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Compartmental Equations Hybrid Model for Modelling Water Pollution Transmission

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ABSTRACT

Water pollution has been identified as one of serious environmental problem that has a negative impact on aquatic animals and plants, terrestrial plants and animals, and human health. Effective pollution management and decision-making require an understanding of the intricate dynamics of water contamination in our environment. There are many workable measures that can be adopted to control the menace. Mathematically, water pollution can be modelled using differential equations through management. In order to describe the pollution of water bodies using a system of differential equations. We deployed compartment models to capture the dynamic of pollution in lakes, rivers, and other water bodies. The model compartmentalizes various forms of water pollution and combines them with purification measures. With this strategy, we showed how water pollutants behave in diverse environmental contexts by providing useful knowledge for putting pollution management measures into practice by solving the compartmental model using the Euler method and the Runge-Kutta of Order 4 numerical method (RK4). The quality of results obtained by applying the two mentioned numerical methods is queried based on how they respond to different values of step size (h), which represents the interval at which the numerical methods approximate the solution trajectory. Our findings demonstrate that both numerical approaches are viable for solving compartmental equations by computing compartment values over a specified time interval. Despite the practicability of both methods, it is noteworthy that Runge-Kutta of order 4 consistently emerges as the more effective numerical method in solving our compartmental model when compared with Euler formula, particularly when step sizes are moderately large. The Runge-Kutta method's robustness and efficiency in accurately approximating solutions over the specified time range make us conclude that it is more preferable to the Euler method for practical implementations of compartmental models with moderately large time steps.

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1. Introduction

Pollution is the expulsion or introduction of man-made and industrial waste by-products or substances into the environment that are susceptible to causing threats to human health, damaging living resources, disrupting ecological systems and quality environment [1,2]. Water is regarded as a fundamental need for life. It is an important part of our bodies and keeps us alive. Without adequate water, the chances of man and other living things in the environment surviving will be jeopardized [3]. In our everyday lives, water is helpful and needful. Water from rivers, lakes, and lagoons has been utilised for irrigation of farm plants, domestic usage, and industrial usage. However, these greatest resources that nature has provided to us have become polluted as a result of human activity [4]. Water pollution occurs when harmful liquids like oil, pesticides, and insecticides are discharged from industries, humans, institutions, and health centres into water bodies. The presence of these pollutants disrupts aquatic ecosystems, interferes with biodiversity, and degrades the quality of water supplies for industrial, agricultural, and domestic purposes such as cooking, drinking, and bathing [5]. It can also promote the development of water-borne diseases like dysentery, malaria, typhoid, cholera, amoebiasis, hookworm, and giardiasis to mention a few [6,7]. Adequate efforts to protect the environment against water pollution begin with effective monitoring of pollutants. One of the very workable measures to monitor pollution mathematically is the use of differential equations. This is achieved by describing the pollution of water using a system of differential equations. A compartmental model is introduced to capture the dynamics of pollution in lakes, rivers, and other bodies of water [8].

Mathematical modelling is series of intelligent activities that helps in turning implementation-related problems into manageable mathematical symbols, relations, equations, and formulae. Numerical and theoretical analysis provides thoughts, solutions, and deductions for the original application [9,10], The use of mathematical models to capture intrigue information is widespread across many academic fields, including the social sciences, agriculture, medicine, and business, to mention but a few. Stochastic or deterministic models, linear or non-linear models, and even dynamical models like chaos and neural networks are options for mathematical models that can be deployed. In epidemiology, the success of mathematical models has been recorded in the past to diagnose, treat, and forecast epidemic outbreaks [11]. Epidemiological models, such as the SIS, SIR, and SEIR, have been deployed to provide accurate approximations for stakeholders and policy makers to facilitate and determine what is needed to control diseases [12]. In the mathematical modelling of infectious diseases to capture the trend in disease dynamics, it can be noted that the majority of infectious diseases require a combination of containment, isolation, quarantine, vaccines, medicine, and many more to slow the transmission of disease [13]. Recent years have witnessed the use of mathematical models to study the dynamics of water contamination and pollution. A compartment model may also be used to analyse the dynamics of water pollution in a system. The compartments here stand in for various components of pollutants that are present or move back and forth [14].

To fully understand the transmission of water pollution, numerous scientists and scholars have proposed many models to capture the intrigues and dynamics of water pollution. Study conducted by Agusto and Bamigbola [15] proposed the application of the Crank-Nicolson numerical approach to numerically solve the mathematical models for water contamination in Nigeria. The end result demonstrates that in every instance, the pollutant concentration drops more quickly. A mathematical model has been deployed to model the dispersal of contaminants via forest resources with the best possible management measures [16]. The outcome demonstrates that, both directly via harvesting and indirectly through pollution, wood-based businesses lower the density of forest resources.

Industries other than wood-based ones only have an indirect impact on forest resources. This proposed increasing the amount of forest resources and installing less. This advocated increasing the amount of forest resources while reducing the number of industries per person. Finite Element Method (FEM), was used to solve a model for the dispersion of river pollution using the concentration of pollutant as variables [17].

Mathematical modelling is an essential tool for understanding the dynamics of water pollution. Using such intuition, researchers can stimulate the behaviour and spread of pollutants in water bodies and investigate the effectiveness of different mitigation strategies mathematically [18,19]. Robust and good modelling techniques are essential in forecasting pollutant behaviour while creating efficient mitigation methods to overcome the threat of water pollution. To effectively handle this problem, this research will utilise a compartmental model to determine the impact of soluble and insoluble pollutants, modifying the variables of the compartmental model to include pollution rate, transmission rate, treatment rate, and many more. In the past, less attention has been given to finding the solutions of compartmental models using the numerical method of the ODE method. Furthermore, we employed the compartmentalization approach and applied numerical techniques to solve the compartmental equations. In particular, we used both the Euler method and Runge-Kutta order 4 numerical methods to see how well numerical methods worked at solving these kinds of compartmental models and to see how well the numerical methods themselves worked. Based on the trend in the obtained solutions, while both methods are practical, it's worth highlighting that the Runge-Kutta method of order 4 consistently proves to be the more effective numerical approach for solving our compartmental model, especially when dealing with moderately large step sizes [20]. The Runge-Kutta method of 4th order demonstrates robustness and efficiency in precisely approximating solutions over the specified interval, leading us to infer that the Runge-Kutta method of 4th order is the preferred choice over the Euler method for practical implementations of compartmental models with moderately large time steps.

2. Mathematical Formulation of the Model

Model formulation is an essential component in conceptualizing a modelling problem; it calls for the selection of appropriate variables to describe the major components and features of water pollutants and determine the physical or chemical interaction between the components. The system description will facilitate and allow us to envisage and comprehend the abstractions in the components within the system while providing information that will aid in making proper assumptions regarding major components of the underlying system we are trying to model. The variables are categorized into compartments that describe the physical attributes of the components, such compartments define the rate of change of pollution in a lake as the difference between the rate at which pollution enters the water body and the rate at which pollution leaves the lake [21]. This can be modified as the rate of change of pollutant in the water bodies, as the difference between the rates of pollution in water bodies and the rate at which pollutants depart the water body in the case where the water is stagnant. Figure 1 is an illustration of the movement of water pollutants into running water. The water pollutants used in this research are made up of two categories of pollutants, which are categorized as soluble and insoluble pollutants.

