

Computational Study and Sensitivity Analysis for Quality Modelling in Water Distribution Systems

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Abstract:

In this paper, forward water quality modelling and the associated unsteady sensitivity equations, are solved in Water Distribution Systems (WDS). A new algorithm is proposed, allowing to approximate the solution of these equations. We propose a time splitting method to separate and solve efficiently each phenomenon such as convection and chemical reaction. This numerical approach allows a simultaneous solving of the direct problem and the sensitivity equations. A special attention is also focused on the advection problem. Thus, a Total Variation Diminishing (TVD) scheme is applied to assure an accurate approximation of the mass transport in pipes. The general model presented in this study, permits to do a global sensitivity analysis of the system. It is essential for better conditioning of the parameters calibration. The methodology is illustrated on two pipes networks and the importance of the sensitivity analysis is showed while a fitting process on a real network.

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Introduction

The quality of water supplied by a distribution network depends directly on the tracking of many indicators. In particular, residence times, origin tracking and concentration in disinfectant such as accounts among the most significative ones. Their knowledge ensures drinking water to be disinfected without gustative unpleasantness. Obtaining these indicators is based on solving mathematical models including physical parameters. The values assigned to these ones are often only rough estimations. Indeed, kinetic parameters involved in disinfectant bulk and wall reaction, are rarely known constants. So, 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 shifted to other plausible values. 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 of previous works, the finite difference methods were used. The sensitivity analysis is then, less accurate compared to the solution chosen in this paper: *the direct method of sensitivity equations*. The structure of the last ones, very close of the forward problem, allows to solve them *simultaneously* with the water quality problem. In this paper we present an new approach to solve this coupled problem.

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: convection, chemical reaction, diffusion is considered separately from the others.

Then, a special attention should be focused on the convection modelling as a dominant factor in our system.

These last ten years, many authors have used different techniques: Eulerian method

(fixed grid), Lagrangian (deforming grid) method, or method of characteristics (MOC) to solve this process in quality modelling. Rossman and Boulos (1996) concluded that Eulerian methods are as accurate as Lagrangian ones except for sharp concentration fronts. So, According to these remark we set up an Eulerian Total Variation Diminishing (TVD) scheme. This approach is appropriate for smooth variation of concentration fronts. Furthermore, using the TVD techniques, it easily overcomes the oscillations due to classical Eulerian schemes.

The paper is organized as follows: Next section describes a physical transport-reaction problem in WDS. We detail the time splitting method, validated by a numerical comparison with other approaches. Sensitivity equations are then derived from the direct problem and the description of the computational algorithms to solve the global model is described. Next, application of the model to three illustrative network examples is performed. A simple network that the results are easily checked by the reader, a benchmark one from the Epanet 2 distribution (U.S. Environmental Protection Agency, 2002) and real network used to show the importance of a sensitivity analysis for the parameters calibrations, are then studied. Finally, concluding remarks are presented.

Water quality in WDS

Water quality modelling consists in estimating the following quality indicators : concentration in disinfectant (chlorine), residence time and source tracking. In this work we consider the above quality indicator as the constituents. The propagation of these constituents (quality indicators) in WDS essentially consists in solving on 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 is described by a

one dimensional hyperbolic Partial Differential Equation (PDE) of the form:

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

where C denotes the constituent considered within the pipe and u the flow velocity in the pipe, depending only the time variable and given by the network hydraulic solution. σ is a reaction function describing each indicators. The change in concentration in the pipe is described by a kinetic rate expression of the form:

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

where α is the order of reaction and k is the overall decay constant (Powell and West, 2000). Likewise, residence time and the source of water are tracked by setting the reaction term:

$$\begin{cases} \sigma(t, x) = -1, \\ \sigma(t, x) = 0. \end{cases} \quad (3)$$

Residence time is described by the first expression. The second expresses the water source tracking which is very useful for the trace of bacteria.

A WDS is mainly composed of pipes, tank, reservoir, and junction nodes. Water arriving at a junction from different origins is supposed to be mixed perfectly and instantaneously. At each node, the resulting concentration is therefore the flow-weighted average of the incoming ones. This average has many properties in common with the the first kirchoff law. It is a straight consequence of the mass conservation. Since no masse can be lost in the junction.

Junction mixing

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 : exit unit normal.

Γ : boundary volume Ω .

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

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

Assuming that we have a control volume small enough to have no reaction.

$$\partial_t C + \text{div}(C\vec{U}) = 0.$$

Integrating on a control volume and using the theorem of divergence, it comes :

$$\frac{d}{dt} \int_{\Omega} C d\Omega + \int_{\partial\Gamma} C\vec{U} \cdot \nu d\Gamma = 0 \quad \text{then} \quad \int_{\partial\Gamma} C\vec{U} \cdot \nu d\Gamma = 0.$$

So, at each node n , the 1D resulting constituent is therefore the flow-weighted average of the incoming ones

$$\begin{cases} C_n(t) = \frac{\sum_{i \in N_{in}} q_i C_i(t)}{\sum_{i \in N_{in}} q_i}, & q_i = u_i * S_{c_i}, \\ C_n(0) = C_{n_{t_0}}, \end{cases} \quad (4)$$

