APPLICABILITY OF LONGITUDINAL DISPERSION COEFFICIENT FORMULAS IN 1-D NUMERICAL MODELING OF SOLUTE TRANSPORT IN OPEN CHANNELS

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Abstract

One-dimensional (1-D) numerical models of solute transport in open channels 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 some of existing dispersion formulas can be used in 1-D numerical modeling of solute transport. The 1-D numerical modeling used here is the open source MASCARET numerical tool. The water quality component of this tool simulates solute transport processes, consisting of advection, diffusion and mass reduction/generation by physical, chemical and biological mechanisms. Dispersion coefficient formulas proposed by Elder (1959), Fisher (1975), McQuivey and Keefer (1974), Magazine et al. (1988), Koussis and Rodriguez-Mirasol (1998), Seo and Cheong (1998), Deng et al. (2001) and Kashefipur and Falconer (2002) are tested by simulating laboratory experimental cases under uniform flow and the transport of tritium in the Loire River over the period July 1st 1999 to December 31th 1999. Comparisons between computed and measured concentrations show that formulas proposed by Elder and Fisher rank as the best predictors for the entire range of laboratory experiments, while better predictions are provided by the formula of Seo and Cheong for the field case under unsteady flow.

Introduction

Solute transport in open channels is an important topic in many industrial and environmental projects. Because solute transport is multi-physical processes (e.g. advection, mixing, exchange with dead zones, physical, chemical and biological processes), resolution of the equations that govern the problem is a very complex task. Analytical solutions have been proposed for hypothetical cases under simplified geometry, flow and solute transport conditions (e.g. prismatic shape, steady and uniform flow, instantaneous injection) (De Smedt, 2006). The application of these solutions to field cases with complex characteristics is questionable. Generally, 1-D models are widely employed in engineering studies, because they require the least amount of data, and the numerical scheme used for solving the water and solute transport equations are more stable and offer gains in computational efficiency over 2- and 3-D models.

Regarding the computation of solute transport, 1-D models rely on the classical advection-dispersion equation, which brings the longitudinal diffusion coefficient, D_L, as unknown parameter to be determined. In most models, D_L is assumed time and space invariant and calibrated using field tracer studies. This can be expensive and time-consuming, especially for large rivers, and the diffusion coefficient estimate is valid only for the particular stream reach and the flow conditions for which the tracer experiment was conducted. To cater so such shortcomings, various empirical formulas have been proposed, derived from different assumptions and tested with 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 (Kashefipour and Falconer, 2002).

Performance of some empirical formulas was investigated by many authors, e.g. Seo and Cheong (1998), Kashefipour and Falconer (2002), Wallis and Manson (2004), Tayfur and Signh (2005), and Riahi-Madvar et al. (2009), by comparing calculated and measured tracer concentration distributions. In most cases the advection-dispersion equation was solved assuming averaged flow variables in river reaches, which requires the flow to be steady and uniform in the river reach, and the channel bed geometry to be prismatic. In this work we make a step forward and investigate the suitability of existing dispersion coefficient formulas in 1-D modeling of solute transport under both uniform and non-uniform flow conditions. We restrict our attention to nonreactive solute transport without transient storage or exchange with hyporheic zones. We use the 1-D, open source MASCARET modeling tool, developed at EDF-R&D (Electricité De France-Recherche & Développement), for simulating flow and solute transport in open channel networks. The water quality component of this tool incorporates dispersion coefficient formulas

proposed by Elder (1959), Fisher (1975), McQuivey and Keefer (1974), Magazine et al. (1988), Koussis and Rodriguez-Mirasol (1998), Seo and Cheong (1998), Deng et al. (2001) and Kashefipur and Falconer (2002). These formulas are used within the modeling tool to simulate solute transport in three laboratory experimental cases under uniform flow, and the transport of tritium along the Loire River (France) within the period July 1st 1999 to December 31th 1999.

Formulation of the problem

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 framework of the IAEA-project EMRAS (Goutal et al., 2008).

