19th International Conference on
TRANSPORT AND SEDIMENTATION OF SOLID PARTICLES
24-27 September 2019, Cape Town, South Africa

ON THE INFLUENCE OF NUMERICAL METHODS FOR THE ADVECTION DISPERSION MODEL ON ESTIMATED LONGITUDINAL DISPERSION COEFFICIENTS

[1]Davy D. Silavwe, [2]Steve G. Wallis and [3]Isobel C. Brink

[1]Department of Civil Engineering, The Copperbelt University, P.O Box 21692, Kitwe, Zambia: Email: ddsilavwe@cbu.ac.zm; [2]School of Energy, Geoscience, Infrastructure and Society, Heriot-Watt University, Riccarton, Edinburgh, EH14 4AS, UK. Email: s.g.wallis@hw.ac.uk; [3]Department of Civil Engineering, Stellenbosch University, Stellenbosch, Cape Town, South Africa. Email: icbrink@sun.ac.za.

The study concerned the computation of dispersion coefficients for a small stream using numerical solutions of the advection-dispersion model and observed temporal solute concentration profiles. Application of the model to simulate the physical processes of solute transport in streams, in most practical situations, requires the use of a numerical solution with appropriate values of the parameters. The selection of a proper value of the dispersion coefficient is the basic task. Computation of the physical dispersion coefficient using numerical schemes by optimization may include artificial mixing caused by truncation terms. Hence, an error analysis using the modified equation approach complements the results obtained by optimisation. Additionally, the optimisation results can be influenced by the relative significance of the transport processes, characterised by the Peclet number (P_e). Four numerical schemes were used: Back-Time/Centred-Space, Crank-Nicolson, Implicit QUICK and QUICKEST. Optimal parameter values were obtained for several values of P_e by changing the magnitude of the space step. Reference values were obtained using a routing procedure. Optimised dispersion coefficients showed the presence, or absence, of artificial mixing in the numerical solutions in agreement with the error analysis for $P_e < 5.0$. Thus only Crank-Nicolson and QUICKEST were reliable in this range of P_e. To different degrees, all the methods gave unreliable physical dispersion coefficients for P_e values greater than 6.0. None of the schemes is recommended for use at larger P_e: instead, the space step should be reduced so that $P_e < 5$.
KEYWORDS: Dispersion coefficient, artificial mixing, numerical methods, optimisation, Peclet number, modified equation.

NOTATION

C	Concentration (µg/l)
D_n	Numerical dispersion (m^2/s)
K	Physical dispersion coefficient (m^2/s)
K_n	Numerical dispersion coefficient (m^2/s)
P_e	Peclet number
t	Time (s)
Δt	Time step (s)
v	Cross-section average velocity of flow (m/s)
x	Longitudinal coordinate direction (m)
Δx	Space step (m)

ISSN 0867-7964 ISBN 978-83-7717-323-7 DOI 10.30825/4.12-29.2019

1. INTRODUCTION

The advection-dispersion model (AD-model) is investigated by estimating the dispersion coefficient using numerical methods. Various numerical solutions of the AD-model have been proposed using finite difference and finite volume approaches. These solutions have varying properties related to stability, consistency and accuracy (Abbott and Basco, 1989; Versteeg and Malalasekera, 2007), and not all of them are equally suitable (Wallis, 2007; Szymkiewicz, 2010). Basically, numerical methods are derived from a Taylor series expansion and a truncation error is always present. Mathematically, such terms introduce errors commonly known as numerical diffusion and numerical dispersion (Szymkiewicz, 2010). In the context of the application of the AD-model to mixing in rivers, the numerical diffusion enhances the physical dispersion. Since, physically, diffusion and dispersion are different processes, and dispersion has two quite different meanings to mathematicians and water-quality modellers, here we use the term artificial mixing when discussing the effects of numerical diffusion and numerical dispersion.

