

A Numerical and Analytical Framework for Estimating Water Pollution in A 3-D Aquatic Region Using Diffusion Model with Du Fort Frankel and Adomian Decomposition Methods

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Abstract: Water pollution is an important environmental issue that affects human health, aquatic habitats, and the sustainability of natural resources. Reliable mathematical models that can forecast the behaviour of pollutants in three-dimension (3-D) water systems are needed to address this issue. In this study, a 3-D diffusion model is used to determine the periodic and location-based fluctuation of the pollutant concentration in water. Investigating the slow increase in pollution levels in a 3-D area and evaluating the precision of analytical and numerical approaches to diffusion-based pollution problems are the objectives of this work. Two approaches are used to accomplish this: the Adomian Decomposition Method (ADM), which is an analytical approach, and the Du Fort Frankel (DF) scheme, which is a numerical approach. Initial and boundary conditions required for the modelling are provided by experimented data (Exp. data) from a 3-D cuboid tank filled with water and introduced with an iodized salt water solution as the pollutant. Direct monitoring of pollution dispersion across time and space is made possible by this configuration, producing useful data for confirming the mathematical models. The results of the experiment verify that the levels of pollutants rise with time at each location in the 3-D region. When comparing the outcomes of the DF approach with Exp. data and ADM, an insignificant difference, measured in parts per million (PPM), is observed, demonstrating the reliability and strength of the suggested model. This study is important because it combines mathematical models and realistic observations to examine pollution of water in 3-D. The results show that the model is accurate and applicable to both controlled experiments and larger-scale water systems. Additionally, this work advances the mathematical solutions for diffusion equations and offers useful information for sustainable resource use, pollution control, and water quality evaluation.

Keywords Water pollution · 3-D Diffusion equation · Du Fort Frankel method · Adomian Decomposition method

Mathematics Subject Classification 35K57 · 65N06

I. Introduction

One of the essential components of the earth is water. Approximately two-thirds of the surface of the earth is covered with it. Most of the world's population, especially humans, rely on freshwater for survival [21]. People today look for water that is both sufficient and of high quality [1, 2]. Residential and industrial water contamination caused by human activities is a significant concern in a lot of countries [4]. An estimated 25 million people each year pass away due to the severe effects of water contamination. As a result, the water quality issue is grabbing massive attention across the world [3]. Water pollution can be categorized in multiple ways, arising from changes in water's physical, chemical, and biological characteristics that harm living organisms. Mainly caused by human actions, this pollution negatively affects both human health and the quality of the environment's water [1, 22]. Two methods, numerical and analytical, can address water pollution issues. Various numerical and analytical techniques are available for solving mathematical equations related to water pollution problems.

This research employs a 3-D diffusion mathematical model to predict water pollution levels over a specified time with assuming a constant diffusion rate. The model considers water as the pollute and an iodized salt-water solution as the pollutant. A 3-D cuboid is created with uniformly spaced grid points in all directions, and experimental data on water pollution, measured in parts per million (PPM), is gathered from each grid point at regular time intervals. The initial and boundary conditions for the mathematical model are derived from the collected data. Two mathematical methods, namely the DF (DF) numerical method and the Adomian Decomposition analytical method, are utilized to estimate water pollution levels. A comparative analysis between DF Vs. ADM and Exp. data is conducted to evaluate their accuracy and determine any potential errors.

Related Work

Through the use of mathematical models of differential equations, **A.K. Misra, J.B. Shukla, and Peeyush Chandra** [6] examined the simultaneous impacts of saturation and water pollution on the concentration of the dissolved oxygen (DO) in a body of water. The transportation of water pollution concentration was predicted by **Zainab Yahya, Hanani Johari, and Nursalasawati Rusli** [1] using 1-D advection-diffusion model and resolved by the Finite Difference Method (FTCS techniques and an Implicit Crank Nicolson techniques). The second-order Lax-Wendorff method and Finite Time Central Space (FTCS) were used by **Nigar Sultana and Laek Sazzad Andallah** [7] to solve the 1-D advection-diffusion equation for determining the

concentration of water pollution in rivers as well as the pollutant in rivers at different times and locations. The 1-D advection-diffusion model was derived by **Abbas Parsaie, Amir Hamzeh Haghiabi** [12], **Safia Meddah, Omar Hireche, Mohamed Hadjel, and Abdelkader Saidane** [13]. This model was utilized in [12] to simulate the spread of pollution in rivers using the Finite Volume Method and Artificial Neural Network (ANN) and to estimate the longitudinal dispersion coefficient. The maximum concentration for a certain length of time and the estimation of the longitudinal dispersion of pollutants were determined in [13] using the Transmission Line Matrix Method. A research work was enlarged by adding some parameters to the 1-D Advection diffusion model by **Delong Wan, Huiping Zeng** [8], **Nonparent Pochai, J. J. H. Miller, L. J. Crane, and Suwon Tangmanee**, [9], **Tsegaye Simon, Purnachandra Rao Koya** [10], **R. V. Waghmare and S. B. Kiwne** [11]. The Pollution Index Method was employed in [8] to forecast the water quality using several parameters. This model was used in [9] to assess the expense of purifying water and calculate the concentration of pollutants using the finite element method. The dynamics of river pollution were examined in [10], and the numerical solution was found utilizing the Splitting Method, the Crank-Nicolson Method, and the Runge-Kutta Method. In this case, the diffusion and reaction terms were separated using the splitting approach, and the numerical solution was found using the Crank-Nicolson and Runge-Kutta methods. The analytical method was employed in [11] to determine the system's solution. **C. A. Poffal, J. R. Zabadal, and S. B. Leite** [5] expanded on a study utilizing a 2-dimensional Advection-Diffusion model and addressed the dispersion of substances and microorganisms in rivers and lakes through the application of a new analytical technique (iterative method).

II. Proposed Methodology

The proposed mathematical approach addresses the problem of water pollution which is described in Fig. 1.

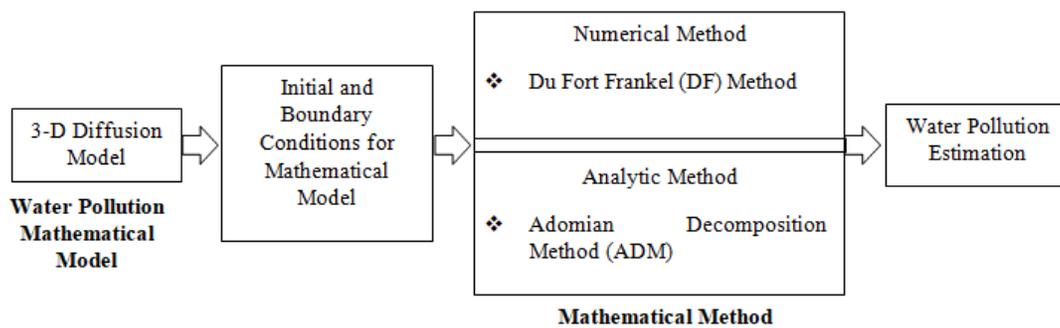


Fig. 1 Mathematical method for 3-D water pollution estimation

Water Pollution Mathematical Model

The mathematical model for estimating water pollution is constructed based on the diffusion model in 3-D region. The rate at which pollution concentration varies concerning time t at different 3-D location in x, y, z direction is mathematically formulated as in Eq. (1).

