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Numerical Simulation of Lake Pollution Model via Crank-Nicolson Finite Difference Scheme

Auwal Ahmad[a] and Auwal Abdullahi[a*]

[a]*Department of Mathematics and Statistics, Federal University of Kashere, Gombe State*

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ABSTRACT

Lake pollution has become a serious challenge considering the number of infectious diseases caused by contaminated water. To understand more about the concentration of pollutant released in a lake, this study formulates a partial differential equation (PDE) model of parabolic type, discretized via the Crank-Nicolson scheme. The accuracy of the formulated scheme was ascertained through the Von Neumann analysis. Our numerical simulation reveals that the concentration of pollutants spreads exponentially at each time steps.

1. Introduction

Water has many impacts on different living organisms including plants, animals and humans. For example, it serves as home for aquatic animals (Moss *et al*., 1996). Humans use water for domestic purposes, cultivation of crops and power generation (Salma, 2019). However, due to many activities of humans resulting in industrial waste, refuge and sewage, water is always being polluted. This poses serious threats to humans' health causing diseases such as dysentery, typhoid and cholera (Agusto and Bamigbola, 2007). Lake pollution also affects other living organisms as well as their environments (Nopparat, 2017). Uncontrolled discharge of crude oil, for example, causes a large-scale loss of many species like fish and marine plants rendering the whole affected area less attractive for any agricultural activities. In addition, a huge amount of money has been proposed for effective control measures of water pollution.

Lake pollution is a complex problem whose thorough understanding requires the application of many techniques from different fields of interest including mathematics (Yan *et al.,* 2024). Even though other disciplines like freshwater ecology and reservoir engineering are actively involved in eradicating the problem of water pollution, mathematics is enriched with different tools capable of increasing our understanding of such a problem (Nava and Guevara-Jordan, 2023; Frei and Singh, 2024). The mathematics that can be used in this study is the simulation of PDEs through finite differences. PDEs have immensely contributed to understanding many problems in both physical and life sciences. This includes the study of travelling waves of wild dogs spreading rabies (Chan, 1984), and the contact tracing of individuals infected by Covid-19 (Majid et al., 2021).

Finite differences have been found to be useful in understanding many real-world problems. For example, Hanani et al. (2005) used Crank-Nicolson method to uncover unconditional stability of the proposed numerical schemes. Chaturvedi et al. (2015) also devised a Crank-Nicolson scheme for the solution of heat equation wherein the method is reported to be unconditionally stable. A similar study investigating the stability of a parabolic PDE was also conducted through the Crank-Nicolson approach (Cael and Seekeell, 2016). The control measures of water pollution were examined using the implicit finite difference scheme (Nopparat and Witsarut, 2016).

This work is motivated by the results presented in the aforementioned studies. Thus, the aim of the study is twofold: (1) to formulate and analyze the lake pollution model through Crank-Nicolson scheme and the Von Neumann stability technique, and (2) to numerically estimate the concentration of pollutants in a lake.

2. Lake Pollution Modelling

* Corresponding author. Tel.: +2348065201563
E-mail address: auwal.abdullahi247@gmail.com (Abdullahi A.)
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In this section, we formulate the lake pollution model, discretize it and test the convergence of the schemes.

2.1 Model Formulation

In order to develop the model of interest, we begin by presenting the following compartmental diagram:

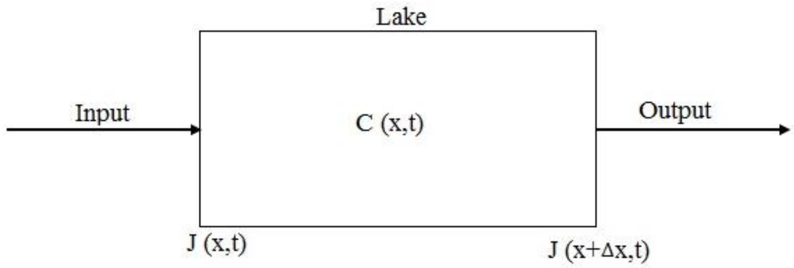

Figure 1: The compartmental diagram of lake pollution model

The flux in and flux out are respectively $J(x,t)$ and $J(x+\Delta x,t)$ while $C(x,t)$ stands for the concentration of pollutants in the lake.

