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Numerical and Analytical Method based Mathematical Approach to Estimate Water Pollution over 3-D Region

Tarjani Naik, Mukesh Patel, Rachna Patel

Abstract:** One of the major environmental issues is water pollution, which harms aquatic ecosystems, human health, and the sustainability of natural resources. To solve this problem, reliable mathematical models are required that can predict the behaviour of pollutants in three-dimensional (3-D) water systems. In this study, the temporal and spatial fluctuations of pollutant concentration in water are estimated using a 3-D diffusion model. The work's goals are to investigate the gradual rise in pollution levels in a 3-D region and assess the accuracy of analytical and numerical methods for addressing diffusion-based pollution issues. Two distinct mathematical techniques are employed to determine the level of pollution in water at a 3-D location: the Crank-Nicolson (C-N) method, a numerical method, and the Adomian Decomposition Method (ADM), an analytical method. The data collected from an experiment conducted in a 3-D cuboid tank, where water serves as the medium and iodised saltwater solution as the pollutant, are used to derive the initial and boundary conditions for the presented mathematical approaches. The dispersion of pollutants over time and space can be directly observed in this experiment, yielding crucial data for validating the mathematical model. The results of the experiments show that during all the time intervals, there is a rise in water pollution at all 3-D locations. Furthermore, the insignificant error in the form of parts per million (PPM) difference obtained when comparing the outcomes of the C-N with Experimental data (Exp. data) and ADM methodologies demonstrates the effectiveness of the proposed mathematical model. The benefit of this research lies in the use of mathematical approaches and experimental data to investigate water pollution in a 3-D region. The study demonstrates the validity of the proposed model and its ability to forecast the spread of pollution in water accurately. This method is also applicable to larger water systems than the experimental tank. The research enhances mathematical solutions to diffusion equations and provides valuable insights for developing pollution control measures, assessing water quality, and promoting sustainable water management.

***Keywords:** Water Pollution · 3-D Diffusion Equation · Crank-Nicolson Method · Adomian Decomposition Method Mathematics Subject Classification: 35K57· 65N06*

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Nomenclature:
ADM: Adomian Decomposition Method
PPM: Parts Per Million
FTCS: Finite-Time Central Space
ANN: artificial neural network
TDS: Total Dissolved Solids
MAE: Mean Absolute Error
C-N: Crank-Nicolson

I. INTRODUCTION

One essential element of the earth is water; two-thirds of its surface is covered by it. Most people, particularly humans, rely on freshwater to ensure their growth [14]. In today's world, people want water that is sufficient in quantity and of superior quality [1]. Residential and industrial human activity-related water pollution is a serious issue in many nations [4]. An estimated 25 million people die from water pollution each year. Therefore, the issue of water quality is gaining huge attention worldwide [3].

There are multiple ways to characterize water pollution. Water pollution occurs when the physical, chemical, and biological aspects of water are altered in a manner that negatively impacts living organisms. Human activity is the leading cause of water contamination, harming both human health and the quality of the environment's water [16].

There are two approaches, numerical and analytical, that can be employed to address the issue of water pollution, and several techniques exist for solving mathematical equations related to this problem.

In this research, a 3-D diffusion mathematical model is used to predict water pollution over a time interval with a constant diffusion rate. This model is demonstrated by considering water as a pollutant and iodised salt-water solution as another pollutant. A 3-D cuboid is prepared with an equidistant grid in all three directions, and the Experiment Is Conducted. data on water pollution in PPM is collected from each grid point of the cuboid over equal time intervals. The initial and boundary conditions are constructed from the experimental data, and two mathematical approaches, the C-N numerical method and the ADM analytical method, have been used to estimate the level of water pollution. Furthermore, their comparative analysis was performed to estimate errors.

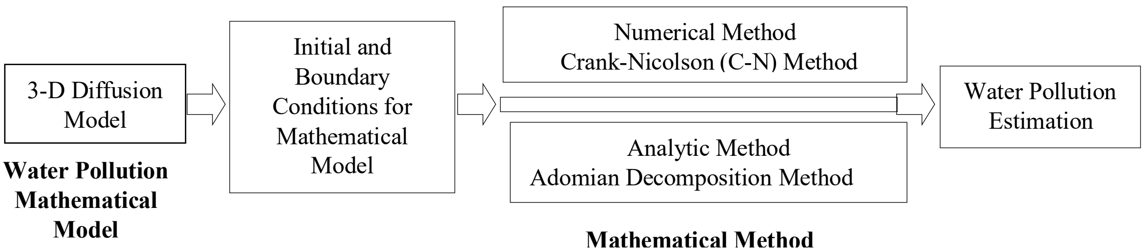
II. RELATED WORK

Chen and Xu [6] developed a 1-D diffusion model to study water pollution in the Tuojiang River Basin. The model was implemented using the finite difference method, along with a Jacobian matrix. Zainab Yahya, Hanani

Johari, and Nursalasawati Rusli [1] employed the one-dimensional advection-diffusion model. She solved it using the Finite Difference Method (FTCS techniques and implicit C-N techniques) to forecast the transportation of water pollution concentration. Nigar Sultana and Laek Sazzad Andallah [7] solved the one-dimensional advection-diffusion equation using the second-order Lax-Wendroff method and Finite-Time Central Space (FTCS) to determine the concentration of water pollution in a river as well as the pollutant in the river at various times and locations. Abbas Parsaie, Amir Hamzeh Haghiabi [12], Omar Hireche, Abdelkader Saidane, Safia Meddah, and Mohamed Hadjel [13] developed a one-dimensional advection-diffusion model. In [12], this model was employed to estimate the longitudinal dispersion coefficient and simulate the transmission of pollution in rivers using the finite volume method and an artificial neural network (ANN). In [13], the Transmission Line Matrix Method was employed to estimate the longitudinal dispersion of pollutants and determine the maximum concentration over time. Delong Wan, Huiping Zeng [8], Tsegaye Simon, Purnachandra Rao Koya [10], R.V. Wagmare, and S.B. Kiwne [11] expanded their research work by adding some parameters to a one-dimensional advection-diffusion model. In [8], the Pollution Index Method was employed to predict water quality based on specific parameters. In [10], the Runge-Kutta, splitting, and C-N methods were applied to calculate the numerical solution and study the dynamics of pollution in rivers. The splitting method separated the diffusion and reaction terms, and the C-N and Runge-Kutta methods were used to find a numerical solution. In [11], the analytical method was used to find the system's solution. Kusuma, Ribal, Mahie, and Aris [5] extended a 1-D advection-diffusion model into a 2-D advection-diffusion model. She utilised a numerical compound finite difference method to investigate pollution levels in Unhas Lake, Indonesia. Saleh, Dimian, and Ibrahim [2] developed a 3-D advection-diffusion model. They employ both analytical methods, such as the Laplace transform, and numerical solutions through the finite difference method. They utilise dimensionless variables to forecast pollutant concentrations in rivers and examine the effectiveness of releasing clean water in reducing pollution levels.

III. PROPOSED METHODOLOGY

The issue of water pollution is addressed by the proposed mathematical method, as shown in Fig. 1.



[Fig.1: Mathematical Method for 3-D Water Pollution Estimation]

A. Water Pollution Mathematical Model

The mathematical model for estimating water pollution is constructed based on the diffusion model in a 3-D region. The mathematical formulation of the rate of change in the concentration of the pollutant with respect to time t at various 3-D locations in the x, y and z directions is given in Eq. (1).

$$\frac{\partial w}{\partial t} = D\left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2}\right) \quad \dots \quad (1)$$

where, $t_0 < t \le t_g, x_0 < x \le x_h, \; y_0 < y \le y_i, \; z_0 < z \le z_j$ and the parameter w is the concentration of the pollutant in x, y, z directions, respectively, t denotes the time, x, y and z denotes directions, and D The diffusion coefficient is constant and the same for all directions.

B. Initial and Boundary Conditions for Mathematical Model

The mathematical model of Eq. (1) has a numerical and analytical solution. $w(x, y, z, t)$ that can be derived using C-N and ADM, respectively. To solve the C-N and ADM methods, initial and boundary conditions are required for space and time. The initial condition for time t is given in Eq. (2).

$$w(x, y, z, t_0) = \emptyset_0(x, y, z) \quad \dots \quad (2)$$

and boundary conditions for x, y and z directions are as follows in Eq. (3)

$$\left.\begin{aligned} w(x_0, y, z, t) &= \Psi_1(y, z, t) \\ w(x_r, y, z, t) &= \Psi_2(y, z, t) \\ w(x, y_0, z, t) &= \Psi_3(x, z, t) \\ w(x, y_s, z, t) &= \Psi_4(x, z, t) \\ w(x, y, z_0, t) &= \Psi_5(x, y, t) \\ w(x, y, z_p, t) &= \Psi_6(x, y, t) \end{aligned}\right\} \quad \dots \quad (3)$$

where, $\emptyset_0, \Psi_1, \Psi_2, \Psi_3, \Psi_4, \Psi_5$ *and* Ψ_6 are known functions.

