A high-resolution method for the depth-integrated solute transport equation based on an unstructured mesh

Jun Kong\textsuperscript{a,b,*}, Pei Xin\textsuperscript{c}, Cheng-Ji Shen\textsuperscript{c}, Zhi-Yao Song\textsuperscript{d}, Ling Li\textsuperscript{a,c}

\textsuperscript{a} State Key Laboratory of Hydrology-Water Resources and Hydraulic Engineering, Hohai University, Nanjing, China
\textsuperscript{b} Nanjing Hydraulic Research Institute, Nanjing, China
\textsuperscript{c} National Centre for Groundwater Research and Training, School of Civil Engineering, The University of Queensland, Queensland, Australia
\textsuperscript{d} Key Laboratory of Virtual Geographic Environment, Ministry of Education, Nanjing Normal University, Nanjing, China

\textbf{Abstract}

This paper presents a high-resolution numerical method for solving mass transport problems involving advection and anisotropic diffusion in shallow water based on unstructured mesh. An alternating operator-splitting technique is adopted to advance the numerical solution with advection and diffusion terms solved separately in two steps. By introducing a new $r$-factor into the Total Variation Diminishing (TVD) limiter, an improved finite-volume method is developed to solve the advection term with significant reduction of numerical diffusion and oscillation errors. In addition, a coordinate transformation is introduced to simplify the diffusion term with the Green-Gauss theorem used to deal with the anisotropic effect based on unstructured mesh. The new scheme is validated against three benchmark cases with separated and combined advection and diffusion transport processes involved. Results show that the scheme performs better than existing methods in predicting the advective transport, particularly when a sharp concentration front is in presence. The model also provides a sound solution for the anisotropic diffusion phenomenon. Anisotropic diffusion has been largely neglected by existing flow models based on unstructured mesh, which usually treat the diffusion process as being isotropic for simplicity. Based on the flow field provided by the ELCIRC model, the developed transport model was successfully applied to simulate the transport of a hypothetical conservative tracer in a bay under the influence of tides.

\textcopyright{} 2012 Elsevier Ltd. All rights reserved.

\section{Introduction}

Numerical simulations of scalar (e.g., solute concentration and temperature) transport in natural water bodies (e.g., river and coastal area) are becoming increasingly useful for assessing water pollution and designing measures to improve water quality in these aquatic environments. Over the past two decades, numerical schemes for scalar transport problems have attracted much attention (Falconer, 1991; Gross et al., 1999; Liang et al., 2010). For most natural systems (e.g., estuary and offshore areas), the horizontal flow is dominant and thus the shallow water equations (SWE) based on the assumption of hydrostatic pressure are often used for predicting the flow dynamics. Linked with the flow model, the scalar transport can be simulated within the two-dimensional (2-D) horizontal plane with the vertical scalar distribution assumed to be uniform.

The new generation of models solving the SWE are mostly based on unstructured mesh and the finite volume method (FVM), e.g., UNTRIM (Casulli and Walters, 2000), FVCOM (Chen et al., 2003), ELCIRC (Zhang et al., 2004), SUNTANS (Fringer et al., 2006) and
CurWaC2D-Sed (Kuang et al., 2011). These models have two main advantages: (1) using unstructured mesh, the models can well simulate real systems with irregular geometries and (2) based on the finite volume method, the models satisfy the conservation principles for primary flow variables (Rossi, 2009).

Both advection and diffusion/dispersion (only diffusion mentioned hereafter) affect the solute transport. When the flow velocity is relatively high, advection tends to predominate; however, diffusion is responsible ultimately for the local mixing of solutes or heat (Ani et al., 2009; Qian et al., 2010). As the diffusion rate coefficient in the longitudinal direction is typically larger by an order of magnitude than that in the transverse direction, diffusion is fundamentally an anisotropic process. For example, in an estuary influenced by both inland freshwater discharge and tidal flow, anisotropic diffusion influences significantly the spread of pollutant after its release and shape of the plume formed (Liang et al., 2010).

In coastal areas influenced by short waves, time-averaged drift may induce anisotropic diffusion and thus influence the pollution concentration distribution (Cea et al., 2011). To accurately predict scalar transport in such water bodies, it is essential to properly simulate anisotropic diffusion in combination with advection. In solving the scalar transport equation numerically, an effective scheme with high precision is needed for approximating the advection terms so that the artificial diffusion and oscillation induced by the numerical approximation can be minimized (Rubio et al., 2008). The “cross wind diffusion” along the transverse direction should be reduced as much as possible to maintain the actual anisotropic diffusion effect. Such a scheme is particularly important for cases where large scalar (concentration or temperature) gradients are encountered. As a traditional method for the advection, the first-order upwind scheme has an advantage in dealing with large scalar gradients including (concentration and temperature) discontinuities; however, this scheme suffers from the artificial diffusion (e.g., Patankar, 1980; de Vahl Davis and Mallinson, 1976). The second-order upwind (SOU) method has been developed to reduce the artificial diffusion effect. However, this method may lead to numerical oscillation in the solution (Hayase et al., 1992). In order to minimize both the artificial diffusion and numerical oscillation, many high-order schemes have been developed, such as the Godunov scheme (Godunov, 1959), approximate Riemann scheme (Roe, 1981), Total Variation Diminishing (TVD) scheme (Harten, 1983) and ENO scheme (Harten et al., 1987). Due to its simplicity and high resolution, the TVD scheme has been widely applied to models based on either structured grids (Gross et al., 1999; Mingham et al., 2001) or unstructured meshes (Barth and Jespersen, 1989; Frink, 1992; Tamamidis, 1995). In the TVD scheme, an r-factor is introduced to determine the TVD flux limiter, designed to reduce the artificial diffusion and numerical oscillation. Various r-factor algorithms have been proposed in terms of the mesh structure and concentration gradient (Darwish and Moukalled, 2003; Casulli and Zanolli, 2005; Li et al., 2008) (detailed comparison of these algorithms are given later). While these algorithms can resolve the problem to some extent, further improvement is still needed, particularly when a sharp concentration or temperature front is in presence (as demonstrated in this paper).

The anisotropic diffusion term also imposes a challenge for the numerical solution. Represented by a full rank tensor, the diffusion coefficients are related to the local flow velocity. Li et al., 2008 adopted a Coupled Lattice Boltzmann method (CLBM) to simulate advection and anisotropic dispersion problems in the shallow water. Liang et al. (2010) solved the diffusion term using a second-order central difference scheme, in combination with a TVD-Mac method for dealing with advection. However, these methods were developed based on structured meshes and cannot be directly incorporated into models using unstructured meshes. Benkhaldoun et al. (2007) developed a finite-volume non-homogeneous Riemann solver (SRNH) incorporating the upwind scheme for fluxes and slope limiters. While it is compatible with unstructured mesh, the solver requires the mesh to be adaptive in order to avoid otherwise large numerical diffusion if a fixed mesh is used, especially when the concentration/temperature gradient is large around the moving fronts. The included mesh regeneration process makes it difficult to link the transport model with existing flow models based on fixed meshes.

