Numerical Simulation of System of Time-Dependent Advection-Diffusion-Reaction Equations Describing River Pollution

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Abstract - In this paper we have studied numerical simulation of a system of time-dependent advection-diffusion-reaction equations describing pollution in a river. The system consists of a pair of coupled equations representing the concentration of dissolved oxygen and that of biochemical oxygen demand or pollutant respectively. The coupling of these equations occurs due to the fact that oxygen and pollutant react with each other that result in producing harmless compounds. In each of the concentration equations both the advection and diffusion terms are linear while the reaction term is non-linear. However, handling of non-linear terms is too difficult to find solutions. Hence in order to make things simpler, the reaction term is separated from the remaining two terms using splitting method. Both the finite element methods, standard Galerkin and Taylor-Galerkin, are applied to solve the advection-diffusion equations. However, Taylor-Galerkin method is preferred to Standard Galerkin whenever advection term dominates otherwise the reverse. Similarly, the time integration methods, particularly an improved Runge-Kutta method of order six, are developed and implemented to solve the system of reaction equations. These numerical methods are successfully applied to a test example consisting of one-dimensional system of advection-diffusion-reaction equations together with Dirichlet boundary condition. Further inferences and discussions are included in the text.

Keywords: Advection-Diffusion-Reaction equation, Biochemical Oxygen Demand, Dissolved Oxygen, Finite Element Method, Pollution, Runge-Kutta of order six, Taylor-Galerkin Method.

1. INTRODUCTION

Advection-Diffusion-Reaction equation (ADRE) is one of the most important and very frequently used mathematical models in science and engineering. It is a partial differential equation that can be derived using the physical laws of mass conservation as well as the mean value theorems of calculus. Advection refers to the movement of a substance due to flow of the medium e.g., water or air. Diffusion accounts the movement of substance from high concentration area to low concentration so as to distribute the substance uniformly in the medium. A chemical reaction is a process leading to the inter conversion of chemical substances. ADR equation is a mathematical model that describes how the concentration of one or more substances e.g., pollutants distributed in a medium or river changes under the influence of these three processes.

The ADR equation can be used to model a wide range of natural phenomenon and explain their dynamics with respect to time. The application of the general advection-diffusion-reaction equations are wide and numerous. For instance, they are used to formulate pollutant transport models in scientific disciplines ranging from atmospheric studies through medical science to chemo taxis [1, 11, 17, 18, and 24].

However, in the present study we have chosen the one-dimensional Streeter-Phelps equation which describing the river self-purification model as a concrete example. Historically, the famous mathematical model used to predict water quality in river is proposed by Streeter H W and Phelps E B in 1925 [3, 14, 18, 19, 21 and 29]. The Streeter-Phelps equation is applied to model the amount of dissolved oxygen (DO) in a stream after waste water is discharged into the stream. This model also enumerates the amount of pollutant at the downstream, for the pollutant travels with the stream velocity in the direction of the flow. When a pollutant is added to water then the amount of dissolved oxygen decreases to a minimum level and then gradually recovers and finally reaches a saturation level [28].

Based on some realistic assumptions Streeter-Phelps model is modified and split into a pair of coupled advection-diffusion-reaction equations representing respectively the concentrations of dissolved oxygen and biochemical oxygen demand. To solve such pair of coupled system on different scales, we have to deal with the operator splitting methods which are used to decouple complicated partial differential equations into simpler equations and are often and widely used to simulate the theoretical models of environmental processes. These methods are developed and successfully applied in [5, 8, 10, 13, and 24]. The idea here is to solve simpler equations using higher order discretization methods and achieve higher efficiency and more exact accuracy. The splitting strategy has been successfully applied to solve and analyze the present model. The model is split or divided into flow and reaction terms. The flow terms represent advective and diffusive transports while reaction term represents chemical transformations.

The advection-diffusion problems can be solved using standard Galerkin finite element method [7, 9, 20, and 26] provided that advection term does not dominate. However, in case of advection dominated problems the standard Galerkin finite element method often results in oscillatory solutions. Taylor-Galerkin method is an alternative to the standard Galerkin and the former can be used to overcome instabilities and inaccuracies of the solution [2, 6, 12, 20, 22, and 23]. Also, the improved Runge-Kutta of order six can be applied to compute the reaction term [4, 25, and 31]. This enables us to get a better understanding on how water quality in river or lake can be predicted and controlled. There are many factors which influence water quality such as dissolved oxygen level, water velocity, pollutant addition, and saturated oxygen concentration. All these factors are required to be included in the model formulation. However, the main consideration here is to predict the interaction between two important and influential factors viz., dissolved oxygen and biochemical oxygen demand concentration.

2. MODEL FORMULATION AND DESCRIPTION

The environmental purification models consider that a body of lake or river can be polluted by many kinds of impurities or substances. These substances will interact among themselves and with also other substances which are not considered as contaminants. The important task here is to model these interactions and is developed as follows:

Let us suppose that a polluted river contains N contaminants with the respective concentrations u_i for all $i = 1, 2, \dots, N$. Then a possible approach to model river purification system corresponding to each of the chemical contaminants lead to the system of equations as

$$\frac{\partial u_i}{\partial t} + \frac{\partial (w u_i)}{\partial x} - D_i \frac{\partial^2 u_i}{\partial x^2} = \left[\frac{q_i}{A} + K_i u_i + C_i\right], \forall\, i = 1,2, \dots, N \qquad (1)$$

In (1), the terms $\frac{\partial (w u_i)}{\partial x}$, $D_i \frac{\partial^2 u_i}{\partial x^2}$ and $\left[\frac{q_i}{A} + K_i u_i + C_i\right]$ respectively represent advection, diffusion and reactions.

The notations and meanings of various components of the models in this section are given in the form of a table as follows:

Variables and Parameters	Meaning
x	Distance along the direction of river
w	Velocity of the river
A	Cross-sectional area of the river
u_i	Concentration of contaminant i
u_1	The concentration of dissolved oxygen
u_2	The concentration of biochemical oxygen demand
q_i	Net rate of addition of the suspension
D_i	Diffusivity coefficient
D_1	The diffusion rates of dissolved oxygen
D_2	The diffusion rates of biochemical oxygen demand
K_i	Emission rate of the contaminant i
K_1	First order reaction rate
K_2	Second order reaction rate
K_0	Permeability to oxygen
h	The effective depth of the imaginary membrane
ω	The concentration of oxygen in the air immediately above the river
λ	Reaeration coefficient
γ	The reaction rate of oxygen and biochemical oxygen demand
C_i	Chemical reaction of contaminant i
t	Time

Table 1: Variables and parameter values

The equation (1) can be termed as coupled, since C_i depends on the concentrations of the remaining $N-1$ contaminants $u_1, u_2, \dots, u_{i-1}, u_{i+1}, \dots, u_N$. Involvement of this many variables and that of coupling make the equation (1) difficult to solve analytically. In order to get rid of this difficulty let us reduce the number of contaminants from N to $k+1$ by combining less important contaminants as follows: Let there be k number of most important contaminants in

the sense that they all exhibit more influence on the river pollution and they be identified with the notations $u_1, \dots, u_k$. The remaining $N-k$ numbers of contaminants are less important in the sense that they all exhibit very less influence on the river pollution independently. However the influence is considerable when all these contaminants are treated combined. Thus, the $N-k$ contaminants $u_{k+1}, \dots, u_N$ can be combined and jointly considered as a single contaminant and let it be denoted by u_{k+1}.