C. Mathematical Method

The diffusion equation can be solved using various analytical and numerical methods. The C-N method is used to obtain a numerical solution, while the ADM is utilized in this research to provide the analytical solution.

i. Crank-Nicolson (C-N) Method [17]

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The C-N method is a finite difference method used to obtain the numerical solution of a mathematical diffusion model. The finite number of grid locations in the x, y and z directions of the 3-D regions where water pollution is estimated in a finite time interval is stated as follows; The grid points (x_a, y_b, z_c, t_d) are given as

$$x_a = x_0 : \delta_x : x_r, \quad a = 0,1,2, \ldots r$$
$$y_b = y_0 : \delta_y : y_s, \quad b = 0,1,2, \ldots s$$
$$z_c = z_0 : \delta_z : z_p, \quad c = 0,1,2, \ldots p \quad \ldots \quad (4)$$
$$t_d = t_0 : \delta_t : t_l, \quad d = 0,1,2, \ldots l$$

Where r, s, p and l are integers and δ_x, δ_y, and δ_z are grid spacing of all three directions, respectively, and δ_t is a time step size and denotes $w(x_a, y_b, z_c, t_d) = w(x, y, z, t)$ in the finite difference approximation.

$$\frac{\partial w}{\partial t} = \frac{w(x,y,z,t+1) - w(x,y,z,t)}{\delta_t}$$ Forward difference for time- space derivative (5)

$$\frac{\partial w}{\partial t} = \frac{w(x,y,z,t) - w(x,y,z,t-1)}{\delta_t}$$ Backward difference for time-space derivative (6)

$$\frac{\partial^2 w}{\partial x^2} = \frac{w(x+1,y,z,t) - 2w(x,y,z,t) + w(x-1,y,z,t)}{{\delta_x}^2}$$ The central difference for space derivative in x-direction (7)

$$\frac{\partial^2 w}{\partial y^2} = \frac{w(x,y+1,z,t) - 2w(x,y,z,t) + w(x,y-1,z,t)}{{\delta_y}^2}$$ The central difference for spatial derivative in y-direction (8)

$$\frac{\partial^2 w}{\partial z^2} = \frac{w(x,y,z+1,t) - 2w(x,y,z,t) + w(x,y,z-1,t)}{{\delta_z}^2}$$ The central difference for spatial derivative in z-direction (9)

Apply Eq. (5), (7) - (9) in Eq. (1),

$$\frac{w(x,y,z,t+1) - w(x,y,z,t)}{\delta_t} = D\left[\frac{w(x+1,y,z,t) - 2w(x,y,z,t) + w(x-1,y,z,t)}{{\delta_x}^2} + \frac{w(x,y+1,z,t) - 2w(x,y,z,t) + w(x,y-1,z,t)}{{\delta_y}^2} + \frac{w(x,y,z+1,t) - 2w(x,y,z,t) + w(x,y,z-1,t)}{{\delta_z}^2}\right] \quad (10)$$

Further, apply Eq. (6), (7) - (9) in Eq. (1),

$$\frac{w(x,y,z,t) - w(x,y,z,t-1)}{\delta_t} = D\left[\frac{w(x+1,y,z,t) - 2w(x,y,z,t) + w(x-1,y,z,t)}{{\delta_x}^2} + \frac{w(x,y+1,z,t) - 2w(x,y,z,t) + w(x,y-1,z,t)}{{\delta_y}^2} + \frac{w(x,y,z+1,t) - 2w(x,y,z,t) + w(x,y,z-1,t)}{{\delta_z}^2}\right] \quad (11)$$

Then, replace t by $t + 1$ in Eq. (11),

$$\frac{w(x,y,z,t+1) - w(x,y,z,t)}{\delta_t} = D\left[\frac{w(x+1,y,z,t+1) - 2w(x,y,z,t+1) + w(x-1,y,z,t+1)}{{\delta_x}^2} + \frac{w(x,y+1,z,t+\delta_t) - 2w(x,y,z,t+1) + w(x,y-1,z,t+1)}{{\delta_y}^2} + \frac{w(x,y,z+1,t+1) - 2w(x,y,z,t+1) + w(x,y,z-1,t+1)}{{\delta_z}^2}\right] \quad (12)$$

Now, add Eq. (10) & (12) and take the same grid spacing for all three directions that $\delta_x = \delta_y = \delta_z = \delta$.

$$w(x,y,z,t+1) - w(x,y,z,t) = \frac{D*\delta_t}{2\delta^2}[w(x+1,y,z,t) + w(x-1,y,z,t) + w(x,y+1,z,t) + w(x,y-1,z,t) + w(x,y,z+1,t) + w(x,y,z-1,t) - 6w(x,y,z,t) + w(x+1,y,z,t+1) + w(x-1,y,z,t+1) + w(x,y+1,z,t+1) + w(x,y-1,z,t+1) + w(x,y,z+1,t+1) + w(x,y,z-1,t+1) - 6w(x,y,z,t+1)] \quad (13)$$

Taking $\frac{D*\delta_t}{\delta^2} = \mu$ in Eq. (13) and simplifying that getting Eq. (14)

$$w(x,y,z,t+1) = \frac{(1-3\,\mu)}{(1+3\,\mu)}w(x,y,z,t) + \frac{\mu}{2(1+3\,\mu)}[w(x+1,y,z,t) + w(x-1,y,z,t) + w(x,y+1,z,t) + w(x,y-1,z,t) + w(x,y,z+1,t) + w(x,y,z-1,t) + w(x+1,y,z,t+1) + w(x-1,y,z,t+1) + w(x,y+1,z,t+1) + w(x,y-1,z,t+1) + w(x,y,z+1,t+1) + w(x,y,z-1,t+1)] \quad (14)$$

This Eq. (14) is the implicit formula for the C-N technique. To get the answer at the $t + 1$ level, it is necessary to finding the solution at some locations of the t-level and $t + 1$ levels. Therefore, this method requires the initial conditions shown in Eq. (2).

D. Adomian Decomposition Method (ADM) [15]

In ADM method, re-write Eq. (1) in the standard operator form as

$$L_t w = D\,(L_{xx}w + L_{yy}w + L_{zz}w) \quad \ldots \quad (15)$$

Were, $L_t = \frac{\partial}{\partial t}$, $L_{xx} = \frac{\partial^2}{\partial x^2}$, $L_{yy} = \frac{\partial^2}{\partial y^2}$, $L_{zz} = \frac{\partial^2}{\partial z^2}$.

Taking the inverse operator of the operator L_t exists and it defined as

$$L_t^{-1}(.) = \int_0^t (.)dt$$

Thus, applying the inverse operator L_t^{-1} to Eq. (15) yields

$$L_t^{-1}\,L_t w(x,y,z,t) = D\,(L_t^{-1}\,L_{xx}w + L_t^{-1}\,L_{yy}w + L_t^{-1}\,L_{zz}w)$$

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$$w(x,y,z,t) - w(x,y,z,0) = D\,(L_t^{-1}\,L_{xx}w + L_t^{-1}\,L_{yy}w + L_t^{-1}\,L_{zz}w)$$

$$w(x,y,z,t) = w(x,y,z,0) + D\,L_t^{-1}\,(L_{xx}w + L_{yy}w + L_{zz}w) \quad (16)$$

In ADM, represent the solution suppose that

$$w(x,y,z,t) = \sum_{n=0}^{\infty} w_n(x,y,z,t) \quad \dots \quad (17)$$

Substituting Eq. (17) into (16), get

$$\sum_{n=0}^{\infty} w_n(x,y,z,t) = w(x,y,z,0) + D\,L_t^{-1}\Big[L_{xx}\sum_{n=0}^{\infty} w_n(x,y,z,t) + L_{yy}\sum_{n=0}^{\infty} w_n(x,y,z,t) + L_{zz}\sum_{n=0}^{\infty} w_n(x,y,z,t)\Big]$$

$$w_0(x,y,z,t) + w_1(x,y,z,t) + \cdots = w(x,y,z,0) + D\,L_t^{-1}\Big[L_{xx}\sum_{n=0}^{\infty} w_n(x,y,z,t) + L_{yy}\sum_{n=0}^{\infty} w(x,y,z,t) + L_{zz}\sum_{n=0}^{\infty} w_n(x,y,z,t)\Big] \quad \dots \quad (18)$$