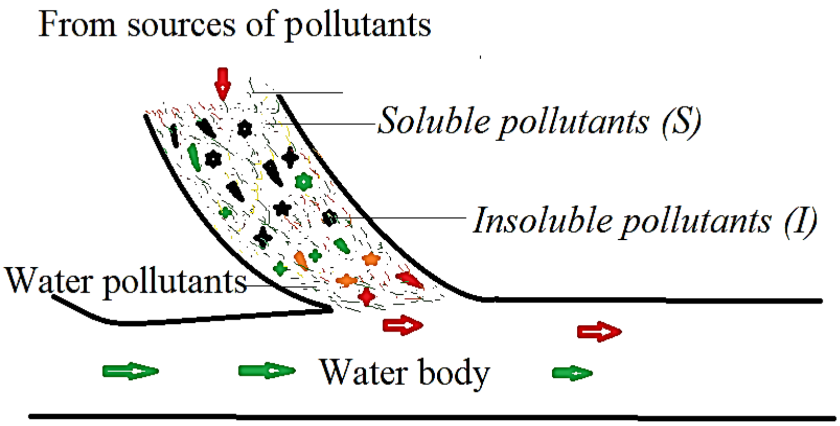


Fig. 1. An illustration of the movement of water pollutants into running water

We investigate the numerical solutions of the modified compartmental model for transmission of water pollution found in the previous study [16]. Our investigation revolves around the use of two popular numerical methods, the Euler method and the Runge-Kutta of order 4 method to solve the compartmental equations in Eq. (1).

The interactions among the compartments shown in Figure 2 leading to the emergence of the following nonlinear ordinary differential equations

$$
\begin{aligned}
W' &= \Lambda - \alpha_1 WS - \alpha_2 WI + \rho\alpha_2 I - \mu W \\
S' &= \alpha_1 WS + \delta I - (\vartheta_1 + \mu) S \\
I' &= \alpha_2 WI - \rho\alpha_2 I - (\delta + \vartheta_2 + \mu) I \\
T' &= \vartheta_1 S + \vartheta_2 I - \mu T
\end{aligned}
\tag{1}
$$

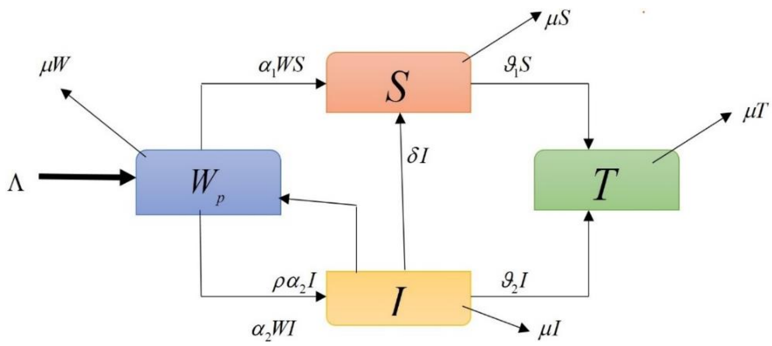


Fig. 2. Illustration of the movement of the agents across the compartments

where Λ is the rate at which pollutants are introduced into the water system over a defined period of time; it signifies the flow or influx of pollutants into the water body from several sources (industries, domestic, and others), and it is measured in concentration per unit time.

α_1 represents the rate of dissolution of soluble water pollutants; it indicates how rapidly the soluble pollutant dissolves and moves within the water.

α_2 represents the rate at which the insoluble pollutants are transported through the water body; this can be influenced by water current, turbulence, and other factors.

μ represents the rate at which pollutants are being taken out of or removed from each individual compartment in the system.

δ represents the rate at which water pollutants that were initially insoluble (not capable of dissolving in water) are transformed into a soluble form through a treatment process.

ρ represents the rate at which initially insoluble water pollutants are converted into forms that contribute to water pollution.

ϑ_1, ϑ_2 are the rate of volume of soluble and insoluble pollutants, respectively, that are subjected to treatment within their respective compartments in the water body.

The compartmental model used in this study is divided into four different compartments. As shown in Eq. (1). W denotes the volume of water pollutants, S denotes the volume of soluble water pollutants, I denotes the volume of insoluble water pollutants, and T is the volume of water treated by removing both soluble and insoluble pollutants. Eq. (1) demonstrates dynamics in each of the compartments, where terms with a negative sign led to a reduction in the volume of the correspondent compartment, while those with positive sign basically led to an increase in the cubic volume of the compartments. The rate of change in each compartment are described using ordinary differential equations, which according to Ziemińska-Stolarska and Skrzypski [22] can be employed to depict the dynamics of activities that take place in surface waters linked to the dissemination of different pollutants, which can pose a lot of danger to human, animal, and plant health. Using the general law of conservation, Eq. (1) can be used to describe each quantity within a non-specified control measure in the compartment as well as the volume of each compartment at a certain point in time. However, since each compartment equation is described in an ODE, we can apply numerical methods to solve the problem to visualize the changes that occur at any interval and the long-term implications of treatment on the water body. The description of the numerical methods to be used is described in Section 4.1 and Section 4.2.

3. Data Source, System and Software Requirement

In this research, we used data from Bonyaha *et al.,* [9] to visualize the dynamic of the system involving water pollution and the movement of entities from one compartment to another. Simulated datasets are artificial datasets that are adopted to imitate real-world instances and can be used to examine how the compartmental model responds in controlled environments. We investigate the dynamics of the system of differential equations in Eq. (1) and the parameter values shown in Table 1, which were extracted from the source. To effectively model the dynamics of the system and reduce the computational burden, we used the MATLAB programming language R2022b version running on Microsoft Windows 10, 8 GB of RAM and a 64-bit multi-core processor. We set $\mathrm{W}(0)=500, \quad I(0)=100 \quad S(0)=400, \text{ and } T(0)=0$ as initial values and other parameters as adopted in Bonyaha *et al.,* [9] and Shah *et al.,* [16]. Table 1 shows other parameters used in the studies.

Table 1
Symbols used and parametric values

Notation	Description	Parameter Value
Λ	Rate of flow of water pollutants into the water	0.8
α_1	Rate of transmission of soluble water pollutants	0.18
α_2	Rate of transmission of insoluble water pollutants	0.02
μ	Rate of removal of water pollutant from each compartment	0.4
δ	Conversion rate of insoluble water pollutants to solute after treatment	0.3
ρ	Rate if conversion of insoluble water pollutants into water pollution	0.25
ϑ_1	Rate of volume of soluble water pollutants treated	0.2
ϑ_2	Rate of volume of insoluble water pollutant treated	0.5

4. Methodology

The compartmental model used in carrying out these numerical comparative studies is a modified version of Shah *et al.,* [16], together with the data and the parameters in a study by Isa *et al.,* [6]. We investigate how the Euler numerical method and the Runge-Kutta method of the 4th-order method behave when used in solving the compartmental model in Eq. (1). Having riven the complex systems into interrelated compartments, the obtained compartmental equations are used to describe and analyse the behaviour of the complex systems. The interactions between the compartments are defined by compartmental equations; as such, each compartmental equation represents a unique component of the system. Here we used the Euler numerical methods and the Runge-Kutta method of order 4 that were described in subsections 4.1 and 4.2, respectively, to see the dynamic of each component in the compartmental models. Figure 3 and Figure 4 depict the flow chart for the methodology used in this study.

4.1 Euler Numerical Method

In the field of computational science and mathematics, the Euler method is also known as the forward Euler method [23]. It is a numerical technique for solving ordinary differential equations (ODEs) when the initial value is known. It is regarded as the simplest Runge-Kutta technique and the most explicit approach for the numerical solution of an ODE [24]. One of the milestones ever reached in continuous time dynamics is the discovery of numerical ODE solutions, since the majority of ODEs cannot be solved analytically. Hence, one of the available options to reveal the trajectory of such solutions is numerical integration. To solve various forms of ODEs properly, a variety of approaches have been proposed. Numerical methods strive to achieve the same goal as analytical methods, and the dynamics of their function closely resemble those of differential equation [25]. Several studies have shown that any first-order ordinary differential equation (ODE) of the form shown in Eq. (2) can be solved using the Euler numerical formula shown in Eq. (3) [26,27].

$$\frac{dy}{dx} = f(x, y), \;\; y(x_0) = y_0 \tag{2}$$

where, $y(x_0) = y_0$ is an initial condition. The Euler method, aside from being a popular technique for solving ordinary differential equations, is also the source from which most of the numerical methods for solving first-order ODEs were derived. The scheme for its implementation is shown in Eq. (3).

