Hydrodynamic Integrated Modelling of Basic Water Quality and Nutrient Transport in Swarna River Basin, Udupi, Karnataka

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Abstract - *After the Streeter-Phelps model the development in technology has caused the increase in number of various water quality models having an increased degree of accuracy and complexity [11]. The enormous progress in the complexity of the model include the change from a one-dimensional model to a complex three-dimensional model with additional computational tools to include process like non-point source pollution, floodplain variation due to the fluxes in waves due to dam break etc. [7]. Surface water from its origin that is the mountains flows towards the catchments carrying along the sediments formed due to the weathering process and from the catchments the water drains through the rivers, lakes, creeks to the ocean which is called the transition zone which contains sediments other than weathered particles like agricultural runoff, waste water etc. [9]. This affects the chemistry of a river as well as causes a variation in the physical and biological structure of a river. [9] Various models can be used to simulate the behaviour of these pollutants and this information can be used to tackle against the present situation of global climatic change in addition, the information on the hydrologic effects of land use is very useful. These models can be helpful for various policy makers in local and federal level to devise certain guidelines to preserve and protect the environmental system and also helps to prepare an appropriate water development plan for the future.*

Key Words: **Streeter-Phelps model, one-dimensional model, water quality models, surface water, pollutant transport, mechanistic models, statistical models, finite difference method, HACH HQ30d multi probe water quality analyser.**

1. INTRODUCTION

A model is defined as "a simplification of reality that is constructed to gain insights into select attributes of a particular physical, biological, economic, or social system." The type of model employed depends upon the field of study like economic, behavioural, physical, engineering design. [3] For example the subsurface flow behaviour taking place in earth can be understood by making a physical model with different soil samples representing the different layers of earth's surface. Even a pollutant behaviour can be understood by injecting a dye into the model and from the observation can be used for further studies of the system. A model can also be developed numerically with the help of a certain mathematical equation which governs the movement of the pollutant or the flow of the system (Mechanistic model) or can be developed based on a collection of data (Statistical model). [6][3] For example the transfer of heat between two media is governed by heat equation. However, a developer can create an equation to model complex systems involving more than one processes having different equations governing each process. So, the model developer ranks the present and future environmental problems related to the study area according to their importance and eliminate the ones which are below in rank with the help of assumptions and develops or finds out the equations which governs those problems with the help of literature and experienced personnel. [2] Thus, these assumptions take away the complexity of a model and thus a model cannot be called an ideal representation of a river. However, a complex model can be as unreliable as a simple model because of over parameterisation [3] and are usually reserved for rivers having greater depth and width and where complex mixing patterns are present along with large requirement of representative data. This limitation itself generates a huge demand of money, time and labour. A model can accommodate the pollutant behaviour of an entire catchment basin or even a simple relationship between two pollutants present in a lake. But the accuracy of the model depends on internal factors like boundary conditions, numerical scheme and spatial and temporal resolution adopted. [5] [3] [10]

In this work, a dynamic integrated modelling of basic water quality and fate of contaminants due to the hydrodynamic transport process present in the river. In this framework, a basic 1-D river water quality model is developed for River Swarna, Udupi district, Karnataka, by using four-point Finite Difference (FD) method.

In this work, a dynamic exposure modelling approach is explained. This kind of modelling method is very beneficial for time-varying effect valuation. Temporal variation of pollutant concentration is a realistic approach due to the fact that most of the physical, chemical and biological change in river depends on it like varying rates of input, dilution, runoff events and sewer overflows. Furthermore, toxicity depends on the duration and frequency of exposure [6], and only such a dynamic exposure model can describe the compliance with the duration and frequency of the exposure concentration [3].

2. STUDY AREA

River Swarna is one of the primary sources of drinking water in Udupi, a district located in the southern coastal part of Karnataka. A population of around 1 lakh generates contamination from agricultural, municipal and industrial activities which introduces significant amount of nutrients and organic materials into the rivers and streams present in the district. Therefore, assessment of the effectiveness of the present alternatives of water management methods of Swarna River is the primary concern.

