Numerical solution for DO transport equation

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An alternate finite difference scheme which is explicit and unconditionally stable has been presented. The scheme overcomes the artificial/numerical dispersion/diffusion error, which is usually encountered when the advection part of the advection dispersion equation is solved using finite difference approximation. The scheme works within certain specified range of time interval \((\Delta t)\) but for spatial grid interval there is no such restriction. The proposed scheme is tested using some hypothetical but rational data. The DO variation with time and distance due to an exponentially decaying source of BOD, are plotted and discussed.

The problem of dissolved oxygen (DO) begins with the oxygen demanding wastes entering a water body which consume the DO contents of the water body. The impact of low DO concentration is consequently reflected through unbalanced ecosystem, fish mortality and other aesthetic nuisance. There may be situations (for example accidental spill of a pollutant or malfunctioning of some process) in which the effect of longitudinal dispersion could not be neglected. In such cases, the quantitative evaluation of mixing and transport of BOD and DO is required to more rationally predict the DO content of a river.

The method to solve the advection-dispersion equation numerically using finite differences by an Eulerian approach has already been reported. The early experiments with finite differences have shown that the Eulerian approach is better suited when the Peclet number is small. In such cases the smoothing effect of dispersion tends to mask the errors in the advective portion of the numerical advective dispersion calculations. However, at the high Peclet number when the advection predominates the error in the finite difference computations based on central difference approximation may result in an artificial diffusion which may be stronger than the natural diffusion. This may result in overshoot, undershoot and negative concentrations. The effect of this error is to smear sharp concentration fronts. For many practical problems, reducing numerical dispersion sufficiently may require an extremely fine grid. Since, this is not always practical, the alternative is to use upstream difference approximations which are capable of eliminating oscillation. Price, Leendertse, Holly and Preissman and Leonard have used upstream centred Eulerian scheme on a dense computational grid but at the expanse of complex algorithm and substantial computational efforts.

An alternative finite difference scheme is presented in this paper which overcomes the above stated errors. The hydraulic parameters such as channel geometry and stream velocity are assumed to vary in longitudinal direction. The unconditionally stable explicit scheme can be applied only for certain specified range of time interval \((\Delta t)\) but the spatial grid interval \((\Delta x)\) is calculated using the time of travel formula.

Differential Equation Representing DO Balance in River

The differential equation representing DO balance in river is developed using principle of conservation which incorporates three phenomena (i) input of oxygen from the atmosphere; (ii) dispersion advection of DO and (iii) decay due to BOD. In developing the equation the following assumptions are used.

- The presented one-dimensional model (i.e. the differential equation) is applied only after the mixing length is over.
- The dispersion coefficient includes the effect of diffusion through longitudinal and turbulent mixing.
- The BOD present is entirely in dissolved form and is decaying according to a first order kinetics.

The transport equation for BOD and its impact on DO would be governed by the following coupled system of equations:

\[
\frac{\partial B}{\partial t} + u(x) \frac{\partial B}{\partial x} = \frac{1}{A(x)} \frac{\partial}{\partial x} \left[ E(x) \cdot A(x) \cdot \frac{\partial B}{\partial x} \right] - K_1 B
\]

\[
\frac{\partial B}{\partial t} + u(x) \frac{\partial B}{\partial x} = \frac{1}{A(x)} \frac{\partial}{\partial x} \left[ E(x) \cdot A(x) \cdot \frac{\partial B}{\partial x} \right] - K_1 B
\]
\[
\frac{\partial C}{\partial t} + u(x) \frac{\partial C}{\partial x} = \frac{1}{A(x)} \frac{\partial}{\partial x} \left[ E(x) \cdot A(x) \cdot \frac{\partial C}{\partial x} \right]
\]

\[+ K_1 B + K_2 (C_s - C) \quad \ldots (2)\]

where \(B(x,t)\) and \(C(x,t)\) are concentration of BOD and DO, respectively, in mg/L, at a distance \(x(\text{m})\) downstream from the outfall at any time \(t(\text{s})\). \(u(x)\) the mean cross-sectional flow velocity (m/s) of the stream, \(E(x)\) the coefficient of longitudinal dispersion (m²/s) at distance \(x\), \(A(x)\) the area of cross-section (m²) at distance \(x\); \(K_1\) the decay rate of BOD (s⁻¹), \(K_2\) the coefficient of reaeration (s⁻¹), and \(C_s\) is the concentration of DO at saturation level (mg/L).

