Modelling depth-integrated contaminant dispersion in the Humber Estuary using a Lagrangian particle technique

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Abstract

A two-dimensional Lagrangian particle model has been established to simulate depth-integrated contaminant dispersion in estuaries and coastal seas. The governing advection-diffusion equation is first rearranged into a Fokker-Planck equation allowing the implementation of a consistent random-walk method to simulate diffusion with a spatially variable diffusivity. The paper then describes a novel particle tracking algorithm which can be used with arbitrary non-orthogonal boundary-fitted coordinate meshes. By definition, the particle tracking method is perfectly conservative and free from numerical diffusion in the classical sense. The scheme is also able to preserve steep concentration fronts enabling accurate simulations of point sources.

1 Introduction

Increasing environmental awareness and the need to predict and improve the water quality in estuaries and coastal seas has led to significant developments in pollution transport modelling. Traditionally, contaminant dispersion has usually been simulated using finite-difference approximations of the standard advection-diffusion equation, expressed in depth-averaged form. However, Eulerian grid based finite-difference methods present a number of problems when applied to advection dominated flow regimes. In particular, grid based methodologies have difficulty modelling point sources of contaminant and steep concentration gradients. Furthermore, in simulations where the pollution does not occupy the whole flow domain, finite-difference schemes are often computationally inefficient compared to particle tracking methods.

The simulation of contaminant dispersion using a particle tracking technique is based upon the simple idea that the pollution may be represented
by discrete particles which are subjected to advection, diffusion and decay. These processes are modelled by the combination of deterministic and stochastic numerical schemes; namely, translation of each particle using an advective velocity derived from the surrounding velocity field and diffusion of each particle using a random-walk technique.

2 Governing equations

The depth-averaged advection-diffusion equation representing the fate of a conservative pollutant can be expressed as

\[
\frac{\partial (cD)}{\partial t} + \frac{\partial (ucD)}{\partial x} + \frac{\partial (vcD)}{\partial y} = \frac{\partial}{\partial x} \left( D \frac{\partial c}{\partial x} \right) + \frac{\partial}{\partial y} \left( D \frac{\partial c}{\partial y} \right) + \frac{\partial}{\partial x} \left( D \Gamma_{xy} \frac{\partial c}{\partial x} \right) + \frac{\partial}{\partial y} \left( D \Gamma_{yy} \frac{\partial c}{\partial y} \right)
\]

(1)

where \( u \) and \( v \) are the depth-averaged velocity components in the \( x \)- and \( y \)-directions, \( D \) is the local water depth, \( c \) is the depth-averaged pollution concentration, and

\[
\Gamma = \begin{bmatrix}
\Gamma_{xx} & \Gamma_{xy} \\
\Gamma_{yx} & \Gamma_{yy}
\end{bmatrix} = \begin{bmatrix}
\Gamma_L & 0 \\
0 & \Gamma_T
\end{bmatrix}
\]

(2)

is the diffusion tensor in the Cartesian and flow-aligned coordinate systems. If \( \theta = \tan^{-1}(v/u) \) is the angle between the local flow direction and the \( x \)-axis, then the Cartesian diffusion coefficients may be evaluated as

\[
\Gamma_{xx} = \Gamma_L \cos^2 \theta + \Gamma_T \sin^2 \theta
\]

(3)

\[
\Gamma_{xy} = (\Gamma_L - \Gamma_T) \sin \theta \cos \theta
\]

(4)

\[
\Gamma_{yy} = \Gamma_L \sin^2 \theta + \Gamma_T \cos^2 \theta
\]

(5)

where \( \Gamma_L \) and \( \Gamma_T \) are the longitudinal and transverse diffusion coefficients measured parallel and perpendicular to the local velocity vector. In the present work, the diffusion coefficients are estimated using Elder’s concept\(^1\).