3. MATERIALS AND METHODS

3.1 Sampling

A reconnaissance survey was conducted along the length of river which was to be later modelled followed by selecting a 2km stretch of river at a location named Herga which was selected based on its uniform hydrological and geometrical properties. Along the 2km stretch 4 sample collection points were selected based on the mixing regime present at those points. And samples were collected from sub-points surrounding each of these 4 points and a weighted average of all these values were taken to obtain a representative value from each point. A sample was collected using a 500 mL tarsons HDPE bottle after been rinsed thoroughly and alternatively using a diluted acid (hydrochloric acid) and distilled water and dried. The bottle was inserted into a depth of 30cm to obtain a sample which has not been diluted to the temperature which has been changed due to the presence of sunlight on the surface.

Fig - 1: Sample Collection - 1- 30 cm deep

3.2 Methods

The input data required for the simulation of the model is classified into (a) hydraulic data (b) reaction constants (c) pollutant load concentration.

3.2.1 Basic Parameter Analysis

Polypropylene bottles (acid-washed, 500-mL capacity) were used to collect water samples at the point where tributaries meet and at the surface of every station. Measurements of water temperature, pH, conductivity, Dissolved Oxygen and Total Dissolved Solids (TDS), Nitrate Nitrogen (NO_3-N) were done in situ using the HACH HQ30d multi probe water quality analyser. Water samples for Nitrogen analysis were stored in 500-mL high-density Polypropylene bottles, previously rinsed with river water two to three times. The analysis for nutrient concentration is carried out within 1 day of sampling to avoid contamination and deterioration. The analysis was carried out using the HACH HQ30d multi probe for nitrates. Physical conditions such as temperature, DO, pH, TDS and conductivity were documented to obtain the current water quality status of the river. Analysis result showed all the parameters are well within the Surface Water Quality Standards.

3.2.2 BOD Analysis

BOD analysis can be carried out using two methods mainly direct method and dilution method. Direct method was preferred for this study as the river water BOD is generally observed to be below 2-3 mg/L and dilution method is usually done for wastewater having high concentration of organics. For the direct method all the water samples were taken in a 300mL BOD bottle and filled with the samples up to the brim. 2 mL of manganous sulphate and alkali-iodide-azide reagent to the BOD bottle and allow the floc to settle down and then add 2 mL of concentrated sulphuric acid and shake well and let the flocs dissolve. Then take 25mL of the sample and titrate it against sodium thiosulphate solution and when the sample colour changes to pale yellow add 2 drops of starch indicator and titrate again till the blue colour disappears. From the volume of sodium thiosulphate consumed and the amount of water sample calculate the concentration of final DO. Initial DO and temperature of the water samples were measured using the HACH MULTIMETER PROBE and from these DO values concentrations of BOD was calculated. Also, value of saturated DO was calculated using the equation

3.3 Hydraulic data measurement

Velocity and depth of the river stretch was carried out experimentally and using the data river water discharge was also calculated. The hydraulic data can also be calculated using the formula

$$\bar{u} = aQ^b \qquad 3.1$$

$$d = cQ^d \qquad 3.2$$

$$A_x = Q\sqrt{u} \qquad 3.3$$

Where u and d are the average cross-sectional velocity and depth of the river and the constants a, b, c and d can be determined from stage-discharge curves or by referring previous literature. [1][4] [12]

3.4 Reaction constants

The present study involves advection-diffusion equation for the nitrate transport and **Streeter-Phelps Equation** for the simulation of BOD and DO behaviour throughout the reach. These equations involve certain reaction coefficients which are calculated using certain equations which are determined by referring previous literature. The reaction constants include Deoxygenation rate, Reoxygenation rate, nitrate variation rate, dispersion coefficient.

