^∞-stable condition) with minimal numerical diffusion.

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 that depends only on time.

Let δx and δt be the space and time step respectively and C_i^n is 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:

$$C_i^{n+1} = \gamma_1 C_{i+1}^n + \gamma_0 C_i^n + \gamma_{-1} C_{i-1}^n + \gamma_{-2} C_{i-2}^n, \tag{11}$$

where the α_k are chosen such that the error

$$e = C(t+\delta t, x) - \sum_{k=-2}^{1} \gamma_k C(t, x+k\delta x),$$

is of order two.

For an unsteady velocity:

$$C_i^{n+1} = C(t+\delta t, x) = C(t,x) - \delta t \frac{\partial C}{\partial x}(t,x)\big[u(t) + \frac{\delta t}{2}\frac{\partial u}{\partial t}(t)\big] + u^2(t)\frac{\delta t^2}{2}\frac{\partial^2 C}{\partial x^2}(t,x) + \mathcal{O}(\delta t^3). \quad (12)$$

The velocity derivative $\dfrac{\partial u}{\partial t}$ in equation (12), is approximated to first order by:

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

such that:

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

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:

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

Thus Eq. (11) can be expressed as:

$$C_i^{n+1} = C_i^n - \lambda u^{n+1/2}(C_{i+1}^n - C_{i-1}^n) + \frac{\lambda^2 u^n u^n}{2}(C_{i+1}^n - 2C_i^n + C_{i-1}^n) - \gamma\lambda(\lambda u^n u^n - u^{n+1/2})(C_{i+1}^n - 3C_i^n + 3C_{i-1}^n - C_{i-2}^n). \quad (13)$$

The scheme represented by Eq. (13) is neither TVD nor L^∞-stable, and may generate instabilities.

The method developed in (Rasetarinera, 1995) is applied to obtain a TVD and L^∞-stable scheme. Eq. (13) is re-written as

$$C_i^{n+1} = C_i^n - \lambda u^{n+1/2}(C_i^n - C_{i-1}^n) - \frac{\lambda(u^{n+1/2} - \lambda u^n u^n)}{2}(C_{i+1}^n - 2C_i^n + C_{i-1}^n) - \gamma\lambda(\lambda u^n u^n - u^{n+1/2})(C_{i+1}^n - 3C_i^n + 3C_{i-1}^n - C_{i-2}^n),$$

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

$$C_i^{n+1} = C_i^n - \lambda u^{n+1/2}\Delta C_{i-1/2}^n - \frac{\lambda(u^{n+1/2}-\lambda u^n u^n)}{2}(\Delta C_{i+1/2}^n - \Delta C_{i-1/2}^n) - \gamma\lambda(\lambda u^n u^n - u^{n+1/2})\big((1-r_{i+1/2}^n)\Delta C_{i+1/2}^n - (1-r_{i-1/2}^n)\Delta C_{i-1/2}^n\big).$$

A TVD scheme is obtained by limiting the numerical flux of the initial Takacs scheme, as been done for Lax-Wendroff scheme (Sweby, 1984) (Rasetarinera, 1995) (it means that, the scheme doesn't generate discontinuities or shocks artificially):

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

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

$$C_i^{n+1} = C_i^n - \lambda u^{n+1/2}\Delta C_{i-1/2}^n - \frac{\lambda}{2}(u^{n+1/2}-\lambda u^n u^n)(\Delta C_{i+1/2}^n - \Delta C_{i-1/2}^n) - \lambda(\lambda u^n u^n - u^{n+1/2})\big(\alpha_{i+1/2}^n(1-r_{i+1/2}^n)\Delta C_{i+1/2}^n - \alpha_{i-1/2}^n(1-r_{i-1/2}^n)\Delta C_{i-1/2}^n\big).$$

So, if $\gamma_{i\pm1/2}^n = min\big(\frac{|1-r_{i\pm1/2}^n|}{2}, \frac{1}{2|1-r_{i\pm1/2}^n|}\big)$ then the scheme (14) is TVD and L^∞-stable under the following CFL condition: $\lambda \parallel u \parallel_\infty \leq 1$. Moreover, it is of second order where the solution is smooth enough except on a neighborhood of critical points. In fact, the main advantage of using a TVD scheme is its capability to take into account discontinuities and shocks. This is not the case for the scheme described by the equation (13).

