Higher order explicit schemes for BOD-DO modelling in open channels

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Abstract

This paper introduces a methodology for developing higher order explicit schemes for the solution of two coupled, one dimensional transport equation describing advection, dispersion and kinetics processes for BOD and DO modeling in open channels. Based on the proposed methodology, four new higher order schemes namely second order nodal, second order cell centered, third order nodal and third order cell centered are developed. Transport of BOD resulting in DO deficit with exponentially decaying BOD input as an upstream boundary condition is simulated with the developed schemes. Results of the proposed schemes are compared with analytical solution for BOD and convolution integral solution for DO. Proposed schemes accurately simulate BOD-DO profiles for the case under consideration.

1 Introduction

Water transports a variety of chemical constituents in natural and man-made water conveyance systems. Their presence in small quantities may results in environmental hazards, and is of prime concern to the environmental engineers. The impact of waste discharges on the dissolved oxygen (DO) is important since water quality standards are expressed in terms of DO. BOD is the measure for characterization of waste discharges and helps in deciding its subsequent impact on DO level in the stream. Two coupled, one dimensional transport equation describing the process of advection, dispersion and kinetics form the basis for the
modeling of biochemical oxygen demand (BOD) and dissolved oxygen (DO) in the streams.

Analytical solutions of transport equation for different cases are available in literature (Adrian and Alshawabkeh [1], Aral and Liao[2], Fisher [7], Li [14], Zoppou and Knight [21]). Almost all available analytical solutions are restricted to simple initial and boundary conditions, coefficients with unrealistically simple functions of space and/or time, uniform flow in prismatic channels, and thereby have a limited practical relevance. Apart from these limitations, the implementation of these analytical solutions often require numerical evaluation of complex convolution integrals (Bennett [3]), which are computationally expensive as compared to numerical solutions of transport equations. Further, due to numerical evaluation of these integrals, the accuracy of analytical solutions can no longer be claimed to be superior to numerical schemes. Hence, for most of the practical applications that involves complex initial and boundary conditions, modelers are forced to resort to the numerical solution of transport equations.

Several numerical approaches such as finite difference, finite volume, essentially non-oscillatory schemes, finite element, finite analytic, Eulerian and Lagrangian and split operator over fixed, variable and/or scattered grids are reported in the literature for the solution of transport equation. Several schemes such as QUICK and QUICKEST (Leonard[12]), Exact Peak Capturing and Essentially Oscillation Free scheme (Yeh and Chang[20]), LAMBDA (McBride and Rutherford [16]), Essentially Non-Oscillatory schemes (Chakravarthy [5]) and split operator schemes have been developed. In the split operator schemes, focus of the research is on the accurate simulation of advective component of transport (Holly and Preissmann [8], Li [13], and, Schohl and Holly [18]). Several other approaches such as upwinding approximation (Dresnack and Dobbins [6]), use of Hermite Polynomials (Holly and Preissmann [8], Yang and Hsu[19]), Lagrangian (Runkel and Chapara[17], Manson and Wallis[15], Bravo [4]), and matched diffusivity (Koussis et al. [9],[10]) also have been put forward.

Numerical solution of differential form of conservation laws has been an area of extensive research since the dawn of computers. Numerous computational algorithms, methods or schemes have been developed, but only a few specific problems could be solved efficiently and accurately (Yeh and Chang [20]). Due to the presence of both hyperbolic (advective process) and parabolic (diffusive process) terms in the transport equations, most of the conventional numerical schemes are vulnerable to spurious damping or oscillations, numerical dispersion, phase errors, peak clipping and/or valley elevating etc. leading to an inaccurate simulation.

A methodology for developing several higher order explicit schemes for an accurate simulation of 1-D pollutant transport in open channels is introduced in this paper. Based on the proposed methodology, four novel schemes are developed for the modeling of BOD-DO transport in open channels with exponentially decaying input. Results of the proposed schemes are compared with analytical solution for BOD and convolution integral solution for DO. It is
observed that proposed schemes accurately simulates BOD-DO profiles for the case under consideration.