$$y_{n+1} = y_n + hf(x_n, y_n). \quad n = 0, 1, 2, . . . \in \mathbf{Z} \tag{3}$$

where *h* is step-size, the difference between consecutive independent variables is calculated using $h = x_{n+1} - x_n$, this can be written as $x_{n+1} = x_n + h$, and from the algebraic perspective slope is defined as $rise/\mathrm{run}$, we can then write $f(x_n, y_n) = \frac{\Delta y}{\Delta x}$, or equivalently, $f(x_n, y_n) = \frac{\Delta y}{h}$, rearranging we have, $\Delta y = hf(x_n, y_n)$ and since our target is to get an expression of the form y_{n+1}, we write $y_{n+1} = \Delta y + y_n$, substituting Δy as shown earlier, and rearranging led to Eq. (3). The Euler method provides substantial solutions to most first-order ODEs. The Euler formula is built around using a known point as a starter and then utilising the tangent line through that point to find new related points. The sequence of these points generated in this pattern will approximate the solution of the analytic solution of the ODE. Although errors during the iterations are a bit higher when compared to other numerical methods, efforts to mitigate the error magnitude have led to modifications of the classical Euler scheme; most of the attempts mainly focus on improving the method's efficiency by reducing the size of errors during iterations. However, findings from research in the field of numerical analysis affirm that the Euler formula is not free from errors when the step size is large but also converges slowly [28]. In this paper, we used the Euler numerical method to solve the compartmental models by treating each compartmental equation as a separate ODE. Such that the system of equations in Eq. (1) can be modified as

$\frac{dW}{dt} = f_w(t_n, W_n, S_n, I_n, T_n)$, $\frac{dS}{dt} = f_s(t_n, W_n, S_n, I_n, T_n)$, $\frac{dW}{dt} = f_I(t_n, W_n, S_n, I_n, T_n)$ and $\frac{dW}{dt} = f_T(t_n, W_n, S_n, I_n, T_n)$

where *W* is the cubic volume of water pollutant, *S* is the cubic volume of soluble water pollutant, *I* is the cubic volume of insoluble water pollutant, and *T* is the treated water pollutant. We transform the compartmental model in Eq. (1) using the Euler formula while taking $h = t_{i+1} - t_i$

$$W_{n+1} = W_n + hf_w(t_n, W_n, S_n, I_n, T_n) = W_n + h(\Lambda - \alpha_1 W_n S_n - \alpha_2 W_n I_n + \rho\alpha_2 I_n - \mu W_n) \tag{4}$$

$$S_{n+1} = S_n + hf_s(t_n, W_n, S_n, I_n, T_n) = S_n + h(\alpha_1 W_n S_n + \delta I_n - (\vartheta_1 + \mu) S_n) \tag{5}$$

$$I_{n+1} = I_n + hf_I(t_n, W_n, S_n, I_n, T_n) = I_n + h(\alpha_2 W_n I_n - \rho\alpha_2 I_n - (\delta + \vartheta_2 + \mu) I_n) \tag{6}$$

$$T_{n+1} = T_n + hf_T(t_n, W_n, S_n, I_n, T_n) = T_n + h(\vartheta_1 S + \vartheta_2 I_n - \mu T_n) \tag{7}$$

Hence, we set $W(0) = W_0$, $S(0) = S_0$, $I(0) = I_0$ and $T(0) = T_0$ as the initial values of each of the compartments at $t = 0$. We choose the time steps as $h = 0.1, 0.01, 0.001$, and we obtain the numerical solutions of $W(t)$, $S(t)$, $I(t)$ and $T(t)$ we compute $W_{n+1}(t_0) = W_n + hf_1(W, S, I, T)$, $S_{n+1}(t_0) = S_n + hf_2(W, S, I, T)$, $I_{n+1}(t_0) = I_n + hf_3(W, S, I, T)$ and $T_{n+1}(t_0) = T_n + hf_4(W, S, I, T)$ with $h = 0.1$. The sequence of results obtained was used in plotting the graphs shown in the results and discussion section, using Eq. (4) to Eq. (7) while varying the value of h and the number of specified iterations; this resulted in the sequence of solutions that represent the dynamics of each compartment at any given time. The source of the initial values used in this research work for all the compartmental equations was obtained from the source indicated in Section 3.

4.1.1 Procedures for solving the compartmental model using Euler model

Step 1: Formulation of the compartmental equations; compartmental model shown in Eq. (1) is made up of four distinct compartments, each compartment is a unique entity within the system (water pollution), and it is described using a differential equation.

Step 2: Step size (*h*) selection or time discretization; time is the independent value in our studies, and the dynamic of each of the entities in the system is investigated with step-size $h = 0.1, h = 0.01$, and $h = 0.01$. The choice of step size is done randomly so as to investigate the dynamics of the compartmental equations by varying the step size for each simulation.

Step 3: Setting of initial values for each of the compartments, at $t = 0$ the set initial values, as presented in Section 3 for each of the compartments.

Step 4: We then compute the value of each of the compartmental equations iteratively; setting the initial values $W_0, S_0, I_0 and\ T_0$ and the parameters in Table 1 to calculate the subsequent values of $W_n, S_n, I_n\ and\ T_n$, where $n = 1,2,3,4,5...$ until the desired time interval. The is done using

$$
\begin{aligned}
W_{n+1}(t) &= W_n(t) + h.f(t_n, W_n, S_n, I_n, T_n) \\
S_{n+1}(t) &= S_n(t) + h.f(t_n, W_n, S_n, I_n, T_n) \\
I_{n+1}(t) &= I_n(t) + h.f(t_n, W_n, S_n, I_n, T_n) \\
T_{n+1}(t) &= T_n(t) + h.f(t_n, W_n, S_n, I_n, T_n)
\end{aligned}
$$

Step 5: Time is updated using the relation $(t_{n+1} = t_n + h)$ at the end of each iteration. This is continued for the predefined number of iterations of defined time interval, subsequent values of each component are computed and recorded.

Step 6: We plot the graphs of sequences of solutions for $W_n, S_n, I_n \text{ and } T_n$ on the y-axis and against the values t on the x-axis for individual methods.

Step 7: Analysis, interpretation, and visualisation of observable trends in the comparative graphs of each approach are carried out.

4.1.2 Pseudocode for the Euler method

1. *Start*
2. *Define the functions in form of compartmental model*

$$
\begin{aligned}
W_{i+1} &= W_i + hf(W_i, S_i, I_i, T_i) \\
S_{i+1} &= S_i + hf(W_i, S_i, I_i, T_i) \\
I_{i+1} &= I_i + hf(W_i, S_i, I_i, T_i) \\
T_{i+1} &= T_i + hf(W_i, S_i, I_i, T_i)
\end{aligned}
$$

3. *Read values of initial conditions* $\left(W_0, S_0, I_0\ and\ T_0\right)$*, compute number of steps* n *and calculation point* t_n
4. *Calculate step size using* $h = \left(t_n - t_0\right)/n$

5. Set $i=0$ *6. Loop* $W_{i+1}=W_i+h*f(W_i,S_i,I_i,T_i)$ $S_{i+1}=S_n+h*f(W_i,S_i,I_i,T_i)$ $I_{i+1}=I_n+h*f(W_i,S_i,I_i,T_i)$ $T_{i+1}=T_n+h*f(W_i,S_i,I_i,T_i)$ $i=i+1$ *while* $i<n$ *7. Display* $(W_i,S_i,I_i\ and\ T_i)$ *as results*   *8. Stop*

4.1.3 Flow chart of Euler numerical method in solving compartmental model

Figure 3 depicts the steps involved in simulating the model. It lays out the initial conditions, step sizes, parameters and defines the flow rates between each of the compartments. It also specifies how the Euler numerical method updates the compartment sizes at each iteration, based on the relationship between the previous solution and current solution.