Now, comparing the Eq. (18) on both sides getting the recurrent relation in the form of as follows

$$w_0(x,y,z,t) = w(x,y,z,t_0) = w(x,y,z,0) = \emptyset_0(x,y,z) \quad \text{(From Eq. (2))}$$

and

$$w_{n+1}(x,y,z,t) = D\,L_t^{-1}\,(L_{xx}w_n(x,y,z,t) + L_{yy}w_n(x,y,z,t) + L_{zz}w_n(x,y,z,t)) \text{ for } n = 0,1,2,\dots$$

From which

$$\left.\begin{aligned} w_1(x,y,z,t) &= D\,L_t^{-1}\begin{pmatrix} L_{xx}w_0(x,y,z,t) \\ +\,L_{yy}w_0(x,y,z,t) \\ +L_{zz}w_0(x,y,z,t) \end{pmatrix} \\ w_2(x,y,z,t) &= D\,L_t^{-1}\begin{pmatrix} L_{xx}w_1(x,y,z,t) \\ +\,L_{yy}w_1(x,y,z,t) \\ +L_{zz}w_1(x,y,z,t) \end{pmatrix} \\ &\vdots \\ w_n(x,y,z,t) &= D\,L_t^{-1}\,(L_{xx}w_{n-1}(x,y,z,t) + L_{yy}w_{n-1}(x,y,z,t) + L_{zz}w_{n-1}(x,y,z,t)) \end{aligned}\right\} \quad \dots \quad (19)$$

Therefore, the estimation of the approximate solution $\emptyset_\gamma$ by using γ-term approximation. That is,

$$\emptyset_\gamma = \sum_{n=0}^{\gamma-1} w_n(x,y,z,t) \quad \dots \quad (20)$$

Therefore, Eq. (20) is the approximate solution of the 3-D diffusion mathematical model.

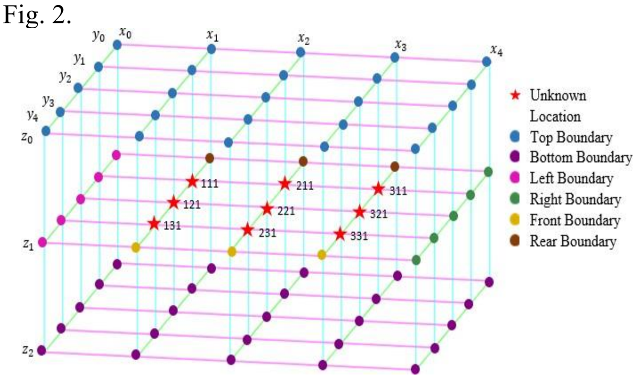
D. Water Pollution Estimation

The level of water pollution at a 3-D grid location is predicted by the C-N mathematical approach over time intervals, and their results are validated through comparison with the ADM approach. Equation (14) employs the C-N approach to estimate the concentration of pollutants in water at various locations over different time periods. It is a 2-level implicit technique, which uses the values of the surrounding locations in the x, y, and z directions of the previous one-time (t) level and the current time $(t+1)$ level to estimate the current time $(t+1)$ level water pollution at a particular location. This technique helps to understand pollution dispersion by simulating the spread of pollutants, such as an iodised salt-water solution, in a water body.

Eq. (20) depicts the concentration of pollutants in water at a specific location (x,y,z) and time t, based on a series solution obtained from the ADM. This formula indicates that the analytical solution is expressed as a sum of terms $w_0, w_1, w_2, \dots, w_{\gamma-1}$.Here, w_0 represents the initial condition, and Eq. (19) is utilized to determine the subsequent terms, $w_1, w_2, \dots, w_{\gamma-1}$. Therefore, this equation provides a method for computing the pollutant concentration over both time and space using a series expansion technique.

IV. EXPERIMENTED RESULTS AND DISCUSSION

According to studies, the majority of previous research has focused on 1-D or 2-D diffusion mathematical models, which have been resolved using a variety of analytical and numerical methods. The proposed research extends the diffusion model into a 3D space to estimate water contamination. Additionally, the researchers used a 3-D dummy cuboid water tank with measurements of $4.25 \times 4.25 \times 2.25$ feet to demonstrate the 3-D water pollution diffusion model. To establish the 3-D grid location in a cuboid tank, a grid structure with a grid spacing of one foot is used in all directions. Each 3-D grid location represents approximately one cubic foot of water volume area, so that the total volume of tank is covered within 75 grid locations. As a result, it is assumed that the amount of pollutant present at a particular location will be consider as the average pollution of one cubic foot water volume area. Thus, this grid setup enables the study of pollution spread in all three directions within the tank. Here, 960 Liters of water are used as a pollutant, and 40 Liters of an iodized salt-water solution are used as a pollutant. The contaminated water is measured by a Total Dissolved Solids (TDS) meter in PPM every 20 minutes. The various types of 3-D grid locations, categorised by their positions within cuboid water tanks, are illustrated in Fig. 2.



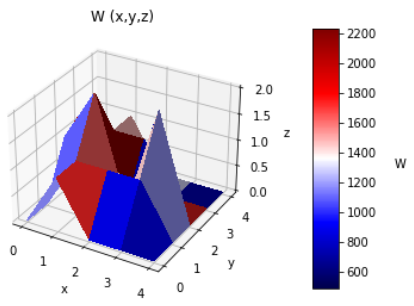
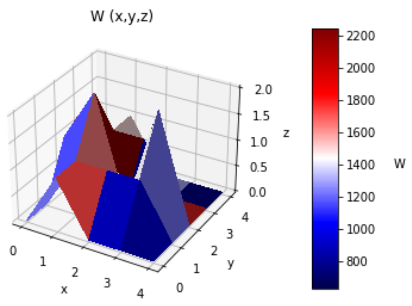
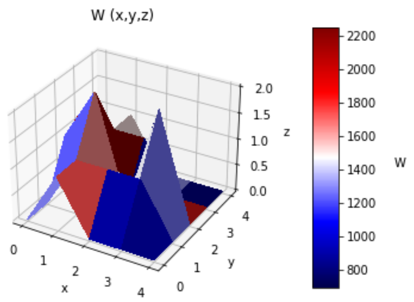
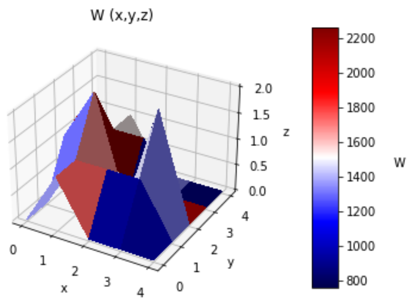
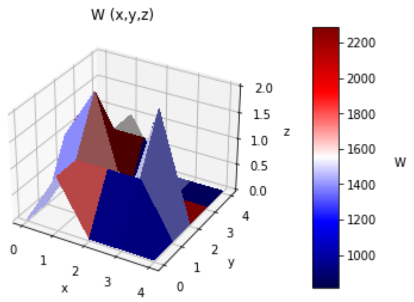
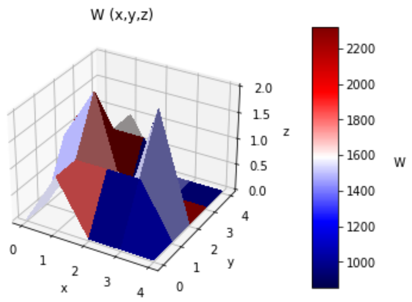
[Fig.2: 3-D Grid Locations]

Here, the range of 3-D grid positions in the x, y and z space directions is set as $r = 4, s = 4, p = 2$ and $l = 5$ respectively in Eq. (4). Therefore, the time interval would be $t_0 \le t \le t_5$ and the space intervals may be defined as $x_0 \le x \le x_4, y_0 \le y \le y_4$ and $z_0 \le z \le z_2$. Moreover, taking into consideration $x_0 = y_0 = z_0 = t_0 = 0, x_4 = y_4 = 4, z_2 = 2$ and $t_5 = 5$The range of various 3-D grid locations can be classified as shown in Table I.

