# Finite difference TVD scheme for modeling two-dimensional advection-dispersion

Y. Guan
*College of Water Resources and Environment, Hohai University, Nanjing, China*

D. Zhang
*Moe's Key Laboratory of Water Resources Development, Hohai University, Nanjing, China*

**Abstract**: This paper describes the development of the stream-tube based dispersion model for modeling contaminant transport in open channels. The operator-splitting technique is employed to separate the 2D contaminant transport equation into the pure advection and pure dispersion equations. Then the total variation diminishing (TVD) schemes are combined with the second-order Lax-Wendroff and third–order QUICKEST explicit finite difference schemes respectively to solve the pure advection equation in order to prevent the occurrence of numerical oscillations. Due to various limiters owning different features, the numerical tests for 1D pure advection and 2D dispersion are conducted to evaluate the performance of different TVD schemes firstly, then the TVD schemes are applied to experimental data for simulating the 2D mixing in a straight trapezoidal channel to test the model capability. Both the numerical tests and model application show that the TVD schemes are very competent for solving the advection-dominated transport problems.

## INTRODUCTION

To predict the contaminant transport in open channel flows, either the analytical or the numerical solutions can be applied. The analytical solution is suitable for straight channels with uniform flow conditions. For natural rivers with such complex geometries as the irregular cross-sections and channel bends, it is impossible to apply the analytical solution. Therefore, it is essential to develop the numerical models for modeling the mixing problems in open channels.

There exist a number of numerical models ranging from the complex 3D to the relatively simple 1D. 1D models are suitable for fully mixing problems over the cross-sections, but inaccurate for the larger river simulations. In addition, 3D models are not favorable for the practical engineering uses due to requiring more input data and computer resources. Therefore the 2D models might be appropriate for simulating the pollutant distribution over the downstream sections. However, due to lacking of secondary flow data in most natural rivers, difficulty arises for calibrating 2D dispersion models. Consequently, 2D advection-dispersion equation has to be further simplified so that it could be probably applied for the practical engineering problems. One popular method for the simplification is using the concept of cumulative discharge to transform the 2D dispersion equation into a simple stream-tube based dispersion model, which the transverse advection term disappeared, but is implicitly considered in the modified lateral dispersion term (Holly, 1975; Guan and Zhang, 2004).

To solve the advection-dispersion equation numerically, the operator-splitting approach is firstly used, and then the Eulerian finite difference method is employed. It is well known that the accurate solution can be easily achieved using central difference scheme for solving the dispersion dominated transport problems, but for the advection dominated problems, numerical diffusions and numerical oscillations are often observed by using most classical numerical schemes. Hence, the accuracy for solving the advection-dispersion equation depends on the application of numerical advection schemes. It is demonstrated that lower order upwind finite difference method is monotonic preserving, but inherent numerical diffusion in its solution (Guan and Zhang, 2004). In contrast, high order methods are more accurate, but produce the numerical oscillations in the solutions because they are no longer monotonic. Moreover, high order methods have difficulty for treating the boundary problems due to more points involved in the interpolations. To combat the unphysical oscillations, the TVD algorithms have been proposed to discrete the strong advection problems, which have been widely applied for the simulation of discontinuity problems. However, there is little investigation on the features of different limiters for modeling the contaminate transport problems.

The purpose of this paper is to investigate the performance of several TVD schemes for modeling the advection-dominated transport problems. First the operator-split approach is employed to separate the advection-dispersion equation into several sub-equations, and then each part is solved using the most suitable numerical scheme. Third, the numerical studies are carried out for the advection dominated 1D and 2D transport problems in order to test features of different TVD schemes, and the performance of different schemes is discussed. The proposed numerical models are also applied to the dispersion experiments to assess the model capability and finally the primary conclusions are drawn.