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

For a variable-level tank, the change in concentration, residence time, source tracking value can be determined also from the mass conservation relationship. Equation (5) assumes that constituents within the tank are completely and instantaneously mixed.

$$\begin{cases} \frac{dC_T}{dt} = \frac{\sum_{i \in N_{in}} q_i (C_i - C_T)}{V_T} + \sigma_T & \text{where} \quad V_T(t) = V_{T_{t_0}} + \int_{t_0}^t (\sum_{i \in N_{in}} q_i - \sum_{j \in N_{out}} q_j) dt, \\ C_T(0) = C_{T_{t_0}} ; V_T(0) = V_{T_{t_0}}, \end{cases} \quad (5)$$

where C_T is the constituent value in the tank and σ_T is the reaction function in the tank. V_T is the water volume inside the tank and N_{out} is the set of pipes taking water out of the tank.

As conclusion, water quality modeling for a network consist in solving for each time step the problems (1) with the mixing relations: (4) et (5), for each water indicators using the well σ function.

Numerical scheme

The aim of this part is to develop a numerical scheme to simulate the quality modelling. Numerical methods for water quality problem already exists and a comparison of some of these models has been proposed in (Rossman and Boulos, 1996). We present here a new efficient method, using a time splitting algorithm associated to a TVD scheme to solve the advection problem.

Time splitting method

The advantage of this approach is the use of a specific numerical solver for each physical phenomenon (e.g., advection, diffusion, chemical reaction) (Yee, 1988) (Sportisse, 2000). This method interacts between solving the advection equation with no source terms and an ordinary differential equation (ODE) modelling chemistry. This splitting method permits one to use the most efficient approach for each stage of the procedure, taking notice of their physical properties and to present better quality of stability.

In this part we detail the Strang's splitting scheme. So, we recall briefly the main equation of the direct problem:

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

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

We divide the overall equation in two EDOs, and we get the two following subproblems:

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

and

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

Let $\mathcal{X}^t w_0$ and $\mathcal{F}^t v_0$ be the respective solution of (7) and (8).

Then a Strang approximation formula (Strang, 1963; Strang, 1968) of the equation (6) can be written

$$\mathcal{S}_1^t = \mathcal{F}^{t/2} \mathcal{X}^t \mathcal{F}^{t/2}. \quad (9)$$

We can change the sequence of successive integration for \mathcal{F}^t and \mathcal{X}^t : $\mathcal{S}_2^t = \mathcal{X}^{t/2} \mathcal{F}^t \mathcal{X}^{t/2}$. The best choice is the Strang formula which starts and ends with reaction parts. It was confirmed by numerical tests and by several authors (Descombes and Massot, 2004).

The usual study of the local error is performed by Taylor series, and we have the following error expression:

$$\|C(t, \cdot) - S_1(t)\|_{L^2} = \mathcal{O}(\delta t^3).$$

Then, the splitting using the Strang Formula is of the 2nd order.

The two processes, advection and reaction being separated, different schemes exist to approximate each problem.

The ODE's for reaction part are solved with an explicit fourth order Runge Kutta method. The other process: advection, is frequently described in water resources. The convection phenomena modelling appears really as a crucial key point. Here the advantage of the operator decomposition is to choose an accurate method to approximate the transport phenomena. In this paper, a TVD scheme is chosen. This scheme preserves positivity solution (L^∞ -stable condition) and decreases the 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 close to the one introduced

by Rasetarinera (1995) is L^∞ -stable and belongs to the family of Takacs schemes. The main difference with the scheme presented by Rasetarinera is the presence of an unsteady velocity depending only on time. The computational technique is described in the following section.

let δx and δt be respectively the space and time step 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:

$$C_i^{m+1} = \gamma_1 C_{i+1}^m + \gamma_0 C_i^m + \gamma_{-1} C_{i-1}^m + \gamma_{-2} C_{i-2}^m, \quad (10)$$

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.

Let's now extend this approach to a variable velocity unsteady problem. Using Taylor series, we get:

$$\begin{aligned} C(t + \delta t, x) &= C(t, x) - \delta t \frac{\partial C}{\partial x}(t, x) \left[u(t) + \frac{\delta t}{2} \frac{\partial u}{\partial t}(t) \right] \\ &\quad + u^2(t) \frac{\delta t^2}{2} \frac{\partial^2 C}{\partial x^2}(t, x) + \mathcal{O}(\delta t^3). \end{aligned} \quad (11)$$

The velocity derivative $\frac{\partial u}{\partial t}$ is approximate at the first order by the following way:

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

Let us write (11) as:

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

After substitutions, it gives

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

where $\lambda = \frac{\delta t}{\delta x}$ 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 the scheme (10) reads:

$$\begin{aligned} C_i^{n+1} = & C_i^n - \lambda u^{n+1/2}(C_{i+1}^n - C_{i-1}^n) + \frac{\lambda^2 u^n u^n}{2}(C_{i+1}^n - 2C_i^n + C_{i-1}^n) \\ & - \gamma\lambda(\lambda u^n u^n - u^{n+1/2})(C_{i+1}^n - 3C_i^n + 3C_{i-1}^n - C_{i-2}^n). \end{aligned} \quad (12)$$

The scheme (12) is neither TVD nor L^∞ -stable, and may generate some instabilities. In this part we use the method developed in (Rasetarinera, 1995) to get TVD and L^∞ -stable scheme.