The numerical errors are also influenced by the numerical grid resolution, which is characterised by numerical properties, namely, the advection number and the dispersion number. Commonly, these properties are characterised in terms of the Peclet number (P_e) which allows one to define the involvement of transport by both advection and dispersion. Numerical problems appear for high values of P_e when the transport is dominated by advection (Abbott and Basco, 1989; Versteeg and Malalasekera, 2007). Therefore, it is important that the properties of a scheme are considered when discretizing the computational domain. In this study, the AD-model was investigated using four Eulerian numerical methods. Also, a routing procedure was used to provide reference values of the physical dispersion coefficient, K. Furthermore, the modified equation approach (Warming and Hyett, 1974; Szymkiewicz, 2010) was used to investigate the presence of artificial mixing in the numerical methods.

2. SOLUTE TRANSPORT MODELLING

This section provides brief background information on the AD-model, the numerical methods used and the modified equation approach.

2.1 THE ADVECTION-DISPERSION MODEL

Mixing in streams is primarily caused by longitudinal dispersion which results from the stretching effect of velocity gradients. In applying the AD-model, the longitudinal dispersion coefficient measures the rate of longitudinal mixing of a solute cloud, and the cross-sectional average velocity defines the rate of downstream movement of the dispersant (Chanson, 2004). Commonly mixing rates and cross-sectional average velocities are assumed constant and the AD-model is written as (Rutherford, 1994),

$$\frac{\partial c}{\partial t} + v\frac{\partial c}{\partial x} - K\frac{\partial^2 c}{\partial x^2} = 0 \qquad (1)$$

The AD-model is applied through its solutions and requires calibration, i.e. estimation of its parameters, v and K (Chanson, 2004). Calibration using a numerical method commonly involves an error, especially in K (Szymkiewicz, 2010). The lack of assessment of the error can result in wrong conclusions about the value of K. Thus, the calibrated value of K may be a combination of its physical value and the error induced by the scheme. Thus, calibration by optimization can result in an incorrect value of the searched K. The issue may be solved if one is able to split the effect of the error from K. Following Warming and Hyett (1974) and Szymkiewicz (2010), the modified equation approach is a helpful tool in this regard. This involves substituting Taylor series expansions into the numerical algorithm and identifying temporal and spatial derivatives that might be a source of numerical error. The approach aims to express the modified AD-model as:

$$\frac{\partial c}{\partial t}+v\frac{\partial c}{\partial x}-K\frac{\partial^2 c}{\partial x^2}=K_n\frac{\partial^2 c}{\partial x^2}+D_n\frac{\partial^3 c}{\partial x^3}+\cdots \qquad (2)$$

The modified AD-model includes additional terms on the right-hand side of Equation (2), which introduce unwanted errors commonly known as numerical diffusion (K_n) and numerical dispersion (D_n). Similar minor errors are introduced by higher order terms. In the application of the model, D_n encourages the appearance of oscillations in numerical solutions (Szymkiewicz, 2010). K_n enhances the physical dispersion causing greater longitudinal spreading (Chapra, 2008, Szymkiewicz 2010). It is important to recognize in the solution the consequences of both K_n and D_n.

Numerical methods are derived by converting the AD-model into algebraic difference equations that can be solved for values not known at incremental points in space and time (Wallis, 2007; Chapra, 2008). Usually, the main challenge is the formulation of an appropriate scheme for the advective contribution to the solution (Versteeg and Malalasekera, 2007; Wallis, 2007). This is influenced by grid discretization which is characterised by non-dimensional numerical properties (Versteeg and Malalasekera, 2007; Wallis, 2007), namely, the advection number, the dispersion number and their ratio, P_e (Abbott and Basco, 1989; Chapra, 2008). P_e $\left(=v\Delta x/K\right)$ defines the relative strength of transport by advection to transport by dispersion. Numerical problems arise for large values of P_e (Szymkiewicz, 2010), depending on the numerical method.