Table I: Types of 3-D grid locations

Types	3-D Grid Locations
Left Boundary	$x = 0\,, 0\ \le\ y\ \le\ 4, 0 < z < 2$
Right Boundary	$x = 4\,, 0\ \le\ y\ \le\ 4, 0 < z < 2$
Rear Boundary	$0 <\ x <\ 4, y = 0, 0 < z < 2$
Front Boundary	$0 <\ x <\ 4, y = 4, 0 < z < 2$
Top Boundary	$0\ \le\ x\ \le\ 4, 0\ \le\ y\ \le 4, z = 0$
Bottom Boundary	$0\ \le\ x\ \le\ 4, 0\ \le\ y\ \le 4, z = 2$
Unknown	$(x_1 = 1) <\ x < (x_3 = 3),$ $(y_1 = 1)\ \le\ y\ \le\ (y_3 = 3),$ $z = (z_1 = 1)$

The mathematical model is simulated in MATLAB with spatial increments of 1 foot in the $x, y, and\ z$ directions and a time step of 1 unit, which corresponds to 20 minutes. The graphical representation of the Exp. data at different time intervals, as *shown* in Fig. 3.

Time	$t = 0$	$t = 1$
		
Range	$495 - 2680\ PPM$	$635 - 2720\ PPM$
Time	$t = 2$	$t = 3$
		
Range	$695 - 2780\ PPM$	$763 - 2840\ PPM$
Time	$t = 4$	$t = 5$
		
Range	$817 - 2920\ PPM$	$858 - 3000\ PPM$

[Fig.3: Water Pollution at 3-D grid Locations of Exp. Data]

Figure 3 illustrates that the water pollution levels at each 3-D grid point increase over time. Initially, at time t=0, the pollution levels range *from* $495 - 2680\ PPM$. After 120 minutes, the range has increased to $858 - 3000\ PPM$.

Now, using the Multi-Poly Regression model on the observed Exp. Based on the data, the necessary initial and boundary conditions for space and time are derived. It can be stated as in Eq. (21) – (27), with their corresponding Mean Absolute Error (MAE) and Standard Deviation of Mean Absolute Error (SD_{MAE}).

Initial and Boundary Conditions	MAE	SD_{MAE}	
Initial Condition for time $t = (t_0 = 0)$ $w(x,y,z,0) = 903.55*z - 71.87*z^2 - 73.67*y - 78.60*y*z + 24.22*y*z^2 + 6.24*y^2 + 5.34*y^2*z - 2.86*y^2*z^2 - 325.08*x - 117.94*x*z + 49.86*x*z^2 + 44.60*x*y + 5.69*x*y*z - 3.57*x*y*z^2 - 3.98*x*y^2 + 0.45*x*y^2*z + 213.34*x^2 - 21.77*x^2*z + 2.06*x^2*z^2 - 19.12*x^2*y + 1.87*x^2*y*z + 0.23*x^2*y^2 - 73.13*x^3 + 0.05*x^3*z + 2.69*x^3*y + 1159.17 + 8.26*x^4;$	0.0014	0.0011	(21)
Left Boundary $w(0,y,z,t) = 50.15*t + 1989.34*z + 4.43*z*t^2 + 2.22*y*t + 0.04*y*t^2 - 128.40*y*z + 9.22*y^2 - 1.04*y^2*t - 0.093*y^3;$	0.0012	0.00076	(22)
Right Boundary $w(4,y,z,t) = -0.12*y*t^2 - 1.22*y^2*t + 958 + 106.32*t + 4.04*t^2 - 47.04*y + 11.88*y*t - 1.44*y^2 - 1.47e - 14*y^3;$	0.0011	0.00085	(23)
Rear Boundary $w(x,0,z,t) = 42.23*t + 1812.02*z + 5.076*z*t^2 - 69.87*x*t - 0.43*x*t^2 - 91.36*x^2 + 21.83*x^2*t + 9.56*x^3;$	0.0012	0.0008	(24)
Front Boundary $w(x,4,z,t) = 40.08*t + 4.8*t^2 + 1504.56*z - 0.27*x*t^2 - 65.76*x*t + 22.35*x^2*t - 76.76*x^2 + 5.88*x^3;$	0.0019	0.0012	(25)
Top Boundary $w(x,y,0,t) = 55.20*t + 4.54*t^2 - 72.73*y + 1.76*y*t + 0.048*y*t^2 + 5.86*y^2 - 0.99*y^2*t - 0.007*y^2*t^2 - 325.096*x - 74.92*x*t - 0.17*x*t^2 + 42.35*x*y + 2.14*x*y*t - 0.0007*x*y*t^2 - 3.51*x*y^2 - 0.046*x*y^2*t + 214.80*x^2 + 22.88*x^2*t - 0.011*x^2*t^2 - 18.21*x^2*y - 0.022*x^2*y*t + 0.13*x^2*y^2 - 74.013*x^3 - 0.087*x^3*t + 2.59*x^3*y + 1159.17 + 8.39*x^4;$	0.0015	0.0012	(26)
Bottom Boundary $w(x,y,2,t) = 2675.5 + 42.94*t + 4.38*t^2 - 130.74*y + 3.02*y*t + 0.002*y*t^2 + 0.025*y^2*t^2 + 4.8*y^2 - 1.18*y^2*t - 353.56*x - 75.64*x*t - 0.34*x*t^2 - 0.023*x*y*t^2 + 39.9*x*y + 2.38*x*y*t - 0.043*x*y^2*t - 2.58*x*y^2 + 0.059*x^2*t^2 + 176.82*x^2 + 23.54*x^2*t - 0.029*x^2*y*t - 15.7*x^2*y + 0.17*x^2*y^2 - 0.27*x^3*t - 73.82*x^3 + 2.82*x^3*y + 8.43*x^4;$	0.0012	0.0009	(27)

In this experiment, it is essential to decide the value of the diffusion rate of the iodized salt-water solution into the water tank volume for the proposed mathematical model. It is based on Fick's first law phenomenon, described in Eq. (28) [18].

$$D = -D_v \frac{dC}{df} \quad \dots \quad (28)$$

Where, D is the diffusion rate, D_v is the diffusivity rate of iodized salt-water solution $\left(\frac{\text{cm}^2}{\text{s}}\right)$ and $\frac{dC}{df}$ is the average concentration gradient. The negative sign in Eq. (28) indicates that the flow moves from areas of high concentration to areas of low concentration.

The diffusivity rate of the iodised salt-water solution is obtained from Eq. (29).

$$D_v = \frac{4\,Vx_c}{\pi d_c^2 NMC_M}\frac{dk}{dt} \quad \dots \quad (29)$$

Where, V is the volume of water in diffusion vessel (Liter (L) or cm^3), x_c is the capillaries' length (cm), d_c is the diameter of capillaries (cm), N is the number of capillaries, M is the molar concentration of iodized salt solution (mol/L), C_M is the slope of conductivity change per unit molar concentration change (μS*L/mol) and $\frac{dk}{dt}$ is the slope of conductivity change per unit time (μS/s).

In this experiment, $V = 2500\ cm^3, x_c = 0.4\ cm, d_c = 0.1\ cm$ and $N = 50$ in this experiment. The iodized salt's molar concentration is

$$M = \frac{w_s}{M_w} \times \frac{1\,(L)}{V_s} \quad \dots \quad (30)$$

Where, w_s is the weight of solute (gm), M_w is the molecular weight of solute (gm/mol) and V_s is the volume of solvent (L).

Here, w_s= 2500 gm iodized salt

$M_w = Na^+ + Cl^- + I^- + Mg^+$(impurity)

= 23+35.5+127+24 = 209.5 gm/mol

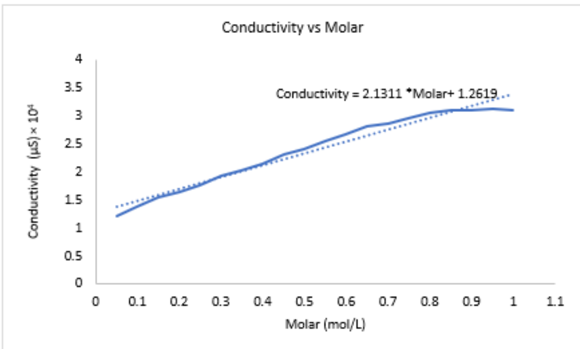
V_s= 40 L

Applying these values into Eq. (30),

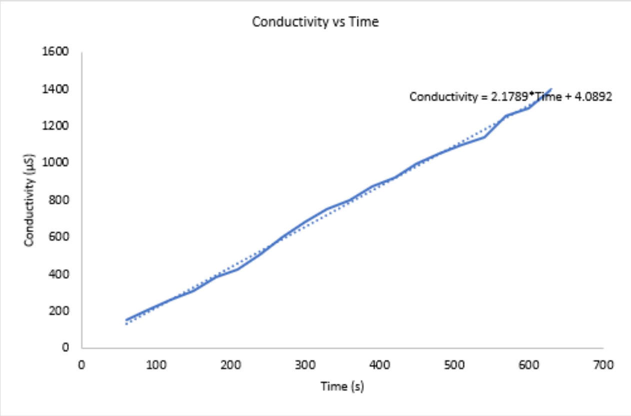
$$M = \frac{2500\ \text{gm}}{209.5\frac{\text{gm}}{\text{mol}}} \times \frac{1\ \text{L}}{40\ \text{L}}$$

$$M = 0.29\ \text{mol/L}$$

The graphs below, in Figs. 4 and 5, show the slopes of conductivity changes per unit of molar concentration change and conductivity changes per unit of time obtained.