Lets us rewrite (12)

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

and let us set $\Delta C_{i+1/2}^n = C_{i+1}^n - C_i^n$ et $r_{i+1/2}^n = \Delta C_{i-1/2}^n / \Delta C_{i+1/2}^n$; we then obtain

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

To have a TVD scheme we limit the numerical flux of the initial Takacs, as it has been done for Lax-Wendroff scheme (Sweby, 1983) (Rasetarinera, 1995).

The method is as follows :

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

where $\phi(r) = 1 - 2\gamma(r)(1 - r)$.

To have $\phi(r)$ in Sweby region we put : $\gamma_{i\pm 1/2}^n = \min\left(\frac{|1-r_{i\pm 1/2}^n|}{2}, \frac{1}{2|1-r_{i\pm 1/2}^n|}\right)$

and the scheme is written as follows

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

So, if $\gamma_{i\pm 1/2}^n = \min\left(\frac{|1-r_{i\pm 1/2}^n|}{2}, \frac{1}{2|1-r_{i\pm 1/2}^n|}\right)$ then the scheme (13) is TVD and L^∞ -stable under CFL condition: $\lambda \|u\|_\infty \leq 1$. Moreover, it is of second order where the solution is smooth enough except on a neighborhood of critical points.

To conclude, 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

In this section, we compare the developed method to well-known comparable techniques on a benchmark case. The compared methods are Lax-Wendroff scheme, θ -scheme, Holly-Preissman method, the Van Leer scheme and the method called hybrid used in Porteau Software (Cemagref, 2004).

Before to describe the numerical tests let's give a brief view of the Porteau Software designed and commercialized in France by the Cemagref. This software is able to model hydraulic flows and also water quality in WDS (Piller, 1996) (Piller, 1997).

This software uses a quality model solver which combines a method of characteristics and a θ -scheme. This coupling thwarts the disadvantages of each method. 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 $\tau = \delta t - \Delta t$:

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

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:

$$Q(t, x) = C^{1-\alpha}(t, x) + (1-\alpha)kt \quad \Leftrightarrow \quad C(t, x) = \left(Q(t, x) - (1-\alpha)kt \right)^{\frac{1}{1-\alpha}} \quad \alpha \neq 1 \quad (13)$$

(13) 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 with a constant flow inside $u = 1m/s$ 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:

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

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

The Method of Characteristics (MOC) is very often used in advection problems. It is initially used in aeronautics to capture shock waves. Furthermore because this method follows the solution on its trajectory, it is very close to Lagrangian method. In the WDS area the Holly-Preissmann technique (Holly and Preissmann, 1977) is

the most usual of this kind of methods. The originality of this concept is the use of an Hermite interpolation formula of the third order, to interpolate the "characteristic foot". This method is very efficient but has two main drawbacks in such WDS problems, 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 important cpu time. In fact for each velocity variation we have to change spatial discretization, and in general case when velocity changes slowly close to 0, the step becomes too small and so the cpu time increases drastically.

Finally, the Van Leer scheme (Van Leer, 1974) using the MUSCL (Monotonic Upstream-centred Scheme for Conservation Laws) approach with a Min-Mod limiter leads to a 2^{nd} order accuracy when the solution is enough smooth. Nevertheless the result, figure 1 (e), is less accurate than the splitting method, because it is more diffusive.

It appears that 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 easy implementation and the low cpu time consuming. The figure 2 compares the cpu time used by the two techniques to compute a one-dimensional unsteady flow in a single pipe. The cpu time advantage of the Splitting-TVD method is well remark in this figure.

Of course, this list of methods is not exhaustive, Eulerian approaches and MOC are not the only methods used in water modelling. Lagrangian methods exist and

perform good results and properties (low cpu time, no diffusion...). Nevertheless, Updating node boundary condition is more technical for these methods (Tzatchkov et al., 2002). Furthermore, they are designed for high velocity variations and not for the usual WDS cases with slight velocity and constituent variations. That's why no comparison is done to this category of methods in this section. However, some validations using Lagrangian methods will be performed in next section for more complex realistic networks.

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 techniques exist to make a 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 the number of parameters and a_j the j th parameter, the main problem with the Dirichlet conditions is to find C_{a_j} for each pipe such as:

$$\left\{ \begin{array}{l} \partial_t C_{a_j} + u(t) \partial_x C_{a_j} + \partial_{a_j} (kC^\alpha) = 0, \\ C_{a_j}(0, x) = 0, \quad \forall x \in \mathbb{R}^+ \\ C_{a_j}(t, 0) = 0, \quad \forall t \geq 0, \\ \text{with } C \text{ verifying the direct problem solution (1),} \end{array} \right. \quad (14)$$

where $C_{a_j} = \frac{\partial C}{\partial a_j}$ is the derivative of C with respect to a_j .

The parameters considered in this paper are: the overall decay coefficient k and the reaction order α . They appear in the concentration equation(2).