2 Governing Equations

One-dimensional multi-species solute transport equation can be written as

\[ \frac{R}{\partial t} \frac{\partial C_A}{\partial t} + u(x,t) \frac{\partial C_A}{\partial x} = \frac{\partial}{\partial x} \left( \epsilon \frac{\partial C_A}{\partial x} \right) + S_A(C_A, C_B) + Q^* C^* \delta(x - x_A) \]  (1)

\[ \frac{R}{\partial t} \frac{\partial C_B}{\partial t} + u(x,t) \frac{\partial C_B}{\partial x} = \frac{\partial}{\partial x} \left( \epsilon \frac{\partial C_B}{\partial x} \right) + S_B(C_A, C_B) + Q^* C^* \delta(x - x_B) \]  (2)

Where, \( C \) = solute concentration; \( t \) = time; \( x \) = spatial coordinate; \( u \) = mean stream velocity in \( x \) direction and is obtained from the flow simulation models; \( \epsilon \) = longitudinal dispersion coefficient; \( Q^* \) = lateral flow; \( C^* \) = concentration of lateral input; \( R \) = sorption term (taken as unity in this case); \( \delta(x - x_A) = \) Dirac delta function; \( S \) = source/sink terms. The subscripts \( A, B \ldots \) refer to the different species of constituents and \( C_A \) and \( C_B \) = respective average BOD and DO deficit concentration. Similarly, for coupled BOD-DO modelling (a special case of multi-species reacting solute transport)

\[
\begin{align*}
S_A &= +k_1 C_A \\
S_B &= +k_1 C_A - k_2 C_B
\end{align*}
\]  (3)

where \( k_1 \) = rate of oxidation of BOD; \( k_2 \) = re-aeration rate coefficient. For this case, both Eqn. (1) and Eqn. (2) along with Eqn. (3) are solved together as coupled system of differential equations. Eqn. (1) or Eqn. (2) can be written as

\[ \frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = \epsilon \frac{\partial^2 C}{\partial x^2} + S(C) \]  (4)

\[ \frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = L(C) \]  (5)

\[ L(C) = \epsilon \frac{\partial^2 C}{\partial x^2} + S(C) \]  (6)

3 Mathematical Formulation

Using difference approximation, (5) can be expressed as,

\[ \left( \frac{\partial C_i}{\partial t} \right) = (u) \frac{C_{i-1} - C_{i+1}}{2\Delta x} + L_i(C) \]  (7)
Set of difference equations for all nodes along with boundary conditions are expressed in the matrix form as,

\[
\frac{dC}{dt} = A^c C + (B + L)
\]  

(9)

In which, \( C = \) nodal concentration vector; \( A^c = \) coefficient matrix; \( B = \) boundary condition matrix; \( L = \) source/sink and diffusion vector. Eqn. (9) can be analytically solved as

\[
C^t = e^{A^c t} + e^{A^c t} \int_0^t e^{-A^c \tau} \left[ (B(\tau) + L(\tau)) \right] d\tau
\]  

(10)

Writing Eqn. (10) at time step \( t+\Delta t \),

\[
C^{t+\Delta t} = e^{A^c (t+\Delta t)} + e^{A^c (t+\Delta t)} \int_0^{t+\Delta t} e^{-A^c \tau} \left[ (B(\tau) + L(\tau)) \right] d\tau
\]  

(11)

Eliminating constant of integration and evaluating integral term using trapezoidal rule,

\[
C^{t+\Delta t} = e^{A^c \Delta t} C^t + \left( I + e^{A^c \Delta t} \right) \frac{(B + L) \Delta t}{2}
\]  

(12)

in which \( I = \) identity matrix. Exponentiation of the matrix \( A^c \Delta t \) results in a dense matrix. There are different ways of computing exponent of a matrix. However, commonly used techniques for matrix exponentiation are not explicit in nature. Performing exact exponentiation of matrix at each time step would be computationally uneconomical and cumbersome. In the proposed methodology, exponent of the matrix is constructed in different ways resulting in different order of approximations.

The proposed methodology makes use of the fact that (1) the structure of the exponentiation of a block diagonal matrix results in a block diagonal matrix of the same structure. (2) The elements of complete exponentiated block diagonal matrix are same as the ones obtained by taking the exponent of individual block matrices. In the present methodology, coefficient matrix \( A^c \Delta t \) is
split in such a way that each matrix consists of smaller \((2 \times 2)\) block diagonal matrix that is exponentiated analytically. Final exponentiated matrices are assembled together to obtain approximation of the matrix \(e^{A^c \Delta t}\). There are different ways of splitting matrices. Depending upon the ways of splitting of coefficient matrix, its exponentiation and assemblage of final expression for approximation of the matrix \(e^{A^c \Delta t}\), higher order explicit methods are developed.