[Fig.4: Conductivity Vs. Molar]



[Fig.5: Conductivity Vs. Time]

Fig. 4 and 5 demonstrate that the molar coefficient reflects the slope of conductivity variation for each unit of molar concentration, with a value of $C_M = 2.1311 \times 10^4\ (\mu S * L)/mol$, while the time coefficient indicates the slope of conductivity change relative to time, represented by $dk/dt = 2.1789\ \mu S/s$. Now, substitute all the values in Eq. (29), obtain that

$$D_v = \frac{4 \times 2500\ \mathrm{cm}^3 \times 0.4\ cm \times 2.1789\ \mu\frac{\mathrm{S}}{\mathrm{s}}}{3.14 \times (0.1)^2 \mathrm{cm}^2 \times 50 \times 0.29\left(\frac{mol}{L}\right) \times 2.1311 \times 10^4 \frac{\mu\mathrm{S}*\mathrm{L}}{\mathrm{mol}}}$$

$$D_v = \frac{8715.6}{0.97028 \times 10^4} \frac{\mathrm{cm}^2}{s}$$

$$D_v = 8982.56 \times 10^{-4} \frac{\mathrm{cm}^2}{s}$$

In the experiment, the z-axis consists of three distinct layers within the range. $0 \le z \le 2$, Namely the 1st layer (Top), 2nd layer (Middle), and 3rd layer (Bottom) of the cuboid tank. Now, the average concentration gradient for the 1^{st} and 2^{nd} layers is

$$\left(\frac{dC}{df}\right)_1 = \frac{c_2 - c_1}{f_2 - f_1} \quad \dots \quad (31)$$

the 2^{nd} and 3^{rd} layers are

$$\left(\frac{dC}{df}\right)_2 = \frac{c_3 - c_2}{f_3 - f_2} \quad \dots \quad (32)$$

where, c_1 is the average of the first layer ($z = 0$) pollution $= 1387.219 \frac{PPM}{cm^3}$, c_2 is the average of the second layer ($z = 1$) pollution $= 1381.575 \frac{PPM}{cm^3}$, c_3 is the average of the third layer ($z = 3$) pollution $= 1372.26 \frac{PPM}{cm^3}$. f_1, f_2 and f_3 are the distance (cm) between the layers. Here, $f_1 = 0$ feet $= 0$ cm, $f_2 = 1$ feet $= 30.48$ cm, $f_3 = 2$ feet $= 60.96$ cm. After all these values are replaced in Eq. (31) and (32), it is obtained that $\left(\frac{dC}{df}\right)_1 = -0.185 \frac{PPM}{cm^4}$ and $\left(\frac{dC}{df}\right)_2 = -0.3056\ PPM/cm^4$. Consequently, the concentration gradient's average value is $\frac{dC}{df} = -0.24 \frac{\mathrm{PPM}}{\mathrm{cm}^4}$. Now, the diffusion coefficient of the iodised salt solution is obtained by substituting each of the necessary values into Eq. (28), which yields Eq. (33).

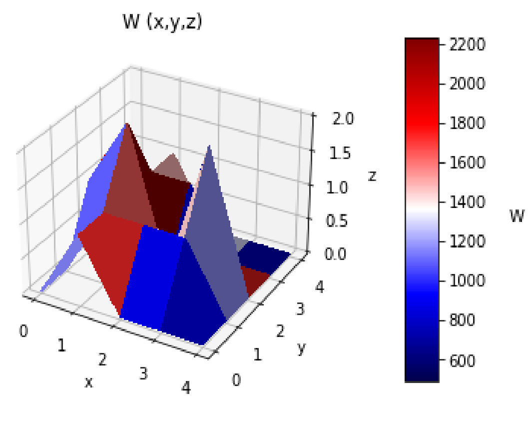
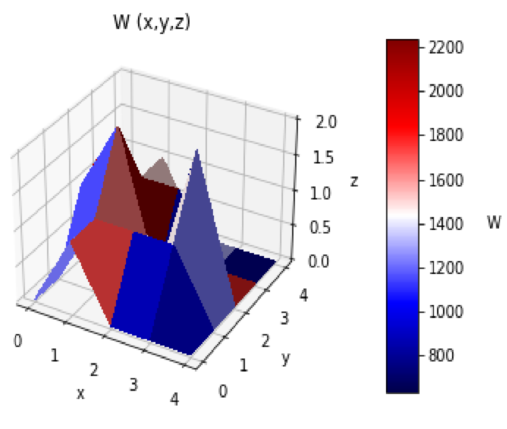
$$D = -8982.56 \times 10^{-4} \frac{\mathrm{cm}^2}{s} \times -0.24 \frac{\mathrm{PPM}}{\mathrm{cm}^4}$$

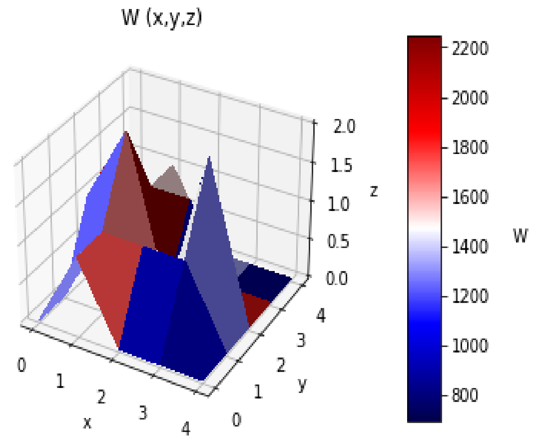
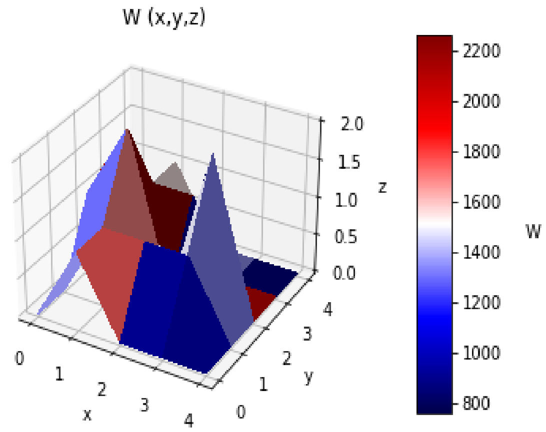
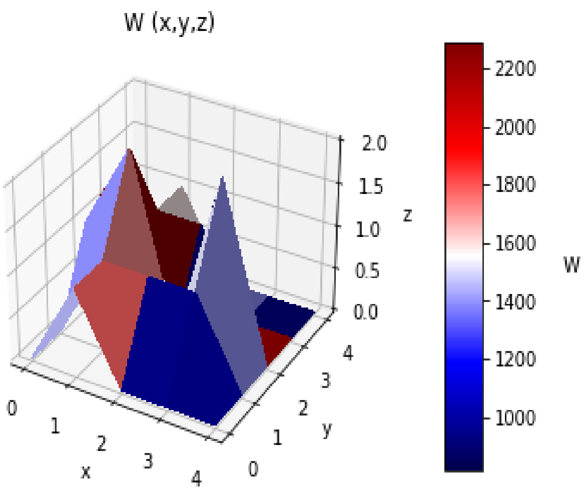
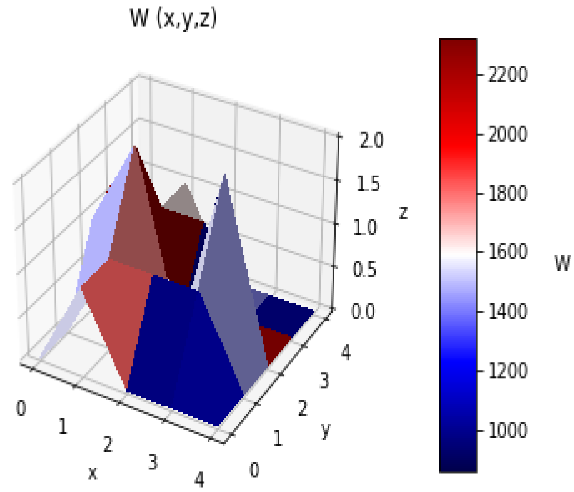
$$D = 2155.8 \times 10^{-4} \frac{\mathrm{PPM}}{\mathrm{cm}^2\ s}$$

$$D = 0.21558 \frac{\mathrm{PPM}}{\mathrm{cm}^2\ s} \quad (33)$$

The suggested mathematical model is implemented in MATLAB, taking into account the following considerations. $\delta_x = \delta_y = \delta_z = 1\ foot, \delta_t = 1$ unit (20 minutes), and a diffusion coefficient $D = 0.21558\ PPM/(cm^2\ s)$ Which is assumed to be uniform in the $x, y, and\ z$ directions.

