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Modeling the transport of physicochemical parameters for water network security

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Abstract

Water quality of water distribution networks may be assessed using models. Single-species transport-reaction equations without interaction between indicators are often sufficient to reproduce the observed values. The objective of this paper is to present a new numerical scheme, which transforms water quality equations into a unique simple transport equation to solve. An advection-reaction equation is derived from incompressible Navier-Stokes for modeling the water temperature in the network. A quality solver was realized using Matlab and validated on small and medium-sized networks. As a result the same subroutine code is called for calculating the evolution of several water quality indicators.

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1. Introduction

The objective of water distribution networks (WDNs) is to supply water to consumers in proper quantity and pressure, with acceptable quality. Security and safety are also important priorities that lead water utilities to install early-warning detection systems. In several collaborative research projects (e.g.: SecurEau (2013) and SMaRT-Online^{WDN} (2013)), such detection systems consist of cheap and non-specific water quality sensors that monitor, for example, temperature, chlorine concentration, and conductivity. Deviations from normal value ranges could

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activate an alarm. Then, the sensor responses and inverse modeling of water quality indicators may be used for source contaminant identification, for the calculation of the contamination plume and for planning of counter-measures. Single-species transport-reaction equations without interaction between indicators are often sufficient to reproduce the observed values in real time. The models are used offline in the SecurEau project and quasi-real time in SMART-Online^{WDN}.

Water quality is classically described with various quality indicators like chlorine concentration, age and origin of water. The propagation of these quality indicators through links is represented by mathematical models and more precisely by three transport-reaction equations, all of them consisting of an advection term and a reaction term. Generically, this reads:

$$\begin{cases} \frac{\partial F}{\partial t}(t,x) + u(t) \frac{\partial F}{\partial x}(t,x) + R(F) = 0 \\ F(0,x) = F_0(x) \\ F(t,0) = \psi(t) \end{cases} \quad \text{with } R(F) = \begin{cases} kF^\alpha(t,x), k>0, \alpha \geq 1 \text{ for chlorine} \\ -1 \text{ for time residence,} \\ 0 \text{ for tracing source.} \end{cases}, \quad (1)$$

Where F is the water quality indicator; u is the velocity function of time; R is the instantaneous rate of reaction; k and α are kinetics constants; F_0 are the initial conditions and Ψ the boundary conditions at the entry point. The dispersion and diffusion term is not considered in this work but has already been used such as in Islam and Chaudhry (1998).

Then, for updating boundary conditions at junction nodes and tanks, we consider perfect mixing at nodes that is complete and instantaneous. In actual fact, imperfect mixing may be observed for some cross or double T- junction geometries (Ho 2008, Romero-Gomez *et al.* 2008, Ung *et al.* 2013, Braun *et al.* 2013). This extension will not be considered here. Therefore, mixing at junction nodes is obtained as the flow-weighted sum of the water quality indicators:

$$F_n = \frac{\sum_{i \in S_{in}} |q_i| F_i}{\sum_{i \in S_{in}} |q_i|} \quad \text{and} \quad \begin{cases} A_n^{upper} = \max_{i \in S_{in}} A_i, \\ A_n^{lower} = \min_{i \in S_{in}} A_i \end{cases} \quad (2)$$

Where F_n is the updated boundary conditions at nodes n; S_{in} is the set of links with flow entering at node n; q_i is the flow rate in link i; and F_i the water quality indicator value just before entering node n. Additionally, for residence time (A^{upper}) upper and (A^{lower}) lower limits are worked out. Finally for tanks, dilution with perfect mixing with reaction is assumed:

$$\begin{cases} \frac{dF_n}{dt} = \frac{\sum_{i \in S_{in}} |q_i| (F_i - F_n)}{V_n} - R(F_n), \\ F_n(0) = F_n^0, \end{cases} \quad (3)$$

With V_n the water volume of the tank n; F_i is the indicator quantity that is entering by link i; and R is the reaction rate similar to than in Eq. (1).

Today, several software solutions are available for water quality, such as Epanet (2013) and Epanet-based software, Piccolo (2013), SynerGee Water (2013), InfoWater (2013), Sir 3S (2013) and Porteau (2013). Porteau is designed and developed by Irstea for hydraulic and quality modeling in WDNs; it uses a different algorithm than in Epanet (Rossman and Boulos, 1996). The hybrid method in the Porteau software (2013) was chosen for this research. It was compared with other usual method (Lax-Wendroff, Holly-Preissman method, theta scheme; and an operator splitting) in Fabrie *et al.* (2010).