This study aims to develop a high-resolution model for resolving advection-diffusion problems based on unstructured mesh and the finite volume method. The scheme is intended to be readily incorporated into existing, widely used flow models (e.g., UNTRIM, ELCIRC and SUNTANS). These “UNTRIM-like” models have shown great promise as the new generation of cross-scale circulation models (Zhang and Baptista, 2008; Kuang et al., 2011). The newly developed transport model can also be integrated into the existing models as a package to expand their capacity in simulating complex flow and solute transport phenomena. The paper is organized as follows: In Section 2, the numerical scheme is developed with the advection and diffusion terms solved separately. In Section 3, we validate the scheme against three benchmark cases involving separated and combined advection and diffusion processes. In Section 4, the presently developed transport model is applied to simulate the transport of a conservative tracer in a bay subjected to the influence of tides. Conclusions are drawn in Section 5.

2. Numerical scheme

The governing equation for scalar transport was first rewritten in an operator-split fashion with advection and diffusion separated in two sets of equations. The finite volume method was then adopted to discretize these equations. An improved r-factor algorithm for the TVD flux limiter was introduced for the advection term while the Gauss theorem was applied to obtain an approximation for the anisotropic diffusion term with a second-order precision. Without losing the generality, the derivation below is based on solute transport and concentration.

2.1. Governing equation and operator-splitting technique

Assuming negligible variations of solute concentration in the vertical direction, one can derive the depth-integrated equation for solute transport subject to advection and diffusion as follows,

\[
\frac{\partial C}{\partial t} + \frac{\partial}{\partial x} \left( v \frac{\partial C}{\partial x} + K_{xx} \frac{\partial C}{\partial y} + K_{xy} \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_{xy} \frac{\partial C}{\partial y} + K_{yy} \frac{\partial C}{\partial y} \right) = \frac{\partial}{\partial x} \left( HC \right) + \frac{\partial}{\partial y} \left( HC \right)
\]

where \( H \) is the water depth [L]; \( C \) is the depth-averaged solute concentration [ML\(^{-1}\)]; \( t \) is the time [T]; \( u \) and \( v \) are the velocity components in the \( x \) and \( y \) directions (Cartesian coordinate system), respectively; \( K_{xx} \), \( K_{xy} \), \( K_{yy} \) and \( K_{xy} \) are the components of the 2-D diffusion coefficient tensor [LT\(^{-2}\)]. The coefficients can be calculated according to Preston (1985).

\[
K_{xx} = K_1 \cos^2(\theta) + K_2 \sin^2(\theta)
\]

(2a)

\[
K_{xy} = K_{yx} = (K_1 - K_2) \cos(\theta) \sin(\theta)
\]

(2b)

\[
K_{yy} = K_1 \sin^2(\theta) + K_2 \cos^2(\theta)
\]

(2c)

where \( \theta \) is the angle of the flow direction with reference to the \( x \) axis [-]; and \( K_1 \) and \( K_2 \) are the diffusion coefficients.
along the longitudinal and transverse directions, respectively. These two diffusion coefficients can be estimated as follows (Elder, 1959),

\[
K_L = \frac{\alpha H \sqrt{g(u^2 + v^2)}}{c}
\]

(3a)

\[
K_T = \frac{\beta H \sqrt{g(u^2 + v^2)}}{c}
\]

(3b)

where \(c\) is the Chezy’s coefficient \([L^{1/2} T^{-1}]\); \(\alpha\) and \(\beta\) are two constant coefficients [-1], with theoretical values close to 5.93 and 0.15 respectively in a fully developed boundary layer of a straight channel (Fischer, 1973). These values increase to 13 and 1.2 respectively as the flow turbulence intensifies (Falconer, 1991). Under these and other conditions, the ratios of \(\alpha / \beta\) and \(K_L / K_T\) are typically much greater than 1, resulting in anisotropic diffusion.

The operator-splitting technique can be used to separate the advective and diffusive transport into two stages, in which different appropriate numerical methods are applied (Valocchi and Malmstead, 1992; Rubio et al., 2008; Liang et al., 2010).

Stage 1: advection

\[
\frac{\partial HC}{\partial t} + \frac{\partial HU_C}{\partial x} + \frac{\partial Hc}{\partial y} = 0
\]

(4a)

which can be rewritten in an operator form as follows,

\[
(HC)^i = L_{Adv}(HC)^n
\]

(4b)

where superscript \(n\) indicates the time step and represents the operator for advection (with subscript Adv) or diffusion (with subscript Diff); \(r\) represents a virtual time step consistent with the updated concentration for the second stage.

Stage 2: diffusion

\[
\frac{\partial HC}{\partial t} + \frac{\partial}{\partial x} \left( HK_{ex} \frac{\partial C}{\partial x} + HK_{ey} \frac{\partial C}{\partial y} \right) + \frac{\partial}{\partial y} \left( HK_{yx} \frac{\partial C}{\partial x} + HK_{yy} \frac{\partial C}{\partial y} \right)
\]

(5a)

which can also be written in an operator form as follows,

\[
(HC)^n+1 = L_{Diff}(HC)^r
\]

(5b)

To improve the accuracy of the solution, we used an alternating operator-splitting procedure as suggested by Liang et al. (2010),

\[
(HC)^n+2 = L_{Adv}L_{Diff}(HC)^n
\]

(6a)

\[
(HC)^n+2 = L_{Diff}L_{Adv}(HC)^n+1
\]

(6b)

2.2. High-resolution scheme for advection

Casulli and Zanolli (2005) proposed an improved upwind scheme for the advection term based on the finite-volume method, which maintains the mass conservation, and satisfies the maximum and minimum principle. The maximum and minimum principle states that without source or sink, the calculated solute concentration value for an element at a new time step should be within the range between the minimum and maximum concentration values among the neighboring elements and itself at the last time step. In this method, the flux across the interface of two neighboring elements is written as the sum of a first-order diffusive upwind term and an anti-diffusion term (Roe, 1983). The concentration value across the interface is determined based on the neighboring values at element centers or vertexes. The advection term can then be written as follows (Casulli and Zanolli, 2005),

\[
P_i^tC_i^t = \Delta t \left[ \sum_{j \in S_i} Q_{ij}^r \frac{C_j^r}{c} - \sum_{j \in S_i} Q_{ij}^r \left( C_{m(i,j)}^n - C_i^r \right) \right]
\]

(7a)

with

\[
Q_{ij}^r = \lambda J_{ij}^r U_{ij}^{r+1}\
\]

(7b)

where \(P\) is the area of the element \([L^2]\) (Fig. 1); \(S_i\) indicates the element such as element triangle IJK and subscript \(j\) indicates the element side such as side IJ, JK and KL (Fig. 1); \(\Delta t\) is the time step size \([T]\); \(\lambda\) is the length of the element side \([L]\); \(S\) represents the element side associated with the flow into and out of the local element \((S^+\) for outward and \(S^-\) for inward); \(\Psi\) is the flux limiter, which is a non-linear function of the \(r\)-factor; \(\zeta\) is implicitness (weighting) factor, typically set to 0.5 (semi-implicit); \(Q\) is the flux across the element side \([L^3 T^{-1}]\) and \(Q_{ij}^{r+1}\) is the combined flux based on fluxes calculated at the previous and present time steps, i.e., \(Q_{ij}^{r+1} = \frac{x}{2} Q_{ij}^r + (1-\frac{x}{2}) Q_{ij}^n\); and \(U\) is the normal velocity \([LT^{-1}]\).