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 put together the decay coefficients in class, $\mathbf{K} = (\mathbf{K}_1, \dots, \mathbf{K}_{n_c})$ 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, (14) can be written as follows for pipe i:

$$\begin{cases} \partial_t C_{\mathbf{K}_j} + u(t)\partial_x C_{\mathbf{K}_j} + \mathbf{K}_i \alpha C^{\alpha-1} C_{\mathbf{K}_j} + C^\alpha \delta_{ij} = 0, & j \leq n_c, \\ \partial_t C_\alpha + u(t)\partial_x C_\alpha + \mathbf{K}_i \alpha C^{\alpha-1} C_\alpha + \mathbf{K}_i C^\alpha \ln C = 0, \\ C_{\mathbf{K}_j}(0, x) = 0, \quad C_\alpha(0, x) = 0, \quad \forall x \in \mathbb{R}^+, \\ C_{\mathbf{K}_j}(t, 0) = 0, \quad C_\alpha(t, 0) = 0, \quad \forall t \geq 0, \\ \text{with } C \text{ verifying the direct problem solution (1),} \end{cases} \quad (15)$$

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

As used the forward problem the time splitting technique is applied in order to separate operators from each others in the sensitivity equations:

$$\begin{cases} \partial_t C_{a_j}(t, x) + [u(t)\partial_x + \mathbf{B}] C_{a_j}(t, x) + f(t, x) = 0, \\ C_{a_j}(0, t) = C_0(t), \end{cases} \quad (16)$$

where f is a source term and $\mathbf{B}(t, x)$ a linear operator. An inhomogeneous, non autonomous ODE with variable coefficients is to be solved. Let be \mathbf{R} the resolvent of the homogeneous equations.

To keep the 2^{nd} order accuracy in general case, the Duhamel formula, is written to provide the exact solution of (16). It follows:

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

Then, the trapezoidal integration gives:

$$\begin{aligned} C_{a_j}(t + \delta t, \cdot) &\approx \mathbf{R}(u(t)\partial_x + \mathbf{B}, t + \delta t, t)C_{a_j}(t, \cdot) + \frac{1}{2}\delta t \left[\mathbf{R}(u(t)\partial_x + \mathbf{B}, t + \delta t, t)f(t) + f(t + \delta t) \right], \\ &\approx \mathbf{R}(u(t)\partial_x + \mathbf{B}, t + \delta t, t) \left[C_{a_j}(t, \cdot) + \frac{1}{2}\delta t f(t) \right] - \frac{1}{2}\delta t f(t + \delta t), \end{aligned}$$

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

The Strang's splitting formula (see Eq. 9) application gives:

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

Finally the solution is written like:

$$C_{a_j}(t + \delta t, \cdot) \approx \mathbf{R}(\mathbf{B}, t + \frac{\delta t}{2}, t)\mathbf{R}(u(t)\partial_x, t + \delta t, t)\mathbf{R}(\mathbf{B}, t + \frac{\delta t}{2}, t) \left[C_{a_j}(t, \cdot) + \frac{1}{2}\delta t f(t) \right] + \frac{1}{2}\delta t f(t + \delta t). \quad (17)$$

With this expression, the 2nd order accuracy is maintained.

To conclude, as the forward problem PDEs and the sensitivity equations have the same pattern with the same terms (advection, reaction and source terms), a splitting technique is implemented for both cases to solve more efficiently each term and to obtain an accurate global solution.

Global scheme

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

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

$$\left\{ \begin{array}{ll} \partial_t C^* + \mathbf{K}_i C^{*\alpha} = 0, & C^*(0) = C_0 \\ \partial_t C_{\mathbf{K}_j}^* + \mathbf{K}_i \alpha C^{*\alpha-1} C_{\mathbf{K}_j}^* + C^{*\alpha} \delta_{ij} = 0 \quad j \leq N_{cl}, & C_{\mathbf{K}_j}^*(0) = C_{\mathbf{K}_j}(0) + \frac{\delta t}{2} f_1(0, x) \\ \partial_t C_\alpha^* + \mathbf{K}_i \alpha C^{*\alpha-1} C_\alpha^* + \mathbf{K}_i C^{*\alpha} \ln C^* = 0, & C_\alpha^*(0) = C_\alpha(0) + \frac{\delta t}{2} f_2(0, x) \\ \partial_t A^* - 1 = 0, & A^*(0) = A_0 \end{array} \right. \quad (18)$$