Dandy *et al.* (2013) studied the advantages and the limitations of the use of water age as a surrogate for water quality in WDN. They worked out the chlorine concentration from the residence time. Their motivation is that the simulation code for residence time may be 30% and 40% faster than for the chlorine concentration because of reaction terms. Their main findings are that in certain situations, water age gives an approximate estimate of water quality and disinfection by-product formation. However, this estimate may be inaccurate due to mixing in tanks and at nodes and is inappropriate for systems with several water sources and/or rechlorination.

The objective of this research is to develop a method that uses the same solver for calculation of single-species water quality indicators. Firstly, the transformation method is explained. It is applicable for the three classical water quality indicators. Then, the temperature formulation is introduced. Next, the solution method is explained. Finally, a discussion is provided and main conclusions are specified.

2. Material and methods

Water quality indicators with an appropriate change of variable can be described by a simple transport equation.

2.1. Transport equation of a wave and application to the water quality indicators

Schematically, a WDN is represented by a graph composed of links connected to nodes. Nodes represent pipe junctions, demand points, tanks, or resources. Firstly, a system of hydraulics equations is solved to work out the velocities in each graph link and the tank volumes.

Rather than solving a specific equation for each graph link for each water quality indicator, the idea is to transform Eq. (1) to be a link transport equation without reaction term as below:

$$\begin{cases} \frac{\partial \lambda}{\partial t}(t, x) + u(t) \frac{\partial \lambda}{\partial x}(t, x) = 0 \\ \lambda(0, x) = \lambda_0(x) = g(F_0(x), 0) \\ \lambda(t, 0) = \phi(t) = g(\psi(t), t) \end{cases} \quad (4)$$

Where lambda is the wave variable; u is the velocity as in Eq. (1) and the BC and IC are determined from Eq. (1) and from the change of variable g. Velocity of propagation $u > 0$ of the wave λ is piecewise constant function with time.

Each transport-reaction of water quality indicators described in Eq. (1) can be transformed in Eq. (4) with an appropriate **change of variable** g given by:

$$\lambda(t,x) = g(F(t,x),t) = \begin{cases} F^{1-\alpha}(t,x) + (1-\alpha)kt, & \text{for chlorine with } \alpha > 1, \\ e^{kt} F(t,x), & \text{for chlorine with } \alpha = 1, \\ F(t,x) - t, & \text{for residence time,} \\ F(t,x), & \text{for tracing source.} \end{cases} \tag{5}$$

This change of variable is the basis for the characteristics method. By the Duhamel formula, the solution of the transport equation (4) may be expressed with regards to the initial conditions as:

$$\lambda(t,x) = \lambda(0,x_0) = \lambda_0(x_0), \text{ with } x_0(t,x) / x_0 = x - \int_0^t u(s) ds \tag{6}$$

Which is useful if x_0 represents a position inside the pipe (*i.e.*, it is positive and less than x). Alternatively, the solution depends on the boundary conditions if a positive t_0 exists such that:

$$\lambda(t,x) = \lambda(t_0,0) = \phi(t_0), \text{ with } t_0(t,x) / x = \int_{t_0}^t u(s) ds \tag{7}$$

It is straightforward to infer the analytic formulae:

$$F(t,x) = g_t^{-1}(\lambda_0(x_0)) = \left(F_0(x)^{1-\alpha} + (\alpha-1)kt \right)^{\frac{1}{1-\alpha}}, \text{ dependency on the IC} \tag{8}$$

$$F(t,x) = g_t^{-1}(\phi(t_0)) = \left(\psi(t_0)^{1-\alpha} + (\alpha-1)k(t-t_0) \right)^{\frac{1}{1-\alpha}}, \text{ dependency on the BC}$$

where $g_t(F) = g(F,t)$ is defined by Eq. (5). Formulae (8) are part of the solving solution for transport in links. Because, the network is not reduced to a simple link, mixing at nodes also has to be considered. Also, the wave boundary conditions at junction nodes are calculated to match Eq. (2). This gives:

$$\lambda_n = g(F_n,t), \text{ with } F_n = \frac{\sum_{i \in S_m} |q_i| g_t^{-1}(\lambda_i)}{\sum_{i \in S_m} |q_i|}, \alpha > 1 \tag{9}$$

When the change of variable (5) is linear with regards to F , this equation reduces to Eq. (2).

