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Applied Mathematics Letters 19 (2006) 1313–1319
Applied Mathematics Letters
www.elsevier.com/locate/aml

Coupled numerical simulation and sensitivity assessment for quality modelling for water distribution systems

G. Gancel[a,b], I. Mortazavi[a,*], O. Piller[b]

[a] *Mathématiques Appliquées de Bordeaux UMR CNRS 5466, Université Bordeaux 1, F-33405 Talence, France*
[b] *CEMAGREF, Bordeaux Regional Center, Hydraulics and Civil Engineering Research Unit, F-33612 Cestas, France*

Received 6 February 2005; accepted 7 July 2005

Abstract

Sensitivity analysis is an important tool which can be used to investigate the stability of a process perturbed by parameter changes and uncertainty impacts. In this work the unsteady sensitivity equations for complex looped pipe networks are solved. Special attention is focused on the coupled version of these equations, with the direct problem. For this purpose a splitting method using a Total Variation Diminishing (TVD) scheme with very good quality of stability is set up and validated on a benchmark pipe network.

Keywords: Sensitivity equation; Water quality; TVD scheme; Distribution network; Splitting method

1. Introduction

Many physical parameters are estimated using empirical techniques. A rigorous analysis of the procedure of modelling of such parameters is necessary. For water distribution systems, sensitivity analyses are used for such studies. They have been sucessfully applied to hydraulic sensitivity [1,2], hydraulic calibration [3] and hydraulic and water quality sampling design [4,5]. Furthermore, this is a key point for inverse problem solving.

One of the most accurate methods for such analysis is developed using the sensitivity equations. They derive from and highly depend on the unsteady advection–reaction equations for quality modelling (direct model).

In this work we propose a method for solving simultaneously the sensitivities with respect to parameters and the direct problem. We present a splitting method based on the Strang Formula [6]. The equations to solve are of the type: *advection–reaction equation with source term*. The advection term is solved with an Eulerian scheme using a Total Variation Diminishing (TVD) criterion and the Ordinary Differential Equations (ODEs) with reaction and source terms are solved with a classical numerical scheme. Our formulation will be able to take into account the stiffness of some problems and also the positivity of the solution.

In the first section, the physical transport–reaction model in quality modelling is presented. Then, sensitivity equations are derived from this model and a solution method based on a splitting method using a TVD scheme from

* Corresponding author.
E-mail address: Iraj.Mortazavi@math.u-bordeaux1.fr (I. Mortazavi).

0893-9659/$ - see front matter © 2006 Published by Elsevier Ltd
doi:10.1016/j.aml.2005.07.012

the family of Takacs is proposed. Finally, some results from a simple case study are presented and compared with those obtained from Cemagref's quality and hydraulic software, Porteau [7], and the well known software in quality modelling, Epanet 2 [8].

2. Physical model

2.1. Direct problem

Establishing the propagation of constituents in Water Distribution Systems (WDS) essentially consists of solving for each pipe an advection equation with a kinetic reaction mechanism and mixing at nodes. The effect of longitudinal dispersion is negligible. The change in constituents due to transport through a pipe is described by a one-dimensional hyperbolic Partial Differential Equation (PDE) of the form

$$\begin{cases} \partial_t C(t,x) + u(t)\partial_x C(t,x) + \sigma(t,x) = 0 \\ C(t=0,x) = C_0(x) \qquad \forall x \in \mathcal{R}^+ \qquad \text{initial condition} \\ C(t,x=0) = \Phi(t) \qquad \forall t \geq 0 \qquad \text{boundary condition} \end{cases} \tag{1}$$

where C denotes the constituent considered within the pipe and u the flow velocity given by the network hydraulic solution. The change in constituents in the pipe is described by a kinetic rate expression of the form

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

where α is the order of reaction and k is the overall decay constant. Likewise, the residence time and the source of water are tracked by setting the reaction terms: respectively $\sigma(t,x) = -1$, $\sigma(t,x) = 0$.

At each node, the water is considered perfectly mixed and a new concentration, age or source is obtained. For the simple nodes the mass conservation relationship yields

$$C(t) = \frac{\sum_k q_{\text{in},k}(t) C_{\text{in},k}(t)}{\sum_k q_{\text{in},k}(t)} \tag{2}$$

where $C_{\text{in},k}$ is the quantity input at this node, $C(t)$ is the mixing quantity result and $q_{\text{in},k}(t)$ is the rate of flow entering this node via link k at the time t. Otherwise the maximum and minimum residence time at each node are calculated as follows:

$$C_{\max}(t) = \max_k C_{\text{in},k}(t); \quad C_{\min}(t) = \min_k C_{\text{in},k}(t).$$

These equations are very useful for giving upper and lower limits for the average residence time calculated by (2).

For a variable-level tank, the change in concentration or age of the water can be determined also from the mass conservation relationship. Eq. (3) assumes that constituents within the tank are completely and instantaneously mixed; this assumption is frequently applied to water:

$$\begin{cases} \dfrac{\mathrm{d}C_T}{\mathrm{d}t} = \dfrac{Q_{\text{in}}(C_{\text{in}} - C_T)}{V_{T_{t_0}} + \int_{t_0}^{t} Q_{\text{in}} - Q_{\text{out}}\mathrm{d}s} + \sigma_T \qquad \sigma_T = kC_T^{\alpha} \quad \text{reaction in the tank} \\ C_T(t=0) = C_T(0) \end{cases} \tag{3}$$

where C_T and V_T are the fully mixed value result and volume of the tank, respectively; $Q_{\text{in}} = \sum_k q_{\text{in},k}$ and $Q_{\text{in}}C_{\text{in}} = \sum_k q_{\text{in},k}C_{\text{in},k}$.

2.2. Sensitivity equations

In quality modelling of the kinetic parameters, the order of reaction and decay constant are hardly known. Sensitivity analysis allows the determination of how "sensitive" our model is to change in the values of these parameters. To carry out this analysis, we use the method of sensitivity equations. These equations are derived from the direct problem.