2.2 NUMERICAL SCHEMES

There are several numerical methods depending on the discretisation approach, the solution method and the order of the scheme, which all have an influence on their performance. Despite that the order gives an intuition into its performance, the modified equation approach summarised above is more revealing. In this study, the AD-model was applied using the following four numerical methods: comments on artificial mixing are taken from the results of the modified equation approach given by Silavwe et al. (2019).

The Back-Time/Centred-Space method (BTCS) is a finite difference scheme in which the transported variable at the new time level is evaluated in terms of other unknown variable values at the new time level, requiring the solution of a set of simultaneous

equations. This method is first-order accurate in time and second-order accurate in space and is unconditionally stable (Chapra, 2008; Szymkiewicz, 2010). The method induces numerical diffusion which depends only on the time step and velocity, i.e. $K_n = \nu^2 \Delta t/2$.

The Implicit QUICK method (IQK) is a finite volume approach with control volume face values of the transported variable expressed in terms of an upstream weighted parabolic interpolation and spatial gradients of the transported variable expressed using linear interpolation (Leonard, 1979; Versteeg and Malalasekera, 2007). The scheme is first-order accurate in time and third-order accurate in space. Its implicit nature offers unconditional stability. The scheme induces the same value of numerical diffusion as the BTCS method.

The Crank-Nicolson method (CN) is a finite difference scheme and it employs a centred-time/centred-space approach, in which values of the transported variable at the new time level are evaluated in terms of variable values from both the old and the new time levels, requiring the solution of a set of simultaneous equations. The scheme is second-order accurate in time and space. The scheme is unconditionally stable (Chapra 2008; Szymkiewicz, 2010) and does not induce numerical diffusion.

The QUICKEST (Leonard, 1979) method (QKST) is a finite volume approach like the QUICK method. It uses upstream weighted parabolic interpolation of the QUICK method (Abbott and Basco 1989, Versteeg and Malalasekera 2007). It is an explicit formulation and includes estimated streaming terms to account for advection and dispersion occurring during the time step (Leonard 1979). The scheme is third-order accurate in space but is conditionally stable (Leonard, 1979). The scheme does not induce numerical diffusion: it is also free from numerical dispersion, unlike the other three schemes.

3. TRACER DATA

The data for the study consisted of concentration-time profiles obtained from twelve experiments conducted on the Murray Burn which flows through the Riccarton campus of Heriot-Watt University in Edinburgh, U.K. (Heron, 2015). The experiments consisted of a gulp release of a known mass of Rhodamine WT tracer at an injection site upstream of two sampling sites at which water samples were collected. The samples were analysed using a Turner Designs Model 10 fluorometer (Heron, 2015). The flow rates for the experiments ranged from 0.017 m^3/s to 0.436 m^3/s. However, only three sets representing low (0.036 m^3/s; Experiment 2), medium (0.084 m^3/s; Experiment 4) and high (0.150 m^3/s; Experiment 11) flow rates were used in this study. The main characteristics of the site were, reach length 184 m, mean width 2.40m and mean slope 0.009 (Heron, 2015).

4. PARAMETER ESTIMATION

Analysis of observed concentration profiles with the numerical solutions of the AD-model to estimate the parameters required an inverse modelling technique. The inverse modelling tools were developed in Excel. Parameter estimation involved optimisation by fitting a predicted profile to the measured data points downstream by optimizing ν and K (Silavwe et al. 2019). To investigate the influence of non-dimensional numerical properties the numerical methods were applied to each data set over a range of space steps (4.00 m to 30.667 m), such that optimisation of the model parameters was observed under different

values of the non-dimensional numerical properties. A routing procedure (SB) was used to determine reference values of K (Singh and Beck, 2003). This employs a semi-analytical convolution integral solution of the AD-model. It only yields solutions in the time domain and is subject to temporal integration numerical errors. Nevertheless, its solutions provide a useful guideline for assessing the results of the other methods.

5. RESULTS AND DISCUSSION

All numerical schemes behaved conservatively, and simulations were stable, except for QKST at small space steps. The results obtained from optimisations were concentration simulations, optimised dispersion coefficients and velocities. Concentration simulations were assessed by the sum of squared errors statistic (SSE) evaluated between observed and modelled concentrations at the downstream boundary of the reach.