To summarize, we proposed a new method that uses the splitting technique to solve the global advection-reaction equation. the TVD scheme is used to solve the important convective term and a Runge Kutta method is applied for the reaction term. The method is named the Splitting-TVD scheme. This numerical scheme seems to have necessary capabilities for the WDS modelling needs. It has Eulerian scheme's robustness but do not cause oscillation at singularity points. A validation of its capabilities is performed in the next section.

Validation for advection reaction problem

The proposed method is first compared to some other Eulerian techniques on a benchmark case. The target is to verify the accuracy of the algorithm for a simple problem with a well-known solution. 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 Porteau Software (Cemagref, 2004). The Porteau Software, designed and commercialized in France by the Cemagref (Piller, 1996) (Piller, 1997), combines the method of characteristics and a θ-scheme. This coupling addresses the disadvantages of each of the separate methods. The step solution: δt, uses two substeps: firstly an exact solving using method of characteristics on step $\Delta t \leq \delta t$ such as $u(t)\Delta t = \delta x,\ t$ fixed. In the linear case ($\alpha = 1$) we get briefly:

$$C(i\delta x, t + \Delta t) = C((i-1)\delta x, t)e^{-k\Delta t}$$

Then the use of a θ-scheme on step $\tau = \delta t - \Delta t$:

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

where $\theta = 1/2$. In the nonlinear case it is more complex due to the approximation of the non linearity. Usually, we use the following change of variable:

$$Q(t,x) = C^{1-\alpha}(t,x) + (1-\alpha)kt \quad \Leftrightarrow \quad C(t,x) = \Big(Q(t,x) - (1-\alpha)kt\Big)^{\frac{1}{1-\alpha}} \quad \alpha \neq 1 \tag{14}$$

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

The other mentioned techniques are quite well-known and the reader can find the algorithmic details about each of them in the literature.

All these techniques are tested on a simple case. The benchmark problem is a single pipe of length 1 m with a constant pipe velocity $u = 1\ m/s$ and a steady chlorine injection at the pipe inlet beginning at time t_1 during a period T and then stopping.

Therefore, the boundary condition is:

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

A comparison between some efficient models for the advection reaction solution is given in the figure 1, where $\delta x = .01$ (100 discretization points).

The Method of Characteristics (MOC), that was initially applied in aeronautics to capture shock waves, is very often used in advection problems. This technique follows the solution on its trajectory like Lagrangian approaches. 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 the "characteristic foot". This method is efficient but has two main drawbacks: its CPU time and the use of solution derivative which creates also oscillations with non smooth solution (Fig.1 (a)).

Alternatively, the well-known Finite Difference Lax-Wendroff scheme figure 1 (b) (second order in time and space, L^2 stable) is efficient for continuous solutions but generates "Overshooting" and "Undershooting" with singularities. Another compared method is an θ-scheme (Fig. 1 (c)). This method suffers from an important numerical diffusion and a positivity condition which may be restrictive for our case.
Figure 1 (d) shows the solution with the Porteau software. This method is very accurate but can lead to high CPU time use for unsteady problems, because its variable space discretization. Finally, the Van Leer scheme (Van Leer, 1974) using the MUSCL (Monotonic Upstream-centred Scheme for Conservation Laws) approach with a Min-Mod limitor leads to a 2^{nd} order accuracy. However, it is less accurate than the splitting method, because it is more diffusive (figure 1 (e)).

The two most accurate approximations are given by the splitting TVD model (Fig. 1 (d)) and the hybrid method (Porteau software) (Cemagref, 2004) (Fig. 1 (e)). Nevertheless, the new Splitting-TVD scheme has two advantages compared to the Porteau software: the simpler implementation and the lesser computational effort.

Figure 2 compares the CPU time used by the two techniques to compute a one-dimensional unsteady flow in a single pipe. The substantially better performance of the Splitting-TVD method is evident especially for small δt.
These comparisons are sufficient for this classical well known case study, to show the efficiency of our proposed method.

