Journal of Hydrology 555 (2017) 323–329

Contents lists available at ScienceDirect

Journal of Hydrology

journal homepage: www.elsevier.com/locate/jhydrol

Research papers

Developing semi-analytical solution for multiple-zone transient storage model with spatially non-uniform storage

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A R T I C L E I N F O

Article history:
Received 25 August 2017
Received in revised form 30 September 2017
Accepted 13 October 2017
Available online 18 October 2017
This manuscript was handled by P. Kitanidis, Editor-in-Chief, with the assistance of Todd C. Rasmussen, Associate Editor

Keywords:
Solute transport
GITT
Multiple transient storage
Spatially non-uniform storage

A B S T R A C T

Transient storages may vary along the stream due to stream hydraulic conditions and the characteristics of storage. Analytical solutions of transient storage models in literature didn't cover the spatially non-uniform storage. A novel integral transform strategy is presented that simultaneously performs integral transforms to the concentrations in the stream and in storage zones by using the single set of eigenfunctions derived from the advection–diffusion equation of the stream. The semi-analytical solution of the multiple-zone transient storage model with the spatially non-uniform storage is obtained by applying the generalized integral transform technique to all partial differential equations in the multiple-zone transient storage model. The derived semi-analytical solution is validated against the field data in literature. Good agreement between the computed data and the field data is obtained. Some illustrative examples are formulated to demonstrate the applications of the present solution. It is shown that solute transport can be greatly affected by the variation of mass exchange coefficient and the ratio of cross-sectional areas. When the ratio of cross-sectional areas is big or the mass exchange coefficient is small, more reaches are recommended to calibrate the parameter.

1. Introduction

Contaminant concentrations in the stream are affected by the flow in the stream and the mass exchange between the stream and storage zones. Bencala and Walters (1983) firstly presented a transient storage model to simulate the concentration in the stream by considering the mass exchange between the stream and a single storage zone. Subsequently, single-zone transient storage models have been widely used to investigate smaller peaks and longer tails in the stream concentration profile (Cheong and Seo, 2003; Dewaide et al., 2016; Fernald et al., 2001; Ge and Boufadel, 2006; Hart, 1995; Morales et al., 2010; Runkel and Broshears, 1991; Runkel and Chapra, 1993; Wörman, 2000; Zaramella et al., 2003). In single-zone transient storage models, a lumped storage zone was assumed. In fact, transient storages are usually categorized into surface transient storages and hyporheic transient storages (Briggs et al., 2009). Since these two kinds of transient storages have different hydraulic and biochemical properties, multiple-zone transient storage models have been developed to consider the effects of multiple storage zones on the concentration in the stream (Anderson and Phanikumar, 2011; Briggs et al., 2009; Briggs et al., 2010; Choi et al., 2000; de Dreuzy and Carrera, 2016; Li et al., 2011; Marion et al., 2008; Neilson et al., 2010; Patrick Wang et al., 2005; Silva et al., 2009; Zaramella et al., 2016).

Transient storage models were usually solved by using the finite difference technique (Choi et al., 2000; Fernald et al., 2001; Runkel and Broshears, 1991; Runkel and Chapra, 1993; Silva et al., 2009). A typical example is the one-dimensional transport with inflow and storage (OTIS) model (Runkel and Broshears, 1991). In OTIS, the stream is divided into one or more reaches and each reach consists of a number of segments. The parameters of transient storage, velocity and diffusion coefficient are stored in the segments. Apparently, although the parameters were not written as explicit functions of spatial coordinate in OTIS, the spatially non-uniform storage throughout the stream was virtually considered because of the definition of segments. A few analytical solutions of transient storage models have been developed by using the Laplace transform technique or the integral transform technique (De Smedt, 2006; De Smedt, 2007; Kazezyılmaz-Alhan, 2008; Qiu et al., 2011). The solutions of De Smedt (2006), De Smedt (2007) and Kazezyılmaz-Alhan (2008) were derived for the constant velocity and diffusion coefficient as well as the spatially uniform storage. The solution of Qiu et al. (2011) considered the variation of the velocity and the diffusion coefficient along the stream while keeping the assumption of spatially uniform storage. However,

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https://doi.org/10.1016/j.jhydrol.2017.10.029
0022-1694/

transient storage varies along the stream due to stream hydraulic conditions and the characteristics of storage such as the sediment component, etc. As pointed out by Briggs et al. (2010), it is of significant importance to determine the variation of the transient storage exchange of solutes along the stream. To the author's knowledge, none has attempted to taken into account the spatially non-uniform storage in the semi-analytical solution of transient storage models.

The purpose of this paper is to derive the semi-analytical solution of the multiple-zone transient storage model with the spatially non-uniform storage. The presented semi-analytical solution is validated against the published experimental data. Some illustrative examples are presented to demonstrate the application of the derived semi-analytical solution.