The introduction of the flux limiter function \(\Psi\) effectively reduces the numerical diffusion error due to the upwind approximation of the advection term. Darwish and Moukalled (2003), Juntasaro and Marquis (2004) and Li et al. (2008) compared different limiters and found that based on the same mesh size, numerical results calculated using the Superbee limiter usually show the best accuracy. Therefore, in this study, the Superbee limiter is adopted (Sweby, 1984) as follows,

\[
\Psi(r) = \max(0, \min(1, 2r), \min(2, r)) \quad \text{with} \quad 0 \leq \Psi \leq 2
\]

(8)

With the substitution of Equation (8) into Equation (7a), it can be found that (1) if \(\Psi = 0\), Equation (7a) returns to the first-order

---

Please cite this article in press as: Kong, J., et al., A high-resolution method for the depth-integrated solute transport equation based on an unstructured mesh, Environmental Modelling & Software (2012), http://dx.doi.org/10.1016/j.envsoft.2012.08.009
upwind scheme; (2) if \( \Psi = 1 \), the second-order central difference scheme will be obtained; and (3) \( \Psi = 2 \) will lead to the first-order downwind formula (Darwish and Moukalled, 2003). The Superbee expression combines the features of the above three numerical schemes with adjustment according to simulated local concentration variations as expressed by the r-factor at each time step. A sound algorithm of the r-factor is fundamental for determining the flux limiter. In the following, we compare four existing algorithms and derive a new r-factor. In theory, \( r \) is determined based on the ratio of the upward concentration difference to the downward concentration difference. For the flow direction from point \( M \) to \( D \) (as illustrated in Fig. 1), \( r \) can be expressed as follows,

\[
F = \frac{C_M - C_U}{C_D - C_M}
\]  

(9)

where \( C_U \) and \( C_D \) are the concentrations, respectively, at nodes \( M \) and \( D \) (note that \( M \) and \( D \) are located at the centers of two neighboring elements, \( IJK \) and \( IRJ \), respectively); \( C_U \) is the concentration at the upwind point \( U \). The distance between points \( U \) and \( M \) is often set to be equal to that between points \( M \) and \( D \), i.e., \( |\mathbf{V}_{M,D}| = |\mathbf{V}_{M,U}| \) (\( \mathbf{V} \) is the displacement vector from the first subscript point to the second subscript point and \( \mathbf{V} \) is the module of the vector, i.e., distance between the two points). If an unstructured mesh is used, \( C_U \) is typically unknown. The calculation of \( C_U \) thus becomes the focus of different r-factor algorithms. Bruner (1996) presented a general r-factor algorithm for the TVD scheme,

\[
r_{\text{Bruner}} = \frac{2|\mathbf{V}_{M,F}|}{|\mathbf{V}_{D} - \mathbf{V}_{M}|} - 1
\]  

(10)

where \( |\mathbf{V}_{M,F}| \) is the displacement vector from point \( M \) to point \( F \); \( \mathbf{V}_{CY} \) is the concentration gradient at point \( M \), which is to be calculated. Bruner (1996) assumed that the distance between points \( U \) and \( M \) is twice that between points \( M \) and \( F \) (Fig. 1; \( F \) is the intersection of lines \( MD \) and \( IL \)). Darwish and Moukalled (2003) pointed out that Bruner’s r-factor cannot recover the TVD condition in the one-dimensional situation and proposed a modification to Equation (10),

\[
r_{\text{Darwish}} = \frac{2|\mathbf{V}_{M,D}|}{|\mathbf{V}_{D} - \mathbf{V}_{M}|} - 1
\]  

(11)

Li et al. (2008) found that if the concentration follows a parabolic distribution along the line passing points \( U, M \) and \( D \), Darwish and Moukalled’s (2003) algorithm can obtain a reasonable \( C_U \) value. However, if the concentration varies exponentially along the line, the calculated \( C_U \) may deviate significantly from the exact value. Subsequently, Li et al. (2008) provided an improved r-factor as follows,

\[
r_{\text{Li}} = \frac{C_M - (C_W + |\mathbf{V}_{W,U} \cdot \mathbf{V}_{W}|)}{|\mathbf{V}_{D} - \mathbf{V}_{M}|}
\]  

(12)

where \( W \) indicates the center of the element which includes point \( U \) (Fig. 1); and \( \mathbf{V}_{W} \) is the local concentration gradient at point \( W \). For the parabolic concentration distributions, Li et al.’s (2008) algorithm is better than Darwish and Moukalled’s (2003). However, both algorithms lead to numerical oscillations when applied to problems with sharp concentration gradients, even if fine grids are used (Li et al., 2008). The reason is that both methods need to calculate the gradient on element centers and the mesh structure tends to lead to an “upwind-biased” rather than full upwind result (Tamamidis, 1995). Furthermore, non-physical overshoots or under-shoots may arise in the vicinity of sharp changes in

the concentration gradient (Woodfield et al., 2004). As an example, we consider here a one-dimensional case shown in Fig. 2: a sharp concentration front moving from the left to the right. The red dotted line indicates the concentration gradient. Based on the method of Li et al. (2008), the value calculated for the upwind point \( U \) is negative. This violates the primary condition on concentration (values equal to or larger than zero) and would lead to oscillatory solutions. To avoid the need for calculating the concentration gradient, Casulli and Zanolli (2005) presented an r-factor algorithm based on the flux-weighted method. For side \( j = s \) where the flow direction is outward, the r-factor is determined as follows,

\[
r_{\text{Casulli}} = \frac{1}{\sum_{i \in S} Q_i} \left[ \frac{\sum_{i \in S} Q_i^n \cdot \mathbf{V}_{i,j} - \sum_{i \in S} Q_i^n \cdot \mathbf{V}_{i,m(i,j)}}{C_{m(i,j)} - C^n_{m(i,j)}} \right]
\]  

(13)

where \( C_{m(i,j)} \) is the concentration at the element centre, with the subscript indicating the element number; \( m(i,j) \) indicates a neighboring element of element \( i \), sharing the same side \( j \). For example, on side \( I \) of element \( IJK \) (Fig. 1), when flow direction is outward, \( C_i \) is represented by \( C_M \) and \( C_{m(i,j)} \) is represented by \( C_D \). On side \( JK \) or \( KL \), if the flow directs to element \( IJK \), \( C_{m(i,j)} \) is represented by \( C_W \) or \( C_C \). The assumption is that the influx is equal to the efflux, which does not necessarily hold for unsteady flow. Furthermore, the scalar value points \( W, G, D \) and \( M \) (Fig. 1) are not aligned in the same direction, inconsistent with the principle of the TVD limiter. This method may result in the “cross-wind diffusion” phenomenon, as shown in later sections.