## 1 GOVERNING EQUATION

The depth-averaged advection-dispersion by using the concept of stream tube in the natural curvilinear coordinate system is written as (Guan et al., 2002):

$$\frac{\partial C}{\partial t}+\frac{U}{h_x}\frac{\partial C}{\partial x}=\frac{1}{Hh_xh_y}\frac{\partial}{\partial x}(\frac{h_y}{h_x}HK_x\frac{\partial C}{\partial x})+\frac{U}{h_x}\frac{1}{Q^2}\frac{\partial}{\partial \eta}(h_xH^2UK_\eta\frac{\partial C}{\partial \eta}) \tag{1}$$

where U is the longitudinal velocity; t is time; C is the contaminant concentration; H is the flow depth; Q is the total discharge of channel; $h_x$ and $h_y$ are the metric coefficients in the longitudinal and transverse directions, respectively; $K_x$ and $K_y$ are the dispersion coefficients in the longitudinal and transverse directions, respectively. For straight channels, $h_x$ and $h_y$ will be unity. The dispersion coefficients can be determined as function of water depth and friction velocity, $K_x = D_xHU_*$ and $K_y = D_yHU_*$; $D_x$ and $D_y$ are the dimensionless mixing coefficients in the longitudinal and transverse directions, respectively. $D_x$ and $D_y$ have to be calibrated.

## 2 NUMERICAL METHOD

To solve the 2D dispersion equation numerically, it requires the numerical methods to be accurate and stable. To meet this goal, the operator-split approach is commonly used for solving the practical mass transport problems (Holly, 1975; Luk et al., 1990). The idea of the split-operator approach is that it separates the 2D advection dispersion equation into the pure advection and pure dispersion sub-equations according to the physical processes; then solves each sub-equation by using the most accurate and efficient numerical methods. If the source and sink terms are not considered, the resulted pure advection and dispersion equations can be expressed as follows according to Guan et al. (2002):

$$\frac{\partial C}{\partial t}+\frac{U}{h_x}\frac{\partial C}{\partial x}=0 \tag{2a}$$

$$\frac{\partial C}{\partial t}=\frac{1}{Hh_xh_y}\frac{\partial}{\partial x}(\frac{h_y}{h_x}HK_x\frac{\partial C}{\partial x}) \tag{2b}$$

$$\frac{\partial C}{\partial t}=\frac{U}{h_x}\frac{1}{Q^2}\frac{\partial}{\partial \eta}(h_xH^2UK_\eta\frac{\partial C}{\partial \eta}) \tag{2c}$$

In 2D shear flows, the longitudinal dispersion will play minor role compared with the longitudinal advection for the transient mixing problems. Therefore, this term can be ignored in the calculation (Luk et al. 1990).

## 3 ADVECTIVE SCHEMES

The numerical approximation for the 1D pure advection equation by using the explicit finite difference method is written in the flux form (Guan and Zhang, 2004)

$$C_i^{n+1}=C_i^n-\alpha_{i+1/2}^nC_r^n+\alpha_{i-1/2}^nC_l^n \tag{3}$$

where $\alpha(x,t)=U\Delta t/\Delta x$ is the Courant number. $s_r$ and $s_l$ are the concentration values at the right and left flux faces, respectively (Fig. 1). They can be determined by explicitly interpolating the concentration values defined at the center of the staggered grid to the flux faces.

The simplest method to approximate the flux value is the first-order upstream interpolation, which is mass conserving, positive and monotonic. It provides stable solution if the Courant number less than unity. But it is inherent of strong numerical diffusion (Guan and Zhang, 2004). The second–order quadratic upwind scheme and other high-order schemes are more accurate, but produce spurious oscillations. In the present study, the Lax-Wendroff scheme and QUICKEST scheme with different flux limiters are applied to solve the advection equation and described in the following subsections.

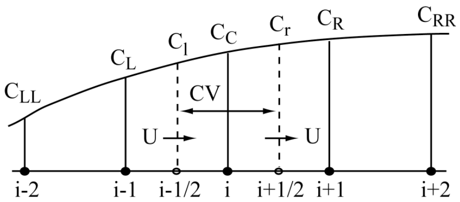


Figure 1. Definition of the control volume

### 3.1 *The TVD Lax-Wendroff scheme*

The Lax-Wendroff scheme is second-order in space and in time. This method often generates the unphysical oscillations in the solutions. Such unphysical oscillation can be interpreted as a poor choice of slopes near the steep gradients. Therefore, suitable slope limiters can be used to eliminate these oscillations and produce the TVD scheme. For the right face value of control volume, the TVD Lax-Wendroff scheme can be expressed in the following flux form