To assess water pollution levels across every point in a 3-D grid over a period of time, apply Eq. (21) – (27) to solve Eq. (1) numerically via the C-N method. It is graphically plotted in Fig. 6.

Time	$t = 0$	$t = 1$
		
Range	495.52 – 2678.80 *PPM*	635.39 – 2722.82 *PPM*
Time	$t = 2$	$t = 3$

<table>
<tr><td></td><td>
</td><td>
</td></tr>
<tr><td>Range</td><td>696.07 − 2778.91 PPM</td><td>763.88 − 2843.78 PPM</td></tr>
<tr><td>Time</td><td>t = 4</td><td>t = 5</td></tr>
<tr><td></td><td>
</td><td>
</td></tr>
<tr><td>Range</td><td>817.91 − 2917.41 PPM</td><td>858.61 − 2999.82 PPM</td></tr>
</table>

[Fig.6: Water Pollution at 3-D Grid Locations by C-N]

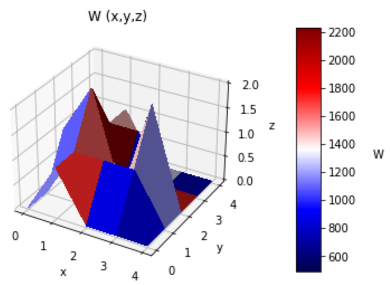
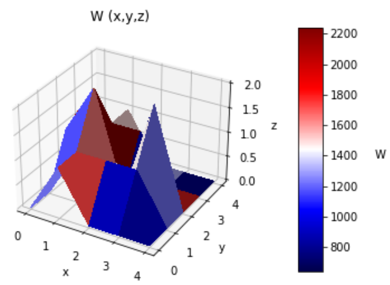
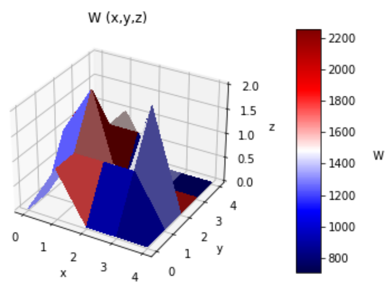
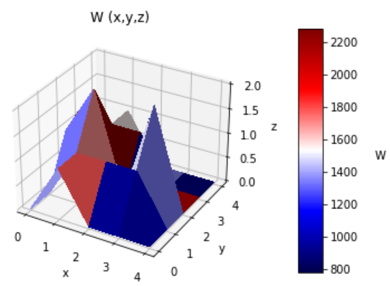
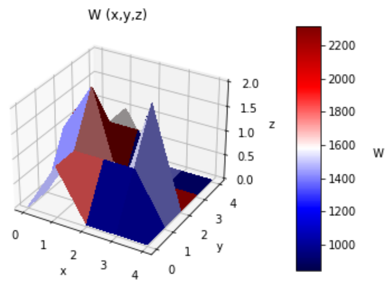
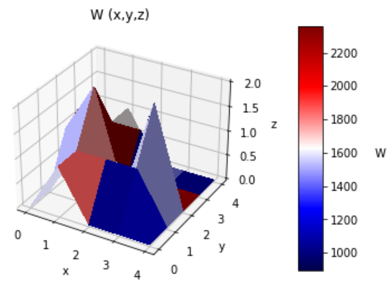
Fig. 6 illustrates that the concentration of pollutant iodised salt-water solution in water tanks at various 3-D grid locations progressively rises over time. The resultant water pollution level in the C-N technique ranges from $495.52 - 2678.80\ PPM$ at the beginning time ($t = 0$) and increases to $858.61 - 2999.82\ PPM$ at time $t = 5$ (120 minutes). There has been a significant increase in water contamination, which is expected to continue rising until it reaches its saturation point.

However, the C-N method gives a numerical solution for the 3-D diffusion model for water pollution, accurately reflecting the phenomena that occurred in real-time during the experiment. Still, another mathematical solution technique should be used to validate the results. Therefore, to obtain the solution of the proposed diffusion model for predicting the amount of water pollution at the exact 3-D location over the same time duration, ADM has been employed as an analytical solution approach.

The analytical solution of Eq. (1), obtained by applying the ADM and using the initial condition given by Eq. (21) at a time ($t = 0$) is expressed in Eq. (34).

$$w(x,y,z,t) = 96.91 * D^2 * t^2 + D * t * (103.8 * x^2 + 9.02 * x * y + 1.207 * x * z - 347 * x - 5.255 * y^2 + 3.736 * y * z + 10.19 * y - 1.586 * z^2 - 32.87 * z + 295.4) + 8.264 * x^4 + 2.692 * x^3 * y + 0.05 * x^3 * z - 73.13 * x^3 + 0.2296 * x^2 * y^2 + 1.868 * x^2 * y * z - 19.112 * x^2 * y + 2.064 * x^2 * z^2 - 21.77 * x^2 * z + 213.3 * x^2 + 0.4536 * x * y^2 * z - 3.979 * x * y^2 - 3.565 * x * y * z^2 + 5.689 * x * y * z + 44.6 * x * y + 49.86 * x * z^2 - 117.9 * x * z - 325.1 * x - 2.857 * y^2 * z^2 + 5.336 * y^2 * z + 6.238 * y^2 + 24.22 * y * z^2 - 78.6 * y * z - 73.67 * y - 71.87 * z^2 + 903.5 * z + 1159; \quad (34)$$

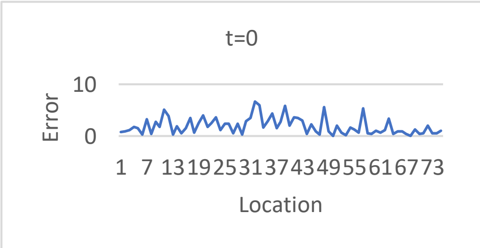
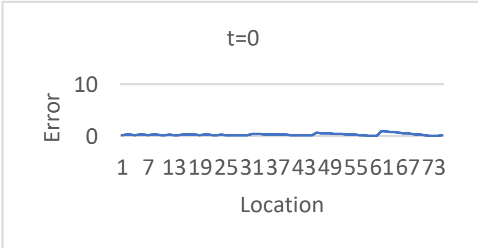
By substituting the values of $x, y, z, and\ t$ in an alternating manner, Eq. (34) is solved, which indicates the water pollution levels at every location within the 3-D grid. Fig. 7 provides a 4-D graphical depiction of the results from the ADM concerning water pollution levels for each 3-D grid location throughout the given time interval.

Time	$t = 0$	$t = 1$
		
Range	$495.50 - 2678.52\ PPM$	$641.86 - 2730.56\ PPM$
Time	$t = 2$	$t = 3$
		
Range	$709.16 - 2791.42\ PPM$	$785.29 - 2861.10\ PPM$
Time	$t = 4$	$t = 5$
		
Range	$848.15 - 2939.60\ PPM$	$897.52 - 3026.91\ PPM$

[Fig.7: Water Pollution at 3-D Grid Locations by ADM]

Fig. 7 demonstrates that, following 120 minutes of testing ($t = 5$), the water pollution level at 3-D grid locations is in the range of $897.52 - 3026.91\ PPM$, having started ($t = 0$) in the range of $495.50 - 2678.52\ PPM$. Additionally, it has been observed that water contamination in various areas increases monotonically with time.

Now, two different approaches, C-N and ADM, have provided numerical and analytical solutions to Eq. (1), respectively. Comparing the C-N results with Experimental Data. Data and ADM results can validate the accuracy of predicting water pollution levels at various 3-D grid locations. The comparison is based on error estimation, calculated as the absolute difference between the water pollution levels at each 3-D grid location over time. The estimated error is displayed graphically in Fig. 8.