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

where, $t_0 \leq t \leq t_1$, $x_0 \leq x \leq x_r$, $y_0 \leq y \leq y_s$, $z_0 \leq z \leq z_p$ and the parameter w indicate the pollutant concentration along the x, y and z direction, while t refers to time, and x, y and z represent directions. The diffusion rate D remains constant across all directions.

Initial and Boundary Conditions for Mathematical Model

The numerical and analytical solution $w(x,y,z,t)$ of the mathematical model described in Eq. (1) is obtained by DF and ADM, respectively, which requires initial and boundary conditions concerning space and time. The initial conditions for time t are as in Eq. (2).

$$\left. \begin{aligned} w_0(x,y,z,t) &= w(x,y,z,t_0) = \phi_0(x,y,z) \\ w_1(x,y,z,t) &= w(x,y,z,t_1) = \phi_1(x,y,z) \end{aligned} \right\} \quad (2)$$

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

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

Where, $\phi_0, \phi_1, \psi_1, \psi_2, \psi_3, \psi_4, \psi_5$ and ψ_6 are known functions.

Mathematical Method

The diffusion equation can be solved using various analytical and numerical techniques. This research utilizes the DF method to obtain numerical solutions and the ADM for the analytical approach.

Du Fort Frankel Method (DF) [17, 18, 19]

The DF Method is a finite difference method used to get a numerical solution for the mathematical diffusion model. The finite number of grid locations in x, y and z directions of 3-D regions at which the water pollution is estimated over a finite time interval is expressed as follows [20];

The grid points (x_a, y_b, z_c, t_d) are given as

$$\left. \begin{aligned} x_a &= x_0 : \delta_x : x_r, & a &= 0, 1, 2, \dots, r \\ y_b &= y_0 : \delta_y : y_s, & b &= 0, 1, 2, \dots, s \\ z_c &= z_0 : \delta_z : z_p, & c &= 0, 1, 2, \dots, p \\ t_d &= t_0 : \delta_t : t_l, & d &= 0, 1, 2, \dots, l \end{aligned} \right\} \tag{4}$$

in which 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. We denote $w(x_a, y_b, z_c, t_d) = w(x, y, z, t)$ in the finite difference approximation.

$\frac{\partial w}{\partial t} = \frac{w(x, y, z, t + 1) - w(x, y, z, t - 1)}{2\delta_t}$	The central difference for time-space derivative	(5)
$\frac{\partial^2 w}{\partial x^2} = \frac{w(x + 1, y, z, t) - 2w(x, y, z, t) + w(x - 1, y, z, t)}{\delta_x^2}$	The spatial derivative's central difference in the x direction	(6)
$\frac{\partial^2 w}{\partial y^2} = \frac{w(x, y + 1, z, t) - 2w(x, y, z, t) + w(x, y - 1, z, t)}{\delta_y^2}$	The spatial derivative's central difference in the y direction	(7)
$\frac{\partial^2 w}{\partial z^2} = \frac{w(x, y, z + 1, t) - 2w(x, y, z, t) + w(x, y, z - 1, t)}{\delta_z^2}$	The spatial derivative's central difference in the z direction	(8)

Applying Eq. (5) - (8) in Eq. (1),

$$\frac{w(x, y, z, t + 1) - w(x, y, z, t - 1)}{2\delta_t} = D \left[\frac{w(x + 1, y, z, t) - 2w(x, y, z, t) + w(x - 1, y, z, t)}{\delta_x^2} + \frac{w(x, y + 1, z, t) - 2w(x, y, z, t) + w(x, y - 1, z, t)}{\delta_y^2} + \frac{w(x, y, z + 1, t) - 2w(x, y, z, t) + w(x, y, z - 1, t)}{\delta_z^2} \right] \tag{9}$$

Consider the same grid spacing in Eq. (9) for all three directions that $\delta_x = \delta_y = \delta_z = \delta$.

$$\begin{aligned} w(x, y, z, t + 1) - w(x, y, z, t - 1) &= \frac{2D\delta_t}{\delta^2} [w(x + 1, y, z, t) + w(x - 1, y, z, t) + w(x, y + 1, z, t) + w(x, y - 1, z, t) + w(x, y, z + 1, t) + w(x, y, z - 1, t) \\ &\quad - 6w(x, y, z, t)] \end{aligned} \tag{10}$$

Letting $\frac{D\delta_t}{\delta^2} = \mu$ in Eq. (10),

$$\begin{aligned} w(x, y, z, t + 1) &= w(x, y, z, t - 1) \\ &\quad + 2\mu [w(x + 1, y, z, t) + w(x - 1, y, z, t) + w(x, y + 1, z, t) + w(x, y - 1, z, t) + w(x, y, z + 1, t) + w(x, y, z - 1, t) \\ &\quad - 6w(x, y, z, t)] \end{aligned} \tag{11}$$

Now, replace $w(x, y, z, t)$ by the mean of the values $w(x, y, z, t + 1)$ and $w(x, y, z, t - 1)$ i.e. $w(x, y, z, t) = \frac{w(x, y, z, t + 1) + w(x, y, z, t - 1)}{2}$ in Eq. (11),

$$\begin{aligned} w(x, y, z, t + 1) &= w(x, y, z, t - 1) \\ &\quad + 2\mu \left[w(x + 1, y, z, t) + w(x - 1, y, z, t) + w(x, y + 1, z, t) + w(x, y - 1, z, t) + w(x, y, z + 1, t) + w(x, y, z - 1, t) \right. \\ &\quad \left. - 6 \left(\frac{w(x, y, z, t + 1) + w(x, y, z, t - 1)}{2} \right) \right] \end{aligned}$$

$$\begin{aligned} (1 + 6\mu) w(x, y, z, t + 1) &= (1 - 6\mu) w(x, y, z, t - 1) \\ &\quad + 2\mu [w(x + 1, y, z, t) + w(x - 1, y, z, t) + w(x, y + 1, z, t) + w(x, y - 1, z, t) + w(x, y, z + 1, t) + w(x, y, z - 1, t)] \end{aligned}$$

Therefore, the following finite difference formula is used by the DF method to solve the 3-D diffusion Eq. (1):

$$w(x,y,z,t+1) = \frac{(1-6\mu)}{(1+6\mu)} w(x,y,z,t-1) + \frac{2\mu}{(1+6\mu)} [w(x+1,y,z,t) + w(x-1,y,z,t) + w(x,y+1,z,t) + w(x,y-1,z,t) + w(x,y,z+1,t) + w(x,y,z-1,t)] \quad (12)$$

This Eq. (12) is the explicit formula of the DF method, and here, finding the solution at the $t+1$ level, requires the solution at some location of t level and $t-1$ level. Therefore, this method requires two initial conditions, shown in Eq. (2).