Governing equations

Assuming a hydrostatic pressure distribution and incompressible flow, the flow hydrodyamics is represented by the shallow water equations. Defining a Cartesian coordinate system (x,y,z), with the x-axis longitudinal, y-axis transversal and the z-axis vertical upward, the system of equations is expressed and vector form as

$$\frac{\partial \mathbf{U}}{\partial t}+\frac{\partial \mathbf{F}(\mathbf{U})}{\partial x}=\mathbf{S}(x,\mathbf{U}) \qquad (1)$$

where t = time, $\mathbf{U}$ = $[A, Q]^T$ = conserved variables, $\mathbf{F}(\mathbf{U})$ = $[Q, Q^2/A+gI_1]^T$ = flux, $\mathbf{S}(x, \mathbf{U})$ = $[q_l, gA(S_0-S_e)+gI_2]^T$ = source terms, A = wetted area, Q = flow discharge, q_l = lateral flow rate per unit length, g = gravitational acceleration, S_0 = longitudinal bed slope, S_e = energy slop computed using Manning-Strickler's equation, I_1 = hydrostatic pres-sure force term (Eq. 2b) and I_2 = a pressure force term that accounts for the forces exerted by the channel walls contractions and expansions (Eq.2c).

$$I_1=\int_0^h (h-\eta)B(x,\eta)\,d\eta \qquad (2a)$$

$$I_2=\int_0^h (h-\eta)\frac{\partial B(x,\eta)}{\partial x}\,d\eta \qquad (2b)$$

where R_h = hydraulic radius, h = flow depth, B = channel width, and h = vertical distance above the channel bottom.

The advection-dispersion equation for solute transport reads

$$\frac{\partial AC}{\partial t}+\frac{\partial (QC)}{\partial x}=\frac{\partial}{\partial x}\left(D_x A\frac{\partial C}{\partial x}\right)+S \qquad (3)$$

where C =solute concentration in the flow, and $S = C_l q_l$ = a source term of the solute with C_l denoting distributed lateral inlet solute concentration per unit length of channel. The dispersion coefficient D_L is prescribed by one out of a range of formulas. Considerable uncertainty exists about its prescription, because DL is closely related to the hydraulics variables, characteristics of the fluid (e.g. viscosity), the sediment transport (e.g. suspension) as well as channel geometry (e.g. cross-sectional shape, planform curvature).

Numerical scheme

Equations 1 and 3 are solved sequentially at each time step. First the flow module is called to provide the time-dependent hydraulic parameters, and then these variables are passed to the water quality module for the solute transport simulation. For a steady flow regime, Eq. (1) is solved using a finite difference scheme. For unsteady subcritical flows, the finite difference Preissmann scheme is employed. For a transient mixed flow regime, a first-order Godunov-type explicit scheme is used.

The advection and dispersion terms are computed independently at each time step. The pure advection equation is solved by a first order finite volume scheme (FV1), which is of higher accuracy compared to finite difference and finite element methods that induce numerical diffusion and oscillatory behavior if advection becomes the dominant transport process. In the second step, an implicit scheme is applied to the pure dispersion equation. Because the numerical scheme is explicit, the time step should be limited by stability conditions. The usual Courant-Friedrichs-Levy (CFL) condition is used, with the Courant number being limited to 0.5. For the solute concentration, the Dirichlet condition is used at the upstream boundary and Neumann condition (i.e. zero-gradient) is imposed at the downstream end.

In this paper, we assess the performance of eight dispersion coefficient formulas proposed by Elder (1959) (noted hereafter E), Fisher (1975) (F), McQuivey and Keefer (1974) (1974) (M&K), 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 Kashefipur and Falconer (2002) (K&F) (Table 1). All formulas are a function of the cross-sectional mean parameters, which are readily obtained from the flow module of MASCARET.