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

$$\left\{ \begin{array}{ll} \partial_t C^\bullet + u(t)\partial_x C^\bullet = 0, & C^\bullet(0) = C^*(\frac{\delta t}{2}) \\ \partial_t C_{\mathbf{K}_j}^\bullet + u(t)\partial_x C_{\mathbf{K}_j}^\bullet = 0, & C_{\mathbf{K}_j}^\bullet(0) = C_{\mathbf{K}_j}^*(\frac{\delta t}{2}) \\ \partial_t C_\alpha^\bullet + u(t)\partial_x C_\alpha^\bullet = 0, & C_\alpha^\bullet(0) = C_\alpha^*(\frac{\delta t}{2}) \\ \partial_t A^\bullet + u(t)\partial_x A^\bullet = 0, & A^\bullet(0) = A^*(\frac{\delta t}{2}) \\ \partial_t S + u(t)\partial_x S = 0, & S(0) = S_0 \end{array} \right. \quad (19)$$

then taking part of the second step the improved reaction and source term equations are solved again on half time step:

$$\left\{ \begin{array}{ll} \partial_t C^\diamond + \mathbf{K}_i C^{\diamond\alpha} = 0, & C^\diamond(0) = C^\bullet(\delta t) \\ \partial_t C_{\mathbf{K}_j}^\diamond + \mathbf{K}_i \alpha C^{\diamond\alpha-1} C_{\mathbf{K}_j}^\diamond + C^{\diamond\alpha} \delta_{ij} = 0 \quad j \leq N_{cl}, & C_{\mathbf{K}_j}^\diamond(0) = C_{\mathbf{K}_j}^\bullet(\delta t) \\ \partial_t C_\alpha^\diamond + \mathbf{K}_i \alpha C^{\diamond\alpha-1} C_\alpha^\diamond + \mathbf{K}_i C^{\diamond\alpha} \ln C^\diamond = 0, & C_\alpha^\diamond(0) = C_\alpha^\bullet(\delta t) \\ \partial_t A^\diamond - 1 = 0, & A^\diamond(0) = A^\bullet(\delta t) \end{array} \right. \quad (20)$$

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 concentration of disinfectant (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. Of course, the above coefficients should be associated to the mixing problem equations (see Eqs. 4, 5).

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

Results and discussion

The applicability of the developed Splitting-TVD technique is tested in this section. Tests are done with three different pipe networks. First a simple case study is considered in which the sensitivity solutions are easily verifiable by the readers. Then,

a comparison with commercialized softwares is performed using the well known real benchmark network from the EPANET 2 distribution. Finally, a validation study for French Network is performed, showing the impact and the necessity of such sensitivity analysis.

A simple case study

To show the validity of the numerical Splitting-TVD scheme, a simple test network found in (Rossman and Boulos, 1996) described by figure 3 is considered. It consists in 6 nodes (including 3 reservoirs and 3 junction nodes) and 6 links. The linear problem with first-order reaction is considered here ($\alpha = 1$) 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 reservoir R1, R2, R3 respectively and hydraulic data are given in table 1. The time step is $\delta t = 300s$ and δx , the space step meets the CFL conditions.

The results for chlorine concentration (see Eqs. 18, 19, 20) are compared with those coming from Porteau, the Cemagref software for water quality modelling (Cemagref, 2004).

Figure. 4 shows the concentration in chlorine calculated by our model and the software Porteau 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. 15). In this graph because the significant concentration of R2, the node 3 is the most sensitive of nodes with respect to k and α . Source concentration and transit time are very influent parameters for sensitivity calculation. If the concentration for all the sources was equal to 100 mg/L, with the same k ($2.4d^{-1}$) the result should be different and node 1 would become the most sensitive with respect to k and α .

Note that at this time, to our knowledge the sensitivity is calculated neither on

Porteau nor on other commercialized softwares. Therefore, this test is very important as the solution is easily verifiable.

In the linear case, the sensitivity with respect to k at node 3 ($C_k(3)$), is:

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

with $(t - t_0) = \frac{L}{u}$ the residence time, L and u the pipe length and velocity into the pipe respectively. Thus,

$$\begin{aligned} C_k(3) &= \frac{3355}{1.74} * 300 e^{-\frac{0.1 * 3355}{3600 * 1.74}} \\ &\approx 5482581 \end{aligned}$$

For the sensitivity with respect to α ($C_\alpha(3)$), we have

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

Thus,

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

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

So it comes:

$$\begin{aligned} C_\alpha(3) &= 300 e^{-\frac{0.1 * 3355}{3600 * 1.74}} * \left[\ln(300) * \frac{-0.1 * 3355}{3600 * 1.74} + \frac{0.1^2 * 3355^2}{2 * 3600^2 * 1.74^2} \right] \\ &\approx -84.82 \end{aligned}$$

$C_k(3)$ and $C_\alpha(3)$ verify exactly the result of sensitivity given by figure 5.

Brushy Plains Network

The next considered network is more complex than the previous one. In this section comparisons are done with Porteau but also with the software: 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).

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 made assuming a first order decay ($\alpha = 1$) and chlorine in the bulk flow occurs with a constant rate: $k = -2.4/day$. The time step is chosen equal to $\delta t = 1min$, that is small enough to have a good solution.

In the 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:

$$C_{k \text{ or } \alpha}^*(N) = \delta t \sum_t |C_{k \text{ or } \alpha}(t)|$$

$$C_{k \text{ or } \alpha}(N) = \frac{C_{k \text{ or } \alpha}^*(N)}{\max_N C_{k \text{ or } \alpha}^*(N)}$$

where $N = 1 \dots$ number of nodes

As the figure 8, shows the two most sensitive nodes with respect to k are node 8 & 19 and with respect to α are node 8 and the tank. The major impact of a little change in α or k is located at these nodes. Thus, the determining positions to measure concentrations, describing the network behaviour are nodes 8, 19 and the tank.