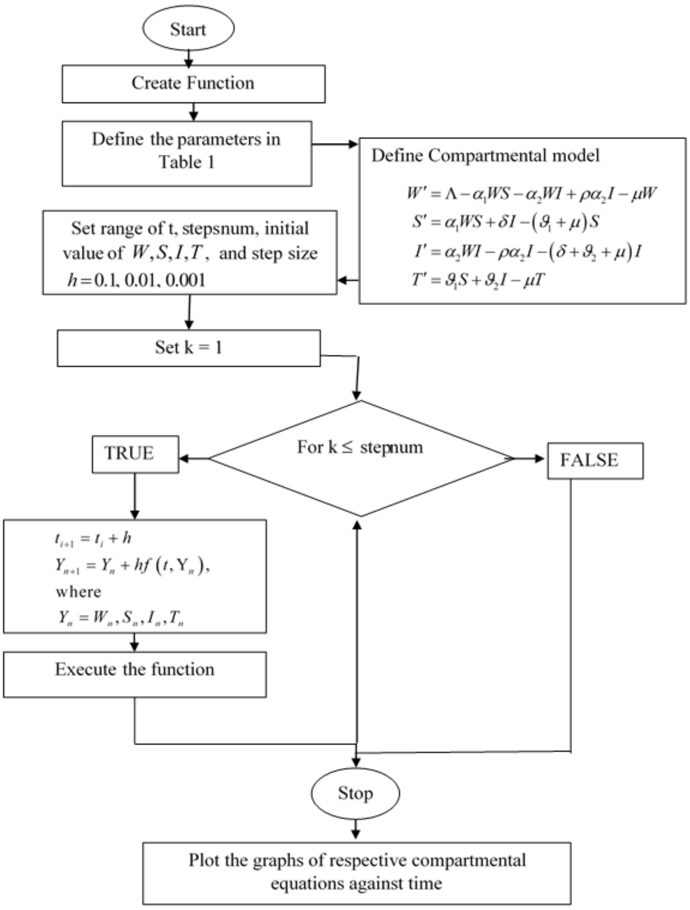


Fig. 3. Flow chart showing Euler method procedures for solving compartmental model

4.2 Runge-Kutta of Order 4 (RK4) Numerical Method

Runge-Kutta is another numerical technique that is well known as an efficient and effective method for solving first-order differential equations with a specified initial condition. The Runge-Kutta technique has the benefit of being the most used numerical method since it provides calculable values, making it especially effective for computing difficult higher-order derivatives [29]. Its provision of better accuracy, when compared to Euler's method in most instances, made it more suitable. Additionally, it is simple to alter the step size for a unique initial value, which cuts down on computation time. Several studies revealed that the Runge-Kutta technique has been deployed in many applications [30,31]. They asserted that the Runge-Kutta fourth-order method (RK4) produced more accurate results. Podisuk [31] asserted in a review of the Euler method, the modified Euler method, and the Runge-Kutta fourth-order method that the Runge-Kutta fourth-order method is the best of the remaining three methods he reviewed. Following the same approach as shown in the Euler method above, we formulate the compartmental model using Runge-Kutta. In general, given that $\frac{dy}{dx} = f(x, y)$ and $y(x_0) = y_0$, Let $n = 0, 1, 2, . . . \in \mathbf{Z}$ and *h* as the step size, the formula to compute the solution of ODE using RK4 is given as

$$y_{n+1} = y_n + \frac{h}{6}\left(k_1 + 2k_2 + 2k_3 + k_4\right). \tag{8}$$

where

$$\begin{aligned}
k_1 &= f(t_i, y_i), \\
k_2 &= f\left(t_i + \frac{h}{2}, y_i + \frac{hk_1}{2}\right), \\
k_3 &= f\left(t_i + \frac{h}{2}, y_i + \frac{hk_2}{2}\right), \\
k_4 &= f\left(t_i + h, y_i + hk_3\right).
\end{aligned}$$

We can approximate the solution at each point using y_{n+1}. We utilized RK4 method to solve the compartmental model from time = 0 to any desired number of times. By modifying the first-order ODE so that, $\frac{dW}{dt} = f_w(t_n, W_n, S_n, I_n, T_n)$, $\frac{dS}{dt} = f_s(t_n, W_n, S_n, I_n, T_n)$, $\frac{dW}{dt} = f_I(t_n, W_n, S_n, I_n, T_n)$ and $\frac{dW}{dt} = f_T(t_n, W_n, S_n, I_n, T_n)$ where W, S, I, T *are* defined above. We transform the compartmental model in Eq. (1) using RK4 and taking $h = t_{i+1} - t_i$ such that

$$W_{n+1} = W_n + \frac{h}{6}\left(k_1^W + 2k_2^W + 2k_3^W + k_4^W\right). \tag{9}$$

where

$$k_1^W = f_W(t_n, \mathrm{W}_\mathrm{n}, S_n, \mathrm{I}_n, T_n) = h(\Lambda - \alpha_1 W_n S_n - \alpha_2 W_n I_n + \rho\alpha_2 I_n - \mu W_n)$$

$$k_2^w = f_W(t_n + \frac{1}{2}\mathrm{h},\ W_n + \frac{1}{2}\mathrm{h}\,k_1^w, S_n + \frac{1}{2}\mathrm{h}\,k_1^s,\ \mathrm{I}_n + \frac{1}{2}\mathrm{h}\,k_1^I, \mathrm{T}_n + \frac{1}{2}\mathrm{h}\,k_1^T)$$
$$= \Lambda - \alpha_1\left(W_n + \frac{1}{2}\mathrm{h}\,k_1^w\right)\left(S_n + \frac{1}{2}\mathrm{h}\,k_1^S\right) - \alpha_2\left(W_n + \frac{1}{2}\mathrm{h}\,k_1^w\right)\left(I_n + \frac{1}{2}\mathrm{h}\,k_1^I\right) + \rho\alpha_2\left(I_n + \frac{1}{2}\mathrm{h}\,k_1^I\right)$$
$$-\mu\left(W_n + \frac{1}{2}\mathrm{h}\,k_1^w\right)$$

$$k_3^W = f_W(t_n + \frac{1}{2}\mathrm{h}, \mathrm{W}_n + \frac{1}{2}\mathrm{h}\,k_2^w,\ S_n + \frac{1}{2}\mathrm{h}\,k_2^s, \mathrm{I}_n + \frac{1}{2}\mathrm{h}\,k_2^I, T_n + \frac{1}{2}\mathrm{h}\,k_2^T)$$
$$= \Lambda - \alpha_1\left(W_n + \frac{1}{2}\mathrm{h}\,k_2^w\right)\left(S_n + \frac{1}{2}\mathrm{h}\,k_2^S\right) - \alpha_2\left(W_n + \frac{1}{2}\mathrm{h}\,k_2^w\right)\left(I_n + \frac{1}{2}\mathrm{h}\,k_2^I\right) + \rho\alpha_2\left(I_n + \frac{1}{2}\mathrm{h}\,k_2^I\right)$$
$$-\mu\left(W_n + \frac{1}{2}\mathrm{h}\,k_2^w\right)$$

$$k_4^W = f_W(t_n + \mathrm{h}, W_n + \mathrm{h}\,k_3^w, S_n + \mathrm{h}\,k_3^s, \mathrm{I}_n + \mathrm{h}\,k_3^I, \mathrm{T}_n + \mathrm{h}\,k_3^R)$$
$$= (\Lambda - \alpha_1\left(W_n + k_3^w\right)\left(S_n + k_3^S\right) - \alpha_2\left(W_n + k_3^w\right)\left(I_n + k_3^I\right) + \rho\alpha_2\left(I_n + k_3^I\right) - \mu\left(W_n + k_3^W\right)$$