Solute transport in laboratory flumes

Herein, we simulate three experimental laboratory cases undertaken by Zulfaquar (1997) at the Civil Engineering Department of Roorkee University, India (Table 2). The experiments covered a laboratory program wherein longitudinal dispersion of a conservative pollutant was investigated under uniform flow conditions. The flume was rectangular, 0.20 m width and 30 m length. The flow was maintained uniform by adjusting a tailgate downstream of the flume. Rhodamine WT was used as a tracer and injected

Table 1: Review of selected longitudinal dispersion formulas

Reference	Formula	Comments/conditions for calibration and verification
Elder (1959) (E)	$D_L = 5.93hV_*$	Uniform flow in an infinitely wide channel Logarithmic vertical-velocity distributions Mixing coefficients for momentum and mass transfer are assumed identical
Fisher (1975) (F)	$D_L = 0.011(V/V_*)^2(B/h)^2hV_*$	Validated using measurements in straight prismatic channels of various regular cross-sectional shapes
McQuivey and Keefer (1974) (M&K)	$D_L = 0.058hV/S_e$	Developed using the similarity between 1-D solute dispersion equation and flow propagation equation Calibrated using field data Flow regime with Froude number lower than 0.5
Magazine et al. (1988) (M)	$D_L = 75.86(0.4V/V_*)^{-1.632}R_hV$	Developed using dimensional analysis Calibrated on the basis of laboratory data sets
Koussis and Rodriguez-Mirasol (1998) (K&R-M)	$D_L = 0.6(B/h)^2hV_*$	Based on the theory and equation proposed by Fischer and von Karman's defect law The value of 0.6 was found by applying a regression analysis on 16 field data.
Seo and Cheong (1998) (S&C)	$D_L = 5.92(V/V_*)^{1.43}(B/h)^{0.62}hV_*$	Developed using dimensional analysis and the one-step Huber method Calibrated and validated using 59 data sets from
Deng et al. (2001) (D)	$D_L = 0.15(V/V_*)^2(B/h)^{1.67}hV_*/(8\varepsilon_t)$ with $\varepsilon_t = 0.145+(V/V_*)(B/h)^{1.38}/3520$	This formula is a revised version of Fisher's equation, integrating a new expression of the transverse mixing coefficient ε_t Valid for $B/h>10$
Kashefipur and Falconer (2002) (K&F)	$D_L = 10.612(V/V_*)hV$ for $B/h>50$ $D_L = [7.428+1.775(V/V_*)^{0.572}(B/h)^{0.62}](V/V_*)hV$ for $B/h<50$	Developed using dimensional analysis coupled with regression analysis Calibrated and validated using 81 data sets from 30 streams in USA

near the upstream end of the flume. Concentration curves were monitored at four locations.

The Strickler coefficient for each run is calibrated using the flow depth, discharge and bed slope (Table 2). Zulfequar (1997) showed that mixing took place over the cross-section at the first location where the concentration was monitored. Therefore, the measured concentration curve at this station is used as Dirichlet condition in the simulations; model-data are compared at the remaining locations. In the numerical runs, the time step is 0.05 s and the space step 0.25 m. For the sake of brevity, we show the results obtained using the two formulas that give the best and worst predictions, respectively.

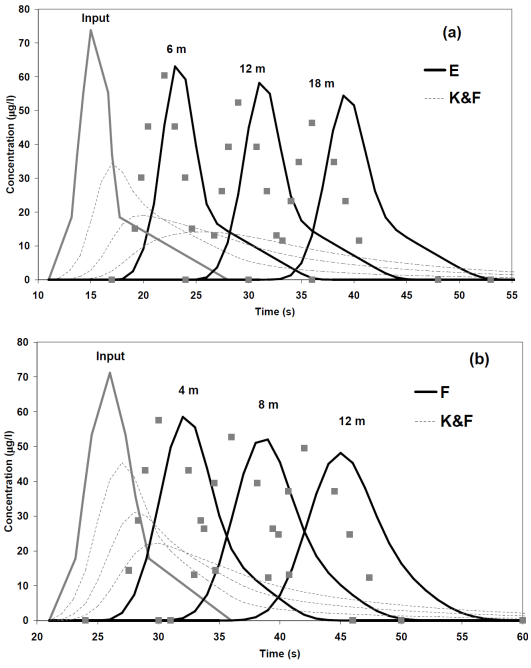
Figure 1 depicts the measured and calculated concentrations at different stations. The performance of one formula depends on the conditions of the experiment. The E formula