3.5 Representation of river network

The river has been represented as a combination of both Plug flow and Stirred tank reactor approach as both the advection and dispersion processes has been considered. If advection transport can be neglected a plug flow approach will be more suitable for the model [1]

3.5.1 Temporal and spatial resolution

The computational stability and accuracy of the model depends upon two important factors like spatial and temporal resolution [1] [4]. A model is actually a scaled down representation of the actual system. As the present study is about the spatial variation of the pollutant concentration spatial resolution has much importance and his resolution should not be too fine or too coarse which will affect the computational stability and accuracy. The river has been divided into 3 reaches of 1km length and each reach has been further divided into grids having each block of size 1x1 cm. there are no specific guidelines for determining temporal resolutions but it should be long enough to eliminate the error of the initial condition.

3.5.2 Time step calculation

The time step should be small enough to ensure computational stability and accuracy of the model results. If the time step is not small enough there is a chance for the solution of the transport equation to go out of bounds. In the present study, the time step has been calculated using the Von-Neumann stability condition. [8]

$$\Delta t = \frac{dx^2}{(V_x * dx + 2 * E_L)} \qquad 3.4$$

3.5.3 Transport processes

The equation is developed after considering a control volume having dimensions Δx, Δy, Δz in corresponding x, y, and z directions. But for simplicity a two-dimensional surface is assumed where the pollutants are moving in x-direction with a velocity V_x.

3.5.4 Advective Transport:

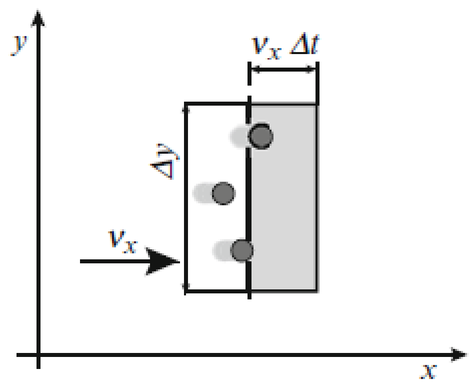

Figure – 2: 2D Plane representing advection process

Due to advection, in the time interval Δt, the mass of the pollutant entering the volume through the face Δy Δz at location x_0 is

$$\Delta y\, \Delta z\, Vx\, Cx\, \Delta t \qquad 3.5$$

And that going out through the face Δy Δz at location x_0 + Δx is

$$\Delta y\, \Delta z\, V_{x0+\Delta x} C_{x0+\Delta x}\, \Delta t \qquad 3.6$$

The difference between the above two quantities is the mass variation in the Δt interval:

$$\Delta y\, \Delta z\, (V_{x0+\Delta x} C_{x0+\Delta x} - Vx\, Cx)\, \Delta t \qquad 3.7$$

Which is equal to the equation

$$\Delta x \Delta y \Delta z\, (C_{t0+\Delta t} - C_{t0}) \qquad 3.8$$

After equating both these equations and dividing it by the dimensions and consider infinitesimal size of the control volume and infinitesimal time scale we obtain the equation for advective transport.

$$-\left(\frac{dC}{dt}\right)_{adv} = \left(\frac{d(V_x C)}{dx}\right) \qquad 3.9$$

Where C is the concentration of the pollutant and the negative sign indicates that the pollutant concentration is decreasing.

3.5.5 Dispersive Transport

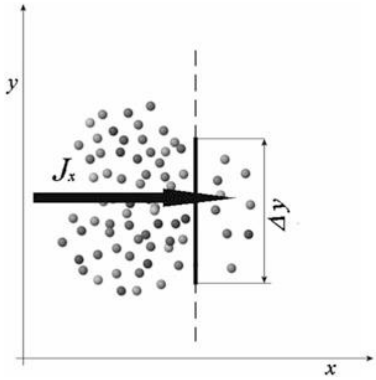

Fig - 1: **2D Plane representing diffusion process**

Similarly, the equation for dispersive transport can be generated from the equation

$$\vec{J} = -E\,\overrightarrow{grad}\,C \qquad 3.10$$

By considering the mass pollutant inflow and outflow through a volume of infinitesimal size and infinitesimal time interval, the following equation can be generated

$$\left(\frac{dC}{dt}\right)_{disp} = E\left(\frac{d^2C}{dx^2}\right) \qquad 3.11$$

3.5.6 Source/Sink (S)

These are additional reaction terms in the equation and can be called Source or a Sink depending upon whether the flow is coming in or going out of the volume. The equation for a source/sink can be represented the same way as advection or diffusion

$$\left(\frac{dC}{dt}\right)_{source/sink} = \pm S \qquad 3.12$$

Here the plus or minus sign depend on whether the equation is considered as a source or a sink.