**Boundary conditions**—Solution of Eqs (1) and (2) require appropriate initial and boundary conditions. A hypothetical case is considered in which the stream is assumed to be free of BOD initially. A BOD source of strength \(B_0\), is considered at the outfall \((x=0)\) which is decaying exponentially with time. It is also assumed that there is no other source of BOD downstream of the outfall except the above stated source of strength \(B_0\).

These consideration leads to the following initial and boundary conditions written in mathematical form.

\[B = 0; \quad C = C_s; \quad t = 0 \quad \ldots (3)\]

\[B = B_0 \exp(-K_1 t); \quad C = C_s - \frac{K_1 B_0}{K_2 - K_1} \left[ \exp(-K_2 t) \right.\]

\[\left. - \exp(-K_1 t) \right]; \quad x = 0 \quad \ldots (3)\]

\[B \to 0; \quad C \to C_s \quad \text{as} \quad x \to \infty \quad \ldots (3)\]

**Simplification for Eqs (1) & (2)—**For the sake of simplicity Eq. (2) is written in terms of DO deficit \(C^* = C_s - C\), which yields Eq. (4)

\[
\frac{\partial C^*}{\partial t} + u(x) \frac{\partial C^*}{\partial x} = \frac{1}{A(x)} \frac{\partial}{\partial x} \left[ E(x) \cdot A(x) \cdot \frac{\partial C^*}{\partial x} \right]
\]

\[+ K_1 B - K_2 C^* \quad \ldots (4)\]

The transformations \(B = b \exp(-K_1 t)\) and \(C^* = c \exp(-K_2 t)\) are used to eliminate unknown source and sink terms from Eqs (1) and (4) giving Eqs (5) and (6)

\[
\frac{\partial b}{\partial t} + u(x) \frac{\partial b}{\partial x} = \frac{1}{A(x)} \frac{\partial}{\partial x} \left[ E(x) \cdot A(x) \cdot \frac{\partial b}{\partial x} \right]
\]

\[+ K_1 b \exp[-(K_1 - K_2) t] \quad \ldots (6)\]

If \(\frac{\partial b}{\partial t} + \frac{V(x) \cdot \partial b}{\partial x} = E(x) \cdot \frac{\partial^2 b}{\partial x^2}\)

\[\ldots (7)\]

\[
\frac{\partial c}{\partial t} + \frac{V(x) \cdot \partial c}{\partial x} = E(x) \cdot \frac{\partial^2 c}{\partial x^2} + K_1 b \exp[-(K_1 - K_2) t]\]

\[\ldots (9)\]

Eq. (7) represents the effective velocity at a point due to the combined action of advection and variable dispersion. The Eqs (5) and (6) are simplified as the effective velocity. The initial boundary conditions for solving Eqs (8) and (9) are accordingly transformed.

**Finite difference technique for the solution of Eqs (8) and (9)—**Since Eq. (9) includes the term representing BOD concentration at any time \(t\) and a distance \(x\), its solution would require the solution of Eq. (8). Therefore, Eq. (8) is solved independently and prior to the solution of Eq. (9), using initial and boundary conditions presented in Eq. (3).

A procedure for solving Eq. (9) is being presented here. Similar methodology may be used to solve Eq. (8).

Eq. (9) is splitted into two parts, i.e., Eqs (10) and (11).

\[
\frac{1}{v(x)} \frac{\partial c}{\partial t} + \frac{\partial c}{\partial x} = K_1 b \exp(K_2 - K_1) t \quad \ldots (10)
\]

and

\[
\frac{\partial c}{\partial t} = E(x) \cdot \frac{\partial^2 c}{\partial x^2} \quad \ldots (11)
\]

The numerical solution of advection Eq. (10) is obtained by discretizing it over a rectangular grid as follows

\[
\frac{1}{v_i} \frac{c_{i+1,n+1} - c_{i,n+1} + c_{i+1,n} - c_{i,n}}{\Delta x_i} = \left[ \frac{1}{\Delta t} \left( \frac{c_{i,n+1} - c_{i,n}}{\Delta x_i} \right) \right] + \left[ \frac{1}{\Delta t} \left( \frac{c_{i+1,n+1} - c_{i+1,n}}{\Delta x_i} \right) \right]
\]

\[+ (1 - \theta) \left[ \frac{1}{\Delta t} \left( \frac{c_{i,n+1} - c_{i,n}}{\Delta x_i} \right) \right]\]
\[
- \frac{K_1 b_{i,n}}{V_i} \times \exp[(K_2 - K_1) n \delta t] = 0 \quad \ldots (12)
\]