In order to make the model (1) physically meaningful let us set $N = 2$ and $k = 1$ and u_1 and u_2 as follows: Let u_1 be the concentration of dissolved oxygen (DO) which is the most important variable in the purification of river. Any substance that consumes oxygen is considered as a pollutant due to the fact that the organisms living in water die without oxygen. Biochemical oxygen demand (BOD) can be defined as the maximum amount of oxygen per unit volume that the pollutant could consume. However, if the pollutants had consumed that much of oxygen, then there would remain no pollutant molecules in the water for the oxygen to combine with. Let the BOD be denoted by u_2.

The present model is built based on the following assumptions: (i) The River flow is with a constant velocity w and it is sufficiently slower so that diffusion along flow of the river is observable. (ii) Certain amount of pollutant elements have been discharged into the river and then ceased the discharge. (iii) BOD can decay only by combining with oxygen or due to combined effects of diffusion and advection. Hence $q_2 = C_2 = 0$ and $C_1 = 0$ since the amount of oxygen is destroyed due to chemical reactions.

With these assumptions, the model (1) simplifies to a purification model as

$$\frac{\partial u_1}{\partial t} + w\frac{\partial u_1}{\partial x} - D_1\frac{\partial^2 u_1}{\partial x^2} = \frac{q_1}{A} - K_1 u_1 \qquad (2)$$

$$\frac{\partial u_2}{\partial t} + w\frac{\partial u_2}{\partial x} - D_2\frac{\partial^2 u_2}{\partial x^2} = -K_2 u_2 \qquad (3)$$

The first equation (2) of the system determines the amount of dissolved oxygen while the second equation (3) determines that of biochemical oxygen demand. In what follows, reasonable assumptions are made and accordingly suitable expressions for q_1 and the first and second order reaction rates K_1 and K_2 are developed.

Let us consider that oxygen diffuses into the river from the air immediately above the water. The interface between air and water behaves like a membrane that is permeable to oxygen in the sense that vertical diffusion near the surface of the river is much less efficient than at the lower levels.

In this scenario it is then suggested that the flux of oxygen into the river is given by $(k_0(\omega - u_1)/h)$[18]. The rate at which oxygen enters the river per unit length is obtained by multiplying $(k_0(\omega - u_1)/h)$ by the average breadth b of the river. Thus,

$$\frac{q_1}{A} = \frac{bk_0(\omega - u_1)}{Ah} = \lambda(\omega - u_1), \qquad (4)$$

Here in (4), $\lambda = \frac{bk_0}{Ah}$ which is a constant and has a dimension of a specific rate i.e. t^{-1}. The expression $\omega - u_1$ denotes the oxygen deficit.

Now to specify K_1 and K_2, the chemical reaction that consumes the river's oxygen may be written symbolically as

$$Oxygen + BOD \rightarrow product \qquad (5)$$

We suppose that the rate at which the reactants, namely oxygen and BOD, convert into product is proportional to their concentration. Moreover, by definition of BOD, they must both convert at the same rate. Thus,

$$-K_1 u_1 = -\gamma u_1 u_2 = -K_2 u_2, \qquad (6)$$ The relations (6) imply that $K_1 = \gamma u_2$ and $K_2 = \gamma u_1$. Combining equations (6) with (2) to (4), we obtain a pair of coupled nonlinear partial differential equations as

$$\frac{\partial u_1}{\partial t} = -w\,\frac{\partial u_1}{\partial x} + D_1\frac{\partial^2 u_1}{\partial x^2} + \lambda(\omega - u_1) - \gamma u_1 u_2 \quad (7)$$

$$\frac{\partial u_2}{\partial t} = -w\,\frac{\partial u_2}{\partial x} + D_2\frac{\partial^2 u_2}{\partial x^2} - \gamma u_1 u_2. \quad (8)$$

The model (7) and (8) is referred to as the modified Streeter-Phelps model. The proposed model is not the Streeter-Phelps model itself, since the original Streeter-Phelps model ignored the diffusive effects, and replaced the deoxygenation term by first order chemical reaction. This has the sizeable benefit of linearizing the problem and permitting an exact solution. However, in the present modified model we included diffusive effects and argue that the river is moderately polluted, and then the second order kinetics is required. Hence, the model is nonlinear and coupled, thus requiring numerical approximation.

The equation (7) represents a mass balance for dissolved oxygen, with addition through the surface at a rate proportional to the degree of saturation of dissolved oxygen $(\omega - u_1)$, and consumption during the oxidation of pollutant $\gamma u_1 u_2$. The BOD concentration u_2 reduces due to its biochemical reaction with dissolved oxygen and its rate of reduction is described by the term $-\gamma u_1 u_2$. Furthermore, the term $-\gamma u_1 u_2$ enables pollution to be removed at a rate proportional solely to the BOD concentration whenever the oxygen levels are higher. However, the same proportionality holds true even when the levels of oxygen concentration is lower. The equation (8) consists of removal of pollutant (BOD) by oxidation $\gamma u_1 u_2$. In order to simplify the equations we will set constant values for all the parameters $w,\ \gamma,\ \omega,\ \lambda,\ D_1$ and D_2 while carrying out simulation study.

3. NUMERICAL METHODS

In this section, different numerical methods have been applied to solve (7) and (8) together with appropriate initial and boundary conditions and parametric values. The independent variable x is restricted to the region $0 \le x \le L$, L being the length of the channel that varies in the interval $[0,\ 1]$. Also the time variable being independent is a non-negative quantity and hence $t \ge 0$.

3.1 Splitting Method

Operator splitting method is widely used to simulate the models of environmental processes. We split the advection-diffusion-reaction equations (7) and (8) into two unsteady sub-problems. The main advantage of splitting is that each sub-problem can be discretized by any convenient and independent methods.

Following this approach we separate the linear advection-diffusion and non-linear reaction terms from equations (7) and (8) to obtain the following:

$$\frac{\partial u_1}{\partial t} = -w\,\frac{\partial u_1}{\partial x} + D_1\frac{\partial^2 u_1}{\partial x^2} \quad (9)$$

$$\frac{\partial u_2}{\partial t} = -w\,\frac{\partial u_2}{\partial x} + D_2\frac{\partial^2 u_2}{\partial x^2} \quad (10)$$

$$\frac{\partial u_1}{\partial t} = \lambda(\omega - u_1) - \gamma u_1 u_2 \quad (11)$$

$$\frac{\partial u_2}{\partial t} = -\gamma u_1 u_2 \quad (12)$$

Advection-diffusion and reaction terms are not commuted here, since reaction term is non-linear. Thus, a splitting error of first order $o(\tau)$ is expected to obtain.