3.5.7 The fundamental equation for pollution transport

The above equations developed after considering all the processes is same for x, y and z directions. For simplicity of the model the equations for y and z directions have been neglected leaving only the equation for x-direction. As not any source or sink is considered in the volume the term for that reaction can also be neglected. So the fundamental equation for pollutant transport can be written as

$$\left(\frac{dC}{dt}\right) = -V_x\left(\frac{dC}{dx}\right) + E_x\left(\frac{d^2C}{dx^2}\right) \qquad 3.13$$

3.5.8 Discretization of the fundamental equation

The fundamental equation (Eqn 3.7) can be transformed into finite terms so that with the help of the efficient computational capacity of an existing software the equation can be solved. Presently the discretized equation can be solved by either of the following ways namely finite difference method, finite element method or finite volume method. [12].The present study has used four-point finite difference approximation to determine the concentrations at each point due to the reasons of simplicity.

3.5.9 Finite difference method

The first step before calculating the concentration using a finite difference approach is to divide the river reach into different boxes or 'grids' and the corner of each of these grids are called nodes at which the concentrations are being calculated. Here the grids are of size 1x1 cm and the area near the first source of pollutant is considered for modelling. The next step for the modeller is to determine the scheme using which the equations are going to be solved. Depending upon the terms involved in the fundamental equation different schemes can be adopted to solve the equation. In the present study, a combination of these scheme is adopted namely forward difference approximation for the concentration varying over the time and backward difference scheme for the advection term and central difference approximation for the diffusion term. [1][4] [12] [3]

3.6 Equations for DO and BOD model

The equations present in Streeter-Phelps model was modified according to the study undertaken [13]. Streeter-Phelps equation consists of first order decay and reaeration under suitable assumptions:

$$\frac{dD}{dt} = k_1L - k_2D$$

For BOD simulation,

$$L = L_o e^{-k1t}$$

Where D is the DO deficit, k_1 is the BOD degradation constant, k_2 is the atmospheric reaeration constant, L is the BOD concentration (mg/L) at time t, L_0 is the ultimate BOD (mg/L), and t is the hydraulic retention time.
Substituting L in deficit equation,

$$D = \frac{k1Lo}{k2 - k1}\left(e^{-k1t} - e^{-k2t}\right) + D_0.e^{-k2t}$$

Where D_0 is initial DO deficit
Carbonaceous and nitrogenous demand is included in the ammonia decay equation.

$$\frac{dD}{dt} = k_1 L - k_2 D + k_3 N \qquad 3.17$$

For NH_3-N Simulation,

$$N = N0e^{-k3t} \qquad 3.18$$

For DO deficit for each calculation,

$$D = \frac{k1Lo}{k_2 - k_1}\left(e^{-k_1 t} - e^{-k_2 t}\right) + \frac{k_3 No}{k_2 - k_3}\left(e^{k_3 t} - e^{-k_2 t}\right) + Do.e^{-k_2 t} \qquad 3.19$$

Where k_3, ammonia degradation is constant, N is the ammonia–nitrogen concentration (mg/L), and N_0 is the ultimate ammonia–nitrogen concentration (mg/L). The rate constantsk_1, k_2 and k_3 are usually determined at 20℃.

$$kT = k20 * \theta^{(T-20)} \qquad 3.20$$

Where k^{20} is the degradation constant at 20℃, k_T is the degradation constant at temperature T, and θ is the temperature correction coefficient. θ is 1.047 for the BOD, 1.047 for the NH_3– N, and 1.024 for the Reoxygenation constants which are obtained from literature. The Reoxygenation constant k_2, may be calculated using following equations,

3.6.1 O'Connor – Dobbins

$$k_2 = 3.93\frac{U^{0.5}}{H^{1.5}} \qquad 3.21$$

H (m) < 0:61

3.6.2 Owens – Gibbs

$$k2 = 5.32\frac{U^{0.67}}{H^{1.85}} \qquad 3.22$$

H (m) > 0:61m and H (m) > $3.45U^{2.5}$.