In Eq. (12), the variable \( \delta x \) is the spatial grid distance computed as \( \delta x = V_i \delta t \), \( V_i \) being the effective velocity at \( i \)th grid. Rearrangement of Eq. (12) gives the explicit finite difference scheme which is unconditionally stable.

\[
C_{i+1,n+1} = A_1 C_{i,n} + A_2 C_{i,n+1} + A_3 C_{i+1,n} + A_4 b_{i,n}
\quad \ldots (13)
\]

In Eq. (13)
\[
A_1 = (1 + 2\theta)/(3 - 2\theta)
\]
\[
A_2 = (1 - 2\theta)/(3 - 2\theta)
\]
and
\[
A_3 = 2K_1 \delta t[(K_1 - K_2) n \delta t]/(3 - 2\theta)
\]

Expansion of \( C_{i+1,n+1}, C_{i,n+1}, C_{i+1,n}, \) etc. by means of Taylor’s theorem in terms of \( C_{i,n} \) upto second order term and their substitution in Eq. (13) would yield.

\[
\frac{\partial c}{\partial t} + V(x) \frac{\partial c}{\partial x} = K_1 b \exp((K_2 - K_1) t)
\]
\[
+ \left[ \frac{V^2(x) \delta t(1 - 2\theta)}{2} \right] \frac{\partial^2 c}{\partial x^2}
\quad \ldots (14)
\]

Comparison of Eqs (10) and (14) suggest that the second non-zero term on R.H.S. denotes the error arising due to approximation of differential equation by finite differences. This term gives the effect of diffusion generally known as artificial or numerical diffusion/dispersion. Further, it is observed that the parameter \( \theta \) representing the weighted average, can be chosen in such a way that the coefficient of second term on R.H.S. in Eq. (14) represents the physical dispersion coefficient \( E \) in a particular grid, i.e., \( E = [V^2 \delta t(1 - 2\theta)/2] \). This yields,

\[
\theta = 0.5 - \frac{E}{V^2 \delta t} = 0.5 - \frac{1}{\rho H} \quad \ldots (15)
\]

Since, \( \theta \) must be positive, Eq. (15) suggests that \( 0 < \theta < 0.5 \). Thus if \( \theta \) is taken as in Eq. (15), only the advection Eq. (10) need to be solved for the solution of Eq. (9). The neglected third order terms are much smaller in magnitude as compared to the first term on R.H.S. of Eq. (14).

For a particular study reach, the time interval \( (\delta t) \) is chosen in a way so that it may satisfy \( \delta t \geq 2E/V^2 \).

The grid size \( \delta x \) is to be computed at each grid according to \( \delta x = V_i \delta t \). This advantageously ensures positiveness of the coefficients \( A_1, A_2, A_3 \) and \( A_4 \) for all computed values of \( \delta x \).

Numerical solutions are first computed for \( i = 1 \) at \( x_i = \delta x_{i-1} \) using initial and boundary conditions for \( i = n \delta t, n > 1 \) till the steady state is reached. The solution is then, advanced to \( x_{i+1} = x_i + \delta x_i \).

**Results and Discussions**

The proposed scheme is used to predict the DO concentration downstream of the source, which is decaying exponentially with time with rate \( K_1 \). Following theoretical but rational data is used.

The area of the river cross-section is assumed to vary linearly in the longitudinal direction as \( A(x) = A_0 + ax \), in which \( A_0 \) is taken as 200 m\(^2\) and \( a = \pm 0.003 \) m (ref. 9). The river flow rate \( Q (= 200 \text{ m}^3/\text{s}) \) is assumed to be constant throughout the study reach. The stream velocity \( u(x) \) (m/s) is computed as \( u(x) = Q/A(x) \).