Following the method outlined by Józsa\(^2\), the advection-diffusion equation is rewritten in a form which can be interpreted from a particle tracking perspective. This is accomplished by introducing a new concentration variable, \( C = Dc \). Equation (1) can thus be rewritten after algebraic manipulation as

\[
\frac{\partial C}{\partial t} + \frac{\partial (UC)}{\partial x} + \frac{\partial (VC)}{\partial y} = \frac{\partial^2 (\Gamma_{xx} C)}{\partial x^2} + 2 \frac{\partial^2 (\Gamma_{xy} C)}{\partial x \partial y} + \frac{\partial^2 (\Gamma_{yy} C)}{\partial y^2}
\]

(6)

in which
If \( C \) is considered as a probability density function, then eqn. (6) is identical to the Fokker-Planck equation. The modified advection velocities presented in eqns. (7) & (8) allow the particle tracking scheme to simulate diffusion using a consistent random-walk technique. Without this modification, the particles would accumulate in regions of low diffusivity (Hunter et al.\(^3\)).

3 Numerical scheme

To facilitate an accurate representation of the complex flow domains found in coastal regions, the numerical model is based upon a boundary-fitted non-orthogonal grid. Following Thompson et al., a smooth curvilinear grid is generated by solving a pair of elliptic Poisson equations:

\[
\begin{align*}
\xi_{xx} + \xi_{yy} &= P(\xi, \eta) \\
\eta_{xx} + \eta_{yy} &= Q(\xi, \eta)
\end{align*}
\]

relating the physical \((x, y)\) coordinates to the transformed \((\xi, \eta)\) coordinates. (Here, the subscripts denote the usual shorthand notation for partial differentiation). The functions \( P \) and \( Q \) are the so-called ‘attraction operators’ or ‘control functions’ which can be used to alter the internal structure of the curvilinear mesh. After interchanging the dependent and independent variables, eqn. (9) may be rewritten as a quasi-linear elliptic system:

\[
\begin{align*}
\alpha x_{\xi \xi} - 2\beta x_{\xi \eta} + \gamma x_{\eta \eta} + J^2(Px_{\xi} + Qx_{\eta}) &= 0 \\
\alpha y_{\xi \xi} - 2\beta y_{\xi \eta} + \gamma y_{\eta \eta} + J^2(Py_{\xi} + Qy_{\eta}) &= 0
\end{align*}
\]

where

\[
\alpha = x_{\eta}^2 + y_{\eta}^2, \quad \beta = x_{\xi}x_{\eta} + y_{\xi}y_{\eta}, \quad \gamma = x_{\xi}^2 + y_{\xi}^2
\]

and \( J \) is the Jacobian of the transformation, given by \( J = x_{\xi}y_{\eta} - x_{\eta}y_{\xi} \). The mapping expressions shown in (10) are rewritten as finite-differences and solved using successive-over-relaxation to find a one-to-one mapping between the transformed \((\xi, \eta)\) plane and the physical \((x, y)\) plane.

Before solving the governing advection-diffusion equation, it is first necessary to decide upon a particular grid configuration on which to represent all constants and variables appertaining to the pollution transport model. The staggered computational grid used in the present work is shown in Figure 1.
Particle movement takes place under the action of both advection and diffusion each time step. In order to translate the particles due to pure advection, it is necessary to calculate the modified advection velocities presented in eqns. (7) & (8) at each particle position. Since the variation in diffusivity from cell to cell is generally quite small, then in the present scheme the derivative terms in eqns. (7) & (8) are assumed constant for all particles within the same cell during a time step. These derivatives are with respect to the Cartesian coordinate system and before it is possible to calculate them on the non-orthogonal boundary-fitted grid they must be transformed and expressed in terms of the curvilinear coordinates ($\xi, \eta$). The transformation is performed according to the numerical mapping formulae presented by Thompson et al.$^4$:

$$
\begin{align*}
\frac{\partial f}{\partial x} &= f_x = \frac{\partial (f, y)}{\partial (\xi, \eta)} + \frac{\partial (x, y)}{\partial (\xi, \eta)} = \frac{1}{J} (y \frac{f_\xi}{f_\eta} - x \frac{f_\xi}{f_\eta}) \\
\frac{\partial f}{\partial y} &= f_y = \frac{\partial (x, f)}{\partial (\xi, \eta)} + \frac{\partial (x, y)}{\partial (\xi, \eta)} = \frac{1}{J} (x \frac{f_\eta}{f_\xi} - f_x) 
\end{align*}
$$