Figure 1 shows a composite plot of the simulated concentration profiles from all four methods and the observed profile of Experiment 11 for one value of P_e, namely, 9.070. Similar results were observed for Experiments 2 and 4. Figure 1 shows that all simulated profiles are distorted, being characterised by undershoots and more spreading than the observed data, reflecting errors due to numerical dispersion at high P_e. At much lower P_e there was very little difference between the simulated profiles from the four methods.

Figure 2 shows a plot of the SSE against P_e for Experiment 11. Similar results were observed from Experiments 2 and 4. In general, simulation errors increased with increasing P_e for all the numerical methods. Generally, the finite difference methods gave higher simulation errors than finite volume methods. This reflects the order of accuracy of the methods described earlier.

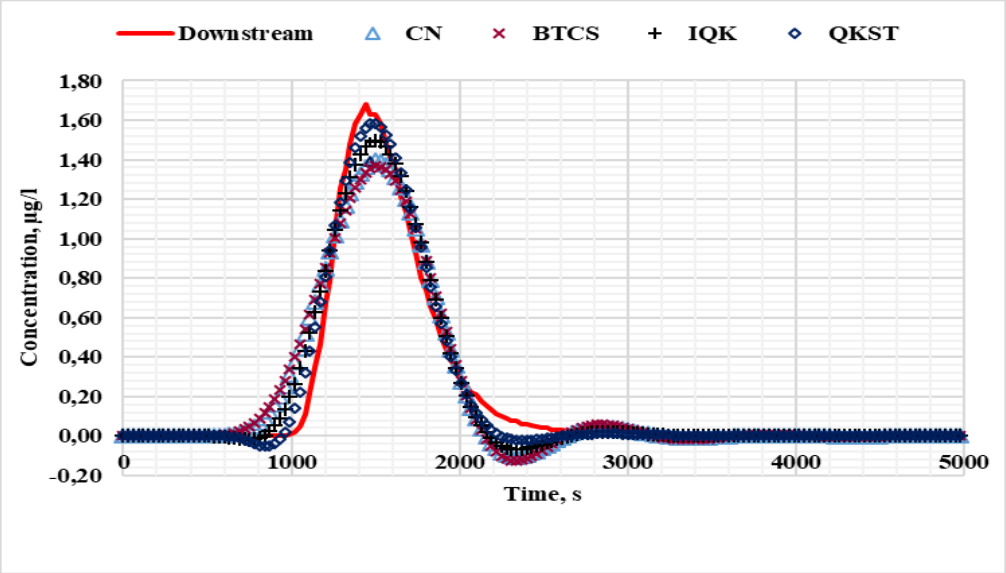

Figure 1. Simulation results for the four numerical methods $P_e = 9.1$, Experiment 11.

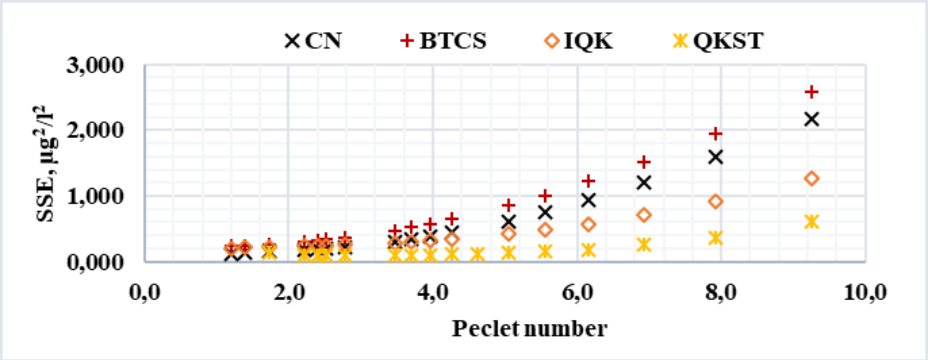

Figure 2. Plot of the sum of squared errors versus Peclet number, Experiment 11.

