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Analysis of Numerical Stability and Step Size Bounds of the Fourth-Order Runge-Kutta in Solving the SEIR Epidemiological Model

Azka Aufa Khoiri[1*] , Oksigeno Phanca Perdana[1], Sri Purwani[2]

[1]Master Program in Mathematics, Faculty of Mathematics and Natural Sciences, Universitas Padjadjaran, Indonesia, 45363

[2]Department of Mathematics, Faculty of Mathematics and Natural Sciences, Universitas Padjadjaran, Indonesia, 45363

E-mail address: azka22005@mail.unpad.ac.id

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ABSTRACT

Mathematical modeling, particularly the SEIR (Susceptible, Exposed, Infected, Recovered) compartmental model, has become an essential tool for understanding the dynamics of infectious disease spread. However, the resulting system of nonlinear ordinary differential equations (ODE) generally lacks analytical solutions, thus requiring numerical approaches. This study analyzes the numerical stability limit and the positivity condition of the fourth-order Runge-Kutta method (RK4) when applied to the SEIR epidemiological model with vaccination intervention. Through a local linearization approach using the Jacobian matrix, the dominant eigenvalues of the system are computed to formulate the RK4 stability limit. Additionally, a more restrictive positivity condition is formulated to prevent the emergence of negative populations, which are biologically meaningless. Numerical simulations are conducted using epidemiological parameters representing an aggressive disease transmission and various time step sizes. The results show that the RK4 numerical stability limit provides a relatively loose upper bound on the step size, whereas the positivity condition yields a much stricter bound. Simulations with small step sizes produce stable and positive solutions; however, when the step size exceeds the positivity limit, sharp oscillations emerge, eventually leading to negative population values, causing the solution to lose its biological meaning. This study concludes that satisfying the numerical stability limit alone is insufficient, and the positivity condition must be prioritized as a criterion in selecting the time step size for epidemiological simulations using the RK4 method.

***Keywords*:** SEIR model, fourth-order Runge-Kutta method, numerical stability, positivity of solution, Jacobian analysis.

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1. INTRODUCTION

Mathematical modeling is a crucial tool for understanding the dynamics of infectious disease spread and formulating public health intervention policies [1]. The foundation of these epidemiological compartmental models was first pioneered by the research of Kermack and McKendrick between 1927 and 1933 [2][3]. One of the most effective frameworks is the SEIR (Susceptible, Exposed, Infected, Recovered) compartmental model, which represents the biological characteristic of an incubation period or latent phase before an individual becomes infectious and transmits the disease [4][5][6]. Therefore, the SEIR approach is highly relevant for application to diseases with specific incubation periods, such as chickenpox, influenza, SARS, and COVID-19 [5]. However, this model produces a complex system of nonlinear ordinary differential equations (ODE) that generally lacks closed-form analytical solutions, thus requiring numerical approaches to approximate the solutions [7].

The fourth-order Runge-Kutta method (RK4) is one of the most widely used algorithms because it offers a balance between computational efficiency and high accuracy [8]. Theoretically, the RK4 method has fourth-order accuracy, which is proven to be far better and more precise than other basic numerical methods, such as the Euler method and Heun's method [9][10]. Nevertheless, the use of RK4 in epidemiological simulations often overlooks fundamental aspects of numerical analysis, namely absolute stability and the positivity condition of the solution [11]. Biologically, population variables must not be negative; however, mathematically, explicit methods such as RK4 can produce unstable solutions or negative values if the chosen discretization step size h exceeds a certain limit derived from the eigenvalues of the system [11]. To mitigate these computational limitations, various nonstandard finite difference (NSFD) schemes and structure-preserving methods have been proposed in recent literature to guarantee the positivity of numerical solutions [12][13][14].

Therefore, this study aims to analyze the theoretical limit of the step size h in the SEIR model. Through a local linearization approach using the Jacobian matrix, the eigenvalues of the system obtained will be used to formulate the positivity condition of the fourth-order Runge-Kutta method. This is important to ensure that the simulation results are not only mathematically accurate but also biologically consistent.

2. MATERIALS AND METHODS

This section explains the theoretical foundation used in this research. The discussion begins with the formulation of the SEIR epidemiological model representing the dynamics of disease transmission. Furthermore, the Fourth-Order Runge-Kutta algorithm used to solve the formulated model is explained.

2.1. SEIR Model

The selection of the SEIR epidemiological model in this study is based on the biological characteristics of infectious diseases that possess a latent period. This model divides the total population (N) into four compartments over time t, namely Susceptible (S), the population of vulnerable individuals, Exposed (E), the population of individuals in the incubation period, Infected (I), the population of infected individuals, and Recovered (R), the population of individuals who have recovered.

The presence of the Exposed (E) compartment makes the SEIR model more representative for modeling epidemic dynamics compared to the basic SIR model. Therefore, this study constructs the SEIR model by modifying the basic SIR model proposed in [15]. This modification integrates the assumptions from [8] and includes an intervention parameter in the form of a vaccination rate. The transition flow of population dynamics among compartments is visualized in Figure 1.