The concentration of the pollutants in the lake can be described by the equation below

$$\frac{\partial \mathrm{C(x,t)}}{\partial t}\Delta x = f(x,t)\Delta x + J(x,t) - J(x+\Delta x,t)$$

Dividing through by Δx, we get

$$\frac{\partial \mathrm{C(x,t)}}{\partial t} = \mathrm{f(x,t)} - \left[\frac{(\mathrm{J(x+\Delta x,t) - J(x,t)})}{\Delta x}\right].$$

Taking the limit as $\Delta x \to 0$ changes the above equation to

$$\frac{\partial \mathrm{C(x,t)}}{\partial t} = \mathrm{f(x,t)} - \frac{\partial \mathrm{J}}{\partial x}. \quad (1)$$

The above equation represents for the law of conservation. We now write the expression of J as

$$J = \frac{F}{A}\frac{\partial \mathrm{C}}{\partial t}, \quad (2)$$

where F is the rate at which water flow and A is the area of the compartment.

Substituting equation (2) into equation (1), we get

$$\frac{\partial \mathrm{C(x,t)}}{\partial t} = \mathrm{f(x,t)} - \frac{\partial}{\partial x}\left[\frac{F}{A}\frac{\partial \mathrm{C}}{\partial t}\right].$$

The above equation can be rewritten as

$$\frac{\partial \mathrm{C(x,t)}}{\partial t} = \mathrm{f(x,t)} - \frac{F}{A}\frac{\partial^2 C}{\partial x^2}. \quad (3)$$

We arbitrarily choose the growth function to be exponential

$$\mathrm{f(x,\,t)} = \alpha \mathrm{C(x,t)}.$$

Then equation (3) becomes

$$\frac{\partial \mathrm{C(x,t)}}{\partial t} = \alpha \mathrm{C(x,t)} - \frac{F}{A}\frac{\partial^2 C}{\partial x^2}, \quad (4)$$

which is the proposed lake pollution model to be considered in this study.

2.2 Model Discretization

While the time derivative is discretized by the forward difference formula, the central difference formula is used to discretize the spatial derivative

$$\frac{\partial \mathrm{C(x,t)}}{\partial \mathrm{t}} = \frac{\mathrm{C}_i^{j+1} - \mathrm{C}_i^{j}}{\Delta t} \quad (5)$$

$$\frac{\partial^2 C}{\partial x^2} = \frac{C_{i+1}^{j} - 2C_i^{j} + C_{i-1}^{j}}{(\Delta x)^2} \quad (6)$$

$$\frac{\partial^2 C}{\partial x^2} = \frac{C_{i+1}^{j+1} - 2C_i^{j+1} + C_{i-1}^{j+1}}{(\Delta x)^2} \quad (7)$$

Substituting Equations (5), (6) and (7) into Equation (4), we write the numerical scheme for the Crank-Nicolson as follows

$$\frac{C_i^{j+1}-C_i^j}{\Delta t} = \propto \left[\frac{1}{2}\left(C_i^{j+1}+C_i^j\right)\right] - \frac{F}{A}\left[\frac{1}{2}\left[\left(\frac{C_{i+1}^j-2C_i^j+C_{i-1}^j}{(\Delta x)^2}\right)+\left(\frac{C_{i+1}^{j+1}-2C_i^{j+1}+C_{i-1}^{j+1}}{(\Delta x)^2}\right)\right]\right],$$

where $\beta = \frac{\propto\Delta t}{2}$ and $\lambda = \frac{F\Delta t}{2A(\Delta x)^2}$.

Thus, we further simplify the above equation to obtain the required Crank-Nicolson scheme

$$\lambda C_{i+1}^{j+1} + (1-\beta-2\lambda)C_i^{j+1} + \lambda C_{i-1}^{j+1} = -\lambda C_{i+1}^{j} + (1+\beta+2\lambda)C_i^j - \lambda C_{i-1}^{j}. \quad (8)$$

2.3 Stability Analysis of the Lake Pollution Model

We now state and prove the theorem regarding the stability of lake pollution model.

