THE METHOD OF LINES FOR SOLUTION OF ONE-DIMENSIONAL DIFFUSION-REACTION EQUATION DESCRIBING CONCENTRATION OF DISSOLVED OXYGEN IN A POLLUTED RIVER

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Abstract

The present paper addresses a diffusion-reaction equation describing the dynamics of dissolved oxygen in a polluted stream of a river. The diffusion-reaction equation is a mass-balanced partial differential equation which relates the concentration of dissolved oxygen with the effect of other natural processes, viz. diffusion, natural aeration and reaction with pollutants. The well-known method of lines is used to solve the one-dimensional non-steady state case with Dirichlet boundary conditions. The study is motivated by the miserable condition of most of the rivers in India. Water pollution has now become a global concern and this study furnishes a better apprehension of complex phenomenon of maintaining desired level of oxygen and will aid water resource management.

Keywords: *Advection, Diffusion, Diffusion-Reaction equation, method of lines, river-pollution, aeration.*

INTRODUCTION

Dissolved Oxygen (DO) is one of the most important water quality indicators, which is essential for the survival of aquatic animals as well as for the decomposition of biological pollutants. In the presence of pollutants, various chemical processes results in the change of concentration of DO and this can be modelled mathematically using diffusion-reaction equation. It is a second-order parabolic partial differential equation (PDE), since the characteristics depends on both spatial and time co-ordinates. Diffusion means the spreading of matter from high concentration region to low concentration region in order to distribute it uniformly. Reaction refers to the chemical process due to which the matter is transformed into each other.

In this study, a mathematical model devised by Hussain et al. [3] is studied in detail. The actual model was solved analytically for zero diffusion case. Here, a relatively recent numerical approach Method of Lines (MOL) is used to solve the more complex case including diffusion. The MOL approximation replaces PDE with an initial value Ordinary Differential Equation (ODE) system [5]. The basic idea is to replace the spatial (boundary value) derivatives in PDE with algebraic approximations, like finite difference approximation or finite element approximation. Consequently, only the initial-value variable, time, remains as the independent variable. The system of ODE thus formed can be solved by using existing, well-established numerical methods.

The standard equation describing concentration of DO was formulated by Chapra [1], which is based on the study of Ohio River done by Streeter and Phelps [8]. This model has been amended in various ways [4, 6, 7] to incorporate different phenomena that occur naturally in a stream of river. Various numerical [2, 6] and analytical methods [3, 4, 9] are used to solve this equation for both steady and non-steady case.

THE GOVERNING EQUATION

The variations of concentration of DO in a river [3], $C(x,t)$ with position x (m) and time t (days) in presence of biological pollutants can be expressed in one-dimension as:

$$\frac{\partial\big(AC(x,t)\big)}{\partial t} = D\frac{\partial^2(AC(x,t))}{\partial x^2} - \frac{\partial(vAC(x,t))}{\partial x} + \alpha(S-C) - q \qquad (1)$$

$$0 \le x \le L, \qquad t \ge 0$$

where

L is the polluted length of river (m),

A is the cross-sectional area of the river (m^2),

D is the diffusion coefficient of DO in x-direction (m^2 day^{-1}),

v is the velocity of water in x-direction (m day^{-1}),

α is the mass transfer of oxygen from air to water(m^2 day^{-1}), and

S is the saturated oxygen concentration (kg m^{-3}),

q is net oxygen decay rate in the presence of biological pollutants (kg $m^{-1}day^{-1}$).

For the above model, it is assumed that the advection along the river can be neglected i.e. v = 0, because most non-perennial rivers in India remains stagnant during non-monsoon period. So, equation (1) simplifies to diffusion – reaction (D-R) equation as follows:

$$\frac{\partial\big(AC(x,t)\big)}{\partial t} = D\frac{\partial^2(AC(x,t))}{\partial x^2} + \alpha(S-C) - q \tag{2}$$

The first term of right side, $D\frac{\partial^2(AC(x,t))}{\partial x^2}$ represent diffusion of oxygen, $\alpha(S-C)$ is the oxygen deficit term which become active only when the oxygen level drops below saturation level and q refers to the sink (decrease) in quantity of oxygen in the presence of pollutant. Assuming cross-sectional area to be uniform all along the stream, equation (2) reduces to

$$\frac{\partial\big(C(x,t)\big)}{\partial t} = D\frac{\partial^2(C(x,t))}{\partial x^2} + \frac{\alpha}{A}(S-C) - \frac{q}{A}$$

We can write this as

$$C_t = DC_{xx} + \frac{\alpha}{A}(S-C) - \frac{q}{A} \tag{3}$$

For the purpose of its numerical solution, the independent variables are restricted to the region $0 \le x \le 1,\ t \ge 0.$ The initial conditions are considered as $C(x,t=0) =$ S.