Table 2: Flow parameters in Zulfequar's experiments

Exp.	Bed slope	Discharge (m^3/s)	Flow depth (m)	Velocity (m)
Zul1	0.004546	0.01053	0.0700	0.7521
Zul2	0.002470	0.01558	0.1243	0.6267
Zul3	0.001480	0.01442	0.1388	0.5195

yields the best model-data fit for Zul1 and Zul3 experiments with a relative error of peak concentration ΔC^p smaller than 11% and a relative error of phase ΔT^p smaller than 7.5%(T denotes the arrival time of the peak). The F formula provides much better predictions for Zul2 experiment with ΔC^p = 1.7% and ΔT^p = 7.2% (ΔC^p = 4.8% and ΔT^p = 7.2% for the E formula). In general, E and F formulas rank as the best predictors for the entire range of experimental conditions, followed by K&R-M and M formulas. These four formulas produce the same trend as the observed data, but the peak concentration arrives systematically late compared to measurements (with a relative error of phase ΔT^p that does not exceed 8%).

Equations providing the less satisfactory predictions at least for one experiment are M&K, S&C, D and K&F formulas with ΔC^p > 40%, systematically underpredicting concentrations. The arrival time of the peak obtained by M&K formula (ΔT^p < 8.5%) and D formula (ΔT^p < 3.6%) is, however, in good agreement with measurements; less satisfactory predictions are provided by S&C (ΔT^p < 16.3%) and K&F (ΔT^p < 29%) formulas.



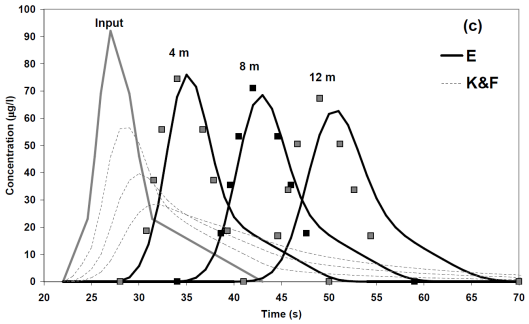


Figure 1. Comparison between computed and measured concentrations at three locations. Symbols= measurements, lines= numerical predictions. (a) Zul1t; (b) Zul2; (b) Zul3

Transport of tritium in the Middle Loire River

Herein, we assess the performance of the formulas by simulating the transport of tritium in the Middle Loire River (France) under unsteady flow conditions during the period July 1st 1999 to December 31th 1999.

The Loire River is the longest river in France with a length of 1012 km. Its drainage area represents 117,000 km^2, that is one fifth of France's area. The reach studied is the Middle Loire River, which extends from Belleville sur Loire to MontJean sur Loire, a linear of 350 km (Fig. 2). This reach has an average width and slope of about 800 m and 0.0004, respectively. The Middle Loire River is characterized by highly variable hydrologic regime: very low discharge during the summer and high magnitude flows in winter and spring. Four main tributary streams feed the river: Vienne, Indre and Cher on the left side and Maine on the right side. Four Nuclear Power Plants (NPP), Belleville, Saint Laurent, Dampierre and Chinon, are located along the Middle Loire River and one NPP, Civaux, is located along the Vienne River. These NPP generate low-activity radioactive liquid waste, including tritium, which is released into the river in a controlled way.