Adomian Decomposition Method (ADM) [14, 15, 16, 24]

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

$$L_t w = D (L_{xx} w + L_{yy} w + L_{zz} w) \quad (13)$$

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

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

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

Thus, applying the inverse operator L_t^{-1} to Eq. (13) yields

$$\begin{aligned} L_t^{-1} L_t w(x,y,z,t) &= D (L_t^{-1} L_{xx} w + L_t^{-1} L_{yy} w + L_t^{-1} L_{zz} w) \\ w(x,y,z,t) - w(x,y,z,0) &= D (L_t^{-1} L_{xx} w + L_t^{-1} L_{yy} w + L_t^{-1} L_{zz} w) \\ w(x,y,z,t) &= w(x,y,z,0) + D L_t^{-1} (L_{xx} w + L_{yy} w + L_{zz} w) \end{aligned} \quad (14)$$

In ADM, represent the solution suppose that

$$w(x,y,z,t) = \sum_{n=0}^{\infty} w_n(x,y,z,t) \quad (15)$$

Substituting Eq. (15) into (14), getting that

$$\begin{aligned} \sum_{n=0}^{\infty} w_n(x,y,z,t) &= w(x,y,z,0) + D L_t^{-1} \left[L_{xx} \sum_{n=0}^{\infty} w_n(x,y,z,t) + L_{yy} \sum_{n=0}^{\infty} w_n(x,y,z,t) + L_{zz} \sum_{n=0}^{\infty} w_n(x,y,z,t) \right] \\ w_0(x,y,z,t) + w_1(x,y,z,t) + \dots &= w(x,y,z,0) + D L_t^{-1} \left[L_{xx} \sum_{n=0}^{\infty} w_n(x,y,z,t) + L_{yy} \sum_{n=0}^{\infty} w_n(x,y,z,t) + L_{zz} \sum_{n=0}^{\infty} w_n(x,y,z,t) \right] \end{aligned} \quad (16)$$

Now, comparing the Eq. (16) on both sides getting the recurrent relation in the form of as follows

$$w_0(x,y,z,t) = w(x,y,z,t_0) = w(x,y,z,0) = \phi_0(x,y,z) \text{ (From Eq. (2))}$$

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

$$\left. \begin{aligned} w_1(x,y,z,t) &= D L_t^{-1} (L_{xx} w_0(x,y,z,t) + L_{yy} w_0(x,y,z,t) + L_{zz} w_0(x,y,z,t)) \\ w_2(x,y,z,t) &= D L_t^{-1} (L_{xx} w_1(x,y,z,t) + L_{yy} w_1(x,y,z,t) + L_{zz} w_1(x,y,z,t)) \\ &\vdots \\ w_n(x,y,z,t) &= D L_t^{-1} (L_{xx} w_{n-1}(x,y,z,t) + L_{yy} w_{n-1}(x,y,z,t) + L_{zz} w_{n-1}(x,y,z,t)) \end{aligned} \right\} \quad (17)$$

Therefore, the estimation of the approximate solution ϕ_γ by using γ -term approximation. That is,

$$\phi_\gamma = \sum_{n=0}^{\gamma-1} w_n(x,y,z,t) \quad (18)$$

Therefore, Eq. (18) is the approximate solution of the 3-D diffusion mathematical model.

Water Pollution Estimation

The DF mathematical approach estimates the water pollution level at a 3-D grid location over a time interval, whose result is validated by comparing it with the ADM approach. Eq. (12) estimates the pollutant concentration in water at different locations over time by the DF method. It is a 3-level explicit method, in which the current time $(t + 1)$ water pollution level at a particular location is estimated by using the surrounding locations' value in x, y and z directions of the previous one-time level (t) and the respective location value of the last two-time level $(t - 1)$. This method simulates the spread of pollutants, such as an iodized salt-water solution, in a water body, helping us understand how contamination disperses.

Eq. (18) represents the pollutant concentration in water at any given point (x, y, z) and time t , using a series solution derived from the ADM. The formula states that the analytical solution is a sum of the terms $w_0, w_1, w_2, \dots, w_{\gamma-1}$. Here, w_0 is an initial condition, and Eq. (17) is used to calculate the remaining terms, $w_1, w_2, \dots, w_{\gamma-1}$. Thus, this equation provides a way to calculate the concentration of pollutants over time and space using a series expansion approach.

III. Experimented Result and Discussion

It is examined that the existing research mainly focused on either 1-D or 2-D diffusion mathematical models solved by different numerical and analytical approaches. The proposed work extends the diffusion model into a 3-D region to estimate water pollution. Furthermore, researchers have demonstrated the 3-D water pollution diffusion model in a 3-D dummy cuboid water tank having dimensions $4.25 \times 4.25 \times 2.25$ feet. A 3-D grid structure with a 1 feet grid distance apart is used in the cuboid tank to define 3-D grid locations. Each 3-D grid location represents approximately one cubic feet 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 helps to study the pollution spreads in all three directions inside the tank. Here, 960 litres (L) of water are used in a tank as a pollute, whereas 40-litres iodized salt-water solution is used as a pollutant, and the polluted water is measured in Parts Per Million (PPM) by Total Dissolved solids (TDS) meter over every 20 minutes of the time interval. The different types of 3-D grid locations based on their respective position in the cuboid water tank are represented in Fig. 2.

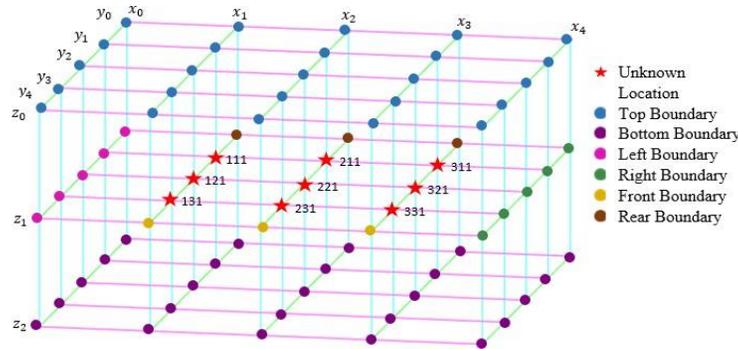


Fig. 2 3-D Grid Locations

Here, the 3-D grid locations in x, y and z space direction are set as $r = 4, s = 4, p = 2$ and $l = 5$ respectively in Eq. (4) so that the space intervals can be defined as; $x_0 \leq x \leq x_4, y_0 \leq y \leq y_4, z_0 \leq z \leq z_2$ and the time interval would be $t_0 \leq t \leq t_5$. Furthermore, considering $x_0 = y_0 = z_0 = t_0 = 0, x_4 = y_4 = 4, z_2 = 2$ and $t_5 = 5$, the range of different types of 3-D grid locations can be classified as in the Table 1.

Table 1 Types of 3-D grid locations

Types	3-D grid locations
Left Boundary	$x = 0, 0 \leq y \leq 4, 0 < z < 2$
Right Boundary	$x = 4, 0 \leq y \leq 4, 0 < z < 2$
Rear Boundary	$0 < x < 4, y = 0, 0 < z < 2$
Front Boundary	$0 < x < 4, y = 4, 0 < z < 2$
Top Boundary	$0 \leq x \leq 4, 0 \leq y \leq 4, z = 0$
Bottom Boundary	$0 \leq x \leq 4, 0 \leq y \leq 4, z = 2$
Unknown	$(x_1 = 1) < x < (x_3 = 3),$

$(y_1 = 1) \leq y \leq (y_3 = 3), z = (z_1 = 1)$
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The mathematical model is executed with spatial increments of 1 foot in the $x, y, and z$ directions and a time step of 1 unit, equivalent to 20 minutes. The visual depiction of the Exp. data at various time intervals is illustrated in Fig. 3.