Following the MUST scheme of Tamamidis (1995), which adopted the concentration difference between vertex and center in the upwind direction to realize the full upwind effect, we developed a new r-factor algorithm using the local element to transfer the upwind information. According to the definition of directional derivative, the upwind virtual point concentration is determined as follows,

\[
C_U = C_M + (C_S - C_M) \frac{\mathbf{V}_{M,U}}{|\mathbf{V}_{M,U}|} = C_M + (C_S - C_M) \frac{\mathbf{V}_{M,D}}{|\mathbf{V}_{M,D}|}
\]  

(14)
With \(|\overline{V_{M,D}}| = |\overline{V_{M,U}}|\), the new r-factor can be derived as follows,

\[
r_{\text{New}} = \frac{C_M - C_U}{C_D - C_M} = \left(\frac{C_M - C_S}{C_D - C_M}\right) \frac{d_{M,D}}{d_{S,M}} \tag{15}
\]

where \(d_{M,D}\) is the distance between points \(M\) and \(D\); \(d_{S,M}\) is the distance between points \(S\) and \(M\); \(C_S\) is the concentration at the intersection point \(S\) between lines \(MU\) and \(KJ\). \(C_S\) can be linearly interpolated by using the vertex values sharing the same side \(KJ\). Concentration at vertex \(K\) \((C_K)\) is also needed in the later anisotropic diffusion calculation and may be determined using the distance-weighted interpolation method, i.e.,

\[
C_K = \frac{\sum_{i=1}^{\text{mne}(K)} C_i}{\sum_{i=1}^{\text{mne}(K)} 1} \tag{16}
\]

where \(\text{mne}(K)\) is the number of elements sharing vertex \(K\); and \(d_i\) is the distance between vertex \(K\) and the center of the neighboring element \(i\) [L]. With the new method, calculation of \(C_U\) is only related to the concentrations at neighboring element nodes through distance-weighted interpolation without involving ambient flow fluxes or concentration gradients. This ensures positive values for \(C_U\) even when sharp concentration gradients are encountered, eliminating possible numerical oscillations in the solution as occurred with the methods of Darwish and Moukalled (2003) and Li et al. (2008). Due to the interpolation involving node \(J\), \(C_U\) is influenced partly by downwind information. To minimize such an effect (in order to maximize the upwind outcome), point \(U\) (i.e., point \(S\)) is required to be located far from the element node \(J\). This requirement is satisfied with typical mesh configurations involving acute angles in the elements, as demonstrated in the first test case presented later. When the mesh size (element side length) is relatively uniform, we can simply use the vertex to replace the point located on the element side, i.e., \(C_S\) replaced by \(C_K\) and \(d_{S,M}\) replaced by \(d_{K,M}\) (Fig. 1). In this case, concentrations at one vertex and two element centers are needed to calculate \(r\).

In the following, the Courant–Friedrichs–Lewy (CFL) stability condition is derived for the numerical solution based on the new algorithm for \(r\). With the substitution of Equations (15) and (7a) can be re-written as follows,

---

**Fig. 3.** Initial concentration distribution (Case 1). Mesh used in the simulation is also shown.

**Fig. 4.** Predicted concentration profiles after one rotation cycle using different algorithms of r-factor. (a) along the line \(y = 40\) m; and (b) along the line \(x = 20\) m (Case 1).

Please cite this article in press as: Kong, J., et al., A high-resolution method for the depth-integrated solute transport equation based on an unstructured mesh, Environmental Modelling & Software (2012), http://dx.doi.org/10.1016/j.envsoft.2012.08.009
\[ P_i H_i^{n+1} = P_i H_i^n - \Delta t \left( \sum_{j \in S_i} Q_j^{n+\xi} C_i^n - \sum_{j \in S_i} Q_j^{n+\xi} C_{m(i,j)}^n \right) \]
\[ - \frac{\Delta t}{2} \sum_{j \in S_i} \frac{dM_j}{ds_M} Q_j^{n+\xi} \left| C_i^n - C_j^n \right| \]
\[ - \frac{\Delta t}{2} \sum_{j \in S_i} \frac{dM_j}{ds_M} Q_j^{n+\xi} \left| C_{m(i,j)}^n - C_j^n \right| \] (17a)

or,
\[ P_i H_i^{n+1} = P_i H_i^n - \Delta t \left( \sum_{j \in S_i} Q_j^{n+\xi} \right) - \frac{\Delta t}{2} \sum_{j \in S_i} \frac{dM_j}{ds_M} Q_j^{n+\xi} \]
\[ + \frac{\Delta t}{2} \sum_{j \in S_i} \frac{dM_j}{ds_M} Q_j^{n+\xi} \left| C_{m(i,j)}^n - C_j^n \right| \]
\[ + \frac{\Delta t}{2} \sum_{j \in S_i} \frac{dM_j}{ds_M} Q_j^{n+\xi} \left| C_i^n - C_j^n \right| \] (17b)

It is worth noting that the implicitness factor \( \xi \) should be in accordance with that used in the flow model so that the sum of the coefficients of formula (17b) is equal to the right-hand side of the difference continuity equation (Casulli and Walters, 2000; Zhang and Baptista, 2008; Fringer et al., 2006).

\[ P_i H_i^{n+1} = P_i H_i^n - \Delta t \sum_{j \in S_i} Q_j^{n+\xi} + \Delta t \sum_{j \in S_i} Q_j^{n+\xi} \] (18)

The sum of right-hand side terms in Equation (18) represents the water volume in each element at the new time step. When the sum is negative, the element is dry and the transport equation is not solved. Then both water volume and scalar (concentration) value are set to zero. When the sum is positive, the transport module is activated. Such a method has been successfully applied in simulating saltwater intrusion based on the ELCRIC flow model (Wang et al., 2008) and revised HSPF model (Sen Bai, 2010), respectively.

According to the definition of the limiter function (Equation (8)), we have \( 0 \leq \psi_j^n \leq 2 \) and \( 0 \leq \psi_j^n / r_j^n \leq 2 \). Therefore, the terms associated with \( C_m^{n(i,j)} \) and \( C_S \) in Equation (17) are positive. To comply with the maximum and minimum principle, the term in front of \( C_i^n \) should also be positive, i.e.,

\[ P_i H_i^n - \Delta t \left[ \sum_{j \in S_i} Q_j^{n+\xi} + \frac{1}{2} \sum_{j \in S_i} \frac{dM_j}{ds_M} Q_j^{n+\xi} \right] - \frac{1}{2} \sum_{j \in S_i} \psi_j^n Q_j^{n+\xi} \geq 0 \] (19a)

The condition expressed by Equation (19a) is for stable solutions based on the numerical approximation of the advection term. The associated constraint on the time step (\( \Delta t_{Adv} \)) is thus given by

\[ \Delta t_{Adv} \leq \frac{P_i H_i^n}{\sum_{j \in S_i} Q_j^{n+\xi} + \frac{1}{2} \sum_{j \in S_i} \frac{dM_j}{ds_M} Q_j^{n+\xi} - \frac{1}{2} \sum_{j \in S_i} \psi_j^n Q_j^{n+\xi}} \] (19b)

Because \( 1 / 2 \sum_{j \in S_i} \psi_j^n / r_j^n \geq 0 \) and \( 0 \leq \psi_j^n / r_j^n \leq 2 \), Equation (19b) can be simplified as follows,

\[ \Delta t_{Adv} \leq \frac{P_i H_i^n}{\sum_{j \in S_i} \left( 1 + \frac{dM_j}{ds_M} \right) Q_j^{n+\xi}} \] (19c)

Fig. 5. Three kinds of triangle meshes used for the sensitivity analysis.
Clearly, this inequality is related to the local mesh structure. If the mesh is nearly uniform, then $1 + \frac{dM}{dS, M}$ is close to 2. The limiting condition on the time step is similar to that given by Casulli and Zanolli (2005) without considering the diffusion term; but the present scheme achieves better precision in dealing with problems involving large concentration gradients, compared with those using different algorithms of $r$-factor (as demonstrated later).