3.2 The Finite Element Method

In order to discretize equations (9) and (10) subsequently, we first discretize the following mathematical model describing the advection and diffusion processes in the one-dimensional time dependent advection-diffusion equation together with initial and boundary conditions

$$\frac{\partial u}{\partial t} + w\,\frac{\partial u}{\partial x} - D\frac{\partial^2 u}{\partial x^2} = 0,\quad 0 \le x \le L,\ t > 0 \quad (13)$$

$$u(x,0) = u_0(x),\ 0 \le x \le L \quad (14)$$

$$u(0,t) = f(t), \quad u(L,t) = h(t), \ t > 0. \tag{15}$$

Here in (14) and (15), $u(x,0)$ is the initial concentration distribution of pollutant at time $t = 0$; $u(0,t)$ is fixed concentration of pollutant at $x = 0$; and $u(L,t)$ is fixed concentration of pollutant at the location $x = L$ for all times.

The varational formulation for the problem (13) reads as follows: For every time interval $I_n = (t_{n-1}, t_n]$ find $u(x,t)$, $t \in I_n$ such that

$$\int_{t_{n-1}}^{t_n} \int_0^L v(x) \left(\frac{\partial u}{\partial t} + w \frac{\partial u}{\partial x} - D \frac{\partial^2 u}{\partial x^2} \right) dx dt = 0 \tag{16}$$

where $v(x)$ is arbitrary test function. On applying integration by parts with equation (15) on the second order derivative in (13) and after simplification it reduces to the form

$$\int_{t_{n-1}}^{t_n} \left[\int_0^L \left(\frac{\partial u}{\partial t} v + w \frac{\partial u}{\partial x} v + D \frac{\partial u}{\partial x} \frac{\partial v}{\partial x} \right) dx \right] dt = 0, \forall v: v(0,t) = v(1,t) = 0. \tag{17}$$

A piecewise linear Galerkin approximation: For each time interval $I_n = (t_{n-1}, t_n]$ with

step size $k = t_n - t_{n-1}$, let

$$u(x,t) = u_{n-1}(x)\varphi_{n-1}(t) + u_n(x)\varphi_n(t) \tag{18}$$

where $\varphi_n(t) = \frac{t - t_n}{k}$, $\varphi_{n-1}(t) = \frac{t_{n-1} - t}{k}$ and

$$u_n(x) = u_{n,1}\varphi_1(x) + u_{n,2}\varphi_2(x) + \ldots + u_{n,m}\varphi_m(x). \tag{19}$$

In (18), u is piecewise linear function with respect to both space and time variables. By the Galerkin approach, we choose the test function to be the same as the basis function. Hence the unknowns are the coefficients $u_{n,k}$ satisfying discrete variational formulation as

$$\int_{t_{n-1}}^{t_n} \left[\int_0^L \left(\frac{\partial u}{\partial t} \varphi_j + w \frac{\partial u}{\partial x} \varphi_j + D \frac{\partial u}{\partial x} \frac{\partial \varphi_j}{\partial x} \right) dx \right] dt = 0. \tag{20}$$

Here j refers to the number of nodes in an element and $j = 1, 2, \ldots, m$.

Further, on substituting the step size $k = t_n - t_{n-1}$ and the space variables $u_n = u(x_n)$ and $u_{n-1} = u(x_{n-1})$ the equation (18) takes the form as

$$\dot{u}(x,t) = u_{n-1}(x)\varphi_{n-1}'(t) + u_n(x)\varphi_n'(t) = \frac{u_n - u_{n-1}}{k} \tag{21}$$

Also differentiation of (18) with respect to x gives

$$u'(x,t) = u'_{n-1}(x)\varphi_{n-1}(t) + u_n'(x)\varphi_n(t) \tag{22}$$

Up on inserting (21) and (22) and using the values of definite integrals $\int_{t_{n-1}}^{t_n} dt = k$ and $\int_{t_{n-1}}^{t_n} \varphi_n dt = \int_{t_{n-1}}^{t_n} \varphi_{n-1} dt = \frac{k}{2}$ the equation (20) takes the form as

$$\int_0^L u_n \varphi_j dx - \int_0^L u_{n-1}\varphi_j dx + w\frac{k}{2} \int_0^L u'_{n-1}\varphi_j dx + w\frac{k}{2} \int_0^L u'_n \varphi_j dx + D\frac{k}{2} \int_0^L u'_{n-1} \varphi'_j dx + D\frac{k}{2} \int_0^L u'_n \varphi'_j dx = 0. \tag{23}$$

This can be written in the compact form as Crank-Nicolson system (CNS)

$$\left(M + \frac{k}{2}(wA_a + DA_d) \right) u_n = \left(M - \frac{k}{2}(wA_a + DA_d) \right) u_{n-1}$$

Also, its solution u_n are given by

$$u_n = \left(M + \frac{k}{2}(wA_a + DA_d)\right)^{-1}\left(M - \frac{k}{2}(wA_a + DA_d)\right)u_{n-1}. \qquad (24)$$

Here $u_n = [u_{n,1}, u_{n,2}, \ldots, u_{n,m}]^T$. For each given the vector u_{n-1}, $\forall n = 1, 2, \ldots, N$ CNS is used to compute the $m-$ dimensional vector u_n.

To compute the stiffness matrices of diffusion term A_d, the advection term A_a, and the mass matrix M, let us differentiate (19) to obtain

$$u'_n(x) = u_{n,1}\varphi'_1(x) + u_{n,2}\varphi'_2(x) + \ldots + u_{n,m}\varphi'_m(x).$$

Thus, we have

$$A_d u_n = \int_0^L u'_n \varphi'_j dx = \left(\int_0^L \varphi'_j \varphi'_1\right) u_{n,1}dx +$$

$$\left(\int_0^L \varphi'_j \varphi'_2\right) u_{n,2}dx + \ldots + \left(\int_0^L \varphi'_j \varphi'_m\right) u_{n,m}dx,$$

By using the linear piecewise function $\varphi_j(x)$ with uniform mesh.

$$\varphi_j(x) = \begin{cases} \frac{x - x_{j-1}}{h}, & for \ x_{j-1} \le x \le x_j \\ \frac{x_{j+1} - x}{h}, & for \ x_j \le x \le x_{j+1} \\ 0, & otherwise \end{cases} \qquad (25)$$