NUMERICAL SOLUTION – METHOD OF LINES

The Dirichlet boundary conditions are taken as $C(x=0,t) =$ S and $C(x=1,t) = S$. Also, without loss of generality, parametric values are chosen as $D = 0.2, A = 100, \alpha = 5.5, S = 0.01$ and $q = 1$.

Descretization of Spatial Axis

The method begins by dividing the considered domain ($0 \le x \le 1$) in N elements. For this case, let N=20, so the length of each element $\Delta x = h = \frac{1}{20} = 0.05$.

Approximation of Spatial Derivative

Now, an approximation is required for the second order spatial derivative C_{xx}. Here, the most-common *central-difference* approximation, derived from Taylor's series can be used as

$$C_{xx} = \frac{C_{i+1} - 2C_i + C_{i-1}}{h^2} + O(h^2)$$

$$\forall i = 1,2,\dots,N.$$

The term $O(h^2)$ denotes the truncation error.

Problem statement

Assuming the truncation error to be negligible, equation (3) can be written as

$$\frac{dC}{dt} = D\frac{C_{i+1} - 2C_i + C_{i-1}}{h^2} + \frac{\alpha}{A}(S - C) - \frac{q}{A} \tag{4}$$

The Dirichlet boundary conditions at $x = 0$ is transformed to $C_1 = S$, and at $x = 1$, it can be written as $C_N = S$.

Also, the initial condition becomes $C_i = S$.

In this way equation (3) has transformed into a system of $N - 1$ linear first order differential equations and can be written in matrix form as

$$\frac{d\boldsymbol{C}}{dt} = D'\boldsymbol{C} + b + \frac{\alpha}{A}S - \frac{q}{A} \tag{5}$$

where

$$D' = \frac{D}{h^2}\begin{bmatrix} -2-\alpha' & 1 & 0 & \cdots & 0 & 0 & 0 \\ 1 & -2-\alpha' & 1 & \cdots & 0 & 0 & 0 \\ 0 & 1 & -2-\alpha' & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -2-\alpha' & 1 & 0 \\ 0 & 0 & 0 & \cdots & 1 & -2-\alpha' & 1 \\ 0 & 0 & 0 & \cdots & 0 & 1 & -2-\alpha' \end{bmatrix}$$

is a matrix of order $(N - 1) \times (N - 1)$ with $\alpha' = \frac{\alpha}{A}$, the vector of unknowns

$$\boldsymbol{C} = [\, C_1 \quad C_2 \quad C_3 \quad \cdots \quad C_{N-1}]'$$

and b is a column vector of order $(N - 1) \times 1$, which is of the form

$$b = \frac{D}{h^2}[C_0 \quad 0 \quad \cdots \quad 0 \quad C_N]'$$

.

Numerical Simulation

Let the time interval for integration be $0 \leq t \leq 2$, which is again divided into N equal intervals. This system of ODE, with initial and boundary conditions has been implemented in MATLAB [5] and the following *Figure 1* was generated:

