Asian Journal of Water, Environment and Pollution, Vol. 4, No. 2, pp. 11-15.

Water Quality Modelling by Numerical Solution of ADE Using An Integrated Model

S.M. Kashefipour*, A.A. Tavakoli and R.A. Falconer[1]

Water Sciences Engineering Faculty, Shahid Chamran University, Ahwaz, Khozestan, Iran
[1]Civil Engineering Department, Cardiff University, Cardiff, Wales, UK
✉ Kashefipour@excite.com

Received May 10, 2006; revised and accepted February 18, 2007

Abstract: Sediment and solute transport processes are the most important existing problems in the coastal, estuarine and riverine waters. Prediction of these processes may be carried out using the numerical solution of the partial differential and dynamic Advective–Diffusion Equation (ADE). The type of the numerical solution is considerably effective on the stability and accuracy of the solution. In this paper an integrated new and effective scheme has been presented, combining two different numerical methods including ULTIMATE QUICKEST (UQ) and finite difference central scheme for solving ADE. This integrated model was verified using a standard example, and was then successfully applied to predict the suspended sediment concentrations in the Humber river (UK).

Key words: Numerical modelling, sediment and solute transport, ULTIMATE QUICKEST scheme, advective diffusion equation.

Introduction

One of the main concerns amongst the current problems in riverine and estuarine waters is sediment and solute transport processes and the negative impacts of these processes on the local habitat. Deposition of fine sediments along rivers and riverine deltas cause a restriction to navigation and can exacerbate flooding problems. Moreover, high sediment concentrations can be effective on high turbidity levels and as a result reducing light penetration. The cohesive sediments are also the main factor for transporting heavy metals, which are mostly poisonous materials for the environments. Biological pollutants such as different types of coliform may have considerable negative effects on the coastal and river environments and also on human health. Consideration of all of the above mentioned problems, caused by sedimentation, erosion and solute transport, highlights the importance of being able to predict sediment and solute transport processes in natural and artificial channels.

Numerical models provide a valuable tool for predicting flow, pollutant and sediment transport processes and are increasingly applied by river engineers and environmental managers. Accurate numerical model predictions of sediment and/or pollutant concentrations can assist in the planning, design and management of the structures related to the river basins and irrigation and drainage networks. Since numerical models provide only an approximate solution to the governing partial differential equations involved, the accuracy, stability and flexibility of the solution would be very important. Using the higher order finite difference accurate schemes has become popular. However, for the advective dominant flows, numerical oscillations may occur in regions of high concentration gradients (for example near sewer outfalls) resulting in unrealistic phenomenon, arising in the form of negative concentrations. One way to eliminate these numerical oscillations is to apply a limiter function to bind the solution (Cahyono, 1992), with this being added

* Corresponding Author

to a highly accurate scheme, such as QUICKEST for solving ADE (Leonard, 1979). Leonard (1991) introduced a limiter, namely ULTIMATE and added to the QUICKEST scheme to bind the numerical solution. Lin and Falconer (1997) applied this scheme in two dimensions to tidal currents. In this paper a new integrated method is introduced combining a central finite difference method (Crank-Nicklson Method) and UQ scheme (Abbott and Basco, 1997).

Numerical Solution of Governing Equations

The 1D unsteady continuity and momentum Saint Venant equations are usually applied to predict velocity, discharge and the other hydraulic parameters (Cunge et al., 1980). These parameters are used in the ADE. Since this research study focused on the numerical solution of the ADE, the Saint Venant equations are not described in this paper.

The 1D unsteady and general form of the ADE may be written as (Kashefipour, 2002):

$$\frac{\partial CA}{\partial t}+\frac{\partial CQ}{\partial x}-\frac{\partial}{\partial x}AD_{\mathrm{x}}\frac{\partial C}{\partial x}=S+\frac{Q_{\mathrm{L}}C_{\mathrm{L}}}{\Delta x} \tag{1}$$

where C = cross-sectional average of sediment or solute concentration, Q = discharge, A = flow cross-section, D_{x} = longitudinal dispersion coefficient, S = source or sink term, Q_{L} = lateral inflow or outflow, C_{L} = sediment or solute concentration of lateral flow, t = time and x = coordinate axis of flow direction. More details about the dispersion coefficients, source and sink terms may be found in Kashefipour and Falconer (2002) and Falconer et al. (2005) respectively. Numerical solution of Equation (1) may be written in the form of:

