ELSEVIER

Water Research 39 (2005) 4287–4298

WATER RESEARCH

www.elsevier.com/locate/watres

Water quality parameter estimation in a distribution system under dynamic state

G.R. Munavalli[1], M.S. Mohan Kumar*

Department of Civil Engineering, Indian Institute of Science, Bangalore 560 012, India

Received 21 August 2003; received in revised form 23 March 2005; accepted 27 July 2005

Abstract

Chlorine maintenance in distribution systems is an issue for water suppliers. The complex pipe geometry in distribution systems, the dynamic flow conditions experienced within them, and the varied nature of chlorine's reactivity make it difficult to predict chlorine levels throughout a water system. Computer-based mathematical models of water quality transport and fate within distribution systems offer a promising tool for predicting chlorine in a cost-effective manner. Nevertheless, the use of water quality models can only be effective and reliable when both hydraulics and the mechanisms of chlorine dissipation within the water system are properly defined. Bulk water decay can be measured experimentally. However, wall reaction rates are more complex to determine and must be deduced from field measurement by comparison with simulation results. The simulation–optimization model presented in this paper provides an effective tool to simplify the chlorine decay model calibration process that is often tedious. The optimization tool is based on the weighted-least-squares method solved by Gauss–Newton technique. Application of the model onto a real-life system shows that quantity, quality and location of measurement nodes play an important role in estimation of parameters.

Keywords: Chlorine decay modeling; Distribution systems; Drinking water; Optimization tool; Wall reaction parameter

1. Introduction

The study of water quality aspects within a municipal water distribution system is of great significance as it plays an important role in assuring a good quality of water to the consumer. The maintenance of residual chlorine is used as key criteria to assess the potability of water in the chlorine fed distribution systems. The spread of chlorine within the distribution system can be best studied by the use of mathematical models due to the complexities arising out of varying hydraulic conditions and non-applicability of universal chlorine reaction kinetics. The spatio-temporal variations in chlorine levels are established using forward simulation water quality model. The reaction parameters constitute a vital component of the input data needed for the realistic simulations using this model. The predicted chlorine concentrations within a distribution system are governed by reaction parameters (classified as overall, bulk and wall). However, the task of assigning these parameters to the pipes individually, globally or zoned is critical. It is generally assumed that chlorine decay in the bulk water entering the distribution system can be described by a

*Corresponding author.
E-mail addresses: gurumunavalli@yahoo.co.in (G.R. Munavalli), msmk@civil.iisc.ernet.in (M.S. Mohan Kumar).
[1]Presently, Faculty, Department of Civil Engineering, Walchand College of Engineering, Sangli 416 415, India.

0043-1354/$ - see front matter © 2005 Elsevier Ltd. All rights reserved.
doi:10.1016/j.watres.2005.07.043

first-order kinetic model. But the bulk decay parameter can also be non first-order and usually determined experimentally by the bottle test. The overall and wall reaction parameters are difficult to measure in the field. Hence the best way of estimating these parameters is through calibration against the field measurements.

Previously, the trial and error procedure (Clark et al., 1995) was used as a calibration approach. But this is too tedious and may not result in the proper estimation of the parameter values. Also very few studies have been reported in the literature on methodical estimation of specific parameters. Zeirolf et al. (1998) illustrated the use of input–output model for chlorine transport to estimate the first-order (global and zoned) wall reaction parameter. The model is applicable only for first-order reaction kinetics, and does not incorporate storage tanks and multiple water quality sources. Al-Omari and Chaudhry (2001) used finite difference procedures for the determination of overall first-order chlorine decay coefficient(s). Munavalli and Mohan Kumar (2003) developed an inverse model, which estimates the various reaction parameters in a multi-source steady-state distribution system. This model is extended herein for parameter estimation under dynamic state. It essentially has the autocalibration procedure consisting of simulation–optimization technique. The Lagrangian forward simulation water quality model is utilized in the model. The developed model, which computes the various reaction parameters in a more direct fashion, is memory efficient, free from numerical diffusion within the length of a segment and avoids the time-consuming trial and error procedure. In the following sections verification, applicability and usefulness of the inverse model are illustrated using real-life distribution systems.