For tanks, a similar equation to Eq. (3) without the reaction term is to be used if g is an affine transformation (that preserves straight lines) *i.e.*, every case except chlorine concentration decay with order different from one. For $\alpha > 1$ the following equation was used:

$$\frac{d}{dt} \lambda_n(t) = \frac{\sum_{i \in S_m} |q_i| [F_i F_n^{-\alpha} - F_n^{1-\alpha}]}{V_n} (1-\alpha) \tag{10}$$

2.2. Temperature calculation in WDNs

We first derive an advection-reaction equation for temperature calculation along pipes. We assume a viscous incompressible fluid and small temperature gradient for consideration of constant fluid properties. With these hypotheses, the local conservation of energy is given by:

$$\rho \frac{de}{dt} = \psi - \nabla \cdot \vec{\phi} \quad (11)$$

Where t represents time [s]; ρ is the water mass density [kg.m^{-3}]; e is the intern energy by unit mass [J.kg^{-1}]; ψ is the dissipation function [$\text{J.m}^{-3}.\text{s}^{-1}$]; and $\vec{\phi}$ is the heat flux density vector [$\text{J.m}^{-2}.\text{s}^{-1}$]. Equation (11) may be rewritten with the temperature variable.

The differential form of Fourier's Law relates the local heat flux density $\vec{\phi}$ to the gradient of temperature:

$$\vec{\phi} = -\lambda \nabla T \quad (12)$$

With λ [$\text{W.m}^{-1}.\text{K}^{-1}$] the thermal conductivity coefficient. Moreover, with the above assumption e is a linear function of the temperature with proportionality coefficient the constant specific heat C [$\text{J.Kg}^{-1}.\text{K}^{-1}$]:

$$e = CT \quad (13)$$

The flow may be assumed axisymmetric, so the velocity vector is given by $V=(V_x, V_r, \theta)$. Equation (11) is expressed according to T using Eqs (12-13); then, thanks to a nondimensionalization each term is analyzed to determine which one is important. This results in only considering axial and radial convections and radial conduction; the dissipation term and the axial conduction are negligible. The conservative form of the energy equation reads:

$$\rho C \left(\frac{\partial T}{\partial t} + \frac{\partial(V_x T)}{\partial x} + \frac{\partial(r V_r T)}{\partial r} \right) = -\frac{1}{r} \frac{\partial}{\partial r} (r \phi_r) \quad (14)$$

Lastly simplification consists of averaging Eq. (14) over the inside cross-sectional area. At the wall, we choose the following Fourier's condition:

$$\vec{\phi} \cdot \vec{n} = \phi_r \Big|_{\Gamma} = \frac{\lambda_w}{R} (T - T_{soil}) \quad (15)$$

Where T_{soil} represents the temperature of the soil; R is the pipe radius; and λ_w is the thermal conductivity coefficient.

The final advection-reaction transport model obtained is given by:

$$\frac{\partial T}{\partial t}(t,x) + u(t) \frac{\partial T}{\partial x}(t,x) + K(T(t,x) - T_{soil}) = 0, \tag{16}$$

$$K = \frac{2\lambda_w}{\rho CR^2} > 0$$

With u the mean value of V_x over the cross-sectional area.

Blokker and Pieterse-Quirijns (2013) used the same equation to predict the water temperature in WDNs. Their conclusion, based on two test cases, is that the soil temperature model is the main parameter to estimate for the prediction. The latter is calculated with a micrometeorology model. They describe a formula to estimate the thermal conductivity coefficient that takes the conduction through the pipe thickness and the water convective process into account. For PVC pipes, the latter water convective term can be neglected.

According to §2.1, we transform Eq. (16) to a transport equation by using a change of variable such as:

$$\lambda(t,x) = e^{Kt} (T(t,x) - T_{soil}) \tag{17}$$

In conclusion, several changes of variables are used to simplify the particular reaction-transport equation to a same advection equation with appropriate initial and boundary conditions. We now explain the wave transport solving of pipe transport equations (4) and perfect mixing at nodes Eqs (9-10).

2.3. Solution method

Hydraulic and transport equations solving was implemented with Matlab. For the quality solver, the “Hybrid method” (Fabrie *et al.*, 2010) was chosen. This consists of a time-splitting method, which combines an exact step by a method of characteristics (MOC) Eq. (6) with an upwind theta-scheme (first-order finite difference and Crank-Nicholson). The grid is shown in Figure 1a. So n_p , the number of spatial intermediary points for the pipe p , is chosen to verify:

$$n_p \Delta t < \frac{L_p}{u_{j,p}} \leq (n_p + 1)\Delta t, u_{j,p} \geq u_{min} > 0 \tag{18}$$

Where u_{min} (e.g., 7 days) is a velocity threshold value to decide if there is advection; L_p is the length of pipe p ; Δt is a transport time step smaller than the hydraulic time step; $u_{j,p}$ is the average velocity in pipe p that is constant for hydraulic time step j . The formula to calculate n_p is given below and δt is chosen to be at maximum:

$$\delta t = \frac{t_{transit}^p}{n_p + 1} \text{ with } \begin{cases} n_p = \text{ceil}\left(\frac{t_{transit}^p}{\delta t}\right) - 1 \\ t_{transit} = \frac{L_p}{u_{j,p}} \end{cases} \tag{19}$$

As a consequence, the time τ for the θ -scheme step (Fig. 1a) is chosen as low as possible.