$$\begin{aligned}&\frac{1}{\Delta t}\left[(CA)_{\mathrm{i}}^{\mathrm{n+1}}-(CA)_{\mathrm{i}}^{\mathrm{n}}\right]\\
&+\frac{1}{\left(x_{\mathrm{i+1/2}}-x_{\mathrm{i-1/2}}\right)}\begin{bmatrix}\theta\left(M_{\mathrm{i+1/2}}^{\mathrm{n+1}}-M_{\mathrm{i-1/2}}^{\mathrm{n+1}}\right)+(1-\theta)\\ \left(M_{\mathrm{i+1/2}}^{\mathrm{n}}-M_{\mathrm{i-1/2}}^{\mathrm{n}}\right)\end{bmatrix}\\
&-\frac{1}{\left(x_{\mathrm{i+1/2}}-x_{\mathrm{i-1/2}}\right)}\begin{bmatrix}\theta\left(N_{\mathrm{i+1/2}}^{\mathrm{n+1}}-N_{\mathrm{i-1/2}}^{\mathrm{n+1}}\right)+(1-\theta)\\ \left(N_{\mathrm{i+1/2}}^{\mathrm{n}}-N_{\mathrm{i-1/2}}^{\mathrm{n}}\right)\end{bmatrix}\\
&=S_{\mathrm{i}}^{\mathrm{n+1}}+\left(\frac{Q_{\mathrm{L}}C_{\mathrm{L}}}{\Delta x}\right)_{\mathrm{i}}^{\mathrm{n+1}}\end{aligned} \tag{2}$$

where $M = CQ$, $N = AD_{\mathrm{x}}\frac{\partial C}{\partial x}$ and $=\theta$ weighing coefficient for splitting the spatial derivatives at the upper and lower time levels. It is clear from Equation (2) that the numerical solution is based on the Crank-Nickelson method, which is an implicit scheme and unconditionally stable. The accuracy of this method is first and second order in time and space respectively. The main disadvantage of this method is numerical oscillation that generally occurs where the sediment or pollutant concentration gradient is high. The QUICKEST scheme is an explicit finite volume method and is third order accurate both in time and space. However, this scheme is only stable for the Courant numbers equal or less than unity (Leonard, 1979).

In the current paper the concentrations at the points $i + 1/2$ and $i - 1/2$, and the faces of a control volume centralised around the node i, were estimated using the ULTIMATE QUICKEST (UQ) scheme. This new scheme, which is a combination of two implicit and explicit schemes, remains implicit and unconditionally stable and also its accuracy is similar to UQ without any numerical oscillations. Therefore, this scheme has the advantages of the UQ and FTCS (Forward in Time and Central in Space) schemes simultaneously.

The coefficient θ plays an important role in stability and accuracy of the solution. According to the amount of Courant number (C_{r}) the stability and accuracy of the model can be controlled by adjusting the amount of θ. The results obtained from this model for the Courant numbers less than unity are very similar to the highly accurate UQ scheme. For the Courant numbers greater than unity the model remains stable and accurate.

Model Application for a Standard Example

Numerical schemes are generally verified using a standard example. Given steady uniform flow with no diffusion, and source or sink term assumed (pure advection). Equation (1) will be turned to the following equation:

$$\frac{\partial C}{\partial t}+U\frac{\partial C}{\partial x}=0 \tag{3}$$

where U = cross-sectional average velocity. The analytical solution of this partial differential equation exists. Thus the results obtained from the proposed model can be compared with the analytical solution. In this example the initial sediment or solute concentrations are assumed with very high spatial gradients, as shown in Figure 1. Since no diffusion is assumed, it is theoretically expected that the amount and magnitude of the concentrations remain constant and the plume forms downstream with

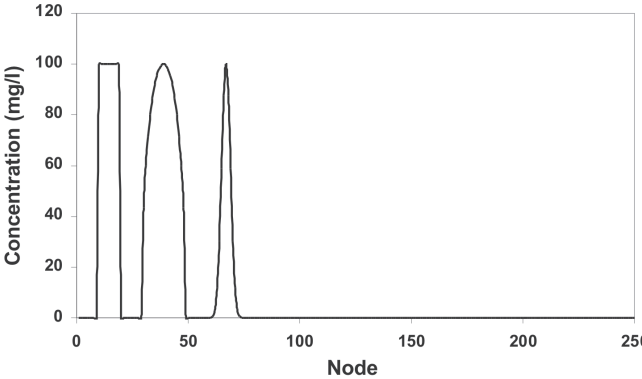

Figure 1: Initial Condition for the standard example.

