Solute Transport Model for Open Channel Flow

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\textbf{ABSTRACT}
A numerical model is expected to become the primary tool in predicting the flow depth of any flood event. Apart from simulating the flood flow, a solute transport model is found to be an important aspect as it could spread by the flood flows. Due to development in computer technology, a two-dimensional (2D) model has become popular in flow modeling and its associated processes such as solute transport. However, in certain cases of modelling the flood event, the modeller would probably face difficulty in resolving the problematic river flow in a 2D manner. Hence, a one-dimensional (1D) model with the ability to deal with complex hydrodynamic flows is needed. This paper presents a 1D solute transport numerical model development. The St. Venant equations for an open channel flow and the advection-diffusion equation are used to simulate both shallow and contaminated flows simultaneously. The model has been validated and the results obtained show a good agreement when compared to the analytical solutions.

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\textbf{1. INTRODUCTION}
Floods are one of the primary hazards affecting Malaysia. With the continuous development in urban areas, the flood risks impact has probably significantly increased. To minimize this impact, computer modelling is expected to become the primary tool in simulating flood flows to predict flow depth. Early warnings of flood events can thus be delivered, especially in urban and commonly flood-ravaged areas. A solute transport model has been found to be an important aspect to be considered as it could be spread by flood flows which then worsens the affected areas. This solute pollutant may be a potential public health risk when associated with urban floods. Thus, a study on the solute transport processes is significant. It may also provide an essential tool in managing water quality and assessing the environmental impact as well.

\textbf{2. THEORETICAL BACKGROUND AND MODEL DEVELOPMENT}
It is common to assume that the 1D channel attached to a floodplain has a rectangular cross-section [1], [2] Equation (1) is the matrix form of 1D SWE’s that is widely used to simulate different types of flow.

\[
\frac{\partial u}{\partial t} + \frac{\partial f}{\partial x} = s
\]

Where \( t \) is time and \( x \) represents the distance along the flow direction. Vector \( u \) contains the flow variables while \( s \) contains the source terms. \( f \) denotes the flux vector in \( x \) direction. For a wide application in modeling the flows Riemann solvers of the SWE’s are of substantial interest (e.g. [3-6]). By adding the solute transport equation to the SWE’s, the integrated model is able to predict the depth-averaged shallow flow and the fate of pollutant. The equation used to predict the pollutant transport is directly inserted into the 1D flow model so that they can be run simultaneously. This scheme is intended to ensure well-balanced and non-negative solutions for the wet-dry front case. Those vectors \( \mathbf{u}, \mathbf{f} \) and \( \mathbf{s} \) and are given in (2).

\[
\mathbf{u} = \begin{bmatrix} u \\ \eta \end{bmatrix} ; \quad \mathbf{f} = \begin{bmatrix} uh \\ uch \\ u^2h + \frac{1}{2}g(\eta^2 - 2\eta\eta_s) \end{bmatrix} ;
\]

\[
\mathbf{s} = -\frac{q}{bh} \frac{\partial b}{\partial x} - C_f |\mathbf{u}| - g\eta \frac{\partial \eta_s}{\partial x}
\]

Where \( q = uh \) gives the unit-width discharge with \( u \) is the depth-averaged velocity while \( h \) is the water depth, \( Zb \) denotes the bed elevation so that \( h = h - Zb \), \( g \) is the gravity acceleration, \( C_f = gn^2/h^{5/3} \) is the coefficient of river roughness while the Mannings’ coefficient is denoted by \( n \).

Besides using the flow depth (h), the free surface water
The concentration is passively transported by the flow. Further assumption is the species are well-mixed vertically in such that the concentration is passively transported by the flow [6].

The 1D model was solved by an explicit finite volume Godunov-type scheme merged with Harten, Lax and van Leer (HLL) Riemann solver. As the advantages of these schemes are numerous, implementation of HLL Riemann solver used to solve the fully 1D SWEs with the source terms accounts for the effects of friction in varying domains. The model is able to handle the wet-dry case over irregular topographic features without producing negative water depth. Denoting \( f \) and \( s \) are the finite volume approximation to the muddling value of \( u(x, t) \) over the cell \( i \) at time \( t \) and at cell interface respectively. Equation (3) is the final simplified explicit time marching formula.

\[
\mathbf{u}^{k+1}_i = \mathbf{u}^k_i - \frac{\Delta t}{\Delta x} \left( f_{i+1/2} - f_{i-1/2} \right) + \Delta x s_i
\]  

(3)

Where the subscript \( i \) denotes the cell index, \( \Delta x \) and \( \Delta t \) are the cell size and time step respectively. \( f_{i+1/2} \) and \( f_{i-1/2} \) are the interface fluxes through the two edges of cell \( i \). During the computation, \( i \) is directly available as all the conserved variables are stored in cell centre. Using the finite volume scheme-Godunov-type, fluxes are evaluated by solving local Riemann problems. In this work, the HLL Riemann solver [9] is adopted to calculate the fluxes as it has the advantage of facilitating wetting and drying. By employing the second-order Runge-Kutta method in (3), the temporal accuracy is improved. Combining the Godunov-type finite volume method with the 2nd-order Runge-Kutta method, the temporal accuracy of the scheme and the time marching formula becomes (4).

\[
\mathbf{u}^{k+1}_i = \mathbf{u}^k_i + 0.5\Delta t \left( K_0(u^k) + K_2(u^2) \right)
\]  

(4)

Where \( K_0 \) is the Runge-Kutta coefficient at predictor and corrector steps. At every time step, the Runge-Kutta coefficients are calculated at two consecutive steps for updating the flow variables with the correct flux and source terms values.