For water at rest in pipe p , $u_p < u_{min}$, the wave value remains the same for the next Δt .

The algorithm for duration of j_{max} consecutive hydraulic time steps j is given in flowchart Figure 1(b). At the starting of a new hydraulic time step, pipes are reordered considering the direction of the flows that will not change for all the period, and the pipes are discretized to satisfy Eq. (19). For each wave transport step n , the boundary conditions are first calculated at the source node with initial condition of Eq. (4) and Eq. (5). Then within an internal loop that explores each pipe given the reordering, the hybrid method is solved and the perfect mixing is carried out at the terminal node. This is done for every wave transport step n and every hydraulic time step j .

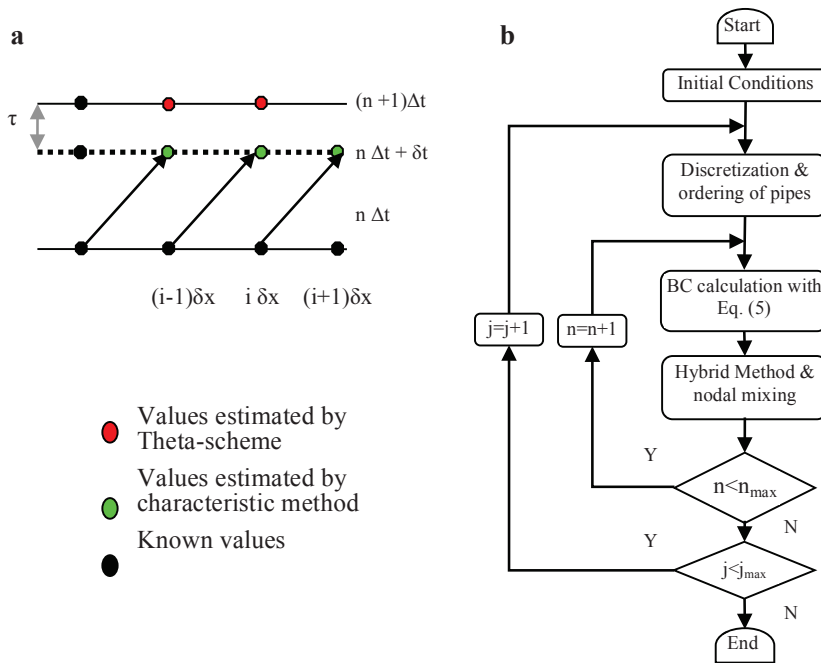


Fig. 1. (a) Grid for Hybrid Method; (b) Flowchart of the transport quality solver.

Therefore, the calculation is divided into two steps: exact resolution by characteristic method on the new time step $\Delta t \leq \delta t$ then using Theta-scheme on the time step $\tau = \delta t - \Delta t$.

3. Method validation and discussions

The results will be shown at the CCWI 2013 conference. These consist of 3 small case studies and a medium-size one. First of all the accuracy is measured and compared to classical transport-reaction equations for existing water quality indicators. This permits the validation of the transport and mixing equations as the solving method. Next, the conditioning such as the stability with regards to stiffer reaction coefficients is assessed. Then execution time is measured. Finally merits of the solution algorithm are discussed.

4. Conclusion

A method that uses the same solver for calculation of single-species water quality indicators is developed in this paper. The main idea is to transform a transport-reaction equation into a unique simple transport equation to solve.

A suitable change of variables is given for the classical water quality indicators that consist of chlorine residual, residence time and source tracking. This could be extended to any single-species indicator as far as the reaction term is a strictly monotone function. As an example, the method is also applied to the temperature. After deriving an advection-conduction equation from Navier-Stokes, the temperature is transformed to a temperature wave.

The solving algorithm consists of a time-splitting method, which combines an exact step by a characteristic method with an upwind Crank-Nicholson scheme. During the MOC time step the water covers a distance that divides the pipe length. For each pipe, this distance is taken as long as possible given the travel time and the periodicity of updating the boundary conditions. The overall two-step scheme is unconditionally stable and accurate to fourth order in time.

Other solution algorithms could be tested (*e.g.* the TVD scheme by Fabrie *et al.*, 2010) and the subroutine code should be changed only once for calculating the evolution of all single-species water quality indicators. This constitutes by design a great advantage for the solver development.

The water quality solver was realized using Matlab and validated on small and medium-sized networks. This permits validation of the solution method, which is at least as accurate as the solution from transport-reaction and is generally obtained faster. The gain in not needing to work out the reaction term is partially compensated by the need to update the boundary conditions.

Future works will be conducted to assess the applicability for large networks.

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