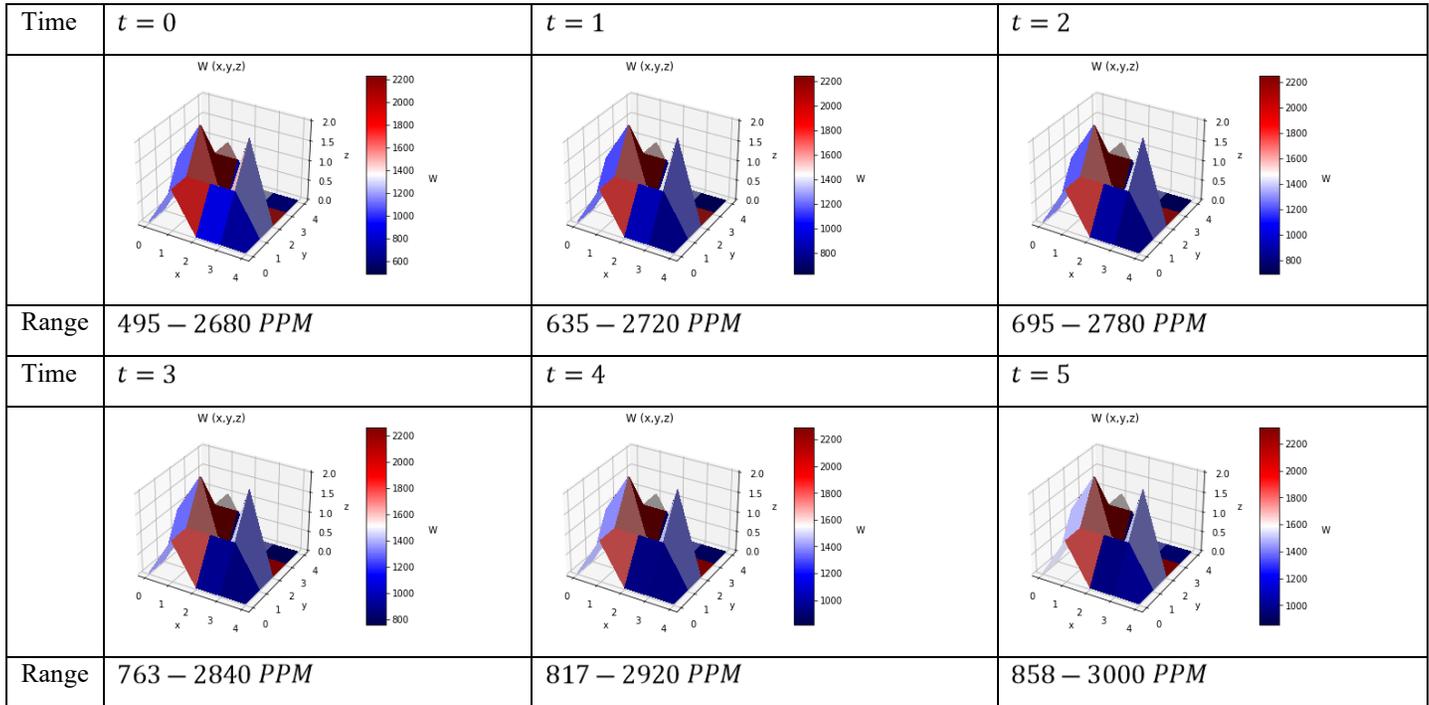


Fig. 3 Water pollution at 3-D grid locations of Exp. data

Fig. 3 shows that the levels of water pollution at each 3-D grid point rise over time. At time $t = 0$, the levels of pollution vary between 495 and 2680 PPM. Following 120 minutes, the range has risen to 858 – 3000 PPM.

The required initial and boundary conditions for time and space are derived using a Multi-Poly Regression model on the obtained Exp. data, which can be expressed as in Eq. (19) – (26) with their respective 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	(19)
Initial Condition for time $t = (t_0 = 1)$ $w(x,y,z,1) = 892.39 * z - 70.96 * z^2 - 70.69 * y - 78.28 * y * z + 25.18 * y * z^2 + 4.60 * y^2 + 6.03 * y^2 * z - 3.31 * y^2 * z^2 - 407.39 * x - 111.71 * x * z + 51.25 * x * z^2 + 46.17 * x * y + 4.81 * x * y * z - 3.44 * x * y * z^2 - 3.35 * x * y^2 + 0.49 * x * y^2 * z + 244.99 * x^2 - 24.97 * x^2 * z + 1.54 * x^2 * z^2 - 19.65 * x^2 * y + 1.94 * x^2 * y * z + 0.11 * x^2 * y^2 - 76.46 * x^3 + 0.58 * x^3 * z + 2.83 * x^3 * y + 1219.93 + 8.63 * x^4;$	0.0012	0.0009	(20)
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	(21)
Right Boundary	0.0011	0.00085	(22)

$w(4,y,z,t) = -0.12 * y * t^2 - 1.22 * y^2 * t + 958 + 106.32 * t + 4.04 * t^2 - 47.04 * y + 11.88 * y * t - 1.44 * y^2 - 1.47e - 14 * y^3;$			
<p>Rear Boundary</p> $w(x,0,z,t) = 42.23 * t + 1812.02 * z + 5.076 * z * t^2 - 69.87 * x * t - 0.43 * x * t^2 - 91.36 * x^2 + 21.83 * x^2 * t + 9.56 * x^3;$	0.0012	0.0008	(23)
<p>Front Boundary</p> $w(x,4,z,t) = 40.08 * t + 4.8 * t^2 + 1504.56 * z - 0.27 * x * t^2 - 65.76 * x * t + 22.35 * x^2 * t - 76.76 * x^2 + 5.88 * x^3;$	0.0019	0.0012	(24)
<p>Top Boundary</p> $w(x,y,0,t) = 55.20 * t + 4.54 * t^2 - 72.73 * y + 1.76 * y * t + 0.048 * y * t^2 + 5.86 * y^2 - 0.99 * y^2 * t - 0.007 * y^2 * t^2 - 325.096 * x - 74.92 * x * t - 0.17 * x * t^2 + 42.35 * x * y + 2.14 * x * y * t - 0.0007 * x * y * t^2 - 3.51 * x * y^2 - 0.046 * x * y^2 * t + 214.80 * x^2 + 22.88 * x^2 * t - 0.011 * x^2 * t^2 - 18.21 * x^2 * y - 0.022 * x^2 * y * t + 0.13 * x^2 * y^2 - 74.013 * x^3 - 0.087 * x^3 * t + 2.59 * x^3 * y + 1159.17 + 8.39 * x^4;$	0.0015	0.0012	(25)
<p>Bottom Boundary</p> $w(x,y,2,t) = 2675.5 + 42.94 * t + 4.38 * t^2 - 130.74 * y + 3.02 * y * t + 0.002 * y * t^2 + 0.025 * y^2 * t^2 + 4.8 * y^2 - 1.18 * y^2 * t - 353.56 * x - 75.64 * x * t - 0.34 * x * t^2 - 0.023 * x * y * t^2 + 39.9 * x * y + 2.38 * x * y * t - 0.043 * x * y^2 * t - 2.58 * x * y^2 + 0.059 * x^2 * t^2 + 176.82 * x^2 + 23.54 * x^2 * t - 0.029 * x^2 * y * t - 15.7 * x^2 * y + 0.17 * x^2 * y^2 - 0.27 * x^3 * t - 73.82 * x^3 + 2.82 * x^3 * y + 8.43 * x^4;$	0.0012	0.0009	(26)

In the experiment of a proposed mathematical model, it is necessary to fix the value of the diffusion rate of the iodized salt-water solution into the volume of the water tank. It is derived based on the phenomena of Fick's first law, which is defined in Eq. (27) [23].

$$D = -D_v \frac{dC}{df} \tag{27}$$

Where, D is the diffusion rate, D_v is the diffusivity value of iodized salt-water solution (cm^2/s), and $\frac{dC}{df}$ is the average concentration gradient. In Eq. (27), the negative sign denotes that the flow proceeds from the area of high concentration to the area of low concentration.