Time	$C - N$ *vs Exp.* Data	$C - N$ *vs ADM*
$t = 0$		

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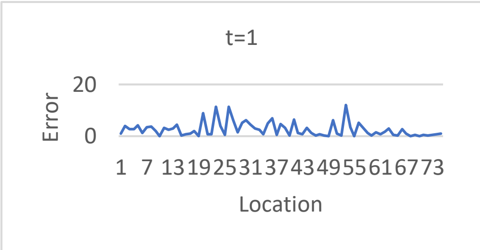
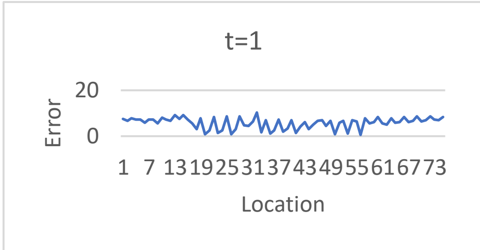
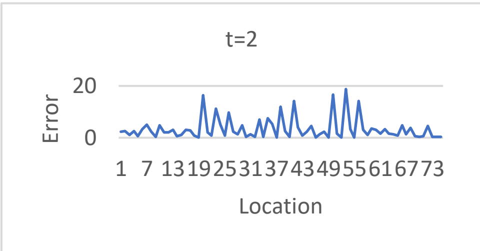
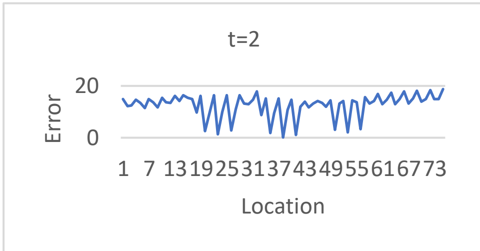
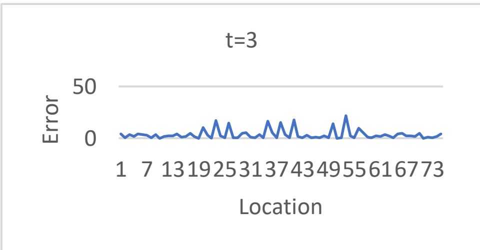
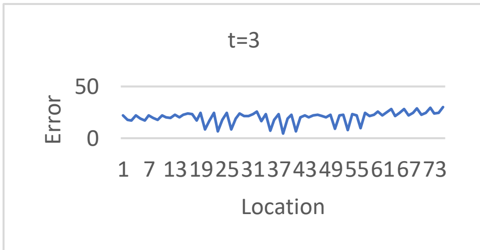
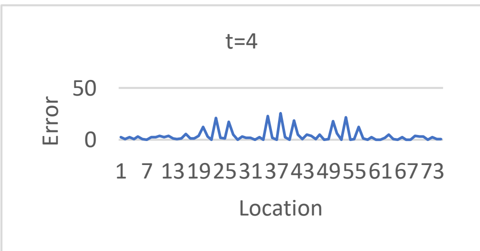
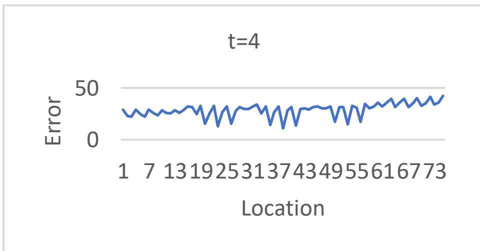
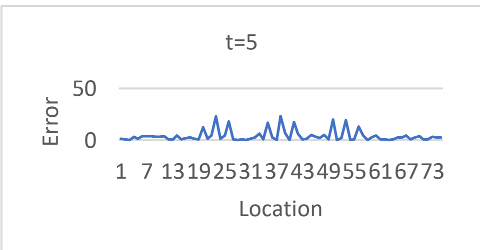
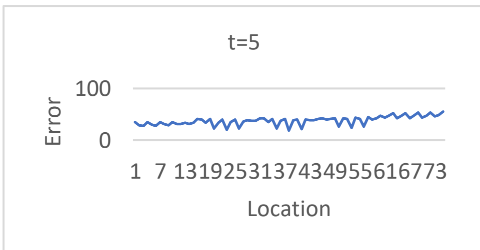
Range	$0.015 - 6.66\ PPM$	$0.019 - 0.94\ PPM$
$t = 1$		
Range	$0.041 - 12.06\ PPM$	$0.59 - 10.32\ PPM$
$t = 2$		
Range	$0.107 - 18.76\ PPM$	$0.13 - 18.77\ PPM$
$t = 3$		
Range	$0.029 - 21.78\ PPM$	$4.51 - 30.11\ PPM$
$t = 4$		
Range	$0.012 - 25.55\ PPM$	$10.99 - 42.31\ PPM$
$t = 5$		
Range	$0.18 - 23.37\ PPM$	$18.72 - 55.37\ PPM$

[Fig.8: Comparative Analysis between C-N Vs. Exp. Data and ADM Results]

Fig. 8 illustrates that the comparative analysis between C-N Vs. Exp. Data is experiencing some minor errors in predicting water contamination at 3-D grid locations at every time interval. It is noticed that the estimated error of C-N Vs. Exp. data are $\leq 25.55\ PPM$. It does not have a significant impact on the water pollution level in terms of PPM, as a change of up to 60 PPM is considered negligible. In comparison, changes above 60 PPM represent a significant increase in water pollution [9] in C-N Vs. At the initial stage, there is an insignificant error at most grid locations. It is also observed that the error occurs between the ranges from $0.019\ PPM\ to\ 55.37\ PPM$ in C-N Vs. ADM.

Also, the analysis of the comparative study between all 75 locations × Six times during the whole duration, it has been observed that the C–N methods error against the ADM method and the Experiment. Data are visually shown in Fig. 9 for both the PPM difference (error) ≤ 60 and > 60.

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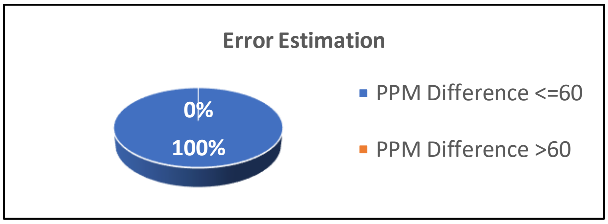
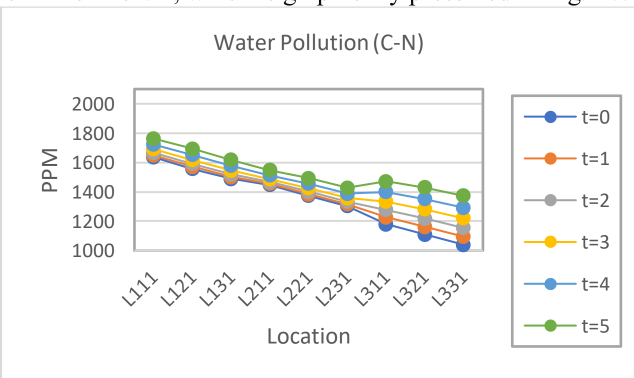


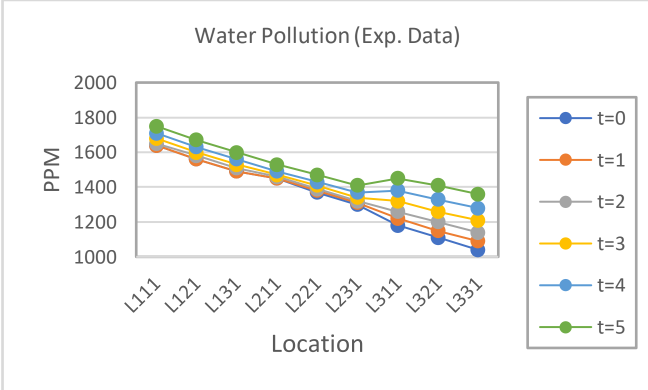
[Fig.9: Error Estimation of C-N Vs. Exp. Data and ADM]

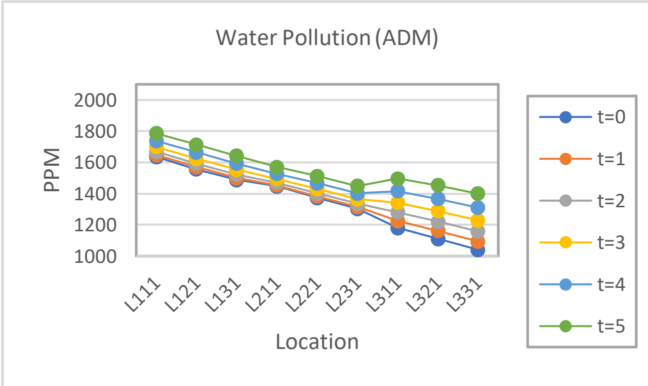
In the comparison between the two C-Ns and the experiment. Data and C-N Vs. ADM, Fig. 9 indicates that 100% of the errors fall below 60 PPM, which does not impact the level of water pollution.