Then, we obtain $A_d = \frac{1}{h}\begin{bmatrix} 2 & -1 & 0 \ldots 0 & 0 & 0 \\ -1 & 2 & -1 \ldots 0 & 0 & 0 \\ . & . & \ldots\ldots & . & . \\ 0 & 0 & 0 \ldots -1 & 2 & -1 \\ 0 & 0 & 0 \ldots 0 & -1 & 2 \end{bmatrix}$

To obtain the stiffness matrix of advection term A_a we have for $j = 1, 2, \ldots, m$ that

$$A_a u_n = \int_0^L u'_n \varphi_j dx = \left(\int_0^L \varphi_j \varphi'_1\right) u_{n,1}dx +$$

$$\left(\int_0^L \varphi_j \varphi'_2\right) u_{n,2}dx + \ldots + \left(\int_0^L \varphi_j \varphi'_m\right) u_{n,m}dx$$

Using the function (25) with uniform mesh it can be obtained that

$$A_a = \frac{1}{2}\begin{bmatrix} 0 & -1 & 0 \ldots 0 & 0 & 0 \\ 1 & 0 & -1 \ldots 0 & 0 & 0 \\ . & . & \ldots\ldots & . & . \\ 0 & 0 & 0 \ldots 1 & 0 & -1 \\ 0 & 0 & 0 \ldots 0 & 1 & 0 \end{bmatrix}$$

Similarly, for all the indices $j = 1, 2, \ldots, m$ the mass matrix M is defined as

$$Mu_n = \int_0^L u_n \varphi_j dx.$$

With the function (25) for uniform partition, we get

$$M = \frac{h}{6}\begin{bmatrix} 4 & 1 & 0 & \dots & 0 & 0 & 0 \\ 1 & 4 & 1 & \dots & 0 & 0 & 0 \\ . & . & . & \dots & . & . & . \\ 0 & 0 & 0 & \dots & 1 & 4 & 1 \\ 0 & 0 & 0 & \dots & 0 & 1 & 4 \end{bmatrix}$$

Following similar procedures as equations from (13) to (25), the numerical solutions of (9) and (10) with the application of Crank-Nicolson method is obtained as

$$u_{1n} = \left(M + \frac{k}{2}(wA_a + D_1A_d)\right)^{-1}\left(M - \frac{k}{2}(wA_a + D_1A_d)\right)u_{1(n-1)} \quad (26a)$$

$$u_{2n} = \left(M + \frac{k}{2}(wA_a + D_2A_d)\right)^{-1}\left(M - \frac{k}{2}(wA_a + D_2A_d)\right)u_{2(n-1)} \quad (26b)$$

The advection-diffusion problems, mentioned in (9) and (10), are said to be advection dominated if the diffusion coefficients D_1 and D_2 are smaller when compared with w. Such problems are often studied in numerical analysis as they are found to have many varieties of applications [13]. In case of all these problems we may observe almost similar numerical behavior as for the pure advection problem. Hence, the discretization of the advection-diffusion equation following finite element and standard Galerkin methods might lead to inaccurate solutions. For that reason Taylor-Galerkin is introduced so that the accuracy might be improved considerably.

3.3 Taylor-Galerkin Method

If the advection term is significantly larger than the diffusion term physically, then advection term dominates and diffusion term is negligible, spreading of the pollutant is almost inexistent, and the patch of pollutant simply moves along the flow of the river.

Since the contribution of the diffusion term $D\frac{\partial^2 u}{\partial x^2}$ is negligible it can be dropped from (13). Thus, the simplified equation after dropping of diffusion term while keeping the conditions given in (14) and (15) approximately reduces to the form as

$$\frac{\partial u}{\partial t} + w\frac{\partial u}{\partial x} = 0, \qquad 0 \le x \le L,\ t > 0 \quad (27)$$

The Taylor-Galerkin method consists of combining the Taylor formula that is truncated to the first order as

$$u(x, t^{n+1}) = u(x, t^n) + \Delta t\frac{\partial u}{\partial t}(x, t^n) + \int_{t^n}^{t^{n+1}}(s - t^n)\frac{\partial^2 u}{\partial t^2}(x,s)ds \quad (28)$$

From (27), we have $\frac{\partial u}{\partial t} = -w\frac{\partial u}{\partial x}$ and also from formulae of derivative we also have $\frac{\partial^2 u}{\partial t^2} = w^2\frac{\partial^2 u}{\partial x^2}$. Up on substituting, (28) then it reduces to

$$u(x, t^{n+1}) = u(x, t^n) - w\Delta t\frac{\partial u}{\partial x}(x, t^n) + w^2\int_{t^n}^{t^{n+1}}(s - t^n)\frac{\partial^2 u}{\partial x^2}(x,s)ds \quad (29)$$

Further, the integral on the right hand side of (29) can be approximated as

$$\int_{t^n}^{t^{n+1}}(s - t^n)\frac{\partial^2 u}{\partial x^2}(x,s)ds \approx \frac{\Delta t^2}{2}\left[\theta\frac{\partial^2 u}{\partial x^2}(x, t^n) + (1 - \theta)\frac{\partial^2 u}{\partial x^2}(x, t^{n+1})\right]. \quad (30)$$

Here $\theta \in [0,1]$ is a parameter. In obtaining (30) we set the values $s = t^n$ and $s = t^{n+1}$. Also, the function $u^n(x)$ is approximated to be the same as $u(x, t^n)$.

At this juncture it is appropriate to consider two remarkable situations: If $\theta = 1$, the resulting semi-discretized scheme is explicit in time and is written as

$$u^{n+1} = u^n - w\Delta t\frac{\partial u}{\partial x} + w^2\frac{\Delta t^2}{2}\frac{\partial^2 u}{\partial x^2}$$

If the space is discretized using finite element method, then Lax-Wendroff finite element schemes might be obtained.

In case of $\theta = 2/3$ the approximation error in (30) becomes $O(\Delta t^4)$. Also the resulting semi-discretized scheme is written as

$$u^{n+1} - w^2 \frac{\Delta t^2}{6} \frac{\partial^2 u^{n+1}}{\partial x^2} = u^n - w\Delta t \frac{\partial u^n}{\partial x} + w^2 \frac{\Delta t^2}{3} \frac{\partial^2 u^n}{\partial x^2} \quad (31)$$

In (31), the truncation error of the semi-discretization in time is $O(\Delta t^3)$. At this point, a discretization in the space using the finite element method leads to Taylor-Galerkin method: for $n = 0,1,...$ find $u^{n+1} \in V$ such that

$$(u^{n+1}, v) - w^2 \frac{\Delta t^2}{6} \left(\frac{\partial^2 u^{n+1}}{\partial x^2}, v\right) = (u^n, v) - w\Delta t \left(\frac{\partial u^n}{\partial x}, v\right) + w^2 \frac{\Delta t^2}{3} \left(\frac{\partial^2 u^n}{\partial x^2}, v\right)$$

After applying the definite integral and the method of integration by parts on the second derivative terms it gives

$$\int_0^L u^{n+1} v dx + w^2 \frac{\Delta t^2}{6} \int_0^L \frac{\partial u^{n+1}}{\partial x} \frac{\partial v}{\partial x} dx = \int_0^L u^n v dx - w\Delta t \int_0^L \frac{\partial u^n}{\partial x} v dx - w^2 \frac{\Delta t^2}{3} \int_0^L \frac{\partial u^{n+1}}{\partial x} \frac{\partial v}{\partial x} dx$$

This yields the linear system

$$u^{n+1} = \left(M + w^2 \frac{\Delta t^2}{6} A_d\right)^{-1} \left(M - w\Delta t A_a - w^2 \frac{\Delta t^2}{3} A_d\right) u^n \quad (32)$$

In (32), M is the mass matrix; A_d and A_a are the stiffness matrices of diffusion and advection terms respectively. Thus, result (32) can be used for solving (9) and (10) when diffusion terms $\frac{\partial^2 u_1}{\partial x^2}$ and $\frac{\partial^2 u_2}{\partial x^2}$ are neglected and helps to make the advection dominated problems stable.