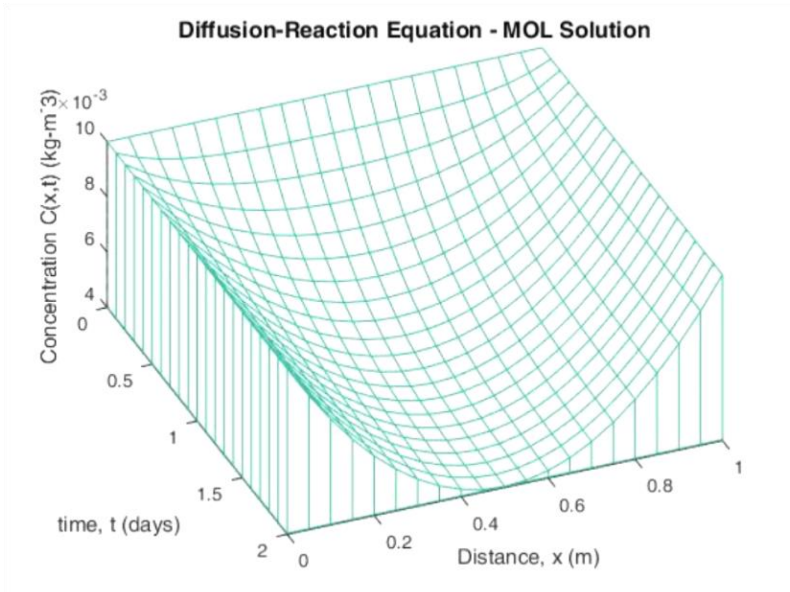

Figure 1 Solution of Equation (3) with $q = 1$

Effect of Decreasing Pollutant Discharge

If the pollutant discharge is controlled to some extent, then there will be a decrease in the oxygen decay rate q. This effect is studied by taking $q = 0.1$, and same iterations are repeated to get the following *Figure 2*.

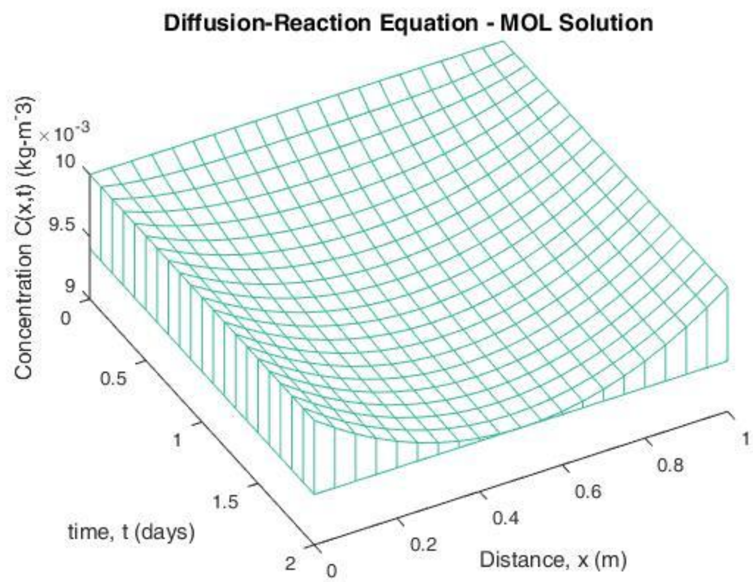

Figure 2 Solution of Equation (3) with $q = 0.1$

INTERPRETATION OF RESULT

The simulation result can be interpreted as: At time $t = 0$, the DO is in its saturated state, but due to the presence of pollutant, oxygen is used to oxidize them. Through oxidation, biological pollutants convert into harmless compounds. As a result, initially there is a decline in the concentration of DO. Simultaneously, the natural aeration process will start which helps DO to again reach at its saturation value. Here, all the observations are along the cross-sectional area of the river, and all variations along the depth and flow direction are ignored.

Figure 2 shows that when less amount of pollutants are discharged into the river, concentration of DO does not drop much and river self-purify itself rapidly. Thus, managing the amount of pollutant addition into the river can considerably improve its water quality.

CONCLUSION

In this study, a one-dimensional diffusion-reaction equation for dissolved oxygen in a river is considered and effect of the presence of pollutant on the concentration of DO is studied in detail. The numerical Method of Lines is used to solve the unsteady case including diffusion.

This method can be preferred over other methods due to non-homogeneous nature of the mathematical model, which makes it difficult to solve analytically. It is observed that, if originally the stream is unpolluted, the dissolved oxygen level remains near saturation. But in the presence of pollutant, oxygen level drops and the natural aeration through atmosphere becomes active helping the oxygen to regain its normal value. The result obtained agrees with the natural variation of DO concentration along the river and can help in maintaining the desired level of oxygen in streams.

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