$$C_r = C_i - \phi_i \frac{1}{2}(1-\alpha_{i+1/2})(C_{i+1} - C_i) \quad (4)$$

where $\phi_i$ is the flux limiter function, which plays an important role in obtaining the monotonic solutions. Certainly, the flux form equation can be taken as the lower first-order upwind scheme plus a high order scheme with limiter. The limiter is supposed to be some sort of function of the regularity of the solution. As a measure of the regularity, the following function is employed

$$r = (C_i - C_{i-1})/(C_{i+1} - C_i) \quad (5)$$

which is called the monotonic monitor. It is apparently that the resulted scheme will be the first-order upwind TVD scheme in case $\phi_i = 0$. If $\phi_i = 1$, it is the Lax-Wendroff non-TVD scheme. If $\phi_i = r$, it is Beam-Warmer scheme. Various oscillation free methods can be achieved by applying a series of limiters. For modeling the hyperbolic equation, the most widely used limiters are the Roe's Superbee limiter, the Minmod limiter, the Woodward limiter, the monotonic limiter of Van Leer, the MUSCL limiter of Van Leer, and et al. It is clearly that a monotonic finite difference method is of TVD property. Certainly, a TVD finite difference method is monotonic preserving and prevents the spurious oscillations.

The flux limiter can be defined as function of r. The Superbee limiter of Roe is defined as

$$\phi_i = \max[0, \min(2r,1), \min(r,2)] \quad (6)$$

in which contains three terms. When Roe's Superbee limiter is used with the second-order LW scheme, the resulting scheme is monotonic preserving because the flux limiter eliminates the nonphysical oscillations present with the LW scheme. Furthermore, the Roe's Superbee limiter is over compressive and is excellent for surface scalar markers.

The Minmod limiter of Roe is expressed as (Harten, 1983).

$$\phi_i = \max(0, \min(1, r)) \quad (7)$$

The Minmod method is diffusive and slow to converge. However, both Minmod and Superbee limiters produce similar results. The monotonic limiter of Van Leer is given as

$$\phi_i = (r + |r|)/(1 + r) \quad (8)$$

The Woodward limiter is expressed as

$$\phi_i = \max[0, \min(2, 2r, 0.5(1 + r))] \quad (9)$$

The MUSCL limiter is similar as the Woodward limiter and defined as

$$\phi_i = \max[0, \min(2, 2r), 0.5(1+r)] \tag{10}$$

These limiters are considerably simple; as a result, they are often used for solving the advection problems. In addition, since $\phi$ determines the value of the anti-diffusion flux, different limiters result in different diffusion. The Minmod and Superbee limiters are the most and least diffusive of all acceptable limiters, respectively. Other limiters lie in between.

### 3.2 *The TVD QUICKIEST scheme*

The QUICKEST scheme was proposed by Leonard (1979), and is third order in space and in time. The interpolation of right face value of control volume using QUICKEST method is

$$C_r = \frac{1}{2}(C_i + C_{i+1}) - \frac{1}{2}\alpha_{i+1/2}(C_{i+1} - C_i) - \frac{1}{6}(1-\alpha_{i+1/2}^2)(C_{i-1} - 2C_i + C_{i+1}) \tag{11}$$

It is stable for simulating strong advection problems because it is third order in time. As previously motioned, the high-order QUICKEST scheme is not monotonic and produces wiggles in the vicinity of abrupt gradient change. The TVD scheme, therefore, have to be applied for the numerical dispersions. In this study, the ULTIMATE universal flux limiter designed by Leonard (1991) for arbitrary high order numerical schemes is combined with the QUICKEST scheme to solve the advection equation. The ULTIMATE has been widely used in mass transport simulations (Guan and Zhang, 2004). For more information about ULTIMATE, it can be found in Leonard (1991).

## 4 NUMERICAL TESTS

To further investigate the numerical properties of different TVD schemes, the numerical tests are carried out. The numerical results depicting various numerical algorithms listed in the previous section with several test problems are presented in this section.

### 4.1 *Test for 1D pure advection*

The numerical experiment for 1D pure advection case is performed in a 2m wide rectangular channel with a uniform flow depth of 15 cm and a mean velocity of 0.5m/s. One typical concentration profile was specified as the initial condition which consists of a step profile, $c(x,0) = 10$ for $5\Delta x \le x \le 35\Delta x$, and a sine-squared profile, $c(x,0) = 10\sin^2[(\pi x)/(20x)]$ for $60\Delta x \le x \le 80\Delta x$.

