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One-dimensional numerical modelling of solute transport in streams: The role of longitudinal dispersion coefficient

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ABSTRACT

One-dimensional (1-D) numerical models of solute transport in streams rely on the advection–dispersion equation, in which the longitudinal dispersion coefficient is an unknown parameter to be calibrated. In this work we investigate the extent to which existing empirical formulations of longitudinal dispersion coefficient can be used in 1-D numerical modelling tools of solute transport under steady and unsteady flow conditions. The 1-D numerical model used here is the open source *Mascaret* tool. Its relevance is illustrated by simulating theoretical cases with known analytical solutions. Ten empirical formulas of longitudinal dispersion coefficient are then tested by simulating eight laboratory experimental cases under steady flow condition and the solute transport in the Middle Loire River (350 km long) under highly variable flow condition (from July 1st 1999 to December 31st 1999). Comparisons between computed and measured breakthrough curves show that Elder (1959), Fischer (1975) and Iwasa and Aya (1991) formulas rank as the best predictors for the experimental cases. For the field case, Seo and Cheong's (1998) formula yields the best model-data agreement, followed by Iwasa and Aya's (1991) formula. The latter formula is, therefore, recommended for the entire range of conditions studied here.

1. Introduction

The ability to predict the transport of contaminants in open channels is a major topic in many industrial and environmental projects, ranging from accidental release of pollutant to the transport of non-point sources. Solute transport is governed by a suite of hydraulic and geochemical processes, such as mixing, exchange with storage zones and biogeochemical reactions. Molecular diffusion, turbulent diffusion and shear dispersion are the fundamental mixing processes in open channels (Boxall and Guymer, 2007). Dispersion in longitudinal, lateral and vertical directions accounts for the effects of spatial differences in velocities (either primary or secondary) over the channel cross-section (Rutherford, 1994). Resolution of the equations that govern solute transport is difficult to achieve especially for field cases under unsteady flow conditions. Analytical solutions have been proposed for idealized cases, such as steady flow and instantaneous injection in prismatic open channels (De Smedt, 2006; Hunt, 2006). The application of these solutions to field cases is, however, questionable.

Numerical models have been employed in engineering studies to predict the travel time and concentration of pollutants. Several 1-D models have been proposed and every model has its advantages and limitations (Cox, 2003). The use of these models requires the hydraulic conditions are correctly simulated and the Fickian assumption is valid (*i.e.* effects of velocity shear are balanced by effects of diffusion, usually dominated by turbulent mixing) (Leibundgut et al., 2009). The development of 1-D models has focused mainly on numerical aspect of the advection–dispersion equation (Russell and Celia, 2002; Rubio et al., 2008; Shen and Phanikumar, 2009) and exchange with dead zones (Bencala and Walters, 1983; Wörman et al., 2002; Anderson and Phanikumar, 2011). Some 1-D models are limited to steady flow conditions (*e.g.* SIMCAT (UK Environment Agency, 2001), QUAL2KW (Pelletier et al., 2006), Multiphysics software COMSOL (Ani et al., 2009)), while other models simulate unsteady flows and solute transport (*e.g.* OTIS (Runkel, 1998), CCHE1D-WQ (Vieira, 2004), MIKE 11 (DHI, 2007), SD model (Deng and Jung, 2009), HEC-RAS (USACE, 2010), ADISTS (Launay et al., 2015)). Generally, validation testing has focused on theoretical cases or simplified river geometries in limited space and time scales (Zerihun et al., 2005).

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Nomenclature

A	wetted area
B	channel width
C	concentration of solute in the flow;
C^p	peak concentrations
C_l	lateral inflow solute concentration per unit length
D_L	longitudinal dispersion coefficient;
F	Froude number
$\mathbf{F}$	flux vector = $[Q, Q^2/A + gI_1]^T$
g	gravitational acceleration
H	flow depth
I_1	hydrostatic pressure force term
I_2	pressure force due to the channel walls contractions and expansions
K_s	Manning–Strickler's coefficient
Q	flow discharge
q_l	lateral flow discharge per unit length
R_e	Reynolds number
R_h	hydraulic radius
R^2	correlation coefficient
s	other point sources besides the lateral inlet solute
S	a source term of the solute = $s + C_l q_l$
$\mathbf{S}$	source term = $[q_l, gA(S_0 - S_e) + gI_2]^T$
S_e	energy slope
S_0	longitudinal bed slope
t	time
T^p	time to peak
T^0	time of starting application
$\mathbf{U}$	conservative hydraulic variables = $[A, Q]^T$
V	flow velocity
V_*	shear velocity
x	longitudinal coordinate
y	lateral coordinate
z	vertical coordinate
z_b	bed elevation
ΔC^p	mean relative error of concentration
ΔC^p	mean relative error of peak concentration
Δt	time step
ΔT^p	mean relative error of phase
Δx	space step
ρ	density of water
ε_t	transverse mixing coefficient