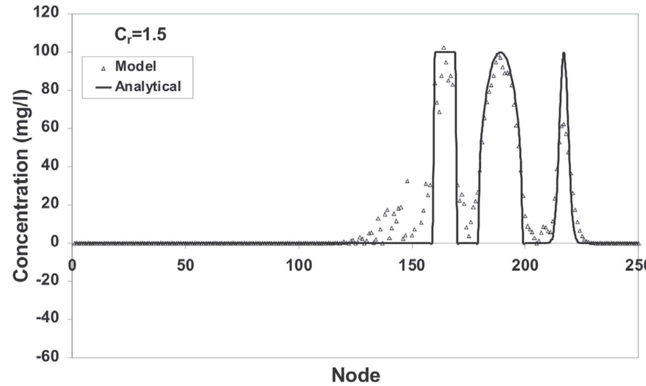

Figure 3: Comparison of the proposed model with the analytical solution for C_r = 1.5.

the same shape of the initial conditions. For a constant Δx after m time steps the plume moves downstream for mC_r nodes, where $C_r = U\dfrac{\Delta t}{\Delta x}$ (Courant number). The analytical solution of Equation (3) has been shown in Figure 2, in which $C_r = 0.5$ and $m = 100$. The results obtained from the implicit central finite difference method ($\theta = 0.5$) and the proposed model are also shown in this figure. As can be seen from this figure, the proposed model was able to accurately estimate the high gradient concentrations without any oscillations. It should be noted that the UQ scheme is as accurate as the proposed model. However, the UQ scheme is only stable for the Courant numbers less than unity, whereas the proposed model remains stable and accurate for Courant numbers more than unity. Figure 3 compares the results obtained from the proposed integrated model and the analytical solution for the $C_r = 1.5$, $m = 100$ and $\theta = 0.05$. This figure shows the accuracy of the model for Courant numbers more than unity. The results obtained from the model for the Courant numbers of 0.5, 1.0 and 1.5 are compared with

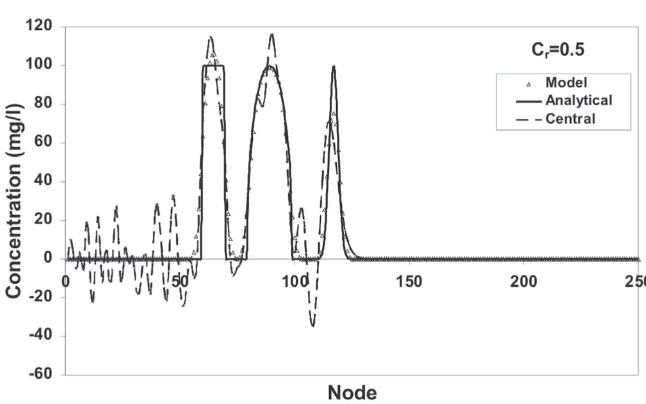

Figure 2: Comparison of the proposed model and central scheme with the analytical solution for C_r = 0.5.

analytical solution using Equation (4). According to this equation for the accurate predictions the coefficient α should be close to unity with a high correlation coefficient (close to unity). The α coefficients and R^2 are computed for the Courant numbers equal to 0.5, 1.0 and 1.5 and are mentioned in Table 1.

$$C_m = \alpha C_P \tag{4}$$

where C_m = measured concentration and C_P = predicted concentration.

Table 1: Comparison of the proposed model and analytical solution using Equation (4)

C_r	α	R^2
0.5	1.028	0.950
1.0	1.019	0.996
1.5	1.058	0.920

Model Application

The proposed integrated model was added to a 1-D hydrodynamic model namely FASTER (Flow and Solute Transport for Estuaries and Rivers), which was developed by the first author (Kashefipour, 2002), and applied for the Ribble river basin to predict the faecal coliform concentrations along the basin. Ribble river and its tributaries are located in the north west of England, UK. More information about the Ribble river modelling may be found in Kashefipour et al. (2002).