3.4 Improved Sixth Order Runge-Kutta Method

Higher order Runge-Kutta methods provide alternatives for avoiding the inefficiencies those are associated with the corresponding fourth-order formulas. Assuming that round-off errors are under control, such a fourth-order approximation requires totally twelve substitutions or functional evaluations. On the other hand, a single application of an improved sixth-order formula requires only eight substitutions. Hence, the application of fourth-order will not be as accurate as that of an improved sixth-order formula. An improved sixth-order formula performs more number of computations in each time step and also, the error decreases very rapidly as step size decreases. Thus, it yields more accurate results and also more economical since it requires less number of substitutions. Therefore, an improved sixth-order formula is preferred to solve the reaction term given in (11) to (12). The algorithm is given as

$$u_6(t_0 + h) = u_0 + \frac{1}{840}[41(k_0 + k_7) + 216(k_2 + k_6) + 27(k_3 + k_5) + 272k_4] \quad (33)$$

Here in (33), the quantities $k_i, \ \forall\, i = 0, 1, \ldots, 7$ represent

$k_0 = hf(t_0, u_0)$

$k_1 = hf\left(t_0 + \frac{1}{9}h, u_0 + \frac{1}{9}k_0\right)$

$k_2 = hf\left(t_0 + \frac{1}{6}h, u_0 + \frac{1}{24}(k_0 + 3k_1)\right)$

$k_3 = hf\left(t_0 + \frac{1}{3}h, u_0 + \frac{1}{6}(k_0 - 3k_1 + 4k_2)\right)$

$k_4 = hf\left(t_0 + \frac{1}{2}h, u_0 + \frac{1}{8}(k_0 + 3k_3)\right)$

$k_5 = hf\left(t_0 + \frac{2}{3}h, u_0 + \frac{1}{9}(17k_0 - 63k_1 + 51k_2 + k_4)\right)$

$$k_6 = hf\left(t_0 + \frac{5}{6}h,\ \ u_0 + \frac{1}{24}(-22k_0 + 33k_1 + 30k_2 - 58\,k_3 + 34\,k_4 + 3\,k_5)\right)$$

$$k_7 = hf\left(t_0 + h,\ \ u_0 + \frac{1}{82}(281k_0 - 243k_1 - 522k_2 + 876\,k_3 - 346\,k_4 - 36k_5 + 72k_6)\right)$$

The reaction term given in (11) – (12) is solved using improved sixth order formula together with initial conditions of u_1 and $u_2$and with the inclusion of parametric values.

4. NUMERICAL SIMULATIONS

For the purpose of present simulation study, let us set initial conditions for DO and BOD terms as $u_1(x,0) = 1\ kgm^{-3}$ and $u_2(x,0) = 6\ kgm^{-3}$ respectively. Similarly, the boundary conditions for DO and BOD can be set as $u_1(0,t) = u_1(1,t) = 0\ kgm^{-3}$ and $u_2(0,t) = u_2(1,t) = 0\ kgm^{-3}$ respectively. Also, we set the parametric values as $\gamma = 1\ day^{-1}$, $\omega = 1\,kgm^{-3}$ and $\lambda = 3\ m^2 day^{-1}$. However, to study the effect of the pollutant transport characteristic parameters w, D_1 and D_2 we will assign varying numerical values. These parameters are assigned different values and they are displayed together with the simulated figures.

4.1. Zero Diffusion

Let us first consider the case when the diffusion is taken to be negligible. That is, $D_1 = 0\ m^2\ day^{-1}$ and $D_2 = 0\ m^2\ day^{-1}$. In this scenario, equations (7) - (8) reduce to

$$\frac{\partial u_1}{\partial t} = -w\,\frac{\partial u_1}{\partial x} + \lambda(\omega - u_1) - \gamma u_1 u_2 \qquad (34)$$

$$\frac{\partial u_2}{\partial t} = -w\,\frac{\partial u_2}{\partial x} - \gamma u_1 u_2, \qquad (35)$$

The initial and boundary conditions are as already mentioned. Furthermore, for this simulation study let us assign $w = 0.0001\ m\ day^{-1}$. Then result is as follows