Sensitivity and Uncertainty

Sensitivity analysis is a main topic in quality modelling. It allows to capture the physical properties in order to solve as well as possible the inverse problem, using the direct method. More precisely this analysis gives the most sensitive nodes where it would be interesting to perform the necessary measures for calibration.
Mainly three approaches have been used for sensitivity analysis: finite differences, automatic differentiation and sensitivity equations. The finite difference techniques that can be used with a large number of commercial softwares 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 parameter, the main problem is to find C_{a_j} for each pipe such as:

$$\begin{cases} \partial_t C_{a_j} + u(t)\partial_x C_{a_j} + \partial_{a_j}(kC^\alpha) = 0, \\ C_{a_j}(0,x) = 0, \quad \forall x \in \mathbb{R}^+ \\ C_{a_j}(t,0) = 0, \quad \forall t \geq 0, \end{cases} \tag{15}$$

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 direct problem ($Eq.$ 1).
The parameters considered in this paper are: the overall decay coefficient k and the reaction order α.

Usually a constant decay coefficient is assigned to the pipes made of the same material with the same age. 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, (15) can be written as follows for pipe i:

$$\begin{cases} \partial_t C_{\mathbf{K}_j} + u(t)\partial_x C_{\mathbf{K}_j} + \mathbf{K}_i \alpha C^{\alpha-1} C_{\mathbf{K}_j} + C^\alpha \delta_{ij} = 0, \quad j \leq n_c, \\ \partial_t C_\alpha + u(t)\partial_x C_\alpha + \mathbf{K}_i \alpha C^{\alpha-1} C_\alpha + \mathbf{K}_i C^\alpha \ln C = 0, \\ C_{\mathbf{K}_j}(0,x) = 0, \quad C_\alpha(0,x) = 0, \quad \forall x \in \mathbb{R}^+, \\ C_{\mathbf{K}_j}(t,0) = 0, \quad C_\alpha(t,0) = 0, \quad \forall t \geq 0, \end{cases} \tag{16}$$

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 the class K_j and α respectively.

As in the state of the direct problem, the time splitting technique is applied in order to separate operators from each others in the sensitivity equations:

$$\begin{cases} \partial_t C_{a_j} t, x) + \big[u(t)\partial_x + \mathrm{B}\big] C_{a_j}(t,x) + f(t,x) = 0, \\ C_{a_j}(0,t) = C_0(t), \end{cases} \tag{17}$$

where f is a source term and $\mathrm{B}(t,x)$ a linear operator. An inhomogeneous, non autonomous ODE with variable coefficients is to be solved. Let $\mathbf{R}$ denote the solution of the homogeneous equations. To preserve 2^{nd} order accuracy in the general case, the Duhamel formula is written to provide the exact solution of (17):

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

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. 10) 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:

$$C_{a_j}(t+\delta t, .) \approx \mathbf{R}(\mathrm{B}, t+\frac{\delta t}{2}, t)\mathbf{R}(u(t)\partial_x, t+\delta t, t)\mathbf{R}(\mathrm{B}, t+\frac{\delta t}{2}, t)\big[C_{a_j}(t, .)+\frac{1}{2}\delta t f(t)\big]+\frac{1}{2}\delta t f(t+\delta t). \tag{18}$$

where the 2^{nd} order accuracy has been maintained.

Global scheme

The global coupled problem allowing the modelling of the water quality and the sensitivity equations on a network may now be started. Because of the time splitting method, the solving on $[0, \delta t]$ is performed in three steps. As already defined, a combination of $\mathcal{X}$ and $\mathcal{F}$ operators is used.

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

$$\begin{cases} \partial_t C^* + \mathbf{K}_i C^{*\alpha} = 0, & C^*(0) = C_0 \\ \partial_t C^*_{\mathbf{K}_j} + \mathbf{K}_i \alpha C^{*\alpha-1} C^*_{\mathbf{K}_j} + C^{*\alpha}\delta_{ij} = 0 \quad j \leq N_{cl}, & C^*_{\mathbf{K}_j}(0) = C_{\mathbf{K}_j}(0) + \frac{\delta t}{2} f_1(0,x) \\ \partial_t C^*_\alpha + \mathbf{K}_i \alpha C^{*\alpha-1} C^*_\alpha + \mathbf{K}_i C^{*\alpha} \ln C^* = 0, & C^*_\alpha(0) = C_\alpha(0) + \frac{\delta t}{2} f_2(0,x) \\ \partial_t A^* - 1 = 0, & A^*(0) = A_0 \end{cases} \tag{19}$$