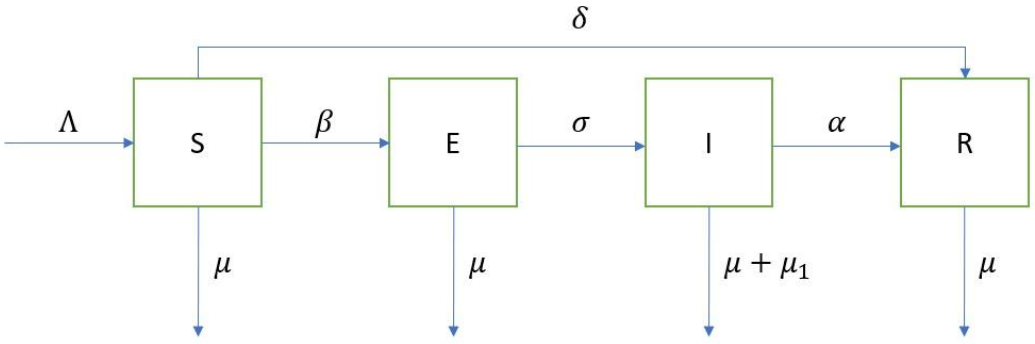

Figure 1. Compartment Diagram of the SEIR Model With Vaccination Intervention.

Based on the compartment diagram above, the rate of change in the number of individuals in each population over time can be formulated into the following system of non-linear Ordinary Differential Equations (ODEs):

$$\frac{dS}{dt} = f_S(t,S,E,I,R) = \Lambda N(t) - \beta S(t)\frac{I(t)}{N(t)} - \mu S(t) - \delta S(t) \quad (1)$$

$$\frac{dE}{dt} = f_E(t,S,E,I,R) = \beta S(t)\frac{I(t)}{N(t)} - \sigma E(t) - \mu E(t) \quad (2)$$

$$\frac{dI}{dt} = f_I(t,S,E,I,R) = \sigma E(t) - \alpha I(t) - \mu_1 I(t) - \mu I(t) \quad (3)$$

$$\frac{dR}{dt} = f_R(t,S,E,I,R) = \delta S(t) + \alpha I(t) - \mu R(t) \quad (4)$$

With the following parameter descriptions:

Λ: Natural birth rate
μ: Natural death rate
β: Infection/transmission rate
σ: Incubation period transition rate
δ: Vaccination rate
α: Recovery rate
μ_1: Disease-induced death rate

2.2. Fourth-Order Runge-Kutta Algorithm

The non-linear ODE system in this study will be solved using the explicit numerical computation method of the Fourth-Order Runge-Kutta (RK4). The general form of the RK4 algorithm for an initial value problem $y' = f(t,y)$ with $y(0) = y_0$ is defined as:

$$y_{n+1} = y_n + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4) \quad (5)$$

where

$$k_1 = f(t_n, y_n)$$
$$k_2 = f\left(t_n + \frac{h}{2}, y_n + \frac{h}{2}k_1\right)$$
$$k_3 = f\left(t_n + \frac{h}{2}, y_n + \frac{h}{2}k_2\right)$$
$$k_4 = f(t_n + h, y_n + hk_3)$$

This algorithm can be used to solve the SEIR model in Equations $(1) - (4)$ by defining the initial value problem:

$$\frac{dy}{dt} = F(t, y), \qquad y(0) = y_0$$

where

$$y(t) = \begin{pmatrix} S(t) \\ E(t) \\ I(t) \\ R(t) \end{pmatrix}, \qquad F(t, y) = \begin{pmatrix} \mathrm{f_S(t, S, E, I, R)} \\ f_E(t, S, E, I, R) \\ f_I(t, S, E, I, R) \\ f_R(t, S, E, I, R) \end{pmatrix}$$

3. RESULTS AND DISCUSSION

3.1. Normalization of the SEIR Model

The SEIR model in Equations $(1) - (4)$ will be normalized to mitigate computational errors such as floating-point overflow and to simplify the search for eigenvalues. By assuming the natural birth rate and natural death rate are balanced ($\Lambda = \mu$), the normalization of the model is carried out through the following steps:

1. The total population at the time of t is defined as $N = S + E + I + R$ so that it is obtained

$$\frac{dN}{dt} = \frac{dS}{dt} + \frac{dE}{dt} + \frac{dI}{dt} + \frac{dR}{dt} = \Lambda N - \mu(S + E + I + R) - \mu_1 I$$
$$\frac{dN}{dt} = -\mu_1 I.$$