Consequently, it can be concluded that the outcomes of the C-N method align with the analytical solution derived from the ADM, Exp. data, and the applied boundary conditions. It demonstrates that the numerical results are validated with both the Exp: data and the analytical ADM results. Therefore, the C-N approach can be relied upon to predict the level of water contamination over time.

There are various kinds of 3-D grid locations, as stated in Table I. The water pollution level at the top, bottom, left, right, rear, and front boundary locations is estimated at each time interval using the boundary conditions provided in Eqs. (22)–(27), whereas the C-N approach is used to calculate the water pollution level at the nine unknown locations. These nine locations can be classified as L_{xyz} : L_{111}, L_{121}, L_{131}, L_{211}, L_{221}, L_{231}, L_{311}, L_{321}, L_{331}. Here, it is necessary to compare the water pollution level calculated by the C-N approach with the experimental results (Exp.). data and the analytical results obtained through the ADM technique at each time interval, which is graphically presented in Fig. 10.



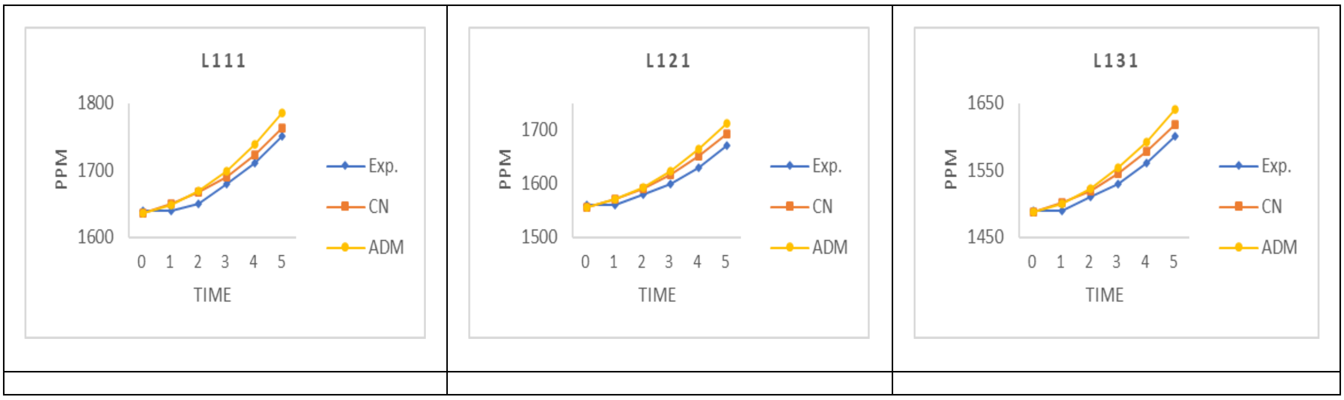




[Fig. 10: C-N, Experimented Data and ADM Result at Nine Unknown Locations]

Fig. 10 demonstrates that, in all the C-N, Exp. Using data and ADM techniques, the level of water pollution at these nine unknown locations has progressively increased over time. Furthermore, at every location, the results generated by the C-N approach match those of Exp. Data and ADM.

Furthermore, each location-wise progression of the level of water pollution over time, as measured by the C-N, Exp. Data and ADM techniques are displayed graphically in Fig. 11. It is observed that the resulting graphs are similar in all cases of unknown locations concerning time, leading to negligible errors in the estimation of the water pollution level.



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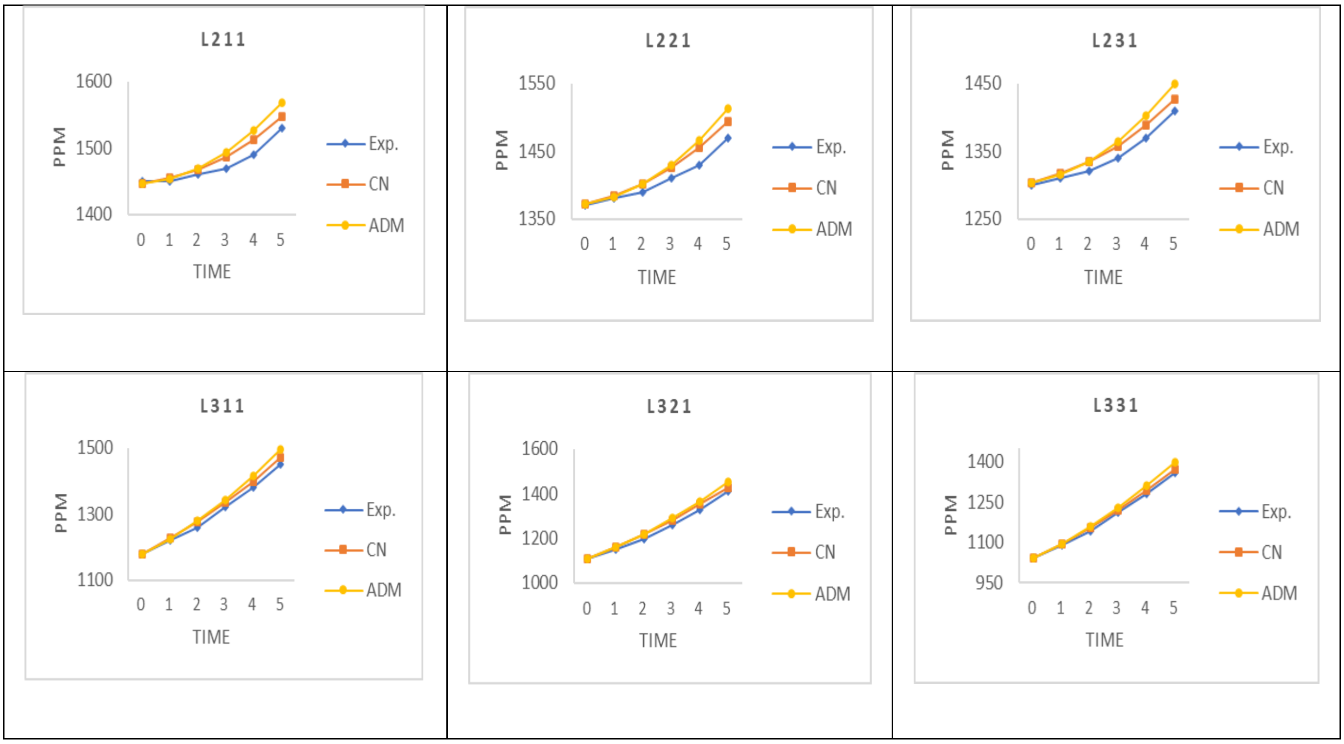

[Fig.11: Water Pollution Level at Unknown Location]

V. CONCLUSION

In this research paper, the water pollution concentration is predicted by using numerical computation. The 3-D mathematical model has been successfully solved using the C-N technique based on simulation data. After evaluating the error with Exp. data and ADM, this method proves to be effective for solving 3-D mathematical models of water pollution. It accurately validated the concentration of water pollution by Exp. data and ADM. Therefore, the water pollution problem can be effectively addressed by utilising the C-N and ADM techniques. This work presents reliable mathematical methods for estimating pollutant concentrations in three-dimensional regions, thereby enhancing our understanding of the dynamics of water contamination.

DECLARATION STATEMENT

I must verify the accuracy of the following information as the article's author.

- **Conflicts of Interest/ Competing Interests:** Based on my understanding, this article has no conflicts of interest.
- **Funding Support:** This article has not been funded by any organizations or agencies. This independence ensures that the research is conducted with objectivity and without any external influence.
- **Ethical Approval and Consent to Participate:** The content of this article does not necessitate ethical approval or consent to participate with supporting documentation.
- **Data Access Statement and Material Availability:** The data that support the findings of this study are available on request from the corresponding author, [*Mukesh Patel, mukesh.mt@gmail.com*]. The data are not publicly available due to [restrictions, e.g. their containing information that could compromise the privacy of research participants]
- **Author's Contributions:** Each author has individually contributed to the article. **Tarjani Naik:** Conceptualization, Methodology / Study design, Validation, Formal analysis, Resources, Investigation, Data curation, Writing – original draft, Writing – review and editing, Visualization. **Mukesh Patel:** Conceptualisation, Validation, Formal analysis, Writing – original draft, Supervision. **Rachna Patel:** Software, Formal analysis, Resources, Data curation.

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