The results at 360s for the grid and time spaces of 1m and 0.4s are shown in Fig. 2. It is clearly seen that the QUICKEST scheme shows some overshoots and undershoots near the discontinuity regions; moreover, the LW scheme not only produces the errors of damping at the peak value of concentration, but also generates significant phase errors. The TVD QUICKEST scheme improves a lot over the QUICKEST to achieve the oscillation free solutions. The TVD LW schemes display similar numerical performance of the limited QUICKEST scheme. However, the Superbee limiter is more suppress and the Minmod is more diffusive. It is shown that the Monotonic, Woodward and MUSCL range between the Superbee and Minmod. Therefore, only the ULTIMATE QUICKEST, the Superbee, Minmod and Woodward limiters with LW are used in the further investigations to illustrate the performance of TVD schemes.

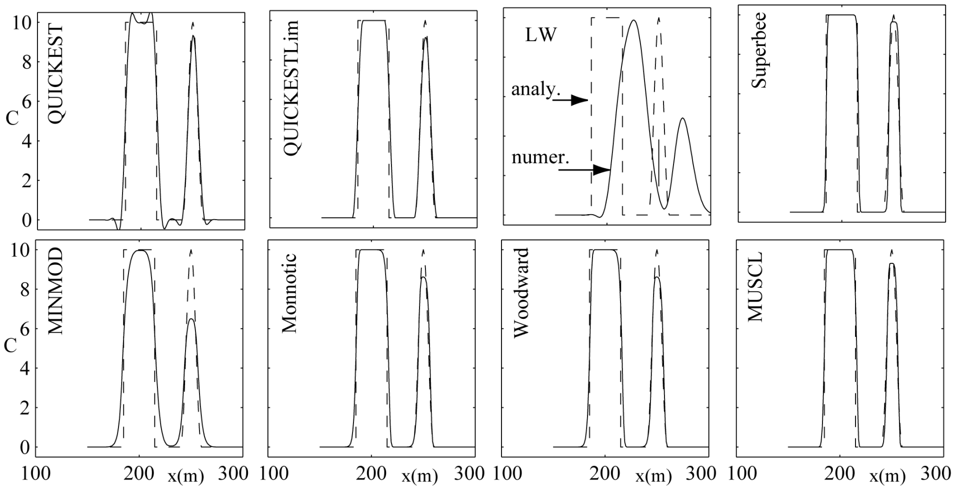


**Figure2. Comparison between the numerical and analytical solutions for 1D advection test.**

## 4.2 *Test for 2D advection-dispersion*

A very long straight rectangular channel of 30 m wide is used for the 2D test. The uniform flow depth is 1 m and the mean velocity is 0.5 m/s. One continuous line source of 0.1 l/s is injected into flow at the channel centerline, and the source concentration is 24 g/l. The analytical solution exists under such simple channel flow conditions (Graf and Altinakar, 1998).

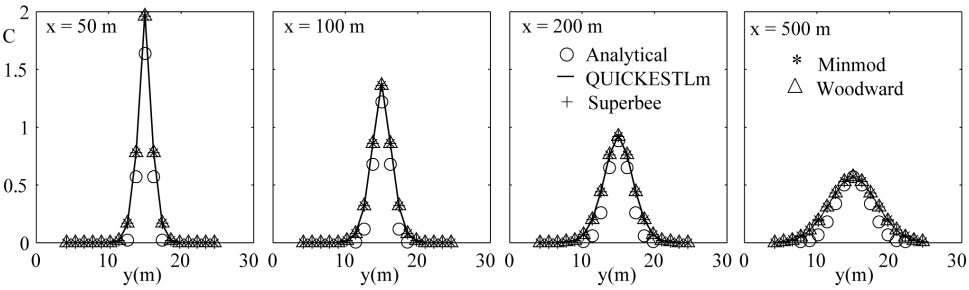


**Figure 3. Comparison between the numerical results and analytical solutions for 2D dispersion test.**

In this test, the concentration distribution obtained from the analytical model at downstream section of 10 m from source is taken as input for the numerical models. The transverse mixing coefficient, $K_y = 0.23HU_*$, is used for both numerical and analytical models. In the numerical model, the dispersion sub equations are solved using the implicit central difference scheme, and the limited QUICKEST and LW schemes are used to solve the advection sub-equation. The simulations from both analytical and numerical models are illustrated in Fig. 3. It is seen that the TVD schemes produce very identical results to each other. As expected that some apparent discrepancies on peak values between the numerical and analytical solutions can be found at the upstream cross-sections. This indicates that the numerical solutions are not very accurate in case the concentration gradient is large. Furthermore, computations show that the numerical model results compare favorably with the analytical solution.