2. Model formulation

The multiple-zone transient storage model includes the transient advection–diffusion equation and some localized mass conservation equations. Taking into account the first-order decay and the generation of solute, the multiple-zone transient storage model can be written as follows

$$\frac{\partial C}{\partial t}=\frac{\partial}{\partial x}\left(D(x)\frac{\partial C}{\partial x}\right)-v(x)\frac{\partial C}{\partial x}-\sum_{i=1}^{M}\alpha_i(x)(C-C_{s,i})-\gamma(x)C+S(x,t) \quad (1)$$

$$\beta_i(x)\frac{\partial C_{s,i}}{\partial t}=\alpha_i(x)(C-C_{s,i});\quad i=1,\cdots M \quad (2)$$

where $C(x,t)$ and $C_{s,i}(x,t)$ are the solute concentration in the stream and in the *ith* storage zone, respectively; $v(x)$ represents the velocity in the stream; $D(x)$ represents the solute dispersion in the stream; $\alpha_i(x)$ is the mass exchange coefficient between the stream and the *ith* storage zone, $\beta_i(x) = A_{s,i}(x)/A(x)$ is the ratio of cross-sectional areas where A(x) and $A_{s,i}(x)$ are the channel cross-sectional area and the storage zone cross-sectional area, $\gamma(x)$ means the first-order decay of solute in the stream, S(x,t) represents the generation of solute in the stream, M is the number of storage zones. In Eqs. (1) and (2), $\alpha_i(x)$ and $\beta_i(x)$ are written explicitly as functions of spatial coordinate x to represent the spatially non-uniform storage.

The inflow boundary condition is given by

$$C(x,t)|_{x=0}=f(t) \quad (3)$$

where f(t) is a function to represent the variation of concentration with time. The outflow boundary condition is given by

$$\left.\frac{\partial C(x,t)}{\partial x}\right|_{x=L}=0 \quad (4)$$

For generality, a concentration distribution is assumed in the stream and in storage zones at the initial time

$$C(x,t)|_{t=0}=g(x) \quad (5)$$

$$C_{s,i}(x,t)\big|_{t=0}=h_i(x);\quad i=1,\cdots M \quad (6)$$

where g(x) and $h_i(x)$ are functions of spatial coordinate.

3. Solution methodology

The Laplace transform technique has been successfully used to solve the transient storage model with constant parameters (De Smedt, 2006; De Smedt, 2007; Kazezyılmaz-Alhan, 2008). When the velocity and the dispersion coefficient in the transient storage model are spatially dependent, the coupled use of the Laplace transform technique and the generalized integral transform technique (GITT) was developed (Qiu et al., 2011). However, for the spatially non-uniform storage the differential equations of $T_n(t)$ (see the definition in Eqs. (16) and (17)) in the paper of Qiu et al. (2011) would become highly complex and is difficult to solve.

In this paper, a full GITT solution strategy is developed to solve the system of Eqs. (1) and (2). GITT was developed by Cotta (1993) to solve heat and fluid flow problem. The solution obtained by GITT is of a general analytical nature (Sphaier et al., 2011). It has been successfully applied to solute transport in porous media (Liu et al., 2000), convection-diffusion problems (Almeida and Cotta, 1995; Cotta, 1990; Cotta et al., 2013), multi-species transport problem (Chen et al., 2012; Pérez Guerrero et al., 2010; Pérez Guerrero et al., 2009). In GITT, a Sturm–Liouville eigenvalue problem is constructed and the eigenfunctions are used to transform the original advection-diffusion equation. Unlike the conventional application of GITT to a single advection-diffusion equation (Sphaier et al., 2011), the system of Eqs. (1) and (2) consists of M+1 partial differential equations. However, only Eq. (1) contains the diffusion term. So, only a single eigenvalue problem can be constructed from Eq. (1), which writes

$$\frac{d^2\varphi_n(x)}{dx^2}+\lambda_n^2\varphi_n(x)=0;\quad n=1,2,\ldots\infty \quad (7)$$

$$\varphi_n(x)|_{x=0}=0 \quad (8)$$

$$\left.\frac{d\varphi_n(x)}{dx}\right|_{x=L}=0 \quad (9)$$

where λ_n is the eigenvalue, $\varphi_n(x)$ is the eigenfunction. The eigenvalue problem (7)-(9) gives the following eigenfunction, eigenvalue and norm

$$\varphi_n(x)=\sin(\lambda_n x) \quad (10)$$

$$\lambda_n=\frac{(2n+1)\pi}{2L} \quad (11)$$

$$N_n=\int_0^L\varphi_n^2(x)dx=\frac{L}{2};\quad n=1,2,\ldots\infty \quad (12)$$

In the derivation of Qiu et al. (2011), integral transform was only performed to C(x, t). In the present full GITT solution strategy, both C(x, t) and $C_{s,i}(x, t)$ are simultaneously transformed by using the eigenfunction $\varphi_n(x)$, which reads

$$U(x,t)=\sum_{n=1}^{K}\frac{1}{N_n^{1/2}}\varphi_n(x)T_n^1(t);\quad K\to\infty \quad (13)$$

$$C_{s,i}(x,t)=\sum_{n=1}^{K}\frac{1}{N_n^{1/2}}\varphi_n(x)T_n^{i+1}(t);\quad i=1,\cdots M;\quad K\to\infty \quad (14)$$

with

$$U(x,t)=C(x,t)-f(t) \quad (15)$$

The existence of Eq. (14) enables the separation of variables of Eq. (2) and the mass exchange term in Eq. (1), which is the crucial step to derive the semi-analytical solution. The boundary condition of C(x,t), i.e., Eq. (3), is inhomogeneous. The introduction of U(x,t) makes the boundary condition of U(x,t) homogeneous, as shown in Eqs. (20) and (21). In the computation, the infinite series in Eqs. (13) and (14) must be truncated at a certain value. K is the number of eigenfunctions and eigenvalues adopted in the infinite series.

The inverse integral transforms can be defined as follows