Theorem 1: The lake pollution model discretized via the Crank-Nicolson scheme is unconditionally stable.

Proof: The above theorem can be proved by the Von-Neumann stability analysis.

Suppose that $C_i^j = w^j e^{I\gamma x_i}$. (9)

We substitute Equation (9) into (8) to get

$$\lambda w^{j+1}e^{I\gamma(x_i+h)} + (2-\beta-2\lambda)w^{j+1}e^{I\gamma x_i} + \lambda w^{j+1}e^{I\gamma(x_i-h)}$$
$$= -\lambda w^j e^{I\gamma(x_i+h)} + (2+\beta+2\lambda)w^j e^{I\gamma x_i} - \lambda w^j e^{I\gamma(x_i-h)}$$
$$\lambda w^{j+1}e^{I\gamma x_i}.e^{I\gamma h} + (2-\beta-2\lambda)w^{j+1}e^{I\gamma x_i} + \lambda w^{j+1}e^{I\gamma x_i}.e^{-I\gamma h}$$
$$= -\lambda w^j e^{I\gamma x_i}.e^{I\gamma h} + (2+\beta+2\lambda)w^j e^{I\gamma x_i} - \lambda w^j e^{I\gamma x_i}.e^{-I\gamma h}.$$

By factoring out $e^{I\gamma x_i}$ we get

$$\lambda w^{j+1}e^{I\gamma h} + (2-\beta-2\lambda)w^{j+1} + \lambda w^{j+1}e^{-I\gamma h} = -\lambda w^j e^{I\gamma h} + (2+\beta+2\lambda)w^j - \lambda w^j e^{-I\gamma h}$$

$$w^{j+1}\left[-4\lambda sin^2\left(\frac{\gamma h}{2}\right)+2-\beta\right] = w^j\left[4\lambda sin^2\left(\frac{\gamma h}{2}\right)+2+\beta\right].$$

Letting $w^{j+1} = kw^j$, we write the above equation as

$$kw^j\left[-4\lambda sin^2\left(\frac{\gamma h}{2}\right)+2-\beta\right] = w^j\left[4\lambda sin^2\left(\frac{\gamma h}{2}\right)+2+\beta\right].$$

By factorizing the above equation and ignoring the constant term, we get

$$k = \frac{1+2\lambda sin^2\left(\frac{\gamma h}{2}\right)}{1-2\lambda sin^2\left(\frac{\gamma h}{2}\right)}$$

The system is stable if and only if the amplification factor satisfies $|k| \leq 1$. We further write the above equation as

$$|k| = \frac{1+q}{1-q},$$

whereby $q = 2\lambda sin^2\left(\frac{\gamma h}{2}\right)$.

Now $\lim_{q\to\infty}|k| = \lim_{q\to\infty}\frac{q\left(\frac{1}{q}+1\right)}{q\left(\frac{1}{q}-1\right)} = \frac{\left(\frac{1}{\infty}+1\right)}{\left(\frac{1}{\infty}-1\right)} = \frac{0+1}{0-1} = -1.$

This shows that $|k| \leq 1$ holds, and the Crank-Nicolson scheme for the lake pollution model is unconditionally stable.

3 Simulation Results

In this section, the numerical scheme derived in the previous section is iteratively used to obtained numerical results for the pollution model.

In order to validate our numerical simulation, the parameter values used for the lake pollution model are reported through similar studies exist in the literature. Thus, Table 1 summarizes all the parameters of the model as well as their sources.

Table 1: Table of Parameter Values

Parameter	Symbol	Value	Source
Initial condition	C_0(x,t)	$\frac{1}{\sqrt{4\pi D}} exp \frac{(-(x-10v)^2)}{4D}$	Nigar and Laek (2022)
Flow rate	F	0.02m/s	Nigar and Laek (2022)

Surface area of the lake	A	$0.46km^2$	Cael and Seekell (2016)
Space step size	Δx	0.05 and 0.025m	Hanani et al. (2018)
Time step	Δt	0.01, 0.025 and 0.005secs	Hanani et al. (2018)
Growth rate	$\propto$	0.1	Adak (2020)

It should note that, in addition to the model parameters listed above, the spatial domain of the $100 \text{ m} \times 200 \text{ m}$ lake, where our numerical simulation is performed, is rescaled to $[0\ \ 1] \times [0\ \ 2]$.