2. Mathematical model

2.1. Forward simulation water quality model

The forward simulation model consists of hydraulic and chlorine transport components which are discussed below.

2.1.1. Hydraulic model

In the present study, the static hydraulic model (of Niranjan Reddy, 1994) is further modified to compute dynamic flows in the pipes using extended period simulation.

2.1.2. Chlorine transport model

When chlorinated water enters the distribution system, chlorine residual tends to dissipate. Three factors that frequently influence chlorine consumption are: (1) reactions with organic and inorganic chemicals (e.g., ammonia, sulfides, ferrous ion, manganous ion, humic material) in the bulk aqueous phase; (2) reactions with biofilm at the pipe wall; and (3) consumption by the corrosion process (Clark, 1998). Chlorine decay in distribution systems is generally considered to be composed of two components viz bulk and wall demands. The chlorine transport model is formulated assuming one-dimensional advection-dominated transport phenomenon within a pipe segment. Thus, the general governing equation for transport of chlorine along the ith pipe is given by

$$\frac{\partial c_{i,t}}{\partial t} = -u_i \frac{\partial c_{i,t}}{\partial x} - R(c_{i,t}), \tag{1}$$

where $c_{i,t}$ is the chlorine concentration in pipe i (mg/L) as a function of distance x and time t; u_i the mean flow velocity in pipe i (m/s) and $R(c_{i,t})$ the reaction rate expression.

$R(c_{i,t})$ represents the combined effect of bulk and wall reactions. The most common combination used is the first-order bulk and first-order wall reaction models. However in this paper, the purpose is to provide a large choice of kinetic models and are discussed in the following paragraphs.

(1) Overall first-order reaction kinetics

$$R(c_{i,t}) = -k_0 c_{i,t}, \tag{2}$$

where k_0 is the overall first-order reaction parameter (d^{-1}).

(2) First-order bulk and first-order wall reactions

$$R(c_{i,t}) = -k_{b,1i} c_{i,t} - \frac{k_{w,1i} k_{fi}}{r_{hi}(k_{w,1i} + k_{fi})} c_{i,t}, \tag{3}$$

where, r_{hi} is the hydraulic radius (m); $k_{w,1i}$ the first-order wall reaction parameter (m/d); $k_{b,1i}$ the first-order bulk decay parameter (d^{-1}) and k_{fi} the mass transfer coefficient (m/d), the expression for the estimation of this parameter is described in detail by Rossman (2000).

(3) First-order bulk and zero-order wall reactions

$$R(c_{i,t}) = -k_{b,1i} c_{i,t} - \mathrm{Min}\left(\frac{k_{fi} c_{i,t}}{r_{hi}}, \frac{k_{w,0i}}{r_{hi}}\right), \tag{4}$$

where $k_{w,0i}$ is the zero-order wall reaction parameter ($mg/m^2\,d$).

(4) Second-order bulk reaction with respect to chlorine only and first-order wall reaction

$$R(c_{i,t}) = -k_{b,2i} c_{i,t}^2 - \frac{k_{w,1i} k_{fi}}{r_{hi}(k_{w,1i} + k_{fi})} c_{i,t}, \tag{5}$$

$k_{b,2i}$ is the second-order bulk decay parameter (L/mg d).

(5) Second-order bulk reaction with respect to chlorine only and zero-order wall reaction

$$R(c_{i,t}) = -k_{b,2i} c_{i,t}(c_{i,t} - C_L) - \frac{k_{w,0i} k_{fi}}{r_{hi}(k_{w,1i} + k_{fi})} c_{i,t}. \tag{6}$$