For soluble pollutants we have

$$S_{n+1} = S_n + \frac{h}{6}\left(k_1^S + 2k_2^S + 2k_3^S + k_4^S\right). \tag{10}$$

where

$$k_1^S = f_s(t_n, \mathrm{W}_n\, S_n, \mathrm{I}_n, T_n) = S_n + h(\alpha_1 W_n S_n + \delta I_n - \left(\vartheta_1 + \mu\right) S_n),$$

$$k_2^S = f_s\left(t_n + \frac{\mathrm{h}}{2}, \mathrm{W}_n + \frac{\mathrm{hk}_1^W}{2} S_n + \frac{\mathrm{hk}_1^S}{2}, \mathrm{I}_n + \frac{\mathrm{hk}_1^I}{2}, T_n + \frac{\mathrm{hk}_1^s}{2}\right)$$
$$= \alpha_1\left(W_n + \frac{hk_1^W}{2}\right)\left(S_n + \frac{hk_1^S}{2}\right) + \delta\left(I_n + \frac{hk_1^I}{2}\right) - \left(\vartheta_1 + \mu\right)\left(S_n + \frac{hk_1^S}{2}\right)$$

$$k_3^S = f_s\left(t_n + \frac{\mathrm{h}}{2}, \mathrm{W}_n + \frac{\mathrm{hk}_2^W}{2} S_n + \frac{\mathrm{hk}_2^S}{2}, \mathrm{I}_n + \frac{\mathrm{hk}_2^I}{2}, T_n + \frac{\mathrm{hk}_2^s}{2}\right)$$
$$= \alpha_1\left(W_n + \frac{hk_2^W}{2}\right)\left(S_n + \frac{hk_2^S}{2}\right) + \delta\left(I_n + \frac{hk_2^I}{2}\right) - \left(\vartheta_1 + \mu\right)\left(S_n + \frac{hk_2^S}{2}\right)$$

$$k_4^S = f_s(t_n + \mathrm{h}, \mathrm{W}_n + hk_3^w, S_n + hk_3^s, \mathrm{I}_n + hk_3^I, \mathrm{T}_n + hk_3^I)$$
$$= \alpha_1\left(W_n + hk_3^W\right)\left(S_n + hk_3^S\right) + \delta\left(I_n + hk_3^I\right) - \left(\vartheta_1 + \mu\right)\left(S_n + hk_3^S\right)$$

For the insoluble pollutant compartment, we have

$$I_{n+1} = I_n + \frac{h}{6}\left(k_1^I + 2k_2^I + 2k_3^I + k_4^I\right), \quad (11)$$

where

$$k_1^I = f_I(t_n, \mathrm{W_n}, S_n, \mathrm{I}_n, T_n) = \alpha_2 W_n I_n - \rho\alpha_2 I_n - \left(\delta + \vartheta_2 + \mu\right) I_n$$

$$k_2^I = f_I\left(t_n + \frac{\mathrm{h}}{2}, \mathrm{W_n} + \frac{\mathrm{hk}_1^w}{2}, S_n + \frac{\mathrm{hk}_1^s}{2}, \mathrm{I_n} + \frac{\mathrm{hk}_1^I}{2}{}_n, \mathrm{T}_n + \frac{\mathrm{hk}_1^T}{2}\right)$$
$$= \alpha_2\left(W_n + \frac{hk_1^W}{2}\right)\left(I_n + \frac{hk_1^I}{2}\right) - \rho\alpha_2\left(I_n + \frac{hk_1^I}{2}\right) - \left(\delta + \vartheta_2 + \mu\right)\left(I_n + \frac{hk_1^I}{2}\right)$$

$$k_3^I = f_I\left(t_n + \frac{h}{2}, \mathrm{W_n} + \frac{hk_2^W}{2}, S_n + \frac{hk_2^W}{2}, \mathrm{I}_n + \frac{hk_2^I}{2}, \mathrm{T}_n + \frac{hk_2^T}{2}\right)$$
$$= \alpha_2\left(W_n + \frac{hk_2^W}{2}\right)\left(I_n + \frac{hk_2^I}{2}\right) - \rho\alpha_2\left(I_n + \frac{hk_2^I}{2}\right) - \left(\delta + \vartheta_2 + \mu\right)\left(I_n + \frac{hk_2^I}{2}\right)$$

$$k_4^I = f_I(t_n + \mathrm{h}, \mathrm{W_n}, S_n, \mathrm{I}_n, \mathrm{T_n}) = \alpha_2\left(W_n + hk_3^W\right)\left(I_n + hk_2^I\right) - \rho\alpha_2\left(I_n + hk_3^I\right) - \left(\delta + \vartheta_2 + \mu\right)\left(I_n + hk_3^I\right)$$

For the rate of treated water pollutant

$$T_{n+1} = T_n + \frac{h}{6}\left(k_1^T + 2k_2^T + 2k_3^T + k_4^T\right). \quad (12)$$

where

$$k_1^T = f_T(t_n, \mathrm{W_n}, S_n, \mathrm{I}_n, \mathrm{R}_n) = \vartheta_1 S_n + \vartheta_2 I_n - \mu T_n$$

$$k_2^T = f_T\left(t_n + \frac{\mathrm{h}}{2}, \mathrm{W_n} + \frac{\mathrm{hk}_1^W}{2}, S_n + \frac{\mathrm{hk}_1^S}{2}, \mathrm{I_n} + \frac{\mathrm{hk}_1^L}{2}, T_n + \frac{\mathrm{hk}_1^T}{2}\right)$$
$$= \vartheta_1\left(S_n + \frac{hk_1^T}{2}\right) + \vartheta_2\left(I_n + \frac{hk_1^I}{2}\right) - \mu\left(T_n + \frac{hk_1^T}{2}\right)$$

$$k_3^T = f_T\left(t_n + \frac{\mathrm{h}}{2}, \mathrm{W_n} + \frac{\mathrm{hk}_2^W}{2}, S_n + \frac{\mathrm{hk}_2^S}{2}, \mathrm{I_n} + \frac{\mathrm{hk}_2^L}{2}, T_n + \frac{\mathrm{hk}_2^T}{2}\right)$$
$$= \vartheta_1\left(S_n + \frac{hk_2^T}{2}\right) + \vartheta_2\left(I_n + \frac{hk_2^I}{2}\right) - \mu\left(T_n + \frac{hk_2^T}{2}\right)$$

$$k_4^T = f_T(t_n + \mathrm{h}, \mathrm{W_n} + \mathrm{hk}_3^T, S_n + \mathrm{hk}_3^T, \mathrm{I}_n + \mathrm{hk}_3^T, \mathrm{T}_n + \mathrm{hk}_3^T)$$
$$= \vartheta_1\left(S_n + hk_3^T\right) + \vartheta_2\left(I_n + hk_3^I\right) - \mu\left(T_n + hk_3^T\right)$$

Setting $W(0) = W_0$, $S(0) = S_0$, $I(0) = I_0$ and $T(0) = T_0$ as the initial values of each of the compartments at $t = 0$, and $h = 0.1$ using the formula $W_{n+1}(t_0) = W_n + hf_1(W,S,I,T)$, $S_{n+1}(t_0) = S_n + hf_2(W,S,I,T)$, $I_{n+1}(t_0) = I_n + hf_3(W,S,I,T)$ and $T_{n+1}(t_0) = T_n + hf_4(W,S,I,T)$.

The sequence of results obtained for $W(\mathrm{t})$, $S(\mathrm{t})$, $I(\mathrm{t})$ and $T(\mathrm{t})$ were deployed in plotting the graphs shown in the result and discussion section. The Eq. (9) to Eq. (12) were reused with value of $h = 0.01$ and 0.001 for a number of specified iterations. This resulted in a sequence of solutions for each compartment that represent the dynamics of each compartment at any given time. The flow chart below shows the procedure used in developing the model, and the graphs showing the dynamics of each of the compartments are shown in Section 5.

4.2.1 Procedures for solving the compartmental model using the Runge–Kutta method of 4th Order

Step 1: The compartmental model consists of four distinct compartments representing unique entities in a water pollution system, each represented by a differential equation in Eq. (1) illustrating their rate of change over time.

Step 2: Selection of an appropriate step size to determine the progression of each of the compartments over a defined time interval. It is done using time discretization, the step-size used in this research are $h = 0.1, h = 0.01$, and $h = 0.01$.