### 3.1 Second order explicit schemes

As discussed above, matrix \(A^c \Delta t\) is split into two block diagonal matrices. Each block of these split block diagonal matrices can be expressed as \(2 \times 2\) matrix. The exponent of \(2 \times 2\) matrices is obtained analytically using Laplace transforms (Kreyszig [11]). Final difference equations are obtained by substituting the exponents of \(2 \times 2\) matrices into block diagonal matrix and assembling them. The details of nodal and cell centered form of methods are discussed below.

Splitting the coefficient matrix \(A^c \Delta t\) in to two block diagonal matrices, \(A^c_{\ell} \Delta t\) and \(A^c_{o} \Delta t\) as,

\[
\begin{bmatrix}
\ldots & \ldots \\
0 & -\alpha \\
\alpha & 0 & -\alpha \\
\alpha & 0 & -\alpha \\
\alpha & 0 & -\alpha \\
0 & \ldots & \ldots \\
\end{bmatrix}
= \begin{bmatrix}
0 \\
\alpha \\
0 \\
0 \\
0 \\
0 \\
\end{bmatrix}
\]

In which, \(\alpha_{c1} = \frac{u \Delta t}{2 \Delta x_i} = \) half the Courant number. Exponentiating each block separately and assembling results in second order accurate approximation of \(e^{A^c \Delta t}\) in space and time.

\[
e^{A^c \Delta t} = e^{(A^c_{\ell} + A^c_{o}) \Delta t} = e^{A^c_{\ell} \Delta t} e^{A^c_{o} \Delta t} + O(\alpha_c^3)
\]

Exponent of each \(2 \times 2\) block of block diagonal matrix is

\[
e^{\alpha_c \Delta t} = \begin{bmatrix}
0 & -\alpha_c \\
\alpha_c & 0
\end{bmatrix} = \begin{bmatrix}
\cos \alpha_c & -\sin \alpha_c \\
\sin \alpha_c & \cos \alpha_c
\end{bmatrix} = \begin{bmatrix}
a & b \\
c & d
\end{bmatrix}
\]

Substitution of Eqn. (15) for each \(2 \times 2\) block of Eqn. (13), exponent of matrices \(A^c_{\ell} \Delta t\) and \(A^c_{o} \Delta t\) as are obtained. Explicit expressions for nodal concentration \(C\)
values at new time level $t + \Delta t$ can be obtained by assembling two matrices. Based on nodal and cell-centered form of Eqn. (7), second and third order schemes are developed, as discussed in the subsequent sections.

### 3.1.1 Second order nodal scheme

Expression for $C$ at the node can be obtained by multiplying matrices $e^{A_i\Delta t}$ and $e^{A_c\Delta t}$ as,

\[
\begin{bmatrix}
C_1 \\
C_2 \\
\vdots \\
C_N
\end{bmatrix} + \Delta t
= \begin{bmatrix}
\cdots & a & b & c & d & \cdots \\
\cdots & a & b & c & d & \cdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots
\end{bmatrix}
\begin{bmatrix}
C_1 \\
C_2 \\
\vdots \\
C_N
\end{bmatrix}
\]

Substituting for $e^{A_i\Delta t}$ in Eqn. (12) and considering appropriate boundary and source/sink terms, unknown $C$ at new time step $t + \Delta t$ are obtained. Above equations for odd node $i$

\[
C_{i+1}^{t+\Delta t} = aC_{i}^t + adY_{i-1}^t + abY_{i-1}^t + bbY_{i+1}^t + \left(L_{i+1}^d + S_i^t + B_i^1 \right) \frac{\Delta t}{2}
\]

and for even nodes $i$,

\[
C_{i+1}^{t+\Delta t} = ccY_{i-2}^t + cdY_{i-1}^t + adY_{i+1}^t + bdY_{i+1}^t + \left(L_{i-1}^d + S_i^t + B_i^1 \right) \frac{\Delta t}{2}
\]

with

\[
Y_i^t = C_i^t + \left(L_{i-1}^d + S_i^t + B_i^1 \right) \frac{\Delta t}{2}
\]

and

\[
a = \cos(\alpha_c)_i, \ b = - \sin(\alpha_c)_i, \ c = \sin(\alpha_c)_i, \ d = \cos(\alpha_c)_i
\]
in which, \( \alpha_c = \frac{u \Delta t}{2 \Delta x} \) = half the flow /advection Courant number; \( L_{i}^d \) = magnitude of diffusion term and is obtained from Eqn. (8); \( S_{i} \) = magnitude of source / sink terms and \( B_{i} \) = boundary terms.