2.3. High-resolution scheme for anisotropic diffusion

As mentioned earlier, we used an alternating operator-splitting procedure suggested by Liang et al. (2010). The details of the separated diffusion calculation are given in this section. In order to simplify the diffusion term, a local coordinate system is introduced at each element side, with the local $X$-axis perpendicular to the element side and the local $Y$-axis parallel to the element side (Fig. 1). It is worth noting that such a local coordinate system has already been used in many recently developed surface water flow models, e.g., UNTRIM (Casulli and Walters, 2000), ELCIRC (Zhang and Baptista, 2008) and SUNTANS (Fringer et al., 2006). If the scalar transport is based on these surface water flow models, the procedure of re-organizing coordinate system is already in place. Related mesh structure information can be used directly by the solute transport model.

With the local coordinate system introduced, the diffusion term on the right side of Equation (5a) can be simplified with only two components included. The concentration at each element centre is obtained as follows,

$$C_{i}^{n+1} = \frac{P_{i}H_{i}^{n+1} C_{i}^{n} + \sum_{j=5} \Gamma_{j} \Delta t}{P_{i}H_{i}^{n+1}}$$

(20)

where $\Gamma$ is the diffusion flux across the element side, given by

$$\Gamma_{j} = H_{j}^{n+1} K_{XX} \frac{\partial C}{\partial X} + H_{j}^{n+1} K_{XY} \frac{\partial C}{\partial Y}$$

(21)

with $\frac{\partial C}{\partial X}$ and $\frac{\partial C}{\partial Y}$ being the concentration gradients across the element side $(j)$, calculated based on the local $X-Y$ coordinate system. To determine these gradients, the Green-Gauss theorem is applied (Barth and Jespersen, 1989; Jawahar and Kamath, 2000), i.e.,

$$\frac{\partial C}{\partial X} = \frac{(C_{D} - C_{M})Y_{I, J} + (C_{J} - C_{I})Y_{D, M}}{2A}$$

(22a)

with

$$Y_{I, J} = Y_{J} - Y_{I} \quad \text{and} \quad Y_{D, M} = Y_{M} - Y_{D}$$

(22b)

where $A$ is the area of the polygon (JMID); $C_{M}$ and $C_{D}$ are concentrations at the center of elements $JKI$ and $JIR$ (Fig. 1), respectively; and $C_{J}$ and $C_{I}$ are the concentrations at vertexes $J$ and $I$, respectively.

Similar to Equation (22), we can obtain the following approximation:

$$\frac{\partial C}{\partial Y} = \frac{(C_{D} - C_{M})X_{I, J} + (C_{J} - C_{I})X_{M, P}}{2A}$$

(23a)

Fig. 6. Predicted concentration profile after one rotation cycle based on different types of meshes. (a) along the line $y = 40$ m; and (b) along the line $x = 20$ m (Case 1).
with

\[ X_{j, I} = X_I - X_j \quad \text{and} \quad X_{M,D} = X_D - X_M \quad (23b) \]

Substituting Equations (22) and (23) into Equation (21) yields,

\[ I_j = H_j K_{XX} \frac{(C_D - C_M) Y_{I,j} + (C_J - C_I) Y_{D,M}}{2A} + H_j K_{XY} \frac{(C_D - C_M) X_{I,j} + (C_J - C_I) X_{M,D}}{2A} \]

\[ = \frac{H_j}{2A} \left[ S(C_D - C_M) + T(C_J - C_I) \right] \quad (24) \]

where

\[ S = K_{XX} Y_{I,j} + K_{XY} X_{I,j} = K_{XX} \lambda_j \quad (25a) \]

\[ T = K_{XX} Y_{D,M} + K_{XY} X_{M,D} \quad (25b) \]

If the anisotropic diffusion effect is neglected (i.e., \( K_{XY} = 0 \)) and points \( M \) and \( D \) are both located at the element orthocenter (i.e., \( Y_{D,M} = 0 \)), \( T \) is reduced to zero (Casulli and Zanolli, 2005). In the present model, \( M \) and \( D \) are set at the geometrical center rather than orthocenter to better reflect the element information, giving a non-zero first term on the right hand side of Equation (25b). The second term \( (K_{XY} X_{M,D}) \) represents the anisotropic diffusion effect.

A similar formulation has been adopted to approximate the diffusion flux within the SRNH scheme (Benkhaldoun et al., 2007) based on the global coordinate system. Following the method of Benkhaldoun et al. (2007), we can derive the following limiting condition on the time step,

\[ \Delta t_{\text{Diff}} \leq \min \left[ \frac{P}{4 \max \{ K_{XX}, K_{XY} \}} \right] \quad (26a) \]

According to Equation (20), the computed concentration at each element centre is also required not to be negative, i.e.,

\[ P_i H_j^{n+1} C_{j}^{n+1} + \sum_{j \in S} I_j \lambda_j \Delta t_{\text{Diff}} \geq 0 \quad (26b) \]

This condition ensures that the maximum and minimum principle is satisfied, an inherent feature of the finite volume method used here. Although a simple inequality cannot be derived from Equation (26b) to express the requirement on the time step, a maximum constraint on the time step would result from the application of this condition to all elements in the model. However, such a constraint is found not to be as stringent as that given by Equation (19c). The final time step used in the simulation should then satisfy the constraints based on both advection and diffusion processes, i.e.,

\[ \Delta t \leq \min \left( \Delta t_{\text{Adv}}, \Delta t_{\text{Diff}} \right) \quad (27) \]

The (maximum) time step allowed for each element \((i)\) given by Equation (27) varies from element to element. In the simulation, the minimum value among all the time steps calculated for all elements is used for computing the next time step solution. So \( \Delta t \) varies with time \((n)\) but not spatially \((i)\).

3. Model verification

Three commonly used benchmark cases were selected to test the present scheme in simulating advection with discontinuous concentration variations (Case 1), advection with continuous concentration variations (Case 2) and advection in combination with anisotropic diffusion (Case 3).