Step 3: Identify initial values W_0, S_0, I_0 and T_0 for each of the entities in the compartment; the value at $t = 0$ the set initial values, as presented in Section 3.

Step 4: The computation of the dynamic of each of the compartmental equations is done iteratively by first finding the values of the k_i $i = 1,2,3,4$ since we are using the Runge-Kutta method of 4th order.

$$k_1^\omega = f(t_i, W_i, S_i, I_i, T_i),$$
$$k_2^\omega = f\left(t_i + \frac{h}{2}, W_i + \frac{hk_1^\omega}{2}, S_i + \frac{hk_1^\omega}{2}, I_i + \frac{hk_1^\omega}{2}, T_i + \frac{hk_1^\omega}{2},\right),$$
$$k_3^\omega = f\left(t_i + \frac{h}{2}, W_i + \frac{hk_2^\omega}{2}, S_i + \frac{hk_2^\omega}{2}, I_i + \frac{hk_2^\omega}{2}, T_i + \frac{hk_2^\omega}{2}\right),$$
$$k_4^\omega = f\left(t_i + h, W_i + hk_3^\omega, S_i + hk_3^\omega, I_i + hk_3^\omega, T_i + hk_3^\omega\right).$$

where $\omega = (W,S,I,T)$ is taking over each of the compartmental equations in the model, each of the compartments is updated using the formula in Eq. (13).

$$W_{n+1} = W_n + \frac{h}{6}\left(k_1^W + 2k_2^W + 2k_3^W + k_4^W\right).$$

$$S_{n+1} = S_n + \frac{h}{6}\left(k_1^S + 2k_2^S + 2k_3^S + k_4^S\right).$$
$$I_{n+1} = I_n + \frac{h}{6}\left(k_1^I + 2k_2^I + 2k_3^I + k_4^I\right).$$
$$T_{n+1} = T_n + \frac{h}{6}\left(k_1^T + 2k_2^T + 2k_3^T + k_4^T\right). \tag{13}$$

Step 5: We update *t* using the relation $(t_{i+1} = t_i + h)$ at the end of each Iteration. We continue the iterations for a predefined number of time (steps), while the subsequent values of each component are computed.

Step 6: We plot the graphs of sequences of solutions for $W_n, S_n, I_n \text{ and } T_n$ on the y-axis and against the values *t* on x-axis for individual methods.

Step 7: Analysis, interpretation, and visualisation of observable trends in the comparative graphs of each approach are carried out.

4.2.2 Pseudocode for the Runge–Kutta method of 4th Order

1. *Start*
2. *Define the functions in form of compartmental model*

$$W_{i+1} = W_i + hf(W_i, S_i, I_i, T_i)$$
$$S_{i+1} = S_i + hf(W_i, S_i, I_i, T_i)$$
$$I_{i+1} = I_i + hf(W_i, S_i, I_i, T_i)$$
$$T_{i+1} = T_i + hf(W_i, S_i, I_i, T_i)$$

3. *Read values of initial conditions* $\left(W_0, S_0, I_0 \; and \; T_0\right)$, *compute number of steps* n *and calculation point* t_n
4. *Calculate step size* $h = \left(t_n - t_0\right)/n$
5. *Set* $i = 0$
6. *Loop*

for $\omega = (W, S.I, T)$

$$k_1^\omega = f(t_0, W_0, \; S_0, \; I_0, T_0)$$
$$k_2^\omega = f\left(t_0 + \frac{\mathrm{h}}{2}, W_0 + \frac{k_1}{2}, S_0 + \frac{k_1}{2}, I_0 + \frac{k_1}{2}, T_0 + \frac{k_1}{2}\right)$$
$$k_3^\omega = f\left(t_0 + \frac{\mathrm{h}}{2}, W_0 + \frac{k_2}{2}, S_0 + \frac{k_2}{2}, I_0 + \frac{k_2}{2}, T_0 + \frac{k_2}{2}\right)$$
$$k_4^\omega = f\left(t_0 + h, W_0 + k_3, S_0 + k_3, I_0 + k_3, T_0 + k_3\right)$$
$$Y_{i+1} = Y_i + \frac{h}{6}\left(k_1^\varpi + 2k_2^\varpi + 2k_3^\varpi + k_4^\varpi\right) \quad Y = \left(W, S, I, T\right)$$

end

$$W_{i+1} = W_i + K^w$$
$$S_{i+1} = S_i + K^S$$
$$I_{i+1} = I_i + K^I$$
$$T_{i+1} = T_i + K^T$$

$i = i + 1$

while $i < n$

7. Display $\left(W_i, S_i, I_i \text{ and } T_i\right)$ *as results*
8. Stop

4.2.3 Flow chart of Runge–Kutta integrated compartmental hybrid model

Figure 4 shows the initial conditions and parameters used in the model development. Additionally, it depicts the iterative process of the 4th-order Runge-Kutta method, where the model equations are discretized and solved over successive time steps. Each step of the flowchart corresponds to a specific calculation involved in the numerical solution, ranging from evaluating the derivative functions, updating the state variables, and advancing the simulation time. Additionally, the flowchart incorporates decision points to handle termination criteria, leading to the effectiveness and convergence of the solution.

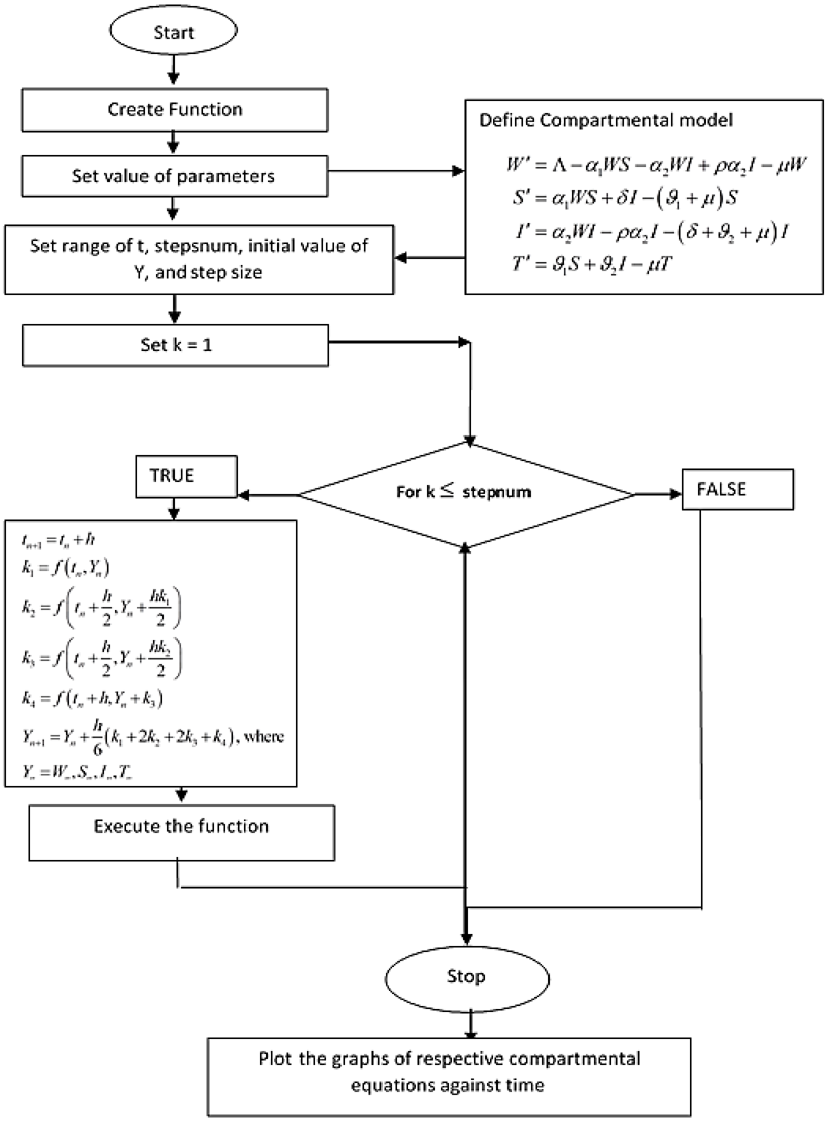
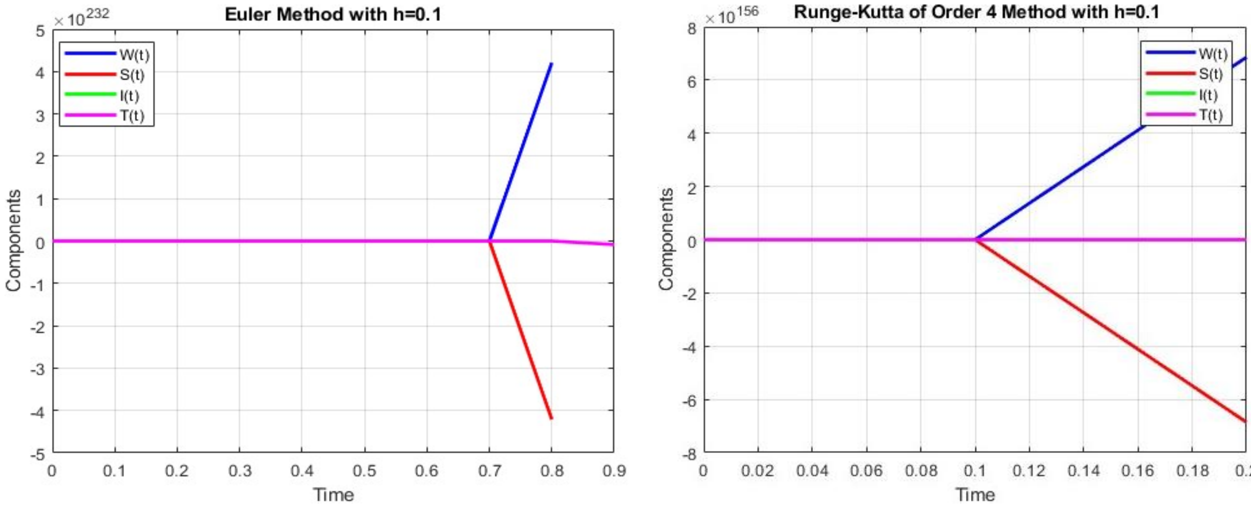