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

$$\begin{cases} \partial_t C^\bullet + u(t)\partial_x C^\bullet = 0, & C^\bullet(0) = C^*(\frac{\delta t}{2}) \\ \partial_t C^\bullet_{\mathbf{K}_j} + u(t)\partial_x C^\bullet_{\mathbf{K}_j} = 0, & C^\bullet_{\mathbf{K}_j}(0) = C^*_{\mathbf{K}_j}(\frac{\delta t}{2}) \\ \partial_t C^\bullet_\alpha + u(t)\partial_x C^\bullet_\alpha = 0, & C^\bullet_\alpha(0) = C^*_\alpha(\frac{\delta t}{2}) \\ \partial_t A^\bullet + u(t)\partial_x A^\bullet = 0, & A^\bullet(0) = A^*(\frac{\delta t}{2}) \\ \partial_t S + u(t)\partial_x S = 0, & S(0) = S_0 \end{cases} \tag{20}$$

Taking part of the second step the improved reaction and source term equations are

solved again on half time step:

$$\begin{cases} \partial_t C^\diamond + \mathbf{K}_i C^{\diamond\alpha} = 0, & C^\diamond(0) = C^\bullet(\delta t) \\ \partial_t C^\diamond_{\mathbf{K}_j} + \mathbf{K}_i \alpha C^{\diamond\alpha-1} C^\diamond_{\mathbf{K}_j} + C^{\diamond\alpha}\delta_{ij} = 0 \quad j \leq N_{cl}, & C^\diamond_{\mathbf{K}_j}(0) = C^\bullet_k(\delta t) \\ \partial_t C^\diamond_\alpha + \mathbf{K}_i \alpha C^{\diamond\alpha-1} C^\diamond_\alpha + \mathbf{K}_i C^{\diamond\alpha} \ln C^\diamond = 0, & C^\diamond_\alpha(0) = C^\bullet_\alpha(\delta t) \\ \partial_t A^\diamond - 1 = 0, & A^\diamond(0) = A^\bullet(\delta t) \end{cases} \tag{21}$$

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 value for the disinfectant concentration (C), the sensitivity coefficients ($C_{\mathbf{K}_j}$, C_α) with respect of $\mathbf{K}_j$ and α, the source tracking (S) and the residence time (A) respectively. The above coefficients should be associated to the mixing problem equations (Eqs. 5, 4). 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 describe 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 French Network 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 consists of 6 nodes (including 3 reservoirs and 3 junction nodes) and 6 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). Constituent

concentrations of 200 mg/L, 300 mg/L, 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.
The results for chlorine concentration (see Eqs. 19, 20, 21) are compared with those obtained with Porteau (Cemagref, 2004).

Figure 4 shows the concentration in chlorine calculated by the proposed model and by the Porteau software at Node 1. No difference appears. Figure. 5 shows the sensitivities with respect to the overall decay constant C_k and reaction order C_α (see Eqs. 16). Because of the large concentration 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 was equal to 100 mg/L and the same k ($2.4d^{-1}$) was 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 modelling 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:

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

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

$$\begin{aligned} C_k(node3) &= \frac{3355}{1.74} * 300\ e^{-\dfrac{0.1*3355}{3600*1.74}} \\ &\approx 5482581 \end{aligned}$$

Setting $w = C^{1-\alpha} + (1-\alpha)kt$, where C is the solution of

$$\partial_t C + u(t)\partial_x C + kC(t,x)^\alpha = 0, \quad with \quad u(t) = Cte,$$

it is easy to show that w satisfies the linear transport equation

$$\partial_t w + u\partial_x w = 0.$$

Moreover, we can write (Gancel, 2006):

$$C(t,x) = \left(C(t_0,0)^{(1-\alpha)} - (1-\alpha)k(t-t_0)\right)^{1/(1-\alpha)} \tag{22}$$

with t_0 as the solution of:

$$X(t) = \int_{t_0}^{t} u(s)ds$$

where $\frac{dX(\tau)}{d\tau} = u(\tau)$ and $X(t) = L$. Then, for $u(t) = u$, we can write again $(t - t_0) = \dfrac{L}{u}$, and hence we have an exact solution for C, we can derive it respect to α.