3.1. Advection in a rotating flow field (case 1)

The movement of a circular solute column in a rotating flow field with diffusion neglected has been often used for testing models’ performance in dealing with advection. The modeled domain is set to be a square of 80 m x 80 m with a background solute concentration of zero. The water depth is assumed to be 1 m.

![Fig. 7. Positions of points S, M and D corresponding to three kinds of meshes.](image)
uniformly. The rotating velocity field with a rotation period of 360 s is given below,

\begin{align}
  u &= \frac{2\pi(y - 40)}{360} \\
  v &= \frac{2\pi(x - 40)}{360}
\end{align}

(28a) (28b)

Initially, one unit concentration is specified within a circle of 7 m in radius centered at the point of \( x = 20 \) m and \( y = 40 \) m (Fig. 3). Under the influence of the rotating flow, the solute column rotates around the flow field center at \( x = 40 \) m and \( y = 40 \) m. Theoretically, the column maintains the circular shape at all times during the rotation. In the model testing, the triangle mesh was used with side length equal to 1 m. The time step was set to 0.2 s.

Models using different algorithms for determining \( r \)-factor were compared based on the same time step and mesh size. It can be seen from Fig. 4 that numerical diffusion was evident in the results given by all schemes after one rotation cycle. Additionally, numerical oscillation also occurred in the results associated with Darwish and Moukalled’s (2003) and Li et al.’s (2008) algorithms. As discussed earlier, in these two algorithms, the \( r \)-factor approaches 2 if the calculated concentration gradient is relatively large. This turns the scheme to a down-wind approximation and causes numerical oscillation in the solution. Although the numerical oscillation was avoided with Casulli and Zanolli’s (2005) algorithm, significant numerical diffusion was evident in the solution—the maximum concentration value decreased with the simulation time. The shape of the concentration field evolved to a circular cone quickly from the initial solute column. In contrast, the present scheme with the new \( r \)-factor algorithm produced the least numerical diffusion in directions perpendicular and parallel to the flow. Simulated concentrations varied symmetrically around the column centre as expected. The numerical oscillation was avoided and the simulated concentration was bounded between its neighboring minimum and maximum values, suggesting that the maximum and minimum principle was held during the simulation.

As mentioned earlier, the concentration for the upwind point \( U \) calculated using the new method is influenced partly by down-wind information depending on the mesh structure, which in turn affects the \( r \)-factor. Thus the accuracy of the solution may be affected by the mesh structure/configuration. A sensitivity analysis on this effect was carried out to better understand the errors associated with the new method. Further simulations were conducted based on three different types of meshes as shown in Fig. 5. Meshes A and B both include right angles in the elements. In Mesh A, each interior node is always connected with six triangular elements. In Mesh B, each interior node is connected with eight elements. Both meshes can be regarded as challenging cases because of the involvement of right angles in the elements. These meshes are rarely adopted in unstructured mesh models and used here only for the purpose of sensitivity analysis. Different from the above two types of meshes, Mesh C is a typical unstructured mesh produced by SMS (http://www.crwr.utexas.edu/gis/gishyd98/byu/sms/smsh.htm). There is no preferred mesh orientation and only acute angles are involved in each element. The element side length is relatively uniform over the domain. Mesh C is widely used in many unstructured mesh models such as FVCOM, ELCIRC and SUNTANS, and has also been used in the above simulation with the results shown in Fig. 4. In the sensitivity analysis, the minimum element side length was set to 1 m for all three types of meshes.

Fig. 8. Comparison between the results before and after the modification of the method with point \( S \) replaced by node \( K \) based on Mesh B shown in Fig. 5. (a) along the line \( y = 40 \) m; and (b) along the line \( x = 20 \) m (Case 1).

Please cite this article in press as: Kong, J., et al., A high-resolution method for the depth-integrated solute transport equation based on an unstructured mesh, Environmental Modelling & Software (2012), http://dx.doi.org/10.1016/j.envsoft.2012.08.009
The results (Fig. 6) show that Meshes A and C delivered much the same, better precision in the numerical predictions, which were closer to the analytical values compared with the results given by Mesh B. The reason is that in Meshes A and C, the upwind point S is very close to the upwind mesh node K (Fig. 7). Thus the upwind information was better captured. In Mesh B, the upwind point S is a relatively far from node K; thus the weighted influence of node J (with downwind information) on S is increased, leading to reduced upwind control. To overcome the shortcoming due to the B-type mesh, we suggest that in equation (15), \( C_S \) can be replaced by \( C_K \) and distance \( d_{S,M} \) by \( d_{K,M} \) - i.e., the upwind point S is actually replaced by node K. With this modification, the precision of the solution with Mesh B is improved as shown in Fig. 8. The modification, however, did not seem to affect the accuracy of the solution with the A-Type and C-Type meshes. Therefore, we suggest that considering the mesh quality and for the purpose of simplicity, the method can also be based on node K instead point S.

We also compared our model with existing models based on structured/unstructured grids, including (1) DIVAST model (Lin and Falconer, 1997) based on the ULTIMATE QUICKEST scheme; (2) HEMAT model (Namin et al., 2004) based on a second-order Godunov Scheme; (3) TVD-Mac model (Liang et al., 2010) based on the TVD-modified MacCormack scheme; and (4) Qian et al.’s (2007) improved QUICK model. Qian et al. (2007) have put forward a physically based limiter to improve the traditional QUICK scheme (Leonard, 1979), which can be easily applied on unstructured mesh. For comparison, the mesh size was also set to 1 m, consistent with

Fig. 9. Predicted concentration profiles after one rotation cycle using different schemes. (a) along the line \( y = 40 \) m; and (b) along the line \( x = 20 \) m (Case 1).

Fig. 10. Predicted concentration distributions after half (a; elapsed time: 180 s) and one (b; elapsed time: 360 s) rotation cycle (Case 1). Mesh used in the simulation is also shown.
those used in other models. Results of models (1), (2) and (3) were extracted from Liang et al. (2010).

The concentration profiles predicted by different models are shown in Fig. 9 (after one rotation cycle). It can be seen that both the present and Qian et al.'s (2007) schemes predicted well the concentration profiles. These two schemes did not lead to much "cross wind diffusion" (Patankar, 1980), compared with the others. The predicted concentration profiles were symmetrical and much close to the exact shape. The present model showed better capability in reducing the transverse diffusion. In Qian et al.'s (2007) model, the Quick scheme is obtained by fitting a quadratic function through points $U$, $M$ and $D$ ($C_F = -1/8C_U + 3/4C_M + 3/8C_D$), which may introduce an artificial diffusion.

The present scheme did not induce much numerical diffusion or oscillation, and reproduced the movement of the circular solute column in the rotating flow field with a 360 s rotation period (Fig. 10). Further tests were conducted with the rotation period reduced to 216 s, 108 s and 36 s (rotation speed increased by 10 times). In order to obtain the solution with acceptable accuracy, small time step sizes were required: 0.1 s, 0.05 s and 0.02 s used respectively. In all cases, the present scheme outperformed the previous ones and simulated well the movement of the circular solute column (results not shown for the purpose of brevity).