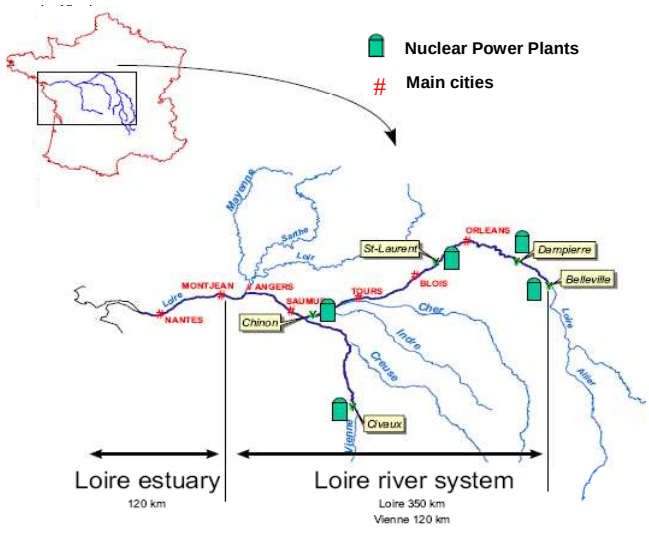


Figure 2. Location map showing the study reach

The Middle Loire River is modeled as one reach with the tributaries Vienne, Indre, Cher and Maine as lateral inflows. The upstream flow rate hydrograph covers the period of July 1st December 31th 1999 with a time step of one hour. The downstream boundary condition is a water stage-flow rate curve. For the solute transport module, the tritium discharge recorded at Belleville NPP during the simulated period with a time step of one hour is specified as the upstream boundary. The tritium releases from Dampierre, Saint Laurent and Chinon NPP on the same period are introduced as lateral injections. The tritium discharge due to release from Civaux NPP is estimated by applying MASCARET to the Vienne River between Civaux NPP and Vienne-Loire junction.

Calibration of the hydraulic module is carried out using measured water level measurements collected along the Middle Loire River at low, medium and high flow discharges. The Strickler coefficient, K_s, is set at 30 $m^{-1/3}/s$. Monitoring of tritium concentration was performed during 1999 at Angers city and used herein for model-data comparison. Finally, the time step in all the numerical runs is 10 s and the space step is 200 m on average.

Figure 3 shows the comparison between the numerical result and measurements at Angers city. The most reliable predictions are provided by S&J formula, which reproduces the magnitude and time-evolution of the concentrations reasonably well; the average relative deviation between the computed and measured values is approximately 43%. This formula is followed by D, K&F formulas with relative errors of 54% and 78%, respectively. The E, M&k and M formulas yield similar predictions, but with much higher relative error (116%) The F and K&R-M formulas display a poor performance; the relative error is particularly high (176%). It should be noted that the performance of the formulas in this case is different from that for the experimental cases of Zulfakar (1997).

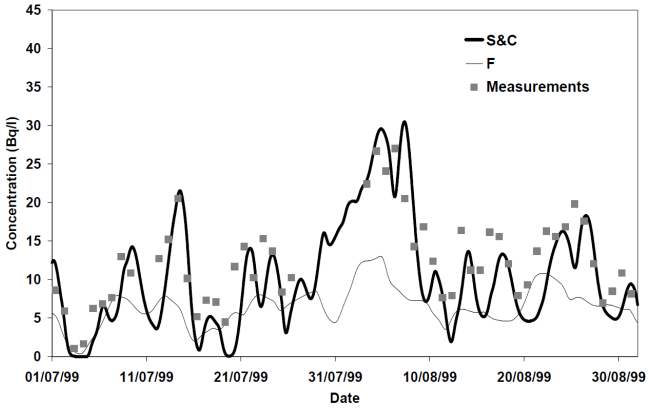
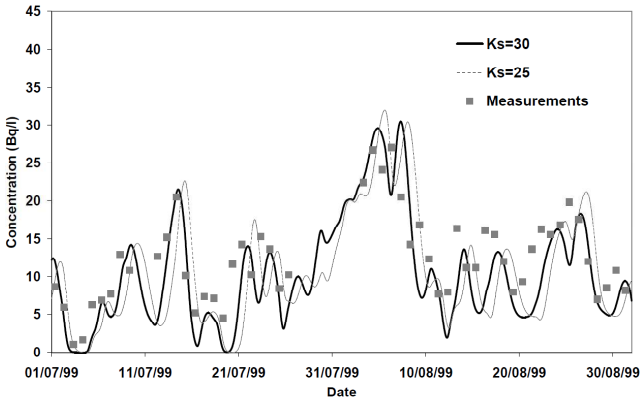


Figure 3: Comparison of model predicted and field observed tritium concentrations at Angers City