In this example, EPANET 2 is the fastest one, only 12s with $\delta t = 30s$ compared to 1 min 27s for Splitting-TVD solver and 4 min 50 s for Porteau. However, as the global scheme (see Eqs 18, 19, 20) shows, the Splitting-TVD solver gives seven results at the same time: Concentration in disinfectant (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: Concentration in disinfectant, average residence time, the trace of bacteria introduced to a node or source tracking. But the program should be run again separately to get any of those results.

The last test is completely different from the others one. No comparison to existing software is done, but the aim of this last section is to demonstrate the importance of the whole work do up to here. Sensitivity analysis is shown as a fundamental study for water quality parameters calibration.

Sensitivity analysis impact on a real network

The main benefit of a sensitivity analysis is the parameters calibration. In fact the knowledge of the sensitivity solution with respect to the parameters is useful to determine decisive place to do future measurements. We show in this part the direct impact of the measurements choice: An accurate data set increases the conditioning of our fitting methods.

Figure 9 shows a real gravity network in France composed of a reservoir, 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 going to be used for the kinetic parameters calibration. This new calibration estimates the water quality parameters k and α .

To fit the kinetic parameters we minimize the deviation between the numerical values and the measurements with a least square method. Different methods exist to solve such problems. In this paper a direct method of Levenberg-Marquardt type is used. Figure. 10 shows the dimensionless objective function of this problem of minimization: find $\hat{x} \in \mathbb{R}^p / \forall x \in \mathbb{R}^p, g(\hat{x}) \leq g(x)$ where

$$g(x) = \frac{1}{2} \left\| C(x) - C^{mes} \right\|_2^2, \quad x = (\mathbf{K}_1, \dots, \mathbf{K}_{n_c}, \alpha), \quad (21)$$

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

Quickly it appears that the fitting of kinetic parameters with sensitive nodes directly 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 unsensitive nodes, the ill-conditioning of the matrix decreases the convergence rate of the solution. Figure. 10 shows that 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 convergence to the solution.

Conclusion

Sensitivity coefficients, $C_{\mathbf{K}}$ and C_{α} , are particularly crucial for kinetic parameter calibration in WDS. They give information for measurement locations useful for parameters estimation.

This paper has presented a new methodology to obtain accurately these coefficients. A general tool solving simultaneously both unsteady transport reaction problem and derived sensitivity equation PDEs is studied. The main 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 the sensitivity equations and direct problem as they have the same pattern.

Among a lot of techniques a Eulerian scheme using the TVD technique was chosen to solve the advection process. It allowed to consider discontinuous solution without oscillations. Validation of the scheme and the numerical accuracy analyses were performed and compared to several techniques like θ -scheme, Holly-Preissman method, the Van Leer scheme and the method "hybrid" used in Porteau Software (Cema-gref, 2004). Furthermore, 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. Tests showed the efficiency and the capability of the approach to calculate the water quality indicator values and sensitivities associated in a network. Then, the actual importance and necessity of sensitivity analysis were shown on a real WDS through a calibration process.

Notation

The following symbols are used in this paper:

- C = constituent value in a pipe; $C = C(t, x)$;
- u = velocity in pipe; $u = u(t)$;
- σ = reaction function; $\sigma = \sigma(t, x)$
- 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;
- σ_T = reaction function in the tank;
- C_i^n = approximate value at the point $(n\delta t, i\delta x)$;
- \mathbf{K}_j = j th 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
R1 1	203	3050	116	1.75	56.54
1 3	152	1830	116	-0.24	-4.31
1 2	152	3660	116	-0.12	-2.25
R2 3	203	3355	116	1.74	56.18
3 2	152	6100	116	0.08	1.37
2 R3	203	1525	116	-2.37	-76.69

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: CPU Time .

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 .