where $f$ denotes a differentiable function of $x$ and $y$. Substitution of the above transformation formulae into all partial derivatives involving $x$ or $y$ in eqns. (7) & (8) leads to

$$
U = u + \frac{1}{JD} \left[ y_\eta \left( \frac{\partial \Gamma_{xx}}{\partial \xi} D + \frac{\partial D}{\partial \xi} \Gamma_{xx} \right) - y_\xi \left( \frac{\partial \Gamma_{xx}}{\partial \eta} D + \frac{\partial D}{\partial \eta} \Gamma_{xx} \right) \\
+ x_\xi \left( \frac{\partial \Gamma_{xy}}{\partial \eta} D + \frac{\partial D}{\partial \eta} \Gamma_{xy} \right) - x_\eta \left( \frac{\partial \Gamma_{xy}}{\partial \xi} D + \frac{\partial D}{\partial \xi} \Gamma_{xy} \right) \right]
$$

and
The cell in which each particle lies is calculated using a method similar to that detailed by Milgram. It is now possible to calculate all derivative terms in eqns. (12) & (13) using central differences about the cell centre. The values of the advective velocities \( u \) and \( v \) are computed using Taylor series expansions up to second order about the nearest non-zero velocity node in the cell containing the particle. If the distances in the \( x \)- and \( y \)-directions between the particle and the nearest non-zero velocity node are denoted by \( \Delta x \) and \( \Delta y \) and if the nodal velocities are represented as \( u_n \) and \( v_n \), then the velocity components at the particle position can be expressed as

\[
\begin{align*}
\frac{3u}{\Delta x} &= \frac{u}{x_n} + \Delta y \frac{\partial u}{\partial y_n} + \frac{\Delta x^2}{2} \frac{\partial^2 u}{\partial x^2_n} + \frac{\Delta y^2}{2} \frac{\partial^2 u}{\partial y^2_n} + \Delta x \Delta y \frac{\partial^2 u}{\partial x \partial y_n} \\
\frac{3v}{\Delta y} &= \frac{v}{y_n} + \Delta x \frac{\partial v}{\partial x_n} + \frac{\Delta y^2}{2} \frac{\partial^2 v}{\partial y^2_n} + \Delta x \Delta y \frac{\partial^2 v}{\partial x \partial y_n}
\end{align*}
\]

Again it is necessary to transform the equations to curvilinear coordinates but this time second derivatives are also required. These are calculated by differentiating eqn. (11) with respect to \( x \) and \( y \). The resulting equations are too long to be presented here, but full details can be found in Pearson & Barber.

Once the modified advection velocities are known, the new particle position due to pure advection can be calculated using a second-order accurate iterative technique which ensures that

\[
\begin{align*}
\frac{x_a(t + \Delta t) - x_a(t)}{\Delta t} &= U^* \\
\frac{y_a(t + \Delta t) - y_a(t)}{\Delta t} &= V^*
\end{align*}
\]

where,

\[
\begin{align*}
U^* &= \frac{U(x_a(t + \Delta t), y_a(t + \Delta t)) + U(x_a(t), y_a(t))}{2} \\
V^* &= \frac{V(x_a(t + \Delta t), y_a(t + \Delta t)) + V(x_a(t), y_a(t))}{2}
\end{align*}
\]

and \( x_a \) and \( y_a \) are the \( x \)- and \( y \)-coordinates of the advected particle position.

At the end of the advection calculation, the resulting particle distribution must undergo diffusion. This is accomplished by adding random velocity...
components to each particle with an appropriate standard deviation. The random longitudinal and transverse velocity components are generated as

\[ u_L' = r_1 \sqrt{\frac{2\Gamma_L}{\Delta t}} \quad , \quad u_T' = r_2 \sqrt{\frac{2\Gamma_T}{\Delta t}} \]  