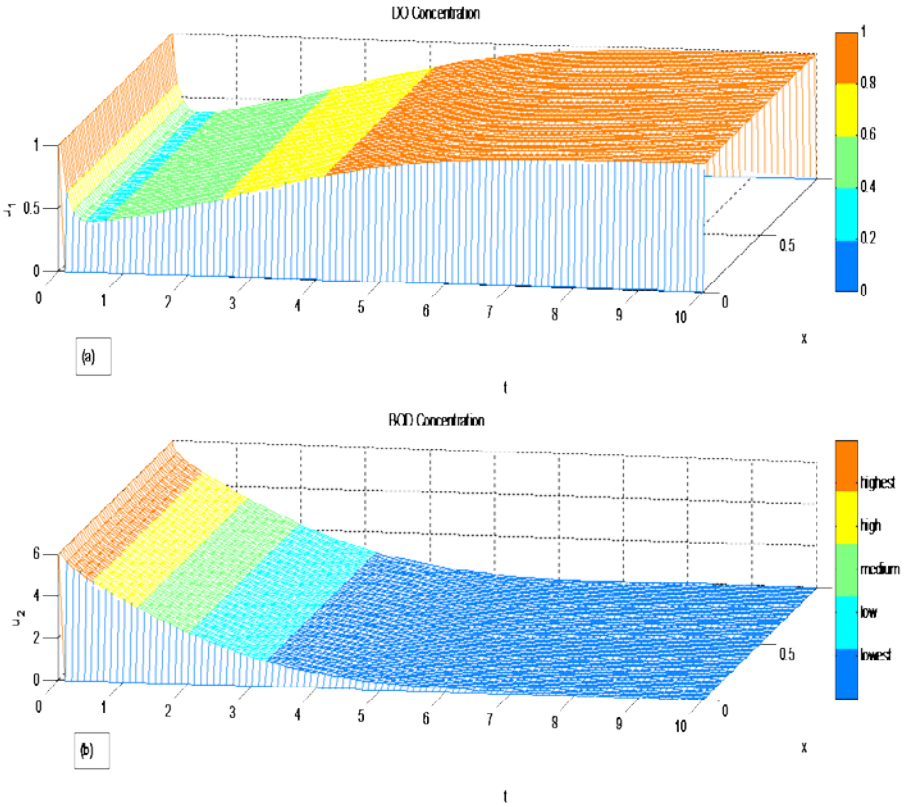

Fig.1. Zero diffusion case for $w = 0.0001\ m\ day^{-1}$

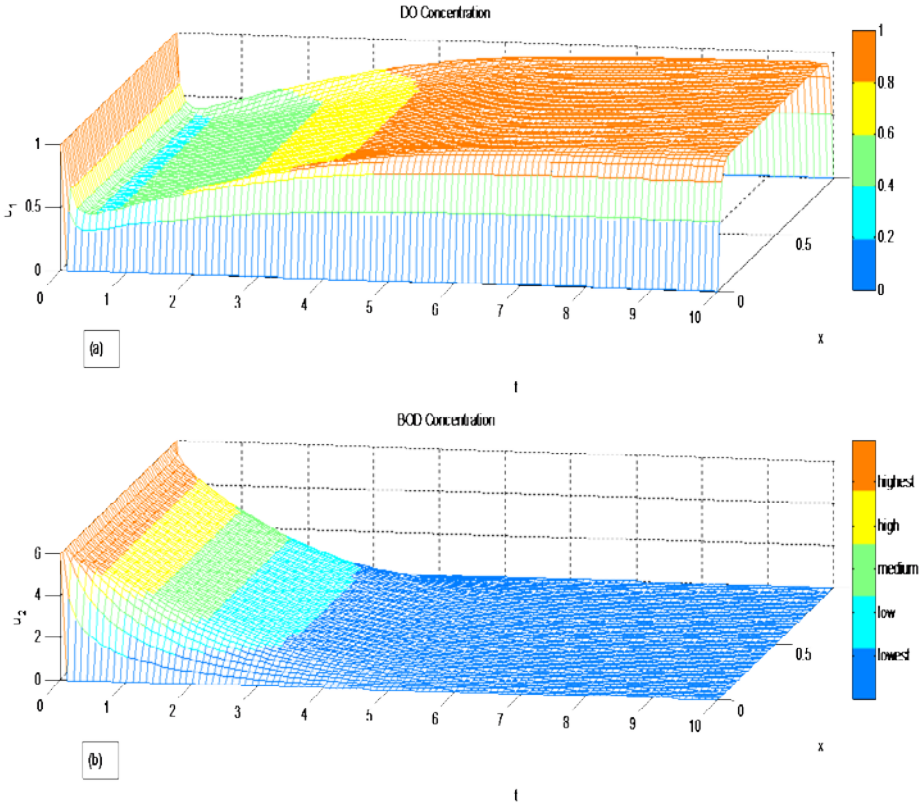

Fig.2. Zero diffusion case for $w = 0.1\ m\ day^{-1}$

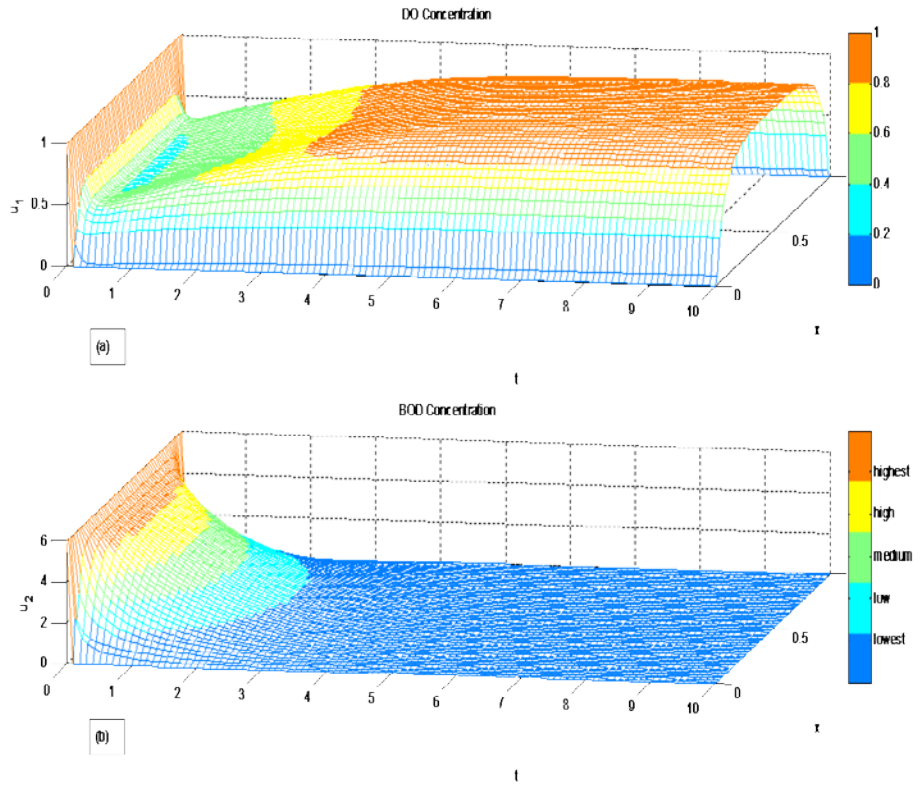

Fig.3. Including diffusion effect for $w = 0.0001 m day^{-1}$, $D_1 = 0.0001 m^2 day^{-1}$ and $D_2 = 0.0001 m^2 day^{-1}$.