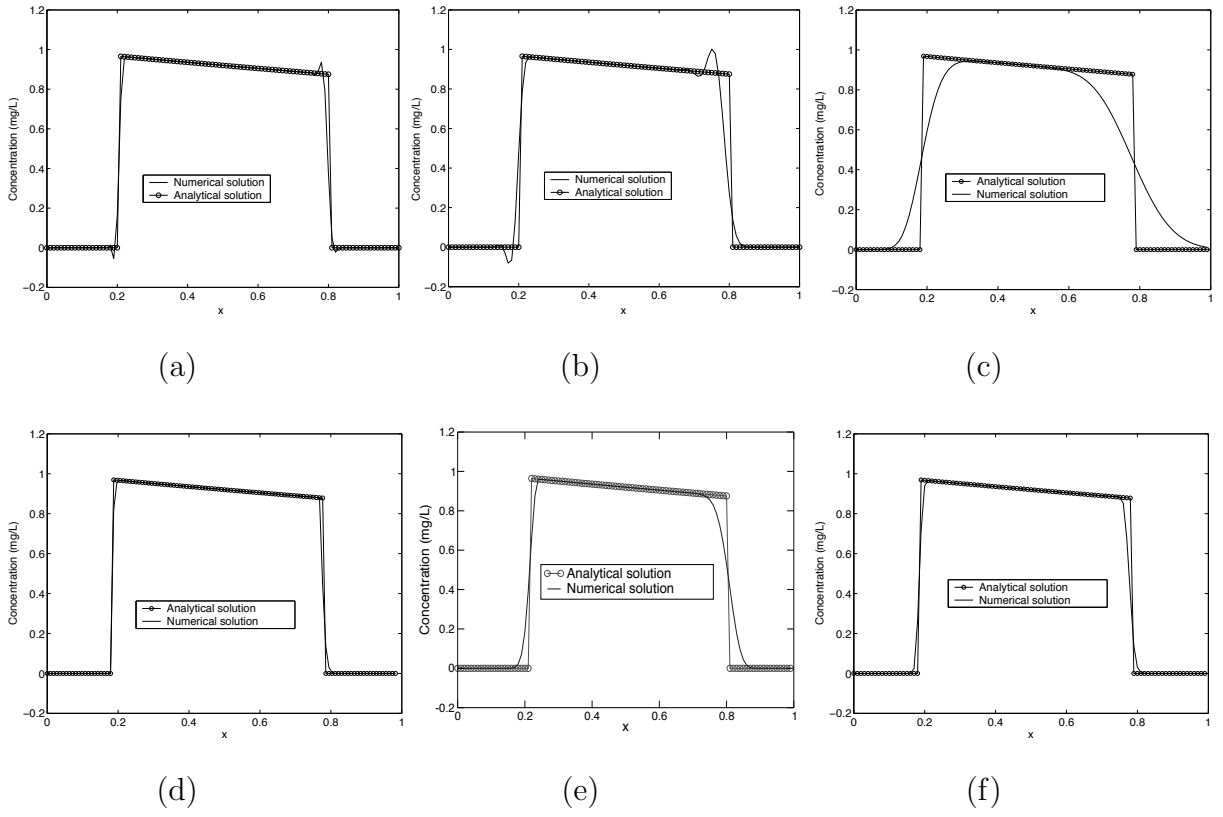


Fig. 1: .

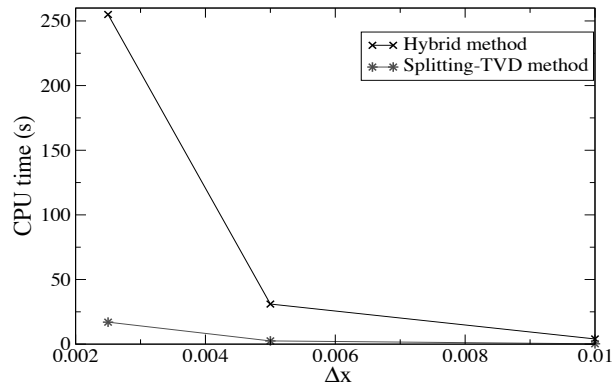


Fig. 2: .

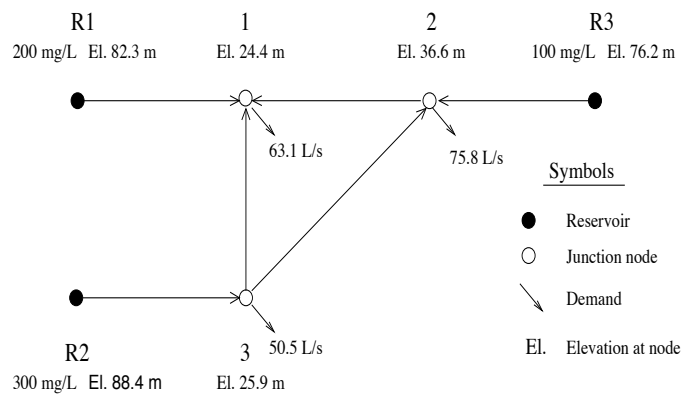


Fig. 3: .

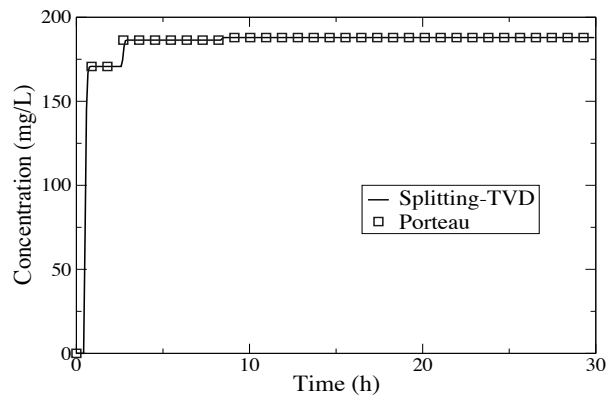


Fig. 4: .