3. Fate of Pollution Model Validation

3.1 Pure Diffusion : Constant Concentration in Various Flow Depth

A 10 m long with a 0.5 m wide rectangular channel with free water surface elevation of 1 m resting with solute concentration \( C = 1 \) mg/L was simulated using the proposed scheme. Fig. 6 illustrates the flow and the bed profile of the channel. The concentration was set to be uniform initially and remain constant as the time increases. The diffusion coefficient, \( D \) was taken as 0.01 m2/s. After 1000 time steps, the concentration, \( C = 1 \) mg/L remained unchanged as in Fig. 1. The uniform results of concentration indicate that the variation of free surface water elevation did not affect the model conservation in mass and momentum [10] and shows that the model can be used to simulate solute transport in a complex topography problem.

![Fig. 1. Comparison of concentration](image)

3.2 Pure Advection : Pollutant Transport in Square Cavity

The first case of pure affection of pollutant transport is as described by \([11]\) and \([12]\). The case was then tested again \([13]\) where the water flowing along a squared channel with dimensions of 9000 m x 9000 m with a bottom slope of -0.001. The Mannings’ roughness coefficient, \( n \) was set to 0.025. A uniform velocity imposed was at 0.5 m/s. The pollution concentration is given by (5) where \( x_1 \) and \( x_2 \) are 1400 m and 2400 m respectively.

\[
C(0, x) = C_1 \exp\left( -\frac{(x-x_1)^2}{\sigma_1^2} \right) + C_2 \exp\left( -\frac{(x-x_2)^2}{\sigma_2^2} \right)
\]  

(5)

Where \( C_1 = 10, C_2 = 6.5 \) and \( \sigma_1 = \sigma_2 = 264 \). No turbulence effect accounted for, thus the constant diffusion coefficient was given as \( D = 0.001 \). Fig. 2 and Fig. 3 shows the plots of pollutant concentration at the initial time and time, \( t = 5235 \) s respectively. A simple inspection shows that at a constant speed of \( u = 0.5 \) m/s, the pollutant shape is conserved along its advection direction. The comparison of numerical results with the analytical results is also satisfactory. From Fig. 2 and Fig. 3, it can be seen that both results show good agreement between numerical scheme and the analytical solutions. The proposed scheme exhibits its attractiveness for the general purpose of pollutant transport modelling. Results obtained also indicate that the scheme may be effective in modelling the pollutant transport in rivers especially for pure advection process.
3.3 Convection–Advection Tests

The test involved a 1D convective–diffusion problem with pollutant suddenly discharged into the river [10]. A discharge, $Q = 5.69 \text{ m}^3/\text{s}$ was imposed with the downstream river depth set to $h = 1.52 \text{ m}$. A 50 g non-degradable contaminant was injected at a location, $x_0 = 10 \text{ m}$ along the channel. The frictional channel has Mannings’ roughness coefficient of $n = 0.01$. Equation (6) is the analytical solution of concentration

$$C = \frac{m}{A} \cdot \frac{1}{\sqrt{4\pi \sigma}} e^{-\left((x-x_0)^2/4\sigma^2\right)}$$

Fig. 4 and Fig. 5 exhibit the solute concentration at different time-steps. From the numerical results, the maximum concentration computed was 0.5982 mg/L. For a longer simulation time, there was a reduction in the maximum concentration value. This can be seen again as in Fig. 5 where with the increase in computational time, the amount of concentration was diluted or mixed well with the flow thus concentration values become lesser. The model can provide good accuracy in the convective-advection problem.

4. CONCLUSIONS

A 1D solute transport model for shallow flow was developed by solving the governing St Venant equations. A Godunov-type finite volume scheme was used to represent the equations. An approximate Riemann solver called Harten Lax vanLeer or HLL scheme was also used to find the direct approximation of fluxes. Meanwhile, higher-order accuracy is achieved using a 2nd Order Runge-Kutta time integration method. The model has been validated against several benchmark tests of solute transport in open channel flow, with good agreement obtained for all tests being considered and this confirms the accuracy of the current 1D model. The species transport model provides a feasible way to understand the nature of environmental flows induced by the underlying dynamics. However, the equation being used only describes passive dynamics of the transported concentration. Thus, an advection-reaction equation is recommended to be taken into account in future investigations.

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