The diffusivity value of iodized salt-water solution can be derived from Eq. (28).

$$D_v = \frac{4 V x_c}{\pi d^2 N M C_M} \frac{dk}{dt} \tag{28}$$

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

In this experiment, $V = 2500 \text{ cm}^3$, $x_c = 0.4 \text{ cm}$, $d = 0.1 \text{ cm}$, $N = 50$. The molar concentration of iodized salt is

$$M = \frac{w_s}{M_w} \times \frac{1 (L)}{V_s} \tag{29}$$

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, $w_s = 2500 \text{ gm}$ iodized salt

$$M_w = Na^+ + Cl^- + I^- + Mg^{+} (\text{impurity})$$

$$= 23 + 35.5 + 127 + 24 = 209.5 \text{ gm/mol}$$

$$V_s = 40 \text{ L}$$

Substituting these values into Eq. (29), that

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

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

The experiment shows that the conductivity of iodized salt water solution is changed as its molar concentration level is vary. Based on the results obtained during experiment the slope of conductivity per unit molar concentration (C_M) is measured from curve fitting of conductivity Vs. molar concentration which is graphically presented in Fig. 4. Furthermore, in the experiment it is observed that the conductivity is varying as the time changed. Based on the experimented results the conductivity changes per unit time ($\frac{dk}{dt}$) is obtained by curve fitting between conductivity Vs. time as graphically presented in Fig. 5.

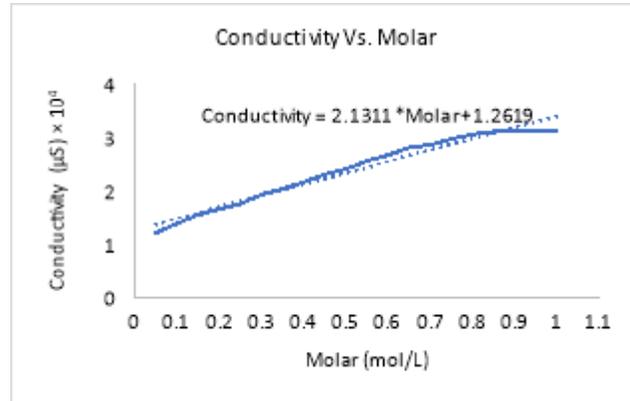


Fig. 4 Conductivity Vs. Molar

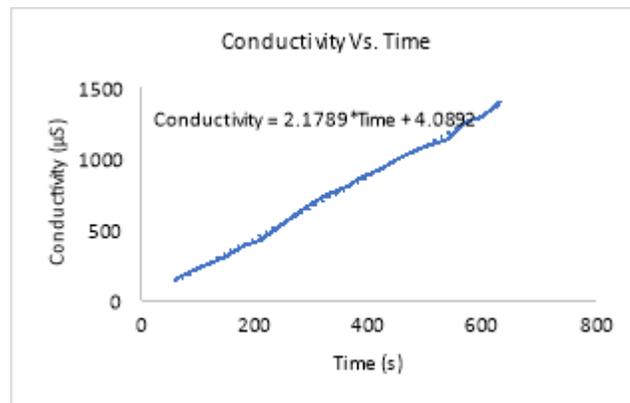


Fig. 5 Conductivity Vs. Time

Fig. 4 and 5 shows that, the coefficient of molar indicates slope of the conductivity change per unit molar concentration $C_M = 2.1311 \times 10^4 \frac{\mu S \cdot L}{mol}$ and the coefficient of time indicated the slope of conductivity change per unit time $\frac{dk}{dt} = 2.1789 \mu S/s$. Now, substituting all the required values in Eq. (28), getting that

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

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

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

In the experiment, the z -axis has three different layers as $0 \leq z \leq 2$ such as 1st layer (Top), 2nd layer (Middle) and 3rd layer (Bottom) of cuboid tank.

Now, the average value of the concentration gradient for 1st and 2nd layer is

$$\left(\frac{dC}{df}\right)_1 = \frac{c_2 - c_1}{f_2 - f_1} \tag{30}$$

and for 2nd and 3rd layer is

$$\left(\frac{dC}{df}\right)_2 = \frac{c_3 - c_2}{f_3 - f_2} \tag{31}$$

where, c_1 is the average of 1st layer ($z = 0$) pollution = $1387.219 \frac{PPM}{cm^3}$, c_2 is the average of 2nd layer ($z = 1$) pollution = $1381.575 \frac{PPM}{cm^3}$, c_3 is the average of 3rd layer ($z = 2$) pollution = $1372.26 \frac{PPM}{cm^3}$. Moreover, f_1, f_2, f_3 are the distance (cm) between layers. Here, $f_1 = 0$ feet = 0 cm, $f_2 = 1$ feet = 30.48 cm, $f_3 = 2$ feet = 60.96 cm. Now, substituting all these values in Eq. (30) and (31), getting that $\left(\frac{dC}{df}\right)_1 = -0.185 \frac{PPM}{cm^4}$ and $\left(\frac{dC}{df}\right)_2 = -0.3056 \frac{PPM}{cm^4}$ whose average value is of $\frac{dC}{df} = -0.24 \frac{PPM}{cm^4}$. By applying all the required values in Eq. (27), gets Eq. (32)

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

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

$$D = 0.21558 \frac{PPM}{cm^2 s} \tag{32}$$

The proposed mathematical model is simulated in MATLAB by considering $\delta_x = \delta_y = \delta_z = 1$ feet, $\delta_t = 1$ unit (20 minutes), and the diffusion rate $D = 0.21558 \frac{PPM}{cm^2 s}$ is considered similar in all the directions x, y and z .

To estimate the water pollution level at each 3-D grid location over a time interval by applying Eq. (19 - 26) as the initial and boundary conditions for the numerical solution of Eq. (1) by DF method, which is graphically represented in Fig. 6.