### 3.1.2 Second order cell centered scheme

Following the above procedure, expression for cell centered values of \( C \) at node \( i \) is obtained.

\[
C_{i}^{t+\Delta t} = 0.5cY_{i-2}^t + acY_{i-1}^t + adY_{i}^t + bdY_{i+1}^t + 0.5bbY_{i+2}^t + \left( L_{i}^d + S_{i}^t + B_{i}^t \right) \frac{\Delta t}{2} \tag{21}
\]

where coefficients \( a, b, c \) and \( d \) are as defined in Eqn. (20) and \( Y \) as defined in Eqn. (19). Unlike the nodal scheme, expression for even and odd nodes is same for cell-centered schemes.

### 3.2 Third order explicit schemes

Following the above procedure, in these schemes the coefficient matrix \( A^c \Delta t \) is split in to three block diagonal matrices. Exponent of these matrices results in to block diagonal matrix. Using exponent of the block matrix, on line of the second order schemes, two third order schemes namely third order nodal and third order cell centered can be developed.

### 4 Application

The above schemes are applied to the following cases of BOD-DO modeling in open channels. Results of the proposed lumped diffusion schemes are compared with the analytical solutions and convolution integrals.

#### 4.1 BOD-DO modeling in uniform flow field

The transport of BOD resulting in DO deficit is studied in this section. Exponentially decaying BOD input is considered as an upstream boundary condition. In this case, a BOD input starts at \( t = 0 \) from an initial value to \( C_{A0} \) and then decays exponentially over time is imposed at the outfall (\( x = 0 \)) as

\[
C_{A}(0, t) = C_{A0} \exp(-k_1 t) \tag{22}
\]

\( C_{A0} \) = peak BOD loading at time \( t = 0 \) and \( x = 0 \) i.e. at the outfall section, \( k_1 \) = rate of oxidation. The stream is semi-infinite and initially free of BOD. Eqn. (22) yields a step input, which is used as upstream boundary condition. The analytical solution of the transport equation for BOD subject to Eqn. (4) is (Koussis et al. [9]).
The DO concentration is obtained from the convolution integral (Bennett [3], Bravo [4]).

\[
\frac{C_A(x,t)}{C_{A_0}} = \frac{1}{\sqrt{\pi}} \exp(\frac{1}{\sqrt{4 \pi \tau}}) \left[ \text{erf} \left( \frac{x - ut}{\sqrt{4 \tau}} \right) + \exp \left( \frac{x + ut}{\sqrt{4 \tau}} \right) \right] \exp \left( \frac{ux}{\varepsilon} \right)
\]

The DO concentration is obtained from the convolution integral (Bennett [3], Bravo [4]).

\[
C_B(x,t) = \int_0^t \frac{u(\tau)}{4 \pi (t - \sigma)^{3/2}} \exp \left( - \frac{z(x,t,\sigma)^2}{4 (t - \sigma)} \right) \left[ C_B(0,\sigma) \exp(-k_2(t-\sigma)) + \frac{C_A(0,\sigma)}{k_2 - k_1} \left[ \exp(-k_1(t-\sigma)) - \exp(-k_2(t-\sigma)) \right] \right] d\sigma
\]

Where \( z = \) Lagrangian distance coordinate used to compute instantaneous unit impulse released at time \( \sigma \), at the upstream boundary. This convolution integral is evaluated numerically, maintaining high accuracy. The stream flow velocity, \( u=1 \text{ m/s, }\varepsilon=216 \text{ m}^2/\text{sec, } k_1=0.2 \text{ day}^{-1}, k_2=0.4 \text{ day}^{-1}, \Delta x = 432 \text{ m} \) and \( \Delta t = 200 \text{ sec.} \) is used. Simulated dimensionless BOD and DO deficit concentrations are compared with analytical and convolution integral solutions for different values of \( x k_1/U \) in Fig. 1.
The dimensionless time $k_{lt}$ is plotted on the abscissa. As BOD gets transported in the stream it decays and disperses, resulting in lowering of peaks. Similarly, DO starts getting consumed as it moves downstream resulting in increase in peak of DO deficit. BOD and DO deficit pollutographs obtained using proposed lumped diffusion schemes are in good agreement with the analytical solution and convolution integral solution, as shown in Fig. 1 (a) and Fig. 1 (b).

5 Closure

A methodology for developing a family of higher order explicit schemes for water quality (BOD-DO) simulation in open channel is introduced. Four new explicit schemes namely, second order nodal, second order cell centered, third order nodal and third order cell centered are developed. From the foregoing discussion and results, it is clear that the proposed schemes can handle all physical, chemical and flow complexity with high degree of accuracy. Proposed methodology can be extended in developing further higher order approximations.

References