Therefore, the sensitivity with respect to α ($C_\alpha(node3)$) is

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

Thus,

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

with $\lim_{\alpha\to 1} C(t,x) = C(t_0,0)e^{-k(t-t_0)}$, yielding

$$\begin{aligned} C_\alpha(node3) &= 300\; e^{-\dfrac{0.1*3355}{3600*1.74}} * [\ln(300) * \frac{-0.1*3355}{3600*1.74} + \frac{0.1^2*3355^2}{2*3600^2*1.74^2}] \\ &\approx -84.82 \end{aligned}$$

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

Brushy Plains Network

The next considered network is more complex. In this section comparisons are made with Porteau but also with EPANET 2. EPANETs water quality simulator uses 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 and Boulos, 1996). It is interesting to explore the computational charaterisitics (CPU time, accuracy etc.) of the proposed approach to an entirely different software in order to solve an engineering example.

Brushy Plains network shown in figure 6 is an example from EPANET 2 (U.S. Environmental Protection Agency, 2002). The network is composed of 41 pipes, 35 junction nodes, 1 storage tank and 1 pumping station. Chlorine transport is modeled assuming a first order decay ($\alpha = 1$) and a constant decay coefficient: $k = -2.4/day$. 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 better compare them 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 $N = 1...$number of nodes

Figure 8 shows that the two most sensitive nodes with respect to k are node 8 and 19 and with respect to α are node 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 behaviour are nodes 8, 19 and the tank.

In this example, EPANET 2 is the fastest, requiring only 12s with $\delta t = 30s$ compared to 1 min 27s for Splitting-TVD solver and 4 min 50 s 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 tracking (S), and two sensitivity results(C_k & C_α) with respect to α and k. Porteau gives also five results at the same time : Concentration in disinfectant, minimum, maximum and average residence time and source tracking. For EPANET 2, it is different because we have only three results that are given separately: disinfectant concentration, average residence time, the trace of bacteria introduced to a node or source tracking. Further, the program needs to be run again

separately to get any of those 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 simultaneously such an analysis. 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 gravity 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 worst 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-square 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

$$g(x) = \frac{1}{2}\left|\left|C(x) - C^{mes}\right|\right|_2^2, \quad x = (\mathbf{K}_1, ..., \mathbf{K}_{n_c}, \alpha), \tag{23}$$

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 method needs the jacobian matrix (sensitivity matrix), mainly used for the "steepest descent". 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 valve, pump or other hydraulic components, accurate measurements are

difficult. It's mainly due to the complex hydraulic flow. Large measurement errors appear, leading to non-realistic solutions.

Conclusion

Sensitivity coefficients, $C_{\mathbf{K}}$ and C_{α}, are particularly crucial for kinetic parameter calibration in WDS. They give information to identify the location of measurements useful for parameters estimation.

This paper has presented a new methodology to estimate accurately these coefficients. A general tool for solving simultaneously both unsteady transport reaction problem and derived sensitivity equation was presented. The method consists in separating the advection operator from the reaction part and source term. A splitting method is then used. This method, more flexible with respect to the choice of the advection scheme, was applied to both the sensitivity equations and the direct problem as these equations have the same structure.

An Eulerian scheme using the TVD technique was chosen to solve the advection process. It allowed to compute discontinuous solution without oscillations. Validation of the scheme and the numerical accuracy analyses were performed and compared to several other standard techniques. An explicit fourth-order Runge-Kutta scheme was used to achieve a good approximation of the reaction and source terms.

Then, the global method could effectively simulate the concentration in disinfectant, age of water, source tracking and the sensitivities in a WDS.

The results were compared to Porteau and EPANET 2 for two case studies and a real benchmark network. The efficiency and the capability of the approach to calculate the water quality indicator values and associated sensitivities were explored. These tests showed that even if EPANET 2 is the fastest software compared to both Eulerian methods, the Splitting-TVD scheme has a higher speed than Porteau (Eulerian). Moreover, we observed that the proposed model provides 7 results at the same time, much more higher than Porteau with 5 and EPANET 2 with 3 simultaneous results. Then, the actual importance and necessity of sensitivity analysis were shown on a

real WDS through a calibration process.