(18)

where \( r_1 \) and \( r_2 \) are independent normally distributed random numbers, each with zero mean and standard deviation of unity. As shown by Hunter et al., it is essential to have a random number generator which returns values that are sufficiently random so that diffusive processes may be simulated accurately. For this reason the routines RAN3 and GASDEV as described by Press et al. are used to provide the normally distributed random numbers. After calculating the longitudinal and transverse diffusive velocities they can be expressed in the Cartesian coordinate system by transformation such that:

\[ u' = u_L' \cos \theta - u_T' \sin \theta \]  

(19)

\[ v' = u_L' \sin \theta + u_T' \cos \theta . \]  

(20)

The final x- and y-coordinates of the particle can now be expressed as

\[
\begin{align*}
  x &= x_a(t + \Delta t) + u'\Delta t \\
  y &= y_a(t + \Delta t) + v'\Delta t .
\end{align*}
\]  

(21)

Any particles which cross a solid boundary are immediately reflected back into the flow domain thus maintaining mass conservation. The method is conservative, front preserving and unconditionally stable although the time step should be limited in order to obtain an accurate representation of the advective transport.

4 Results

The particle tracking algorithm was validated against an analytical test case of pure advection of a circular distribution of particles. The non-orthogonal boundary-fitted mesh used in the study is shown in Figure 2. The domain has a radius of 25 m and is 1 m deep. The fluid was given an anticlockwise angular velocity of 0.04 rads/s about the centre of the domain (0,0), giving a velocity of zero at the centre and 1 m/s at the perimeter. A circular distribution of 10000 particles and 5 m in radius was introduced, initially centred at (0,10). The particles were advected for 1 revolution using a model time step of 0.2 s. The time for one revolution is given by \( 2\pi/0.04 \) which is approximately equal to 157 s. Theoretically, the circular distribution of particles should undergo no deformation. The results for 0.25, 0.5, 0.75 and 1.0 revolutions are given in Figure 2 and were indistinguishable from the analytical solution therefore implying that the advective scheme is phase preserving.
The practical potential of the method is demonstrated by application of the model to a 50 km long section of the Humber Estuary on the east coast of England. The Humber Estuary provides an outlet to the North Sea for the rivers Trent and Ouse, and shipping access to a number of ports including Hull, Immingham and Grimsby. The present work has concentrated on the wider lower part of the estuary where the flow patterns are of a complex two-dimensional nature and tidal effects dominate. Figure 3 shows the extent of the modelled area and the location of velocity observation sites used in model validation, whilst Figure 4 shows the boundary-fitted coordinate system representative of the estuary. For the mesh illustrated, no grid line attraction was necessary and so the control functions, P and Q, in the grid generation equations were set to zero. The depth of the bed below a fixed ‘Chart Datum’ was then calculated at all grid nodes using inverse power interpolation between scattered bathymetry points.

The hydrodynamic calculations providing the velocities to drive the pollution model were solved within the same computer code using the method described by Pearson & Barber. The time step was identical for both models and equalled 12 s. The purpose of the study was to examine the dispersion of pollution from a proposed sewer outfall north of Grimsby. The position of the outfall is shown by the crosshair in Figure 5. Pollution was discharged into the estuary at a rate of 1.25 m³/s beginning 15 minutes after high water and ending 2 hours 15 minutes after high water. The mean pollutant concentration
was set to 1.0 kg/m³ and the particle mass was set to 1 kg. This led to a mass of 15 kg being introduced into the system each time step, equivalent to 15 particles. Thus, in total, 9000 particles were released into the estuary over the two hour period. The position of the plume on the ebb tide, 4.75 hours after high water, is presented in Figure 5 whilst the position of the plume on the flood time, 10 hours after high water, is shown in Figure 6. From the results, it is obvious that very little mixing occurs during the tidal excursion.
Figure 5: Plume transport on ebb tide

Figure 6: Plume transport on flood tide
5 Conclusions

A particle tracking model has been developed for use with non-orthogonal boundary-fitted grids to simulate depth-averaged pollution transport in well mixed estuaries and coastal seas. The method is conservative, front preserving and unconditionally stable although the time step should be limited in order to obtain accurate representation of the advective transport. In the case of practical estuary studies, the number of particles required to obtain accurate quantitative predictions may become prohibitive. However, the method is useful from the qualitative point of view as a means of assessing pollution transport trends and perhaps to assist in contingency planning.

References