The model was also applied to Humber river which is located in the north east of England (Figure 4) for predicting suspended sediment concentrations. The predicted suspended sediment concentrations at a survey point are compared with the corresponding measured

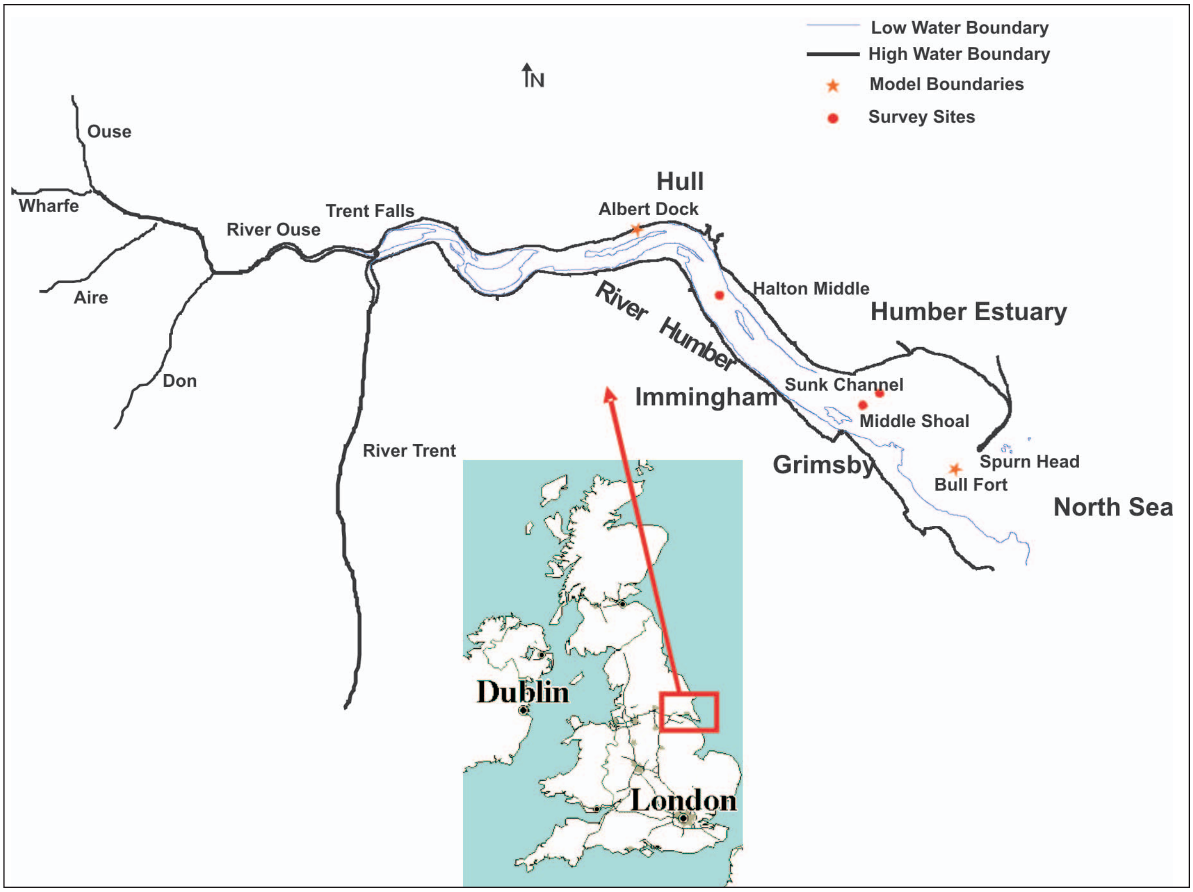

Figure 4: Humber river.