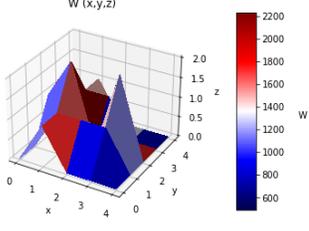
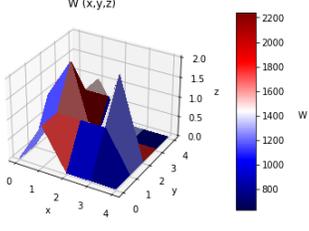
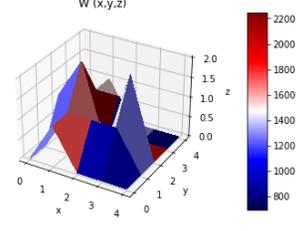
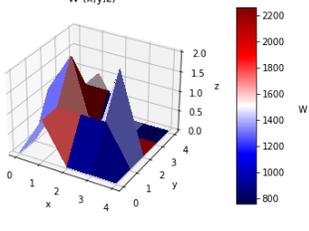
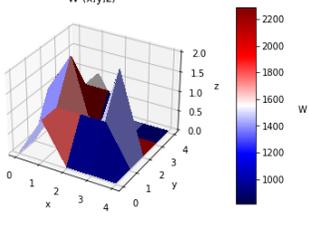
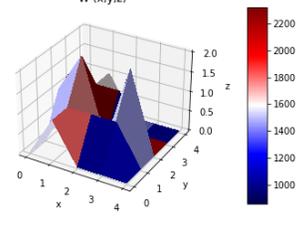
Time	$t = 0$	$t = 1$	$t = 2$
			
Range	495.52 – 2678.80 PPM	635.10 – 2720.87 PPM	696.07 – 2778.91 PPM
Time	$t = 3$	$t = 4$	$t = 5$
			
Range	763.88 – 2843.78 PPM	817.91 – 2917.41 PPM	858.61 – 2999.82 PPM

Fig. 6 Water pollution at 3-D grid locations by DF

Fig. 6 shows that the concentration level of pollutant iodized salt-water solution in water tank at different 3-D grid locations gradually increases over time. In the DF method, the resultant water pollution level has the range of $495.52 - 2678.80 \text{ PPM}$ at the initial time ($t = 0$) that is increased to the range of $858.61 - 2999.82 \text{ PPM}$ at the time $t = 5$ (120 minutes). A significant increment in water pollution to be noted can also be increased as the time passed up to its saturation limit.

Although the DF method has given a numerical solution of the given 3-D diffusion model for water pollution that reflects the real-time phenomena that actually happened during the experiment, another mathematical solution approach should be adopted to validate the obtained results. Thus, ADM has been used as an analytic approach to find the solution of the proposed diffusion model for predicting the level of water pollution at the same 3-D locations at the same time interval.

The required analytical solution of Eq. (1) by applying the ADM approach using the initial condition ($t = 0$) given in Eq. (19) is expressed as in Eq. (33).

$$\begin{aligned}
 w(x,y,z,t) = & 96.91 * D^2 * t^2 + D * t * (103.8 * x^2 + 9.02 * x * y + 1.207 * x * z - 347 * x - 5.255 * y^2 + 3.736 * y * z \\
 & + 10.19 * y - 1.586 * z^2 - 32.87 * z + 295.4) + 8.264 * x^4 + 2.692 * x^3 * y + 0.05 * x^3 * z - 73.13 * x^3 \\
 & + 0.2296 * x^2 * y^2 + 1.868 * x^2 * y * z - 19.112 * x^2 * y + 2.064 * x^2 * z^2 - 21.77 * x^2 * z + 213.3 * x^2 \\
 & + 0.4536 * x * y^2 * z - 3.979 * x * y^2 - 3.565 * x * y * z^2 + 5.689 * x * y * z + 44.6 * x * y + 49.86 * x * z^2 \quad (33) \\
 & - 117.9 * x * z - 325.1 * x - 2.857 * y^2 * z^2 + 5.336 * y^2 * z + 6.238 * y^2 + 24.22 * y * z^2 - 78.6 * y * z \\
 & - 73.67 * y - 71.87 * z^2 + 903.5 * z + 1159;
 \end{aligned}$$

Now, solving Eq. (33) by substituting the value of the diffusion rate D derived in Eq. (32) and x, y, z and t alternating that gives the level of water pollution at all 3-D grid locations. Fig. 7 displays a graphical representation of the ADM's outcomes for the water pollution level at each 3-D grid location over the time period.

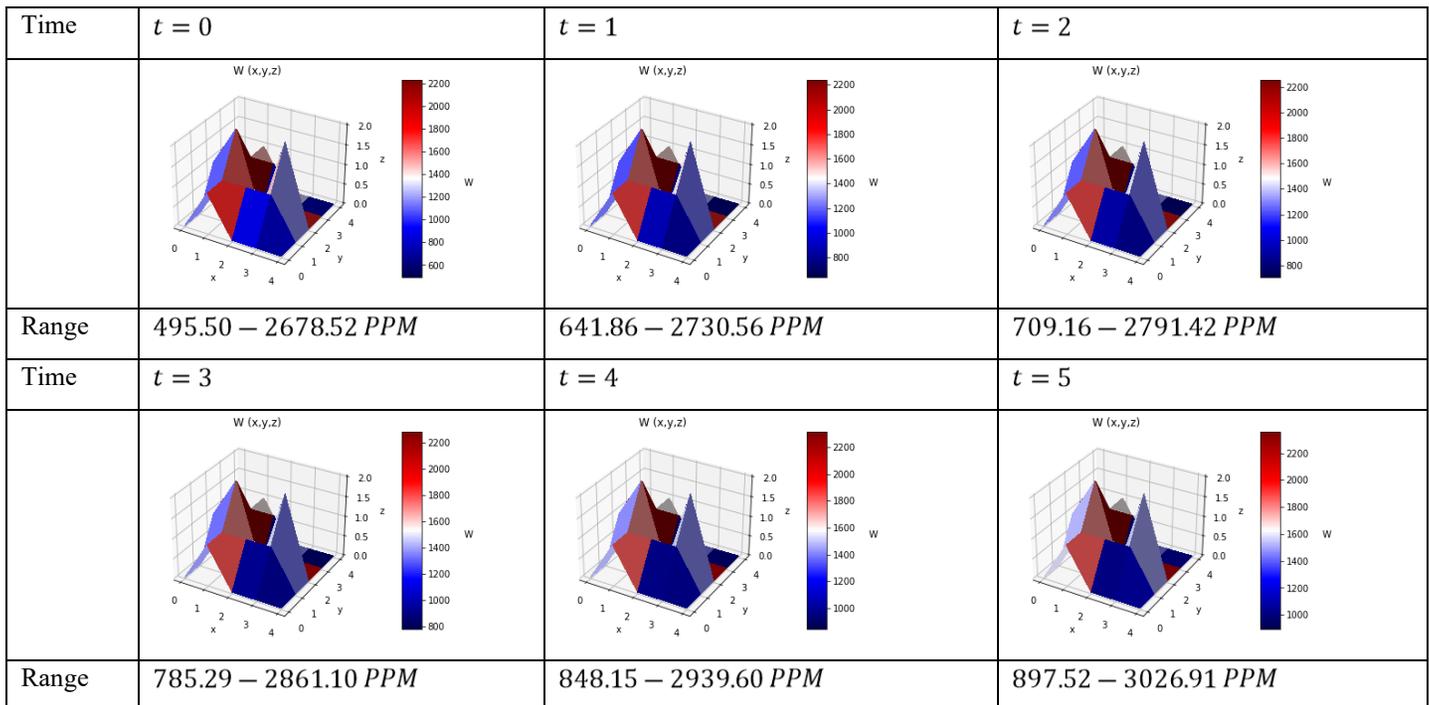
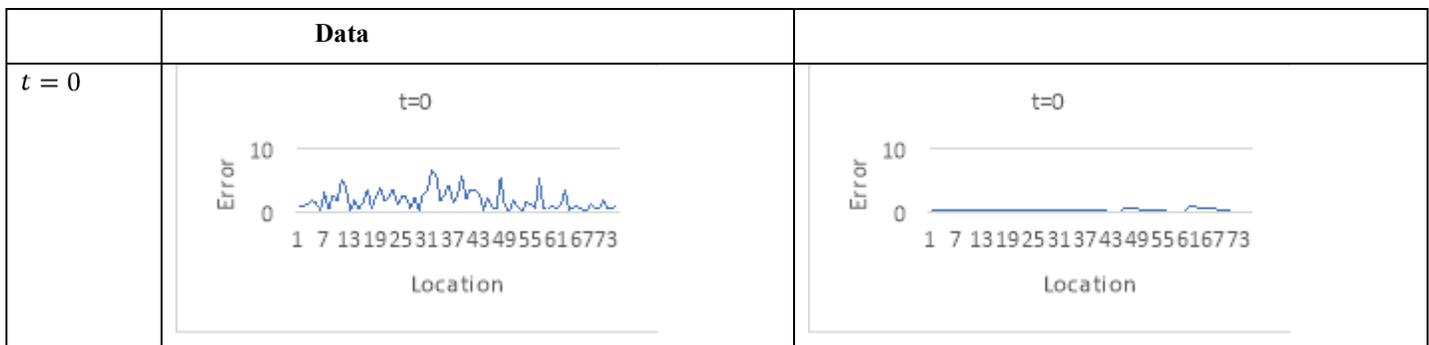