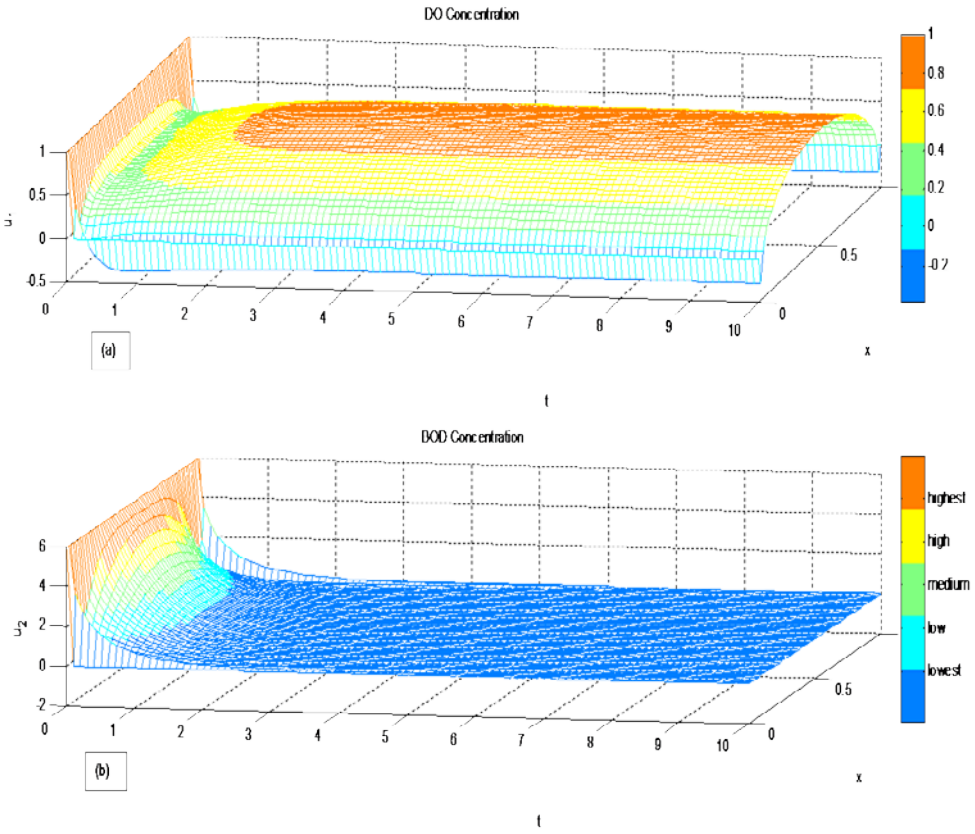

Fig.4. Including diffusion effect for $w = 0.1mday^{-1}$, $D_1 = 0.1m^2day^{-1}$ and $D_2 = 0.1m^2day^{-1}$.

The numerical result for the DO concentration $u_1(x,t)$ is shown in Fig.1 (a). The initial DO concentration is set as $u_1(x,0) = 1\ kg\ m^{-3}$. The DO concentration has the highest concentration at time $t = 0$, due to reaction with BOD and flow of the river it declines slowly and after a while it returns back to its normal value $1kgm^{-3}$ because of the reaeration effect. In Fig.1 (b) we have set initial value for pollution concentration BOD to be $u_2\ (x,0) = 6\ kg\ m^{-3}$. The BOD has the highest concentration at the initial instance $t = 0$. But it declines slowly with the increase of time t, and goes to zero ultimately at the location $x = 1$ downstream. So, clean water is available on the spatial boundary at larger times due to the effects of rapid flow of the river and the self-cleaning effects of the reactive term.

The effect of increased flow velocity is shown in fig. 2(a) and 2(b). We assigned $w = 0.1\ m\ day^{-1}$ while other parametric values remain the same as those values simulated in fig.1. It can be observed from figure 2 that as w increases, the increased BOD zone rapidly decreases and goes to zero in a better speed than figure 1. Also DO decreases because of its reaction with BOD and high flow velocity and after a while it goes to its normal value. Hence, with high velocity the river cleans faster than that of with lower velocity.

4.2. Including Diffusion

The effect on the numerical results when the diffusion is included is shown in figures 3 and 4. We set $w = 0.0001\ m\ day^{-1}$, $D_1 = 0.0001\ m^2\ day^{-1}$ and $D_2 = 0.0001\ m^2\ day^{-1}$ in fig. 3.

Here the figures 3(a) and 3(b) are obtained by the simulation study of the system of equations (7) - (8) with the initial and boundary conditions and parametric values given in section 4. We applied Galerkin finite element method with θ method where $\theta = 1/2$ and it gives the Crank-Nicolson for advection-diffusion term.

We used the peclet number is equal to one unit i.e., $pe = 1$ and hence there is no domination between advection and diffusion terms. For peclet number less than one unit i.e., $pe < 1$, the diffusion term dominates over the advection term and the analysis is given in [28]. For the peclet number greater than one i.e., $pe > 1$, the advection term dominates over the diffusion term and the analysis is given in Figures 1 and 2.

We also applied improved Runge-Kutta method of order six for reaction term of the model (7)-(8). In case when the diffusion term is included, all variations along both the flow direction and depth of the river are ignored. But, the variations at a cross-sectional area of the river of

width one unit i.e., normalized are considered. At time $= 0$, waste water is poured into the water, all over. But we assume that the water at the boundaries cleans. So there, the DO is 1, and the BOD is zero. But then, in addition to the effect of advection term and the self-cleaning effect from the reactive term, we get diffusion of the clean water from the boundaries, which makes the river cleans faster than if we did not have this effect. Comparing figure 1 and figure 3, both DO and BOD concentration profiles of figure 3 has faster changing than figure 1 for the same flow velocity value $w = 0.0001mday^{-1}$.

The effects of increased diffusion coefficients are shown in fig.4 (a) and (b). We give $D_1 = 0.1m^2day^{-1}$ and $D_2 = 0.1m^2day^{-1}$ while other parameter values remain the same values as those values simulated in fig.3. It can be shown that as diffusion coefficients D_1 and D_2 increase, the increased BOD zone is decreases dramatically and tends to zero. And DO also decrease immediately because of reaction with BOD and high diffusion effect and after a while it goes to its normal value.

5. CONCLUSION

In the foregoing sections, we have presented a mathematical model of DO concentration interaction with BOD in the river. The model shown in the form of a coupled pair of nonlinear advection-diffusion-reaction equations, which is required to solve the DO concentration in coupled with BOD at space and time, and have investigated the effects of advection and diffusion on the degradation of BOD in the river. We have also presented efficient numerical methods after splitting the problem into two unsteady sub-problems and solved the splited problems based on the standard Galerkin finite element and Taylor-Galerkin methods with linear piecewise basis function and improved sixth order Runge-Kutta for solving the system model. Two test cases have been performed. These are zero diffusion and including diffusion effects. We have simulated these two test cases by setting some appropriate initial and boundary conditions and parametric values. From the profile of varying advection and diffusion term, we saw that the rate of advection and diffusion is high; the concentration of BOD decreases faster. Thus, this shows that increasing the factors and parameters like DO, river velocity, diffusion and reaction rate helps us to get clean water within a short time by removing biological pollutants or BOD in the river. This model and its solutions will aid in decision support on restrictions to be imposed on farming and urban practices.

REFERENCES

[1] Agusto F. B. and Bamigbola O. M. (2007), Numerical Treatment of the Mathematical Models for Water Pollution, *Journal of Mathematics and Statistics*, Vol. 3, No.4, Pp. 172-180.

[2] Ambrosi D. and Quartapelley L. (1998), A Taylor–Galerkin Method for Simulating Nonlinear Dispersive Water Waves, *Journal of Computational Physics* 146, Pp.546–569.

[3] Brain J. McCartin, Sydney B. and Forrester Jr. (2002), A Fractional Step-Exponentially Fitted Hoscotch Scheme for the Streeter-Phelps Equations of River Self-Purification, *Engineering Computations*, Vol. 19, Pp. 177-189.