Discussion

Previous results showed that for each configuration, better predictions were obtained using a particular formula. However, some discrepancies between measurements and predictions still remain; the best formula does not capture the whole spatial and time variability in concentrations. Apart from the measurements uncertainty, other plausible sources that may impact the numerical predictions include the Strickler coefficient, the space step, and the numerical scheme used for resolving the solute transport equation. To get an insight on the effect of these parameters, additional numerical runs were performed using the Middle Loire case with the S&C formula as baseline run. Performing runs with as pace step of respectively 100 m and 400 m instead of 200 m shows that the predictions are not influenced by he space step; the use of 100 m does not lead to an improvement of the predictions. Regarding the computation of the energy dissipation, we further test a Strickler coefficient Ks of 25 m-1/3/s. The overall model-data fit is slightly affected (Fig 4a); Ks= 30 m-1/3/s provides the best model-data fit. Finally, The numerical treatment of the advection term of the solute transport equation represents the most challenging step of the solution of the advection–diffusion equation. Hence, the sensitivity of the numerical predictions to numerical scheme is evaluated using two additional methods: 2nd order finite volume scheme (FV2) with a superbee limiter function, and method of characteristics (Char.) applied to the conservative form of the advection term. As shown in Fig 4b, the first order finite scheme (FV1) and characteristics method yield similar predictions, slightly different from those given by the 2nd order finite volume scheme (FV2).



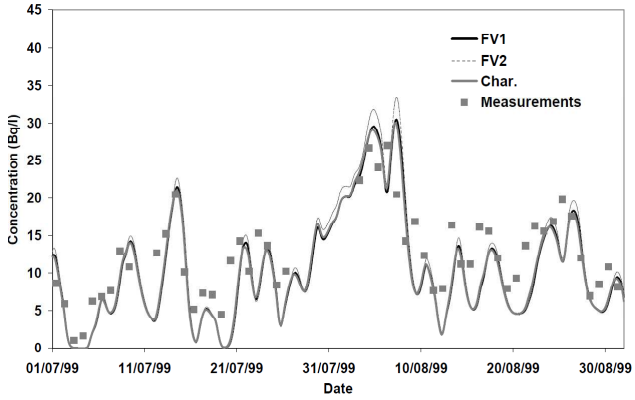


Figure 4: Sensitivity of predictions to changes in (a) Strickler's coefficient, and (b) numerical scheme

Conclusions

The performance of dispersion coefficient formulas was assessed using a 1-D numerical model of flow and solute transport in open channels. The numerical modeling tool, called MASCARET (open source package, http://innovation.edf.com/recherche-et-communaute-scientifique/logiciels/code-mascaret-41197.html), relies on the 1-D shallow water equations and the convection-dispersion equation for the solute transport. We tested eight formulas proposed by Elder (1959), Fisher (1975), McQuivey and Keefer (1974), Magazine et al. (1988), Koussis and Rodriguez-Mirasol (1998), Seo and Cheong (1998), Deng et al. (2001) and Kashefipur and Falconer (2002). Results indicate that the model can predict solute transport in open channels satisfactorily, provided the dispersion coefficient formula is well selected.

Simulating experimental cases of solute transport under steady flow, results show that for each case, better predictions are obtained using a particular formula. Elder (1959) and Fisher (1975) formulas rank as the best predictors for the entire range of conditions of the experiments. In contrast, simulating the transport of tritium in the Middle Loire River over the period of July 1st to December 31th 1999 with highly variable flows, the formula proposed by Seo and Cheong (1998) yields the best predictions. Fisher (1975) and Koussis and Rodriguez-Mirasol (1998) formulas provide the less reliable results.

This work is a first step toward a consistent validation of existing longitudinal dispersion formulas used in 1-D numerical models. Validation of the formulas should be extended to other cases with complex flow regime, cross-sectional geometry (including floodplains, transient storage, hyporheic zones) and reactive pollutants. Nevertheless, the present results highlight how the numerical predictions depend on the formula selected for computing the dispersion coefficient, and more importantly that no "universal" formula can be retained, which have implications for river engineering practice.

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