Fig. 7 Water pollution at 3-D grid locations by ADM

Fig. 7 shows that the water pollution level at 3-D grid locations is initially ($t = 0$) in the range of 495.50 – 2678.52 PPM, and after 120 minutes ($t = 5$), it is in the range of 897.52 – 3026.91 PPM. Also, there has been a monotonically increment in water pollution at different locations with respect to the time interval.

Now, two different approaches, DF and ADM, have given numerical and analytical solutions of Eq. (1), respectively. The comparison between numerical DF outcomes with ADM outcomes and Exp. data can validate the accuracy level of prediction of water pollution levels at different 3-D grid locations. The error estimation criteria are used for the comparison, which can be obtained by taking the absolute difference between the water pollution levels at each 3-D grid location across the time interval. The estimated error is graphically plotted in Fig. 8.



<i>Range</i>	0.015 – 6.661 PPM	0.019 – 0.940 PPM
<i>t = 1</i>		
<i>Range</i>	0.011 – 5.463 PPM	0.042 – 11.520 PPM
<i>t = 2</i>		
<i>Range</i>	0.107 – 11.106 PPM	6.951 – 18.769 PPM
<i>t = 3</i>		
<i>Range</i>	0.029 – 15.487 PPM	12.046 – 30.115 PPM
<i>t = 4</i>		
<i>Range</i>	0.012 – 17.585 PPM	18.963 – 42.315 PPM
<i>t = 5</i>		
<i>Range</i>	0.178 – 15.405 PPM	27.092 – 55.369 PPM

Fig. 8 Comparative analysis between DF Vs. Exp. data and ADM Results

Fig. 8 shows that, the comparative analysis between DF Vs. Exp. data has the error range in between 0.0113 PPM to 17.585 PPM and 0.019 to 55.369 PPM in DF Vs. ADM. Also, the analysis of the comparative study between all 75 locations and six-time intervals during the whole duration, it has been observed that the DF methods error against the Exp. data and ADM method is visually shown in Fig. 9 for both PPM difference (error) ≤ 60 and > 60 .

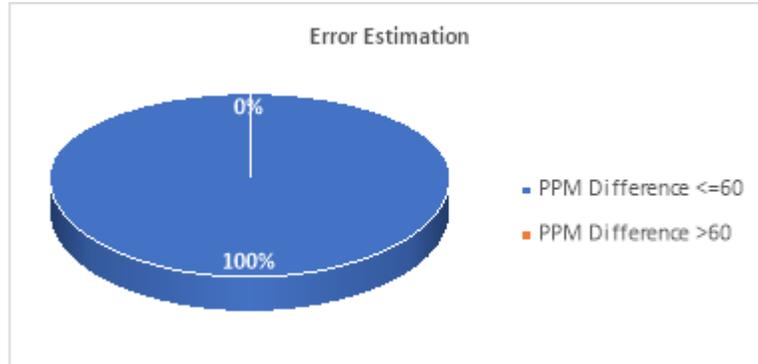
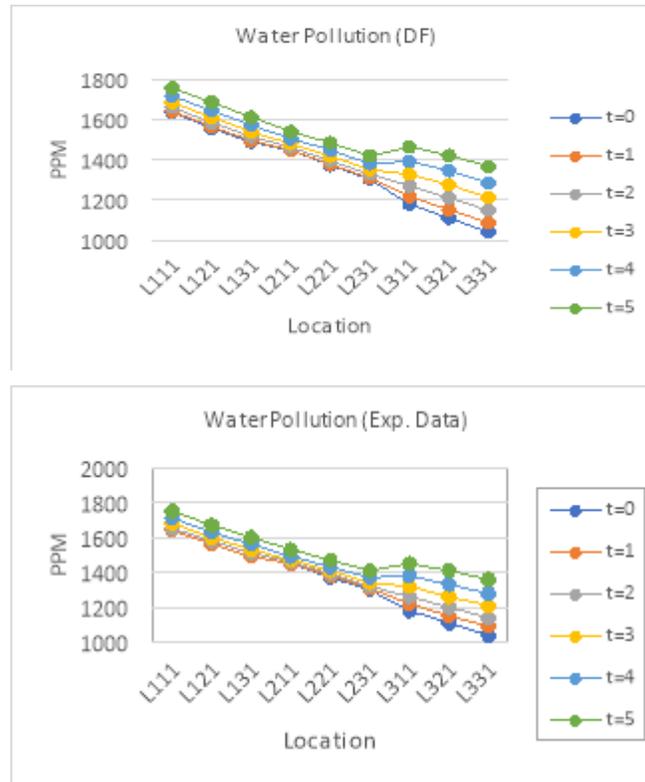


Fig. 9 Error Estimation of DF Vs. Exp. data and ADM

Fig. 9 shows that, in both DF Vs. Exp. data and DF Vs. ADM comparison, 100% of the PPM difference lies under 60 PPM which is highly negligible in the form of PPM because a change of up to 60 PPM is considered a negligible change while above 60 PPM represents a significant change in the level of water pollution [25,26]. As a result, it can be said that 100% of the PPM difference does not affect the water pollution level.

Thus, DF methods results are validated with the Exp. data, the analytical solution obtained by the ADM method and implemented boundary conditions. It concludes that the result obtained by the DF method can be reliable with the Exp. data and the analytical ADM results for predicting water pollution levels over a time interval.

As described in Table 1, there are several types of 3-D grid locations in cuboid water tank. In which, at every time interval, the water pollution level at the top, bottom, left, right, rear and front boundary locations is estimated based on the boundary conditions given in Eq. (21) – (26) while the water pollution level at nine unknown locations is calculated by DF method. These nine locations can be labelled as $L_{xyz} : L_{111}, L_{121}, L_{131}, L_{211}, L_{221}, L_{231}, L_{311}, L_{321}, L_{331}$. Here, it is essential to compare the water pollution level numerically obtained by DF with the Exp. data and the analytical values derived by the ADM approach at each time interval, graphically represented in Fig. 10.