Figures 3 to 5 show plots of optimized K obtained by all numerical methods against P_e for the three experiments. The figures also show the reference K estimated by the SB routing procedure. It should be noted that the values of P_e were calculated using the parameter values from the SB routing procedure so that results could be easily compared.

It can be observed that for $P_e < 5$, the results fall into two noticeable groups. Here, CN and QKST yield optimised dispersion coefficients that agree closely with that given by the SB routing procedure; BTCS and IQK yield values that are considerably lower. This is consistent with the error analysis of the modified equation approach, which predicts the presence of numerical diffusion (K_n). Table 1 shows the calibrated K values (row 2) and the K_n values (row 4) of the BTCS scheme from Experiment 4. Adding these values give results that are close to the SB routing procedure values. Note that for BTCS and IQK the optimised dispersion coefficient is underestimated even as P_e approaches zero because the numerical diffusion, being dependent on Δt, is always present. For $P_e > 6.0$, estimated K for all numerical methods diverge from the value obtained for $P_e < 5.0$. Those from CN and BTCS show a small increase (due to numerical dispersion) whilst those from IQK and QKST show a large decrease (due to numerical diffusion) in estimated K with an increase in P_e. Silavwe et al. (2019) expands on these issues.

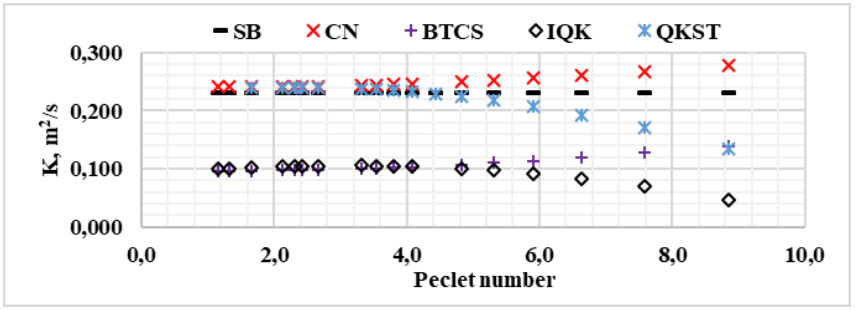

Figure 3. Plot of optimized dispersion coefficients versus Peclet number, Experiment 2.

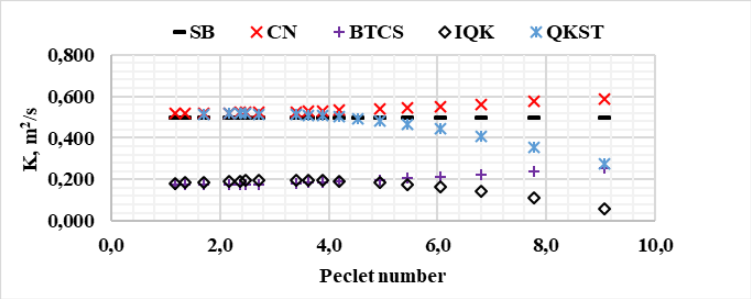

Figure 4. Plot of optimised dispersion coefficient versus Peclet number, Experiment 4.

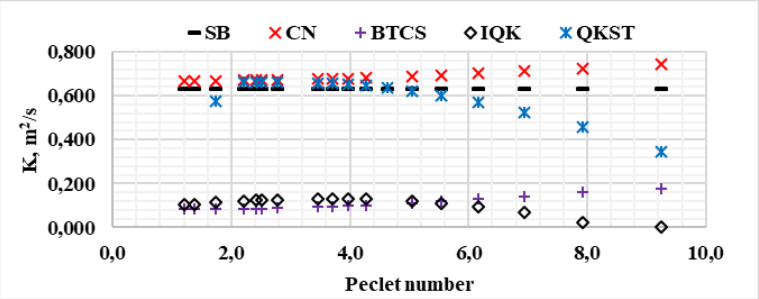

Figure 5. Plot of optimised dispersion coefficient versus Peclet number, Experiment 11.