3.6.3 Churchill:

$$k2 = 5.026\frac{U}{H^{1.67}} \qquad 3.23$$

4. RESULTS AND DISCUSSION

Hydrological measurements, mathematical modelling of pollutant transport and water quality of upstream stretch of River Swarna and various simulations of it has been carried out and the results are discussed below. The field measurements were carried out during monsoon season.

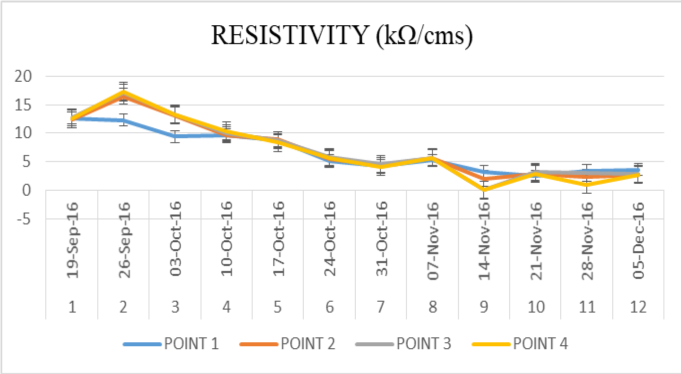

Chart - 1: Resistivity profile of sampling points

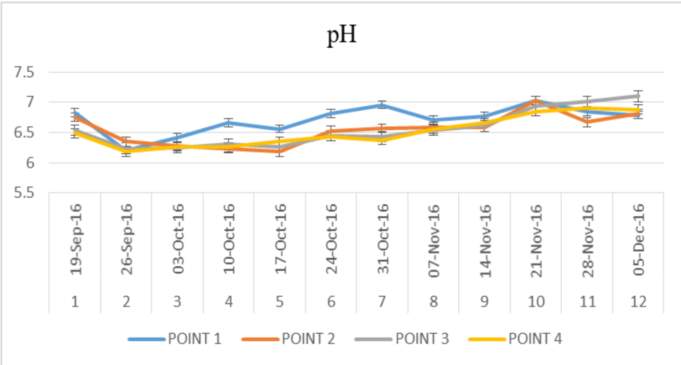

Chart - 2: pH profile of sampling points

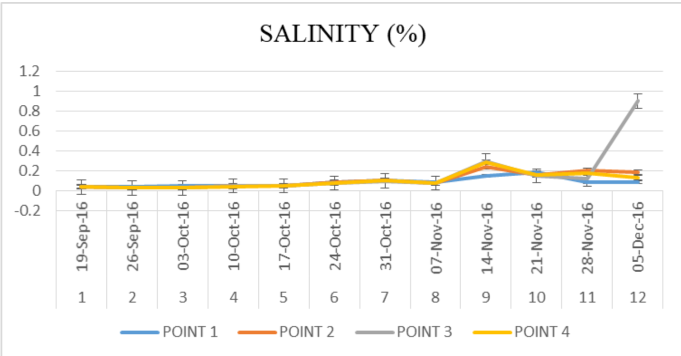

Chart - 3: Salinity profile of sampling points

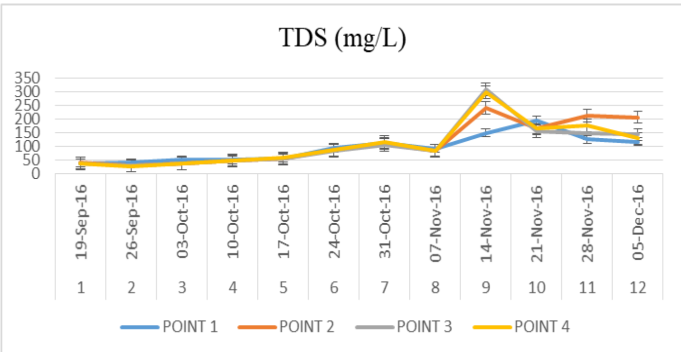

Chart - 4: TDS profile of sampling points

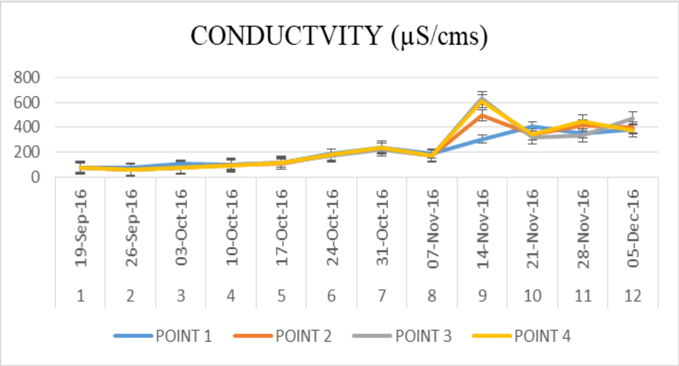

Chart - 5: Conductivity profile of sampling points

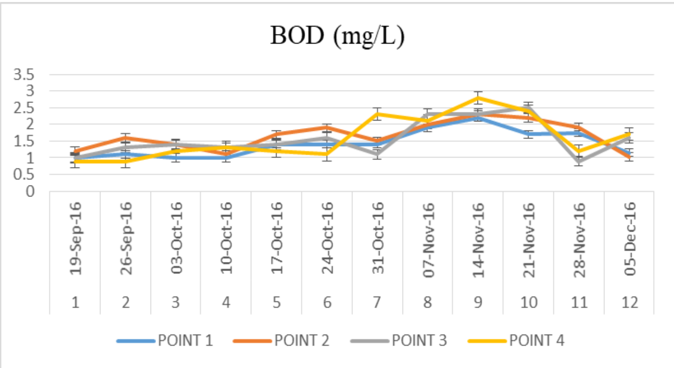

Chart - 6: BOD profile of sampling points

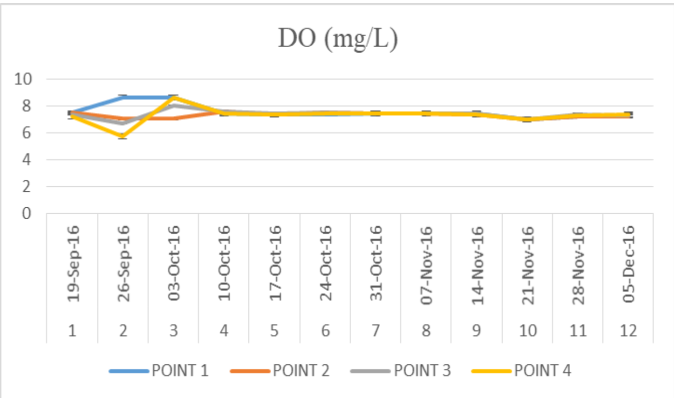

Chart - 7: DO profile of sampling points

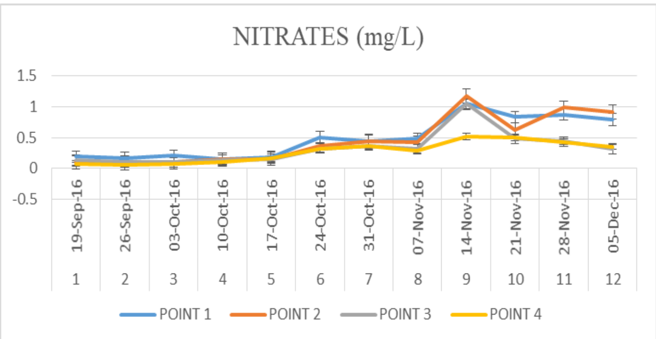

Chart - 8: Nitrate profile of sampling points

4.1 MS-EXCEL MODEL RESULTS

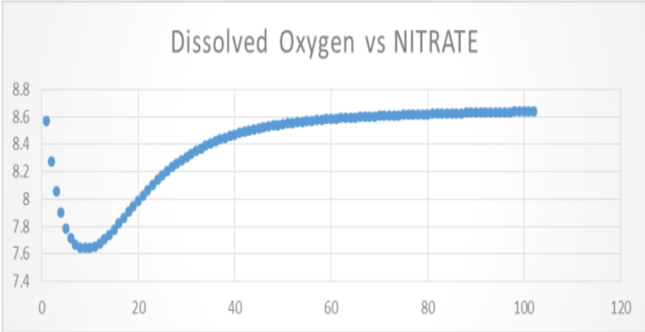

Chart - 9: DO vs Nitrate variation profile