Fig. 4. Flow chart Runge-Kutta method of 4th Order procedures for solving compartmental model

5. Results and Discussion

Using the pseudocodes provided in subsections 4.1.2 and 4.2.2, we obtained the corresponding values of W_n, S_n, I_n *and* T_n as the simulated solutions for both methods, which we deployed to demonstrate the applicability of numerical methods in solving compartmental models and scrutinized the dynamics as well as the behaviour of pollutants in water systems. The compartmental model shown in Eq. (1) and corresponding parameter values detailed in the provided Table 1 were utilized to investigate the responses of water pollutants (W), soluble water pollutants (S), insoluble water pollutants (I), and the rate of treated water pollutants by solving numerically with step sizes ranging from 0.1, 0.01, and 0.001. The discussion of the accuracy of both methods using different step size values is as follows:

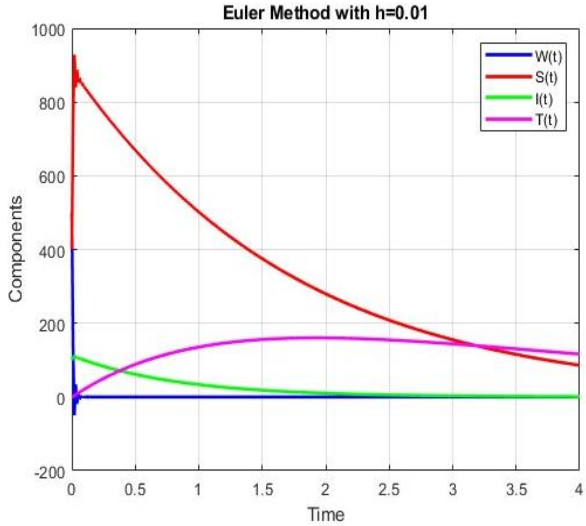
From Figure 5(a) and Figure 5(b), it can be clearly observed that both methods were not able to capture any trend in the data. This can be attributed to the fact that the step size is large, justifying the fact that most numerical techniques work better at approximating the solution of an ODE when the small step size is utilised for each iteration. Overshooting or undershooting might occur if the step size is too large, leading to inaccurate solutions.



(a) Solution with Euler Method (b) Solution with Runge-Kutta order 4

Fig. 5. Compartmental solutions using $h = 0.1$ for Euler method and Runge-Kutta method

In Figure 6(a) and Figure 6(b), we set, $h = 0.01$, Runge-Kutta method approximates the solution better; as seen in Figure 4, the graph of the Runge-Kutta is smoother than that of the Euler method. A closer look at the solution produced by the Euler method shows a negative value for graph $T(t)$ and it has some 'spikes' at the beginning. $W(t)$ attaining some negative values at the beginning invalidates our initial condition. Here, we can only infer that we obtain a better solution when compared with $h = 0.1$. Thus, it can be seen that the Runge-Kutta method provides a better approximated solution when compared to the solution obtained using the Euler method at $h = 0.01$.



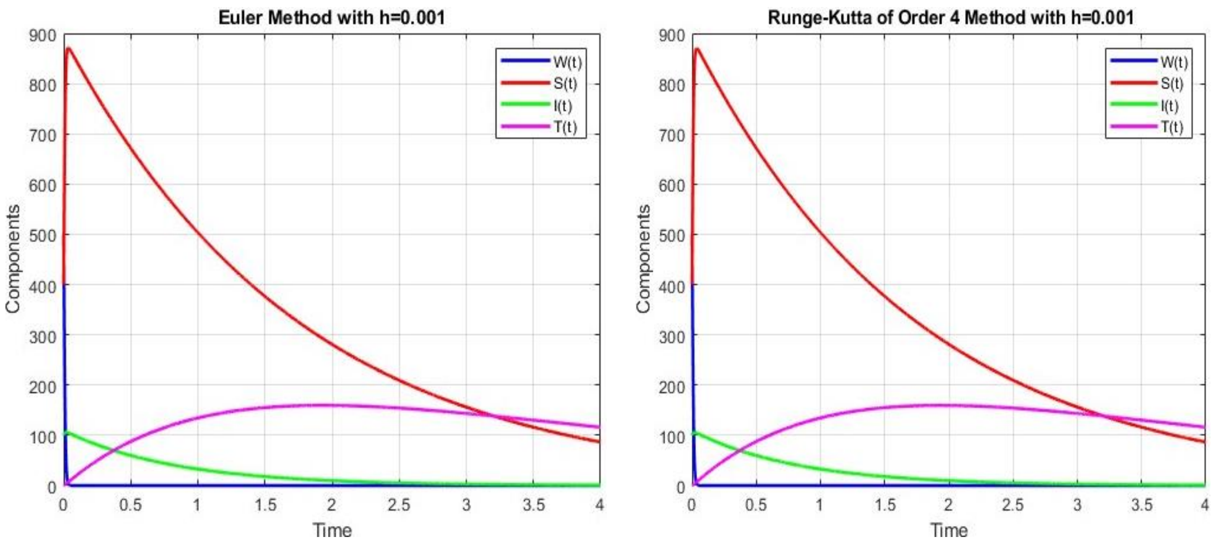
(a) Solution with Euler Method

(b) Solution with Runge-Kutta order 4

Fig. 6. Compartmental solutions using $h = 0.01$ for Euler method and Runge-Kutta method

From Figure 7(a) and Figure 7(b), it can be observed that at $h = 0.001$, the graphs of both methods look similar. Showing the effectiveness of both approaches in providing reasonable approximations when the step size is small, several studies have shown the effectiveness of Runge-Kutta, especially the fourth-order (RK4), as it shows higher accuracy, stability, and versatility [22,24]. They justified their proclamation by citing that the Euler method has an error of order $O(h^2)$ while the Runge-Kutta method has an error of order $O(h^5)$ that is much smaller when compared to the error in the Euler method. We can infer that even with reasonably large step size. The Runge-Kutta method will produce a more accurate result.