# 5 APPLICATION TO EXPERIMENT

The dispersion measurement was carried out in a 25 m long laboratorial trapezoidal flume. The flume surface is 1.2m wide and the bottom is 0.05 m wide (Holly, 1975), hence the flow velocity and water depth vary across the flume. The measured concentrations at downstream section of 7m from source were taken as input to the numerical models, and the lateral mixing coefficient is taken as $0.23HU_*$ in the calculation.

The computed results are illustrated in Fig. 4. The comparison shows that the TVD schemes are also very identical and match quite well with the measurements except the very diffusive Minmod limiter. This indicates that most of the employed TVD schemes are suitable for the contaminant transport simulations except the more diffusive Minmod limiter.

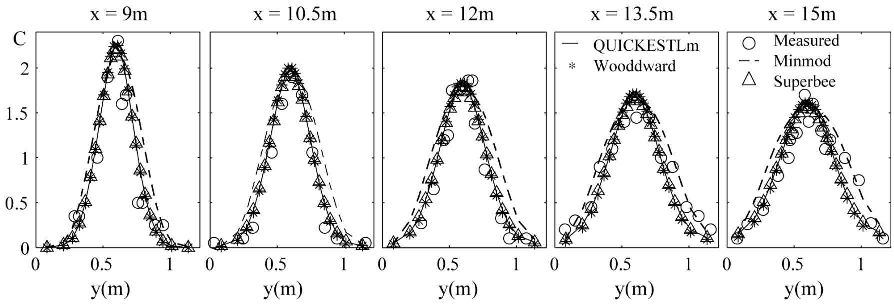


**Figure4. Comparison of model results with the measurements.**

## 6 CONCLUSIONS

In summary, the TVD schemes are combined with the operator-splitting algorithm to solve the 2D advection-dispersion equation in the present study. The numerical test illustrate that the ULTIMATE QUICKEST and limited LW schemes produce the oscillation free solutions. The comparison show that the limited QUICKEST and the limited LW perform very well compared with the exact solutions, moreover, the performance show that the accuracy of TVD schemes are comparable except the diffusive Minmod limiter.

The study indicates that the limited QUICKEST, most performed limited LW algorithms are very favourable for simulating high advection-dominated transport problems because they possess the desirable properties of high accuracy and computational efficiency. In addition, comparable accuracy between the limited QUICKEST and limited LW schemes also indicates that the TVD LW schemes are more attractive for the flow and scalar simulations because they are simple and use less points in the interpolation and easy to be extended for 2D scalar transport and flow simulations, especially for treating the boundary problems.

## REFERENCES

Graf W. H. and Altinakar M. S. 1998. *Fluvial Hydraulics*, West Sussex, Wiley.

Guan Y., Altinakar M. S. and Krishnappan B. G. 2002. Two-dimensional simulation of advection-dispersion in open channel flows, *Proc. 5th Int. Conference on Hydroinformatics*, Cardiff, UK, (1): 226-231.

Guan Y. and Zhang D. 2004. Comparative study of numerical methods to the advection equation, *Proc. 6th Int. Conference on Hydroinformatics*, SG, (1): 134-141.

Harten A. 1983. High resolution schemes for hyperbolic conservation law. *J. Comp. Phys.*, (49): 357-393.

Holly F.M. 1975. *Two-dimensional mass dispersion in rivers*, Colorado State University, Colorado.

Leonard B.P. 1991. The ULTIMATE conservative difference scheme applied to unsteady one-dimensional advection, *Comp. Methods Appli. Mech. Engrg.,* (88): 17-74.

Luk G.K.Y., Lau Y. L. and Watt W. E. 1990, Two-dimensional mixing in rivers with unsteady pollutant source. *ASCE J. Environ. Engrg.*, (116): 105-143.