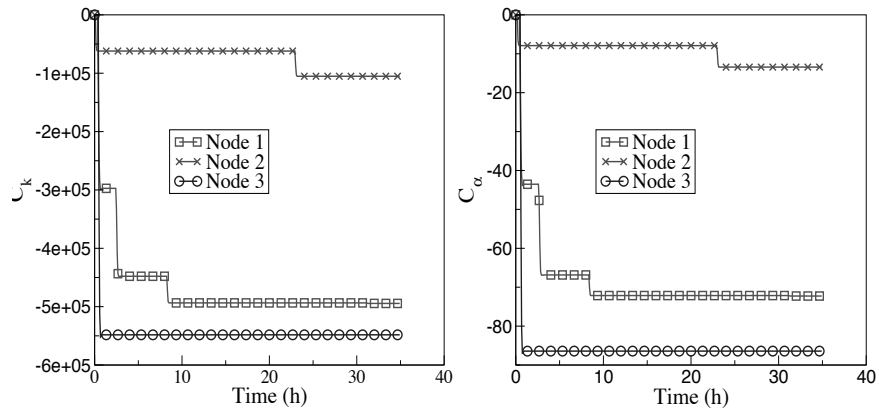


Fig. 5: .

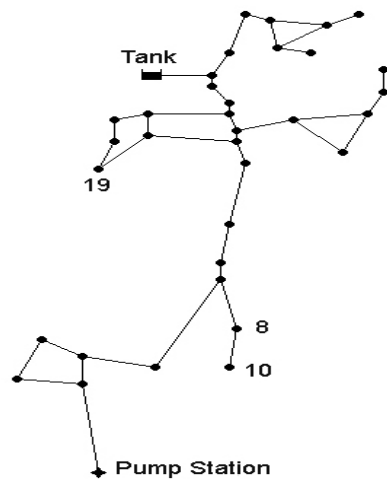


Fig. 6: .

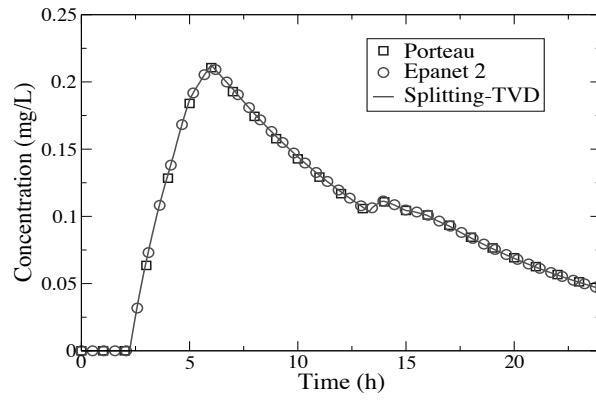


Fig. 7: .

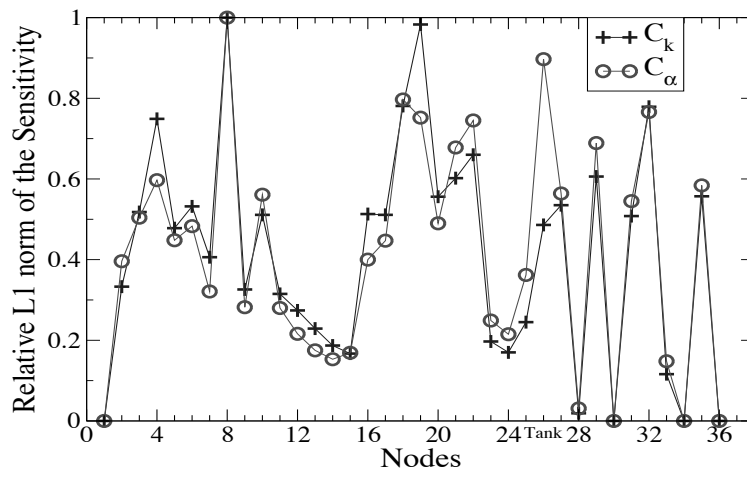


Fig. 8: .

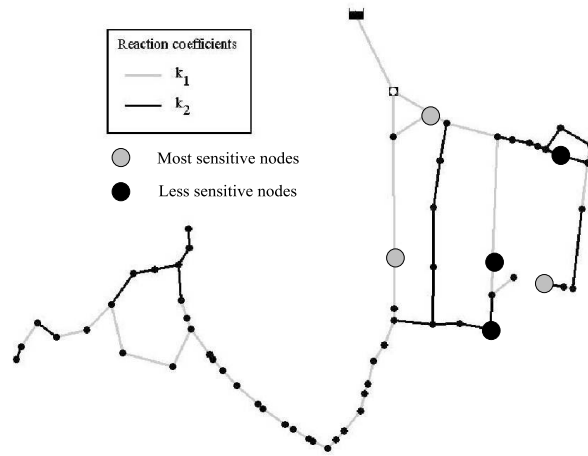


Fig. 9: .

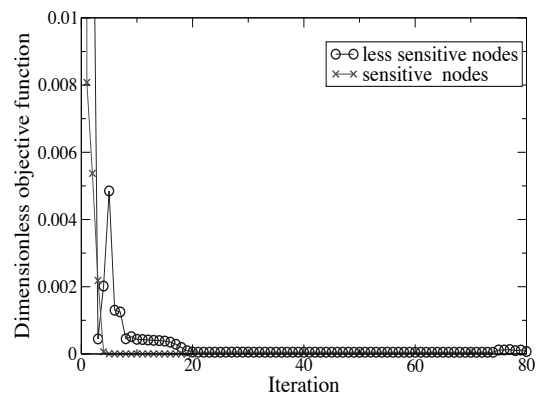


Fig. 10: .