To summarize, the proposed technique in this work is efficient to modelize water quality in WDS. It allows to couple the direct problem with sensitivity equations, and then to optimize the device locations based on the sensitivity coefficients. This approach is useful for an efficient measurement choice and to reduce related errors.

Notation

The following principal symbols are used in this paper:

C = constituent value 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 value 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 tracking; $S = S(t, x)$;

g = objective function;

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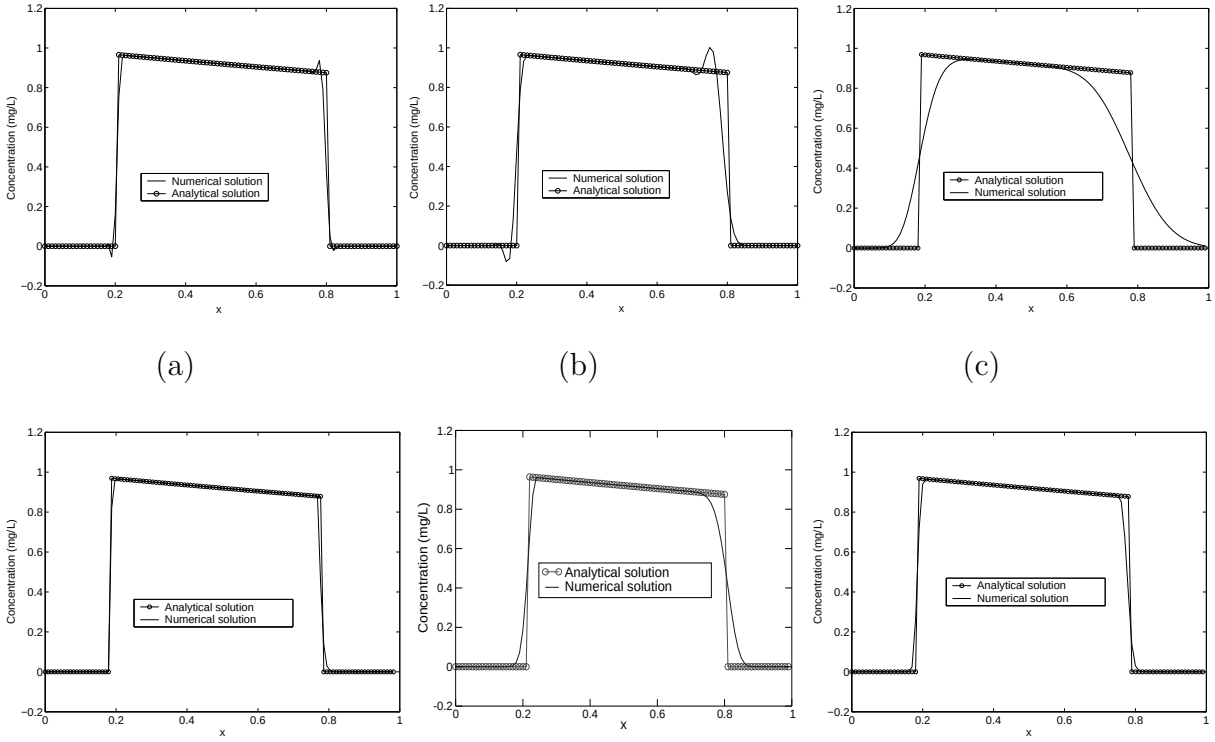
Table. 1: Hydraulic data

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



(a) (b) (c)

(d) (e) (f)

Fig. 1: .

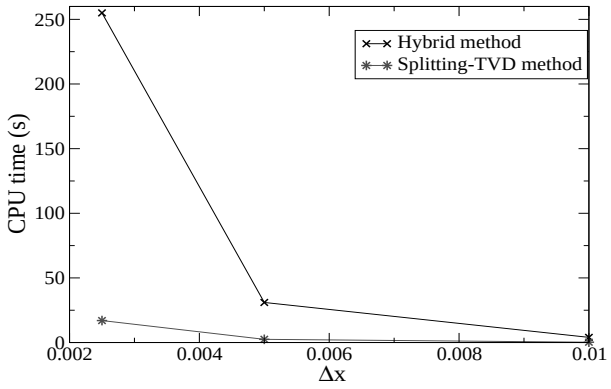


Fig. 2: .