4. The Numerical Simulation of Lake Pollution Model

This section presents key results obtained from our numerical simulation using the Crank-Nicolson scheme. Using the discretized scheme from Equation (8) and the parameter values listed in Table 1, we present our findings. Therefore, the concentration of released pollutants in the lake increases exponentially along the time axis (see the surface plot Figure 1)

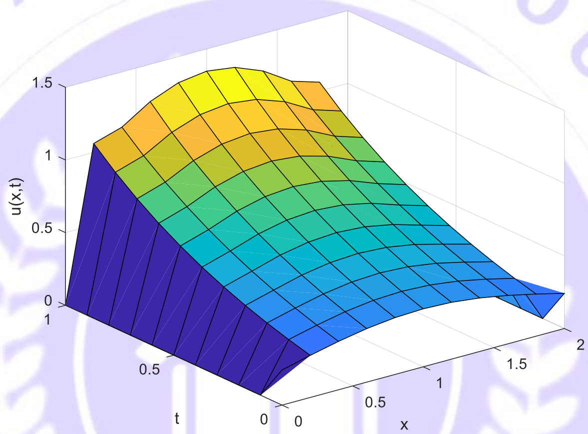

Figure 1: Surface Plots for Crank-Nicolson Scheme

Consequently, the corresponding time course plot generated using the Crank-Nicolson scheme from Equation (8) also indicates that the concentration of the pollutants increases as the number of days progresses (see Figure 2).

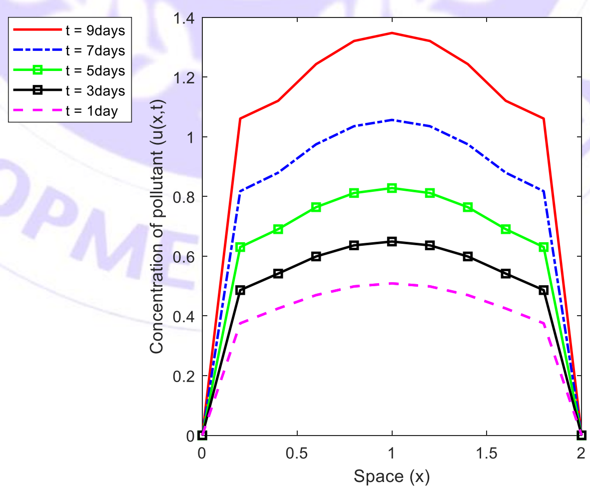

Figure 2: Time course plot for the concentration of pollutants

The concentration of pollutants in the lake increases with the number of days, as observed in the result obtained using Crank-Nicolson scheme with parameter values reported in Table 1.

5. Discussion

Lake pollution is a serious problem affecting most living organisms including humans, plants and animals. Different control strategies have been proposed to control the lake pollution problems. This study, therefore, formulates the partial differential equation model of parabolic type to increase our understanding of the concentration of pollutants when released in the lake. Consequently, our numerical simulation, devised via the Crank-Nicolson scheme, reveals that the concentration of pollutant increases exponentially (see Figure 1). Perhaps, this could be due the exponential growth function incorporated the model.

Even though the released pollutants dissolve faster in the lake, our numerical simulation was able to track their concentrations at each time step precisely on daily basis (see Figure 2). In order to strengthen the finding of this study, the stability of our proposed partial differential equation model has been tested. This has been reported by many authors in different scenarios (see Leon and Austria,1987; Morton, 1971; Omowo and Abhulimen, 2021; Rigal, 1979).

6. Conclusion

This study is concerned with the determination of the concentration of pollutants released in the lake through the formulation of partial differential equation model, discretized by the Crank-Nicolson finite difference approach. Thus, the numerical simulation employed in this study suggests that the concentration of pollutants increases exponentially and it can also be estimated daily. Perhaps this is due to the fact that an exponential growth function has been used in our proposed partial differential equation model. Therefore, further studies are recommended to include different growth functions, such as logistic and growth and Gompertz functions to study the increase of concentration of pollutants in the lake.

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