3.2. Advection in a cyclogenesis flow field (case 2)

To further validate the model's capability of simulating the advection process, the cyclogenesis problem was selected for testing. The cyclogenesis problem reflects the mixing of a warm and a cold front under the influence of an applied rotating flow field (Tamamidis and Assanis, 1993). During the rotation, the concentration gradient increases, especially in the area close to the rotation center. In the Cartesian coordinate, the non-dimensional and constant flow velocity field (shown in Fig. 11a) is described as follows,
Fig. 12. Snapshots of concentration distributions at different times (left columns for the analytical results and right columns for the simulation results). (a) $t = 3$; (b) $t = 6$; and (c) $t = 9$ (Case 2).
\[ u = -\omega y \]  
\[ v = \omega x \]  

where \( \omega \) is the angular velocity of the rotation, given by,

\[ \omega = \frac{Q}{d_{\text{max}}(Q)} \]  

with

\[ d = \sqrt{x^2 + y^2} \]  

\[ Q = \text{sech}^2(d)\tanh(d) \]

where \( d \) is the distance to the centre and \( Q \) is the tangential flow velocity.

This velocity field was used to drive the scalar transport. For an infinite domain, the exact solution of \( C \) is given in a non-dimensional form as follows,

\[ C(x, y, t) = -\tanh\left(0.5y\cos(\omega t) - x\sin(\omega t)\right) \]  

The initial concentration was set according to this analytical solution (with \( t = 0 \)), i.e., \( C(x, y) = -\tanh(0.5y) \) (Fig. 11a). It is worth noting that “negative” concentrations were included in the simulation. However, these “non-physical” concentrations, better seen as relative concentrations, would not affect the model testing results.

The simulation domain was set as a square with the size of \( 80 \times 80 \) (note that the equation has been non-dimensionalized. A refined mesh was used for the centre area with the element size set to 0.05; Away from the centre, the coarse mesh was used with the element size set to 0.1 (Fig. 11b). The simulation time step was set to be 0.01.

Overall, the model predicted well the concentration variations induced by the cyclogenesis flow field (Fig. 12): spatially a vortex forms and the central concentration gradient increases with time, in agreement with the cyclogenesis patterns. Across an observation section \( (y = 0) \) shown in Fig. 13, the concentration oscillates with an increasing wave number as the simulation continues. At the early stage when relatively small concentration gradients are present, models integrating different \( r \)-factor algorithms can all predict well the concentration profile (Fig. 12a). However, the continuing advection process increases the concentration.

![Graph showing variations of global relative error with time](image)

**Fig. 14.** Variations of global relative error with time (Case 2).
gradients and leads to sharp concentration fronts, particularly near the cyclogenesis centre (Figs. 12 and 13). By this stage (Fig. 13b and c), various problems with these models become evident: (1) artificial diffusion inherent in Casulli and Zanolli’s (2005) scheme leads to significant smearing effects, resulting in under-predictions of the concentration variations (gradients) around the cyclogenesis centre (0, 0); (2) Li et al.’s (2008) algorithm leads to numerical oscillation, giving predictions with large differences from the analytical values; and (3) in contrast, the present and Darwish and Moukalled’s (2003) methods agreed better with the analytical solution.

Following Li and Huang (2008), we calculated the global relative error ($E_{g}$) as defined below to quantitatively evaluate the accuracy of different schemes.

$$E_{g} = \sqrt{\frac{\sum |C_i - C_{ai}|^2}{\sum |C_{ai}|^2}}$$

where $C_{i}$ and $C_{ai}$ are, respectively, the concentrations given by the numerical and analytical solutions, $i$ is the number of the observation point. Here, all the points (around 15 thousand) were examined. The results (Fig. 14) show that after 10 unit time, the global relative error related to the present and Darwish and Moukalled’s (2003) algorithms remains close to 0.03. However, predictions by Casulli and Zanolli’s (2005) and Li et al.’s (2008) algorithms involve larger $E_{g}$ values, by almost an order of magnitude. For Li et al.’s (2008) algorithm, $E_{g}$ increases rapidly after 6 unit time, suggesting that this scheme is not suitable for scalar transport problems with large concentration gradients.

In summary, the first two test cases have demonstrated that the present $r$-factor algorithm is robust in dealing with advection scalar transport, involving both small (continuous) (Fig. 12) and large (discontinuous) (Fig. 10) concentration variations.

### 3.3. Advection and anisotropic diffusion in a uniform flow field (case 3)

The scheme was also tested against a case with combined advection and anisotropic diffusion under a uniform flow condition. A certain amount of solute was instantaneously released to the water body and subsequently underwent advection and diffusion transport. An analytical solution for this problem in an infinite domain is available (Liang et al., 2010). The analytical solution in a general form based on flow in an arbitrary direction is given below.

![Fig. 16. Concentration profiles along the flow direction (note: profiles at four different times are plotted together for comparison). The results are for Case 3.](image1)

![Fig. 17. Temporal variations of global relative errors with different $P_t$ numbers (Case 3).](image2)
with,
$$\chi = \frac{[(x - ut - x_0)\cos(\theta) + (y - vt - y_0)\sin(\theta)]^2}{4K_L t} \tag{35b}$$
$$\delta = \frac{[(x - ut - x_0)\sin(\theta) + (y - vt - y_0)\cos(\theta)]^2}{4K_T t} \tag{35c}$$

where $M_s$ is the total amount of mass released [M]; $x_0$ and $y_0$ are the coordinates of the release location [L]; $u$ and $v$ are the flow velocity components [LT$^{-1}$] in the $x$ and $y$ directions, respectively; and $\theta$ is the angle of the flow direction with reference to the $x$ axis.

In the numerical simulation, the domain was specified to be a square with the size of 500 m $\times$ 500 m. $M_s$ and $H$ were set to 988 g and 1 m, respectively. The flow field was defined as $u = v = 0.5$ m/s. The domain was represented by around 144 thousand of triangle elements with the element size set to 2 m. The time step was set to 0.1 s. The Chézy's coefficient was set to 30 m$^{1/2}$/s, and the longitudinal dispersion and transverse diffusion constants to 13 and 1.2 in Equation (3), respectively, giving corresponding dispersion/diffusion coefficients ($K_L$ and $K_T$) equal to 1 m$^2$/s and 0.1 m$^2$/s.

The release point was chosen at $x_0 = 5.9$ m, $y_0 = 5.9$ m. The initial concentration for the numerical simulation was defined using the analytical solution for $t = 50$ s. For comparison, we also simulated the isotropic diffusion with $K_L = K_T = 1$ m$^2$/s. The evolution of the solute concentration is shown in Fig. 15. The model

Fig. 19. Comparison between measured and simulated local flow velocities for location +2 marked in Fig. 18. (a) is for flow speed and (b) for flow direction with respect to the north.
demonstrated significant differences between the anisotropic and isotropic diffusion. The anisotropic diffusion leads to and maintains a solute plume of an elliptical shape with the major axis aligned with the flow direction.