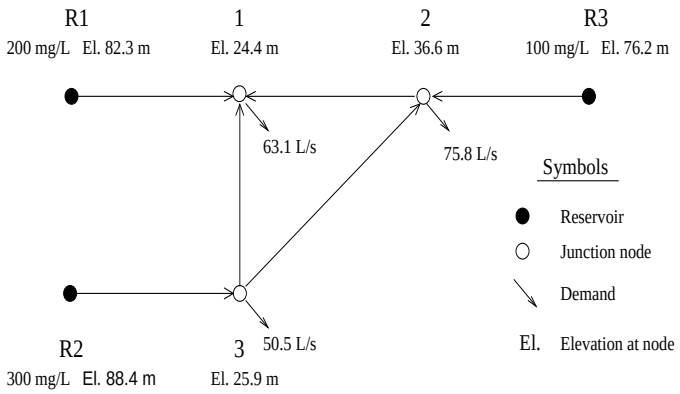


Fig. 3: .

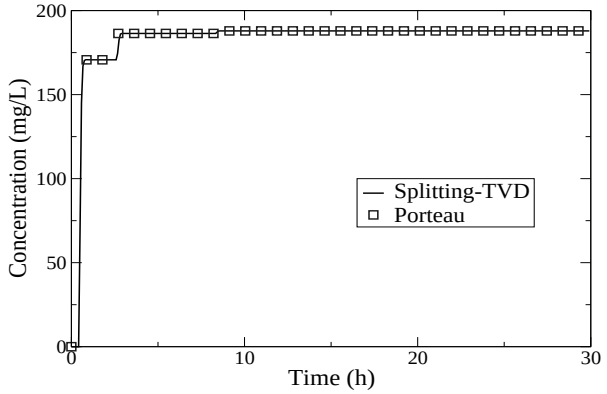


Fig. 4: .

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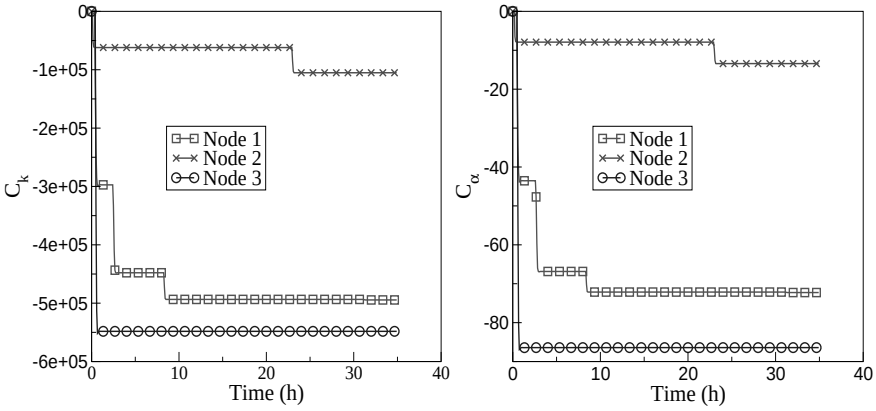
0
-1e+05
-2e+05
-3e+05
-4e+05
-5e+05
-6e+05
C_k
Node 1
Node 2
Node 3
0
10
20
30
40
Time (h)
0
-20
-40
-60
-80
C_α
Node 1
Node 2
Node 3
0
10
20
30
40
Time (h)

Fig. 5: .

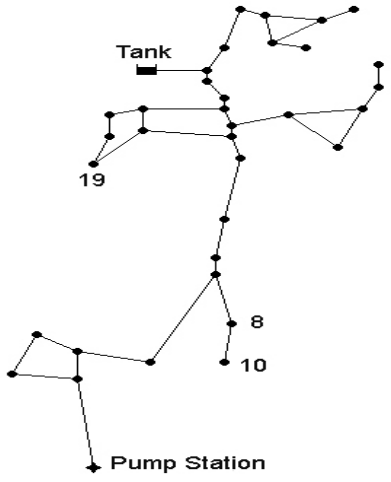
Tank
19
8
10
Pump Station

Fig. 6: .