The coefficient of dispersion \( E(x) \) is determined by the formula developed by Fisher\(^{10}\) for natural streams, \( E(x) = [0.01 u^{-2} w^2/(u^* d)] \), in which \( d \) is the depth (m) of the river assumed to be constant (= 4 mL), \( w \) is the width (m) varying linearly with \( x \) as \( w = 50 + 0.00075 x \), \( m, u^* \) is the friction velocity which is assumed as 0.09 m/s (ref. 10). The \( K_1 \) and \( K_2 \) values are assumed to be 0.3 \( \times 10^{-4} \) /s and 0.4 \( \times 10^{-4} \) /s, respectively, and \( B_0 \) is assumed to be 15.5 mg/L. The DO in the stream at upstream of the wastewater input point is assumed to be at a saturation level of 9.17 mg/L.

The DO concentration variation with time is computed by a repeated application according to the scheme down in Eq. (13), with boundary conditions shown in Eq. (5), for a segment \( \delta x \). Such evaluated values were taken as the input data for the next grid point, and this process was continuously repeated up to the last section of the considered reach. The evaluated values of \( C_{i+1,n+1} \) were transformed into the \( C^*_i, C_{i+1,n+1} \) values through the use of the transformation expression.

Finally, the DO concentration (i.e., \( C_{i+1,n+1} \)) is computed using \( C_{i+1,n+1} = C_0 - C_i^* \).

The concentration of DO at the different distances were computed. The variation in stream velocity leads to different \( \delta x \) values at different grids. The evaluated values of DO are used to prepare DO v/s time plots at these five different distances and along the stream stretch using three different velocity profile, i.e., uniform stream velocity, decreasing stream velocity and increasing stream velocity.
Fig. 1 contains such DO v/s time plots at various distances for a condition in which the stream velocity is assumed uniform at 1 m/s, throughout the considered reach.

In real life situations, the stream velocity is never uniform. Therefore, under conditions of a decreasing effective stream velocity pattern, \( \alpha = 0.003 \), the plots of predicted DO v/s time at distance 8.92, 17.92, 24.90, 31.92 and 38.47 terms, respectively, are depicted in Fig. 2. It is observed that BOD concentration takes some time to arrive at a particular distance up to which time, the concentration of BOD is negligible and the concentration of DO is at saturation level. As the BOD increases, the DO starts to decrease. The point of minimum DO is the critical point. The deficit at this point is known as critical deficit and time to reach this point is the critical concentration time.

A similar exercise was carried out using an increasing velocity profile (i.e. a decreasing stream cross-sectional area pattern) in the application of the proposed scheme for the same data and the plots of DO v/s time at distance 10.03, 16.44, 23.52, 31.99, 43.22 km, respectively, along the stream stretch as shown in Fig. 3. It is observed that due to decreasing stream velocity, the maximum value of BOD occurs much more rapidly when compared to the increasing velocity profile. Consequently the minimum DO occurs at earlier
point and at earlier time compared to the increasing stream velocity profile situation. In other words it may be said that the point of critical deficit shifts towards left or right side of the point of critical deficit shifts towards left or right side of the point of critical concentration in the case of uniform velocity profile, according as the flow velocity is decreasing or increasing. Because in case of decreasing velocity profile the pollutant moves slowly in the stream and, therefore, consumes more DO of stream in the time less than the time that it takes in increasing velocity profile pattern. However, in case of increasing flow velocity the pollutant moves much more faster and, therefore, giving the critical point at a farther distance.

Conclusions

The non-dimensional mixing and attainment of DO along a stream simultaneously due to the advection, dispersion and biochemical decay effects have significance in knowing efficiently the DO variation with time at any distance along a stream. Such predictions can be helpful in predicting the critical conditions of DO in streams. Control measures can also be evolved, if necessary, for the safe survival of the fish and wild life present in the streams. It can make the stream classification more efficient.

The proposed scheme has no restriction on spatial grid size, which is computed after accounting for the velocity variations. In real life situation where the stream velocity varies considerably, the presented scheme can handle the situation more efficiently. The scheme is very sensitive to velocity changes in the stream which are very common in real life situations. The plots amply justify this aspect and manifest the rationality of the effects of velocity changes on the prediction of DO variation with time at any distance along a stream. Further, the scheme incorporates the variation of dispersion effect with longitudinal distance by modifying the stream velocity expression.

Acknowledgement

The financial support provided by C.S.I.R. is gratefully acknowledged.

References

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