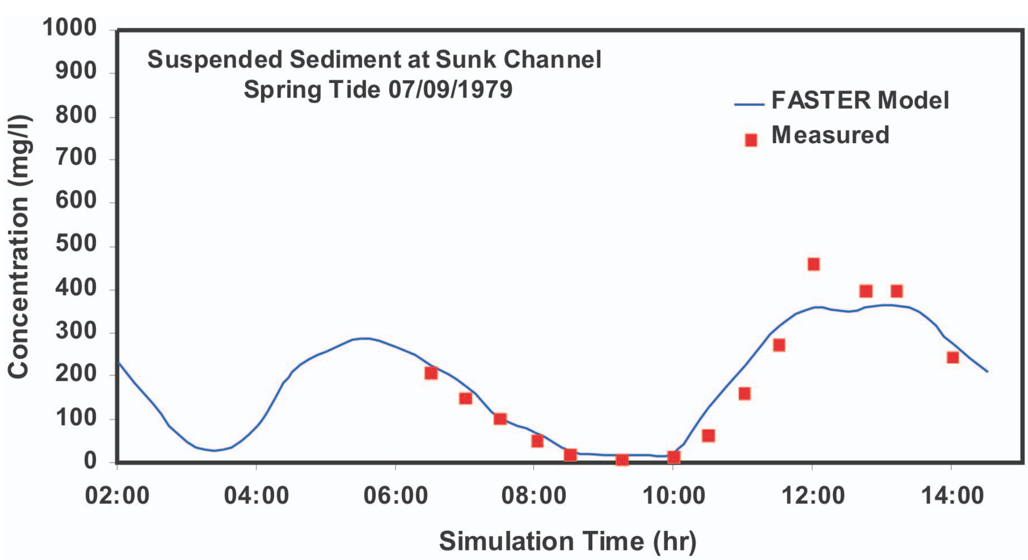

Figure 5: Application of the model for Humber: Comparison of the measured and predicted suspended sediment concentrations.

values in Figure 5. As can be seen from this figure the model was able to accurately predict sediment concentrations. More details relating to these two applications may be found in Kashefipour (2002).

Conclusions

This paper describes the development of an integrated numerical method in which an implicit finite difference central scheme was combined with the ULTIMATE QUICKEST (UQ) scheme. The final model was implicit and unconditionally stable, and the concentrations of the faces of the control volumes centralised around the node i ($i + 1/2$, $i - 1/2$) were computed using the UQ scheme. A coefficient was also applied to split the spatial derivatives on the upper and lower time levels. The stability and accuracy of the model was controlled by this coefficient. Therefore, the model was accurate and stable for the Courant numbers more than unity without any oscillations for the high gradient concentration regions. The model was verified using a standard numerical example and then was successfully applied to the Ribble river basin for predicting faecal coliforms and to the Humber river for predicting suspended sediment concentrations.

References

Abbott, M.B. and D.R. Basco (1997). Computational Fluid Dynamics: An introduction for engineers. Longman Singapore Publishers (Pte) Ltd.

Cahyono (1992). Three-dimensional Numerical Modelling of Sediment Transport Processes in Non-Stratified Estuarine and Coastal Waters. PhD Thesis, University of Bradford, UK.

Cunge, J.A., Holly, F.M. Jr and A. Verwey (1980). Practical Aspects of Computational River Hydraulics. Pitman Publishing Limited, London.

Falconer, R.A., Lin, B. and S.M. Kashefipour (2005). Modelling Water Quality processes in estuaries. *In:* Computational Fluid Dynamics: Applications in Environmental Hydraulics, P.D. Bates, S.N. Lane and R.I. Ferguson, pp. 305-328.

Kashefipour, S.M. (2002). Modelling Flow, Water Quality and Sediment Transport Processes in Riverine Basins. PhD Thesis, University of Cardiff, UK.

Kashefipour, S.M., Lin, B., Harris, E. and R.A. Falconer (2002). Hydro-environmental Modelling for Bathing Water Compliance of an Estuarine Basin. *Water Research*, **36:** 1854-1868.

Kashefipour, S.M. and R.A. Falconer (2002). Longitudinal Dispersion Coefficients in Natural Channels. *Water Research*, **36:** 1596-1608.

Leonard, B.P. (1979). A Stable and Accurate Convective Modelling Procedure Based on Quadratic Upstream Interpolation. *Computer Methods in Applied Mechanics and Engineering*, **19:** 59-98.

Leonard, B.P.(1991). The ULTIMATE Conservative Difference Scheme Applied to Unsteady One-dimensional Advection. *Computer Methods in Applied Mechanics and Engineering*, **88:** 17-74.

Lin, B. and R.A. Falconer (1997). Tidal Flow and Transport Modelling Using ULTIMATE QUICKEST Scheme. *Journal of Hydraulic Engineering*, **123(4):** 303-314.

Asian Journal of Water, Environment and Pollution

Volume 1 Number 1 & 2 **July – December, 2004**

Contents