All 1-D solute transport models rely on the advection–dispersion equation, which brings the longitudinal dispersion coefficient, D_L, as unknown parameter to be determined. This coefficient measures the intensity of longitudinal dispersion, which is the primary mechanism that is responsible for reducing peak concentrations once the cross-sectional mixing is complete (Chen et al., 2009). In most numerical models, D_L is assumed to be time and space invariant, and estimated with field tracer experiments, with values varying within a range of 10^{-1}–10^7 m^2/s (Seo and Cheong, 1998). Field tracer studies can be expensive and time-consuming, especially for large rivers (Shen et al., 2010; Kim, 2012), and the dispersion coefficient estimate is valid for only the stream reach examined and the set of hydraulic conditions during which the tracer experiment was conducted. Therefore, water quality modellers often use semi-analytical and empirical formulations, relating D_L to flow and channel properties. Most formulas were derived from different assumptions and tested using laboratory and field data sets, and when applied to one study case the estimated dispersion coefficients for the different formulas may vary over several orders of magnitude (Rutherford, 1994). Performance of formulations has been usually assessed by comparing calculated and measured dispersion coefficients (Tayfur and Singh, 2005; Sahay, 2011; Etemad-Shahidi and Taghipour, 2012; Zeng and Huai, 2014), with the measured values being deduced from the observed transverse velocity profiles using the volume integral expression (Deng et al., 2001; Seo and Baek, 2004) or from the temporal concentration profiles using statistical approaches such as moments method (Ho et al., 2002; Zhang et al., 2006) and Chatwin method (Chatwin, 1980). Only some authors investigated the accuracy of selected formulas by comparing numerically calculated breakthrough curves with measurements (Kashefipour and Falconer, 2002; Ani et al., 2009). However, they solved the advection–dispersion equation assuming averaged flow variables in the river, which requires the flow to be steady and the bed geometry to be prismatic. The application of longitudinal dispersion coefficient formulas to geometrically non-uniform channels and unsteady flow conditions is therefore still needed.

In this work we make a step forward and investigate the suitability of dispersion coefficient formulas in 1-D modelling of solute transport under steady and unsteady flow conditions. In contrast to many works published in the literature, the performance of each formula is assessed in the current paper by comparing the calculated breakthrough curves of concentration with measurements. We restrict our attention to non-reactive solutes. We use the Mascaret code, which is the 1-D component of the open source Telemac-Mascaret system developed at EDF-R&D (www.opentelemac.org The code incorporates dispersion coefficient formulas proposed by Elder (1959) (noted hereafter E), Fischer (1975) (F), McQuivey and Keefer (1974) (M&K), Liu (1977) (L), Iwasa and Aya (1991) (I&A), Magazine et al. (1988) (M), Koussis and Rodriguez-Mirasol (1998) (K&R-M), Seo and Cheong (1998) (S&C), Deng et al. (2001) (D) and Kashefipour and Falconer (2002) (K&F).

The remainder of the paper is set out as follows: Section 2 presents the modelling framework. A brief background to the investigated dispersion coefficient formulas is provided in Section 3. In Section 4, the performance of the formulas is assessed using eight laboratory experimental cases under steady flow. In Section 5, formulas are applied for simulating solute transport along the 350 km of the Loire River (France) over the period July 1st 1999 to December 31th 1999. A discussion is given in Section 6, followed by conclusions in Section 7.

2. Formulation of the problem and numerical scheme

The description of the modelling tool given herein is brief. *Mascaret* has been extensively applied for simulating flow propagation in open channels, through the framework of the EU-project CADAM (Goutal, 1999), and solute transport through the IAEA-project EMRAS (Goutal et al., 2008). However, the pure advection term of the solute transport equation was solved by the method of characteristics. In all numerical runs (*i.e.* experimental and field cases), we use a second order finite volume scheme (FV2). Its relevance is demonstrated hereafter using two theoretical cases.

2.1. Basic equations for flow

Based on the hydrostatic pressure distribution and incompressible flow assumptions, the flow hydrodynamics is represented by