Table 1

K, ν and K_n for BTCS (Exp. 4, Δt = 30 seconds) for a range of P_e.

Pe	1.2	1.4	1.7	2.2	2.4	2.5	2.7	3.4	3.6	3.9	4.2	4.9	5.4	6.0	6.8	7.8	9.1
K **(m^2/s)**	0.173	0.173	0.173	0.175	0.175	0.176	0.177	0.181	0.183	0.186	0.189	0.199	0.205	0.214	0.225	0.238	0.254
v **(m/s)**	0.150	0.150	0.151	0.151	0.151	0.151	0.152	0.153	0.153	0.153	0.154	0.155	0.156	0.157	0.158	0.160	0.162
K_n **(m^2/s)**	0.339	0.340	0.341	0.343	0.344	0.344	0.345	0.349	0.351	0.353	0.355	0.360	0.364	0.369	0.376	0.384	0.396

6. CONCLUSION

Four numerical methods of the AD-model were applied to observed solute concentration data from three tracer experiments under similar grid resolutions. Optimal dispersion coefficients and velocities were computed over a range of P_e; from 1.2 to 9.1. The behaviour of the methods was generally consistent with the known presence or absence of artificial mixing (derived from the modified equation approach). In this regard, numerical diffusion in BTCS and IQK significantly reduced the computed dispersion coefficient for P_e < 5, whilst computations with CN and QKST, which contain no

numerical diffusion, produced reliable optimised dispersion coefficients in the same P_e range. For $P_e > 6$ results from all methods were poor with errors becoming more prominent with increasing P_e, this being generally consistent with the predictions of the modified equation approach at high P_e. For high P_e optimised dispersion coefficients for CN and BTCS increased from the values in the lower P_e range (due to numerical dispersion) whilst those from IQK and QKST showed a substantial decrease from the values in the lower P_e range (due to numerical diffusion). Consequently, only the CN and QKST schemes are recommended for use for $P_e < 5$. None of the schemes is recommended for use at larger P_e: instead, the space step should be reduced so that $P_e < 5$.

REFERENCES

1. Abbott, M.B., Basco, D.R., 1989. Computational fluid dynamics: an introduction for engineers, Longman Scientific & Technical, Harlow, UK.
2. Chanson, H. 2004. Environmental hydraulics for open channel flows, Elsevier, Oxford, UK.
3. Chapra, S.C., 2008. Surface water-quality modelling, Waveland Press, Long Grove, Ill, USA
4. Heron, A.J., 2015. Pollutant transport in rivers: estimating dispersion coefficients from tracer experiments. MPhil Thesis, Heriot-Watt University, Edinburgh, UK.
5. Leonard, B.P., 1979. A stable and accurate convective modelling procedure based on quadratic upstream interpolation. Comput Method Appl M 19:59–98.
6. Rutherford, J.C. 1994. River mixing, Wiley, Chichester, UK.
7. Silavwe, D.D., Brink, I.C., Wallis, S.G., 2019. Assessment of some numerical methods for estimating the parameters of the one-dimensional advection-dispersion model. Acta Geophysica, 67, 999-1016.
8. Singh, S.K., Beck, M.B. 2003. Dispersion coefficient of streams from tracer experiment data. J Env Eng, ASCE 129:539–546.
9. Szymkiewicz, R., 2010. Numerical modelling in open channel hydraulics, Water Science and Technology Library 83, Springer.
10. Versteeg, H.K., Malalasekera, W., 2007. An introduction to computational fluid dynamics: the finite volume method, Pearson Education Ltd, Harlow, UK.
11. Wallis, S.G., 2007. The numerical solution of the advection-dispersion equation: a review of some basic principles. Acta Geophys 55:85–94.
12. Warming, R.F., Hyett, B.J., 1974. The modified equation approach to the stability and accuracy analysis of finite-difference methods. Journal of Computational Physics 14, 159-179.