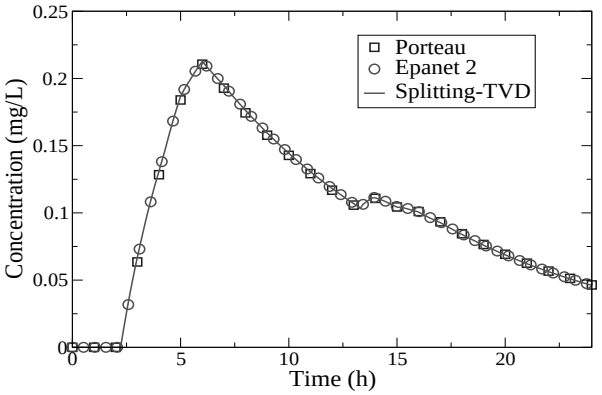
Porteau
Epanet 2
Splitting-TVD
Concentration (mg/L)
Time (h)
0.25
0.2
0.15
0.1
0.05
0
0
5
10
15
20

Fig. 7: .

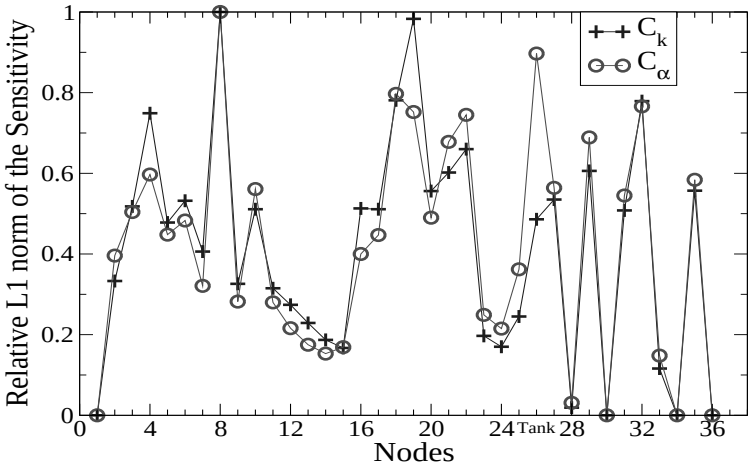
C_k
C_α
Relative L1 norm of the Sensitivity
Nodes
Tank
1
0.8
0.6
0.4
0.2
0
0
4
8
12
16
20
24
28
32
36

Fig. 8: .

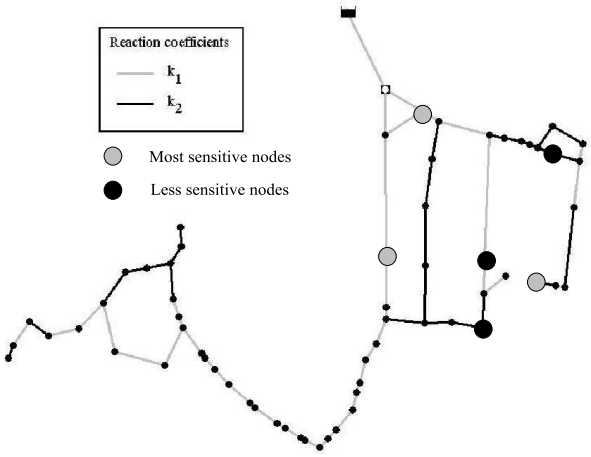
Reaction coefficients
k1
k2
Most sensitive nodes
Less sensitive nodes

Fig. 9: .

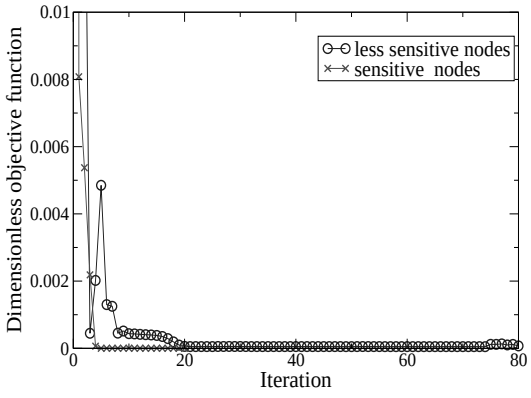
Dimensionless objective function
Iteration
less sensitive nodes
sensitive nodes
0.01
0.008
0.006
0.004
0.002
0
0
20
40
60
80

Fig. 10: .

<http://porteau.cemagref.fr/> (accessed September 2005).

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