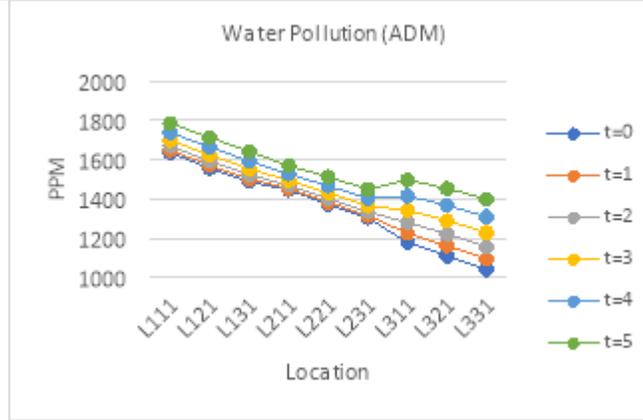


Fig. 10 DF, Exp. data and ADM Result at Nine Unknown Locations

Fig. 10 shows that the water pollution level at these nine unknown locations is gradually rising over a time interval in the cases of DF, Exp. data and ADM approaches. Furthermore, the DF method result is very similar to Exp. data and ADM at all locations. Also, Fig. 11 graphically represents each location-wise progression of water pollution levels over time intervals by DF, Exp. data and ADM approaches.

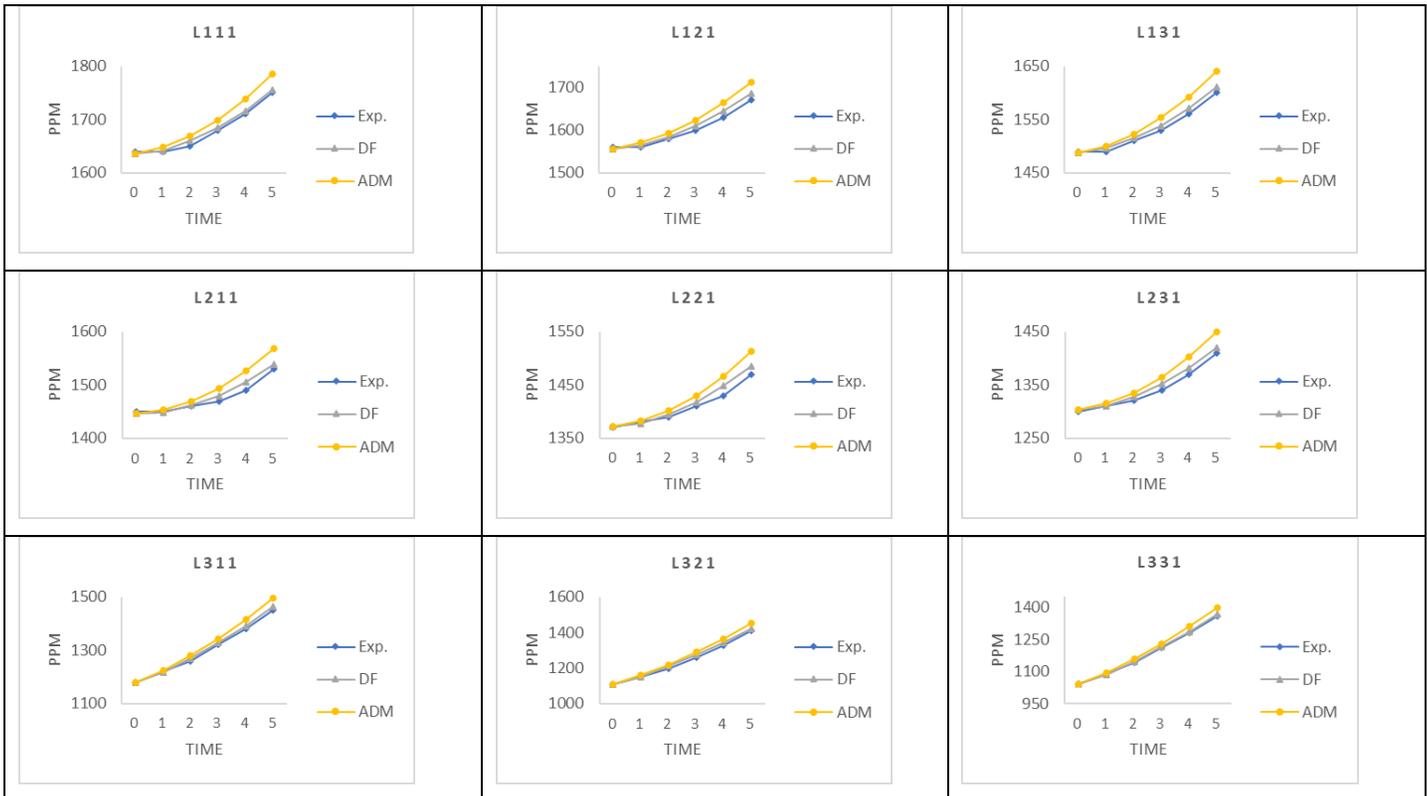


Fig. 11 Water pollution level at unknown Location

Fig.11 shows that, the resultant graphs seem identical in all the cases of unknown locations with respect to time, which leads to negligible errors in the estimation of water pollution levels.

IV. Conclusion

The present research effectively illustrates a mathematical model based on 3-D diffusion model for forecasting the levels of water pollution in a cuboid water tank. A more accurate estimation of the spread of pollutant is made possible by this research's extension of the analysis into three spatial directions. Iodized salt water has been used as the pollutant in the experiment, which produced accurate experimental data for validation. Pollutant concentrations increased gradually over time, according to both analytical outcomes from the ADM and numerical results from the DF approach. During DF approach, in the given time period the water pollution is incremented at minimum range as 363.09 PPM while at maximum range of 321.02 PPM, while in ADM approach the increment was found to be at minimum range 401.67 PPM and at maximum range of 348.39 PPM across the cuboid water tank. According to comparative analysis, it is found that the variations in DF, ADM, and Exp. data are almost identical.

Moreover, the error analysis revealed that the variations in the pollution level in both DF and ADM with Exp. data is less than 60 PPM, which is considered to be insignificant changed in the water pollution level in the form of PPM. This confirms that the DF technique is a trustworthy numerical scheme that aligns with both analytical predictions and experimental results. Overall, a trustworthy framework for predicting water pollution in 3-D regions is offered by the validated 3-D diffusion model. The reliability is confirmed by the high convergence of approaches, and the strategy can be expanded to larger natural water systems for monitoring, pollution prevention, and water quality management.

Declaration of Competing Interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Authors contribution

Tarjani Naik: Conceptualization, Methodology / Study design, Validation, Formal analysis, Resources, Investigation, Data curation, Writing – original draft, Writing – review and editing, Visualization. **Mukesh Patel:** Conceptualization, Conceptualization, Validation, Formal analysis, Writing – original draft, Supervision. **Rachna Patel:** Software, Formal analysis, Resources, Data curation.

Data Availability

The data that support the findings of this study are available on request from the corresponding author, [Mukesh Petel, 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]

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