As expected, the DO concentration decreases gradually and increases back due to natural self-purification phenomenon. Fig. 4.1 shows the variation of DO due to the presence of BOD and Nitrate (NO_3-N) along the upstream stretch of River Swarna. Under steady-state condition, from the model output we can obtain the time taken by the river to nullify the pollutant effect completely.

4.2 POLLUTANT CONCENTRATION VARIATION MODEL USING MATLAB

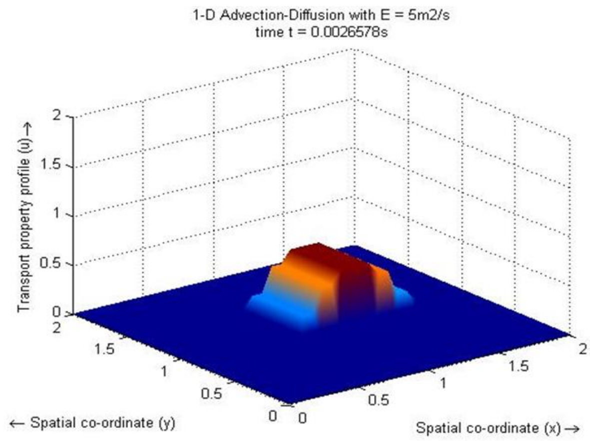

Fig – 4: Initial Condition of Pollutant concentration

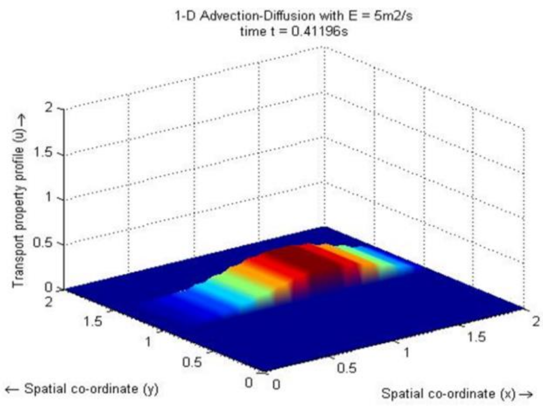

Fig – 5: Final Variation of Pollutant concentration

The concentration is spread over the region because of advection and diffusion and the time elapsed can be observed. The model can be simulated with different time limits and the change in the concentration can be noted corresponding to the time. Also, the model can be simulated by changing the value of dispersion coefficient and other parameters depending upon the river characteristics.

5. CONCLUSION

This study developed a one-dimensional basic water quality model using MS-Excel and a pollutant transport model using Matlab and reviewed their applicability and reproducibility using sensitivity analysis, calibration and verification. Both models can be used to determine the fate and transport of the pollutants in the river. It can satisfactorily identify behavior of conservative and non-conservative pollutants in the river in a one-dimensional pattern. The matlab pollutant transport model is developed for a stretch of 10km of the river which accommodates uniform geometry and hydrological characteristics. The model has been developed using the fundamental steps required to develop a one dimensional model and thus provides a framework to accommodate further components depending upon the complexity of the study taken. Model fit is not adequate for most adverse situations and this can be solved using further observations and data. Discrepancies observed between the simulated and measured results can be attributed to the lack of data obtained, model assumptions adopted and complexity of the model formulated. Both MS Excel water quality model and Matlab pollutant transport model are user friendly and doesn't require extensive collection of input data and hydrological parameters unlike other complex models.

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