[4] Butcher J. C. (2009), On Fifth and Sixth Order Explicit Runge-Kutta Methods: Order Conditions and Order Barriers, *Canadian Applied Mathematics Quarterly*, Vol. 17, No. 3, Pp.1-14.

[5] Chertock A., Kurganov A. and Petrova G. (2006), Fast explicit operator splitting method for convection–diffusion equations, *International Journal for Numerical Methods in Fluids*, doi: 10.1002/fld.1355, http://www.interscience.wiley.com.

[6] Colin O. and Rudgyard M. (2000), Development of High-Order Taylor–Galerkin Schemes for LES, *Journal of Computational Physics* 162, Pp. 338–371, doi:10.1006/jcph.2000.6538, http://www.idealibrary.com.

[7] Evans G., Blackledge J. and Yardely P. (2000), Numerical Methods for Partial Differential Equations, Springer-Verlag, London.

[8] Geiser J. (2016), Multicomponent and Multiscale Systems Theory, Methods and Applications in Engineering, *Springer International Publishing Switzerland*, doi 10.1007/978-3-319-15117-5_2, http://www.springer.com/978-3-319-15116-8.

[9] Hasadsri S. and Maleewong M. (2012), Finite Element Method for Dissolved Oxygen and Biochemical Oxygen Demand in an Open Channel, *Procedia Environmental Sciences*, Vol. 13, Pp. 1019 – 1029, doi:10.1016/j.proenv.2012.01.095.

[10] Holden H., Karlsen K.H., Lie K. and Risebro N.H, (2010), Splitting Methods for Partial Differential Equations with Rough Solutions-Analysis and MATLAB programs, *European Mathematical Society*, ISBN 978-3-03719-078-4.

[11] Holzbecher E. (2007), Environmental Modeling Using Matlab, Springer-Verlag, Berlin Heidelberg.

[12] Huang H. and Huang S. (2011), A High-order Implicit Difference Method for the One-dimensional Convection Diffusion Equation, *Journal of Mathematics Research*, Vol. 3, No. 3, doi:10.5539/jmr.v3n3p135,http://www.ccsenet.org/jmr.

[13] Hundsdorfer W. and Verwer J.G. (2003), Numerical Solution of Time Dependent Advection-Diffusion-Reaction Equations, Springer-Verlag, Berlin Heidelberg.

[14] Hussain S.A., Atshan W.G. and Najam Z.M. (2012), Mathematical Model for the Concentration of Pollution and Dissolved Oxygen in the Diwaniya River (Iraq), *American Journal of Scientific Research*, ISSN 2301-2005 Issue 78, Pp.33-37, http://www.eurojournals.com/ajsr.htm

[15] Kaushik N., Tyagi B. and Jayaraman G. (2012), Modeling of the Dissolved Oxygen in a River with Storage Zone on the Banks, *Applied Mathematics*, Vol. 3, Pp. 699-704, http://dx.doi.org/10.4236/am.2012.37103.

[16] Mahto K. and Kumar I. (2015), The Self Purification Model for Water Pollution, *International Journal Of Mathematics And Statistics Invention (IJMSI)*, Vol. 3, Pp. 17-32, *www.Ijmsi.org*.

[17] Marusic G. (2013), A Study on the Mathematical Modeling of Water Quality in "River-Type" Aquatic Systems, *WSEAS Transactions on Fluid Mechanics*, Vol. 8, Pp. 1-10.

[18] Mesteron-Gibbons, M. (2007), A Concrete Approach to Mathematical Modeling, John Wiley and Sons – Interscience.

[19] Pimpunchat B., Sweatman W.L., Wake G.C., Triampo W. and Parshotam A. (2009), A Mathematical Model for Pollution in River and Its Remediation by Aeration, *Applied Mathematics Letters*, Vol. 22, Pp. 304-8, doi:10.1016/j.aml.2008.03.026.

[20] Quarteroni, A. (2009), Numerical Models for Differential Problems, 4^{th} ed., Springer-Verlag Italia.

[21] Ramalinga Reddy D.V and Sreenivasa Chari A. (2013), A Mathematical Model for Toxic Waste in a River and Its Remediation by Freshening, *International Journal of Innovative Research & Studies*, Vol. 2, Pp. 1-10.

[22] Rathish Kumar B.V. and Mehra M. (2005), Time Accurate Fast Wavelet-Taylor Galerkin Method for Partial Differential Equations, doi:10.1002/num.20092, http://www.interscience.wiley.com

[23] Rathish Kumar B.V and Mehra M. (2005), Wavelet multilayer Taylor Galerkin schemes for hyperbolic and parabolic problems, *Applied Mathematics and Computation 166*, Pp. 312–323.

[24] Sanderson A. R., Meyer M. D., Kirby R. M. and Johnson C.R. (2007), A Frame works for Exploring Numerical Solutions of Advection-Reaction-Diffusion Equations Using a GPU Based Approach, *Computer visual Sci.*, Vol. 10, Pp. 1-16.

[25] Sarafyan D. (1972), Improved Sixth-Order Runge-Kutta Formulas and Approximate Continuous Solution of Ordinary Differential Equations, *Journal of Mathematical Analysis and Applications*, Vol. 40, Pp. 436-445.

[26] Sharma D., Jiwari R. and Kumar S. (2011), Galerkin-Finite Element Method for the Numerical Solution of Advection-Diffusion Equation, *International Journal of Pure and Applied Mathematics*, Vol. 70, No. 3, Pp. 389-399.

[27] Shukla J.B., Misra A.K. and Chandra P. (2008), Mathematical Modeling and Analysis of the Depletion of Dissolved Oxygen in Eutrophied Water Bodies Affected by Organic Pollutants, Nonlinear Analysis: *Real World Applications*, Vol. 9, Pp. 1851-1865, doi:10.1016/j.nonrwa.2007.05.016.

[28] Simon T. and Koya P.R. (2015), Modeling and Numerical Simulation of River Pollution Using Diffusion-Reaction Equation, *American Journal of Applied Mathematics*, Vol. 3, No. 6, Pp. 335-340, doi: 10.11648/j.ajam.20150306.24, http://www.sciencepublishinggroup.com/j/ajam.

[29] Streeter H.W. and Phelps E.B. (1925), A Study of the Pollution and Natural Purification of the Ohio River, *U.S. Public Health Service*, Bulletin No. 146.

[30] Uzunca M. and Karasözen B. (2014), A Matlab Tutorial for Diffusion-Convection-Reaction Equations Using DGFEM, *Middle East Technical University, Ankara, Turkey*, http://iam.metu.edu.tr.

[31] Zingg D.W. and Chisholm T.T. (1999), Runge–Kutta methods for linear ordinary differential equations, *Applied Numerical Mathematics*, Vol. 31, Pp. 227–238.