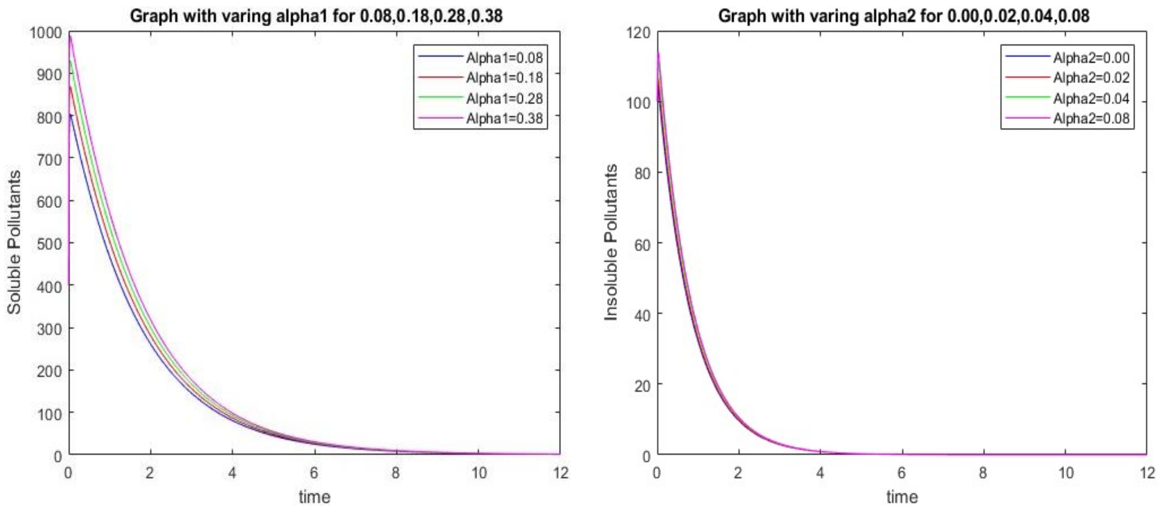
Moreover, from Figure 7(a) and Figure 7(b), it can be seen that as the number of days increases, the concentration of water pollutants does not change much. An indication of equilibrium in the concentration of pollutants as time progresses. Soluble water pollutants increase quickly at first, from 400 mg/l to 900 mg/l, and then decline as the number of day's increases. The sudden increase in soluble water pollution is probably a result of interactions with other pollutants in the water, along with the conversion of insoluble pollutants to solute pollutants. On the other hand, treatment of soluble water pollutants may be responsible for the decline in soluble water pollutants. Also, the curve for insoluble water pollutants slopes downward, justifying the presence of adequate water purification procedures.



(a) Solution with Euler Method
(b) Solution with Runge-Kutta order 4

Fig. 7. Compartmental solutions using $h = 0.001$ for Euler method and Runge-Kutta method

Adequate purification procedures and awareness may contribute to the declining trend in insoluble pollutants, and the conversion of insoluble water pollutants to solutes can also contributed to the decline in it. To clearly visualise the above assumption and hypothesis, we investigate the role plays by the two recruitment agents in our model using Figure 8(a) and Figure 8(b).



(a) Graphs showing perturbation of α_1
(b) Graphs showing perturbation of α_2

Fig. 8. Graph showing solutions of soluble and insoluble compartments with perturbed α_1 *and* α_2 using $h = 0.001$ with Runge-Kutta method of 4th order

One might do a sensitivity analysis and parameter verification to increase the numerical simulation's effectiveness. Sensitivity analysis revolves around how variations in model parameters affect the outcomes of the simulation. Gaining knowledge about important factors and how they affect the model's predictions will help to comprehend how the system behaves. Furthermore, by fitting the simulated results more closely to observable data, parameter estimation techniques may be used to optimise model parameters. Through this iterative process, the simulation's predictive power and accuracy may be improved. The model's dependability and practicality would also be enhanced with the inclusion of real-world data for validation and calibration. It is imperative to investigate the predominant forms of pollution in our studies, namely soluble and insoluble pollutants. These two pollutants contribute massively to the pollution of water bodies. To comprehend the situation and evaluate the implications of the dynamic in water bodies, we alter the parameters that describe the transmission rates of soluble and insoluble pollutants in our compartmental equations. To better grasp the implications, we extended the observation period to 10–12 months and analyzed the effects of varying these transmission rates.

Figure 8(a) illustrates the consequences of different values of the parameter α_1 for 0.08, 0.18, 0.28, and 0.38. Each value produces varying volumes of pollutants available at the 12th month, with (0.08, 1.159) as the lowest and (0.38, 1.5333) highest volume of pollutants, suggesting that implementing better waste disposal policies and purification processes can reduce the transmission rate of soluble water pollutants to a bearable rate. When $\alpha_1 = 0.08$, the available quantity of pollutants in the water has reduced significantly at 12th month compared to the value obtained when α_1 is higher. In a similar manner, Figure 8(b) demonstrates that lower rate of insoluble water contaminants favours treatment and disappearance of pollutants within the water body. This can be achieved by making a policy that disallows unlimited access to activities that can contaminate the water while intensifying treated process, with the value of $\alpha_2 < 0.02$ these pollutants disappear over time.

However, another important thing to be noted here is that an increase in the insoluble water pollutant will facilitate the creation of homes for vectors that can cause diseases, distort ecosystem formation, and cause nuisance to plants and animals, rendering water unfit for consumption and other purposes it is meant for. The combined effect of the impurities in water bodies in the form of soluble and insoluble impurities might increase the turbidity of the water and change the pH of the water, forcing the water to be acidic or alkalinic and causing an increase in live germs with a high tendency to make plants, animals, and humans' sick. This research has demonstrated the effect as a result of the treatment of water pollutants. The decline in both soluble and insoluble pollutants in the water bodies is a result of the treatment compartments, leading to an increase in the volume of water available for usage while preventing disease incidences among the population through water-borne disease in plants and animals. The solution obtained shows good water quality Thus, we can also gain a better understanding of the dynamics of water contamination if the model can incorporate more components, such as changes in the climate, changes in land use, or industrial activity. By adding these elements, the simulation would be more accurate, and the model's predictive power would increase. The model has the potential to be an effective tool for proactive water management plans by including scenarios of anticipated changes in pollution sources and extrapolating existing data patterns.

6. Conclusion

We looked at how the Euler method and the Runge-Kutta methods of order four worked when solving compartmental models related to water pollution transmission. Our main objective revolves around investigation and evaluating the accuracy of these methods in determining which one of them provides a better approximation in the context of the compartment model. The results of our comparison revealed that the Runge-Kutta method outperformed the Euler method in terms of accuracy, even when using a reasonably large step size. This superiority can be attributed to the smaller truncation error associated with the Runge-Kutta method. Therefore, we can confidently state that the Runge-Kutta method is a more reliable approach for solving compartmental models in this specific scenario.

Furthermore, our findings suggest that numerical methods, like the ones utilised in this study, play a crucial role in proffering solutions for differential equations when analytical solutions are difficult or unavailable. Our research demonstrated that numerical methods can produce accurate results, especially when the step size is relatively small. Additionally, we analysed the responses and trends of variations in the solutions obtained for each compartment as the number of days increased. This analysis permitted us to scrutinise the impact of certain parameters on water pollutants. Notably, our study inferred that increasing the treatment rate of both soluble and insoluble water pollutants will facilitate a quicker elimination of pollution from water sources. Overall, our research highlights the significance and trustworthiness of numerical methods in solving complex problems associated with water pollution transmission.

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