Predicted concentration profiles along the flow direction are compared with the analytical solutions at different times as shown in Fig. 16. It can be seen that the locations of the peak solute concentration, controlled by the advection, are not affected by the anisotropic or isotropic diffusion (identical in both cases). Although the longitudinal dispersion coefficient was the same, the solute plumes exhibited much difference due to different transverse diffusion coefficients. With a higher transverse mixing coefficient (the isotropic case), the solute spread and was diluted more quickly along the transverse direction.

Overall, the model reproduced the solute transport behavior as predicted by the analytical solution (Figs. 15 and 16). We further examined the total amount of solute in the simulated domain, with the aim of verifying mass conservation. As expected, the total mass remained unchanged, indicating that the model conserves well the mass.

Further simulations were conducted to examine how the Péclet number \( Pe = \frac{\sqrt{u^2 + v^2} dx}{\sqrt{K_v K_t}} \) affects the accuracy of the numerical scheme. For this purpose, the \( K_v \) value was varied from 0.1 to 1.0 m\(^2\)/s with \( K_t \) unchanged (1.0 m\(^2\)/s). Under these conditions, the ratio of \( K_v \) to \( K_t \) varied from 1 to 10, covering most of the practical situations in surface water flow. It should be noted that the Péclet number represents the relative importance of advection versus diffusion.

As the modeled domain was set to 500 m × 500 m, the domain boundaries affected little the simulated solute transport within the first 600 s, allowing comparison of the numerical results with the analytical solution based on an infinite domain. The global relative errors of the numerical solutions for different Péclet numbers were calculated using Equation (34) for this period. The results show that in all simulations, the errors remain largely constant at relatively low levels after initial increases. This seems to suggest that the error accumulation was insignificant. As the \( Pe \) number decreased, the effect of diffusion became more important in the solute transport, enhancing the mixing and thus reducing further local solute concentration gradients. This led to improved accuracy of the numerical solution (Fig. 17).

4. Application

The presently developed transport model was applied to simulate solute transport in the Quanzhou bay, located on the southeastern coastline of China. The purpose of this application was to demonstrate the capacity of the model in simulating mass transport processes in natural shallow water bodies. Therefore, a non-reactive tracer was considered with a focus on simulating advective and diffusive transport.

The bathymetry of this bay is relatively complex (Fig. 18), with an extensive intertidal zone undergoing periodic wetting and drying during the tidal oscillation. The ELCIRC ocean model (Zhang and Baptista, 2008) was employed to simulate the flow field, which was applied to drive the solute transport. An

---

Please cite this article in press as: Kong, J., et al., A high-resolution method for the depth-integrated solute transport equation based on an unstructured mesh, Environmental Modelling & Software (2012), http://dx.doi.org/10.1016/j.envsoft.2012.08.009
unstructured mesh was used in the model to represent the complex geometry with a minimum side length of 100 m. On the open boundary, tidal sea level was specified according to the local tidal condition: the maximum tidal level is 3.06 m above the mean sea level (MSL) and the minimum tidal level is −3.15 m below the MSL. Flow velocity and water level data collected from five observation points (shown in Fig. 18) were used to validate model predictions with reasonably good agreement obtained. As an example, comparison between predicted and measured flow velocity at one of the observation points is shown in Fig. 19. The simulated velocity field across the whole bay over one tidal period is shown in Fig. 20. During the flooding and ebbing periods the directions of tidal flow on the open boundary were north-east and south-west, respectively. The existence of circulating flow near the coastline increased the complexity of the flow field.

In simulating the solute transport, a pulse of solute input to the bay was assumed at the point \((x = 11.5 \, \text{km} \, \text{and} \, y = 16.4 \, \text{km})\), Fig. 21. The solute input started at a rate of 100 g/s when the tidal sea level reached the maximum and lasted for 1 h. Driven by the tidal flow, the solute plume formed, and oscillated back and forth passing by the shallow shoal and deep channel (Fig. 21).
Simulations were conducted with the solute subjected to isotropic and anisotropic diffusion, respectively. For isotropic diffusion, the dimensionless constants ($\alpha$ and $\beta$) in Equation (3) were both set to 13. For anisotropic diffusion, these two constants were set to 13 and 1.2, respectively. The results show that in the case of isotropic diffusion, the plume area of low concentrations was larger than that due to anisotropic diffusion. This was caused by excessive spreading and associated dilution of the solute plume in the transverse direction under isotropic diffusion. Such a trend was clearly evident at elapsed time $t = 12$ h when the plume reversed the movement back to the source point.

Correspondingly the area of high concentrations decreased compared with the results in the case of anisotropic diffusion as shown in Fig. 21d. To further examine the differences between the two cases, the concentrations at point ($x_0 = 11.6$ km, $y_0 = 15.5$ km) were plotted every half an hour over a tidal period as shown in Fig. 22. Although similar temporal variations were present in both cases, the maximum concentrations differed significantly with a relative difference of 27% (0.008 mg/L for the isotropic case compared with 0.011 mg/L for the anisotropic case). This difference highlights the necessity of considering the physically anisotropic diffusion in simulating solute transport in natural water bodies.

5. Concluding remarks

A high-resolution numerical method based on unstructured mesh has been developed for solving the advection and anisotropic diffusion problem of scalar transport in shallow water. In this method, a new $r$-factor for the Total Variation Diminishing (TVD) limiter is derived to improve the ability of traditional schemes in dealing with the advection. The aim is to reduce the effect of artificial diffusion and oscillation on the solution due to numerical approximations of the advection term. The new method also enables simulations of anisotropic diffusion within unstructured mesh-based models by applying the Green-Gauss theorem to approximate the anisotropic diffusion term based on a local coordinate system.

The new method has been tested against the exact solutions for three benchmark cases with a satisfying outcome. The simulation results agree well with the exact solutions and demonstrate the advantage of this method compared with others. The method was also applied to simulate the transport of a hypothetical conservative tracer in a bay subjected to isotropic and anisotropic diffusion in two different cases, respectively. Results show large differences in the simulated behavior of the plume between the two cases and highlight the need to consider the physically anisotropic diffusion in simulating solute transport in natural water bodies.

Since the method is based on the same finite volume scheme as used in many shallow water hydrodynamics models (e.g., UNTRIM, ELCIRC and SUNITANS), it can be readily incorporated into these models as a package to expand their capacity in simulating complex solute transport phenomena in real systems. The method can be further developed in the future work to incorporate chemical and biological reactions concerning reactive solute transport in natural water.

Acknowledgments

This research was supported by the Australian Research Council (DP0988718), National Natural Science Foundation of China (51009059), the Postdoctoral Research Fund of Jiangsu, China (10022023C) and the Open Fund of State Key Laboratory of Hydrology-Water Resources and Hydraulic Engineering provided by Hohai University (2010491111).

References


Please cite this article in press as: Kong, J., et al., A high-resolution method for the depth-integrated solute transport equation based on an unstructured mesh, Environmental Modelling & Software (2012), http://dx.doi.org/10.1016/j.envsoft.2012.08.009


Please cite this article in press as: Kong, J., et al., A high-resolution method for the depth-integrated solute transport equation based on an unstructured mesh, Environmental Modelling & Software (2012), http://dx.doi.org/10.1016/j.envsoft.2012.08.009