2. Let s, e, i, r be new variables representing the proportions of the Susceptible, Exposed, Infected, and Recovered populations, given by the equations:

$$s(t) = \frac{S(t)}{N(t)}, e(t) = \frac{E(t)}{N(t)}, i(t) = \frac{I(t)}{N(t)}, r(t) = \frac{R(t)}{N(t)}$$

so that the total population proportion is $s + e + i + r = 1$. By differentiating the above equations with respect to t, the following system of equations is obtained:

$$\frac{ds}{dt} = \frac{1}{N(t)}\frac{dS(t)}{dt} + \frac{S(t)}{N^2(t)}\frac{dN}{dt}$$
$$\frac{de}{dt} = \frac{1}{N(t)}\frac{dE(t)}{dt} + \frac{E(t)}{N^2(t)}\frac{dN}{dt}$$
$$\frac{di}{dt} = \frac{1}{N(t)}\frac{dI(t)}{dt} + \frac{I(t)}{N^2(t)}\frac{dN}{dt}$$
$$\frac{dr}{dr} = \frac{1}{N(t)}\frac{dR(t)}{dt} + \frac{R(t)}{N^2(t)}\frac{dN}{dt}$$

Thus, the normalized SEIR model is as follows:

$$\frac{ds}{dt} = \mu - \beta si - (\mu + \delta)s \quad (6)$$
$$\frac{de}{dt} = \beta si - (\sigma + \mu)e \quad (7)$$
$$\frac{di}{dt} = \sigma e - (\alpha + \mu_1 + \mu)i \quad (8)$$
$$\frac{dr}{dt} = \delta s + \alpha i - \mu r \quad (9)$$

3.2. Equilibrium Point and Jacobian Linearization

In this section, a search is conducted for a condition where disease transmission is no longer changing, namely by setting the right-hand side of Equations $(6) - (9)$ to zero:

$$\frac{ds}{dt} = 0, \quad \frac{de}{dt} = 0, \quad \frac{di}{dt} = 0, \quad \frac{dr}{dt} = 0 \quad (10)$$

From the solution of the system of Equations (10), the Disease-Free Equilibrium (DFE) point is obtained, which is the condition when there are no sick or infected individuals ($e = 0, i = 0$) as follows:

$$(s_0, e_0, i_0, r_0) = \left(\frac{\mu}{\mu + \delta}, 0, 0, \frac{\delta}{\mu + \delta}\right) \quad (11)$$

Next, the non-linear ODE system in Equations $(6) - (9)$ will be linearized around the DFE point using a 4×4 Jacobian matrix (J) containing the first-order partial derivatives of each function with respect to its variables. By substituting Equation (11) into the Jacobian matrix, we obtain:

$$J = \begin{pmatrix} -(\mu+\delta) & 0 & -\beta\left(\frac{\mu}{\mu+\delta}\right) & 0 \\ 0 & -(\sigma+\mu) & \beta\left(\frac{\mu}{\mu+\delta}\right) & 0 \\ 0 & \sigma & -(\alpha+\mu_1+\mu) & 0 \\ \delta & 0 & \alpha & -\mu \end{pmatrix}$$

Furthermore, the eigenvalues of the Jacobian matrix J will be determined using the characteristic equation formula:

$$\det(J - \lambda I_4) = 0$$

where I_4 is a 4×4 identity matrix. The above equation yields a 4th-degree polynomial that will be solved computationally using Python. From the four obtained eigenvalues, namely $\lambda_1, \lambda_2, \lambda_3, \lambda_4$, the dominant eigenvalue $\lambda_{max} = \sup_{i=1,2,3,4} \{|\lambda_i|\}$ will be selected to represent the stiffness of the system.

3.3. Stability Analysis and RK4 Positivity Condition

The numerical stability analysis of explicit methods such as RK4 fundamentally relies on the algorithm's evaluation against the standard linear test equation, namely:

$$y' = \lambda y, \qquad y(0) = y_0 \tag{12}$$

where λ is the dominant eigenvalue obtained from the Jacobian matrix in the previous step. To determine the stability boundary region, the RK4 algorithm is used to solve Equation (12). By defining the function $f(t, y) = \lambda y$, the value of each k will be determined:

$$\begin{aligned} k_1 &= f(t_n, y_n) = \lambda y_n \\ k_2 &= f\left(t_n + \frac{h}{2}, y_n + \frac{h}{2}k_1\right) = \lambda y_n \left(1 + \frac{1}{2}h\lambda\right) \\ k_3 &= f\left(t_n + \frac{h}{2}, y_n + \frac{h}{2}k_2\right) = \lambda y_n \left(1 + \frac{h\lambda}{2} + \frac{(h\lambda)^2}{4}\right) \\ k_4 &= f(t_n + h, y_n + hk_3) = \lambda y_n \left(1 + h\lambda + \frac{(h\lambda)^2}{2} + \frac{(h\lambda)^3}{4}\right) \end{aligned}$$

By substituting the respective k values obtained into Equation (5), we obtain:

$$\begin{aligned} y_{n+1} &= y_n + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4) \\ &= y_n + \frac{h}{6}\left(\lambda y_n + 2\lambda y_n \left(1 + \frac{1}{2}h\lambda\right) + 2\lambda y_n \left(1 + \frac{h\lambda}{2} + \frac{(h\lambda)^2}{4}\right)\right. \\ &\qquad \left. + \lambda y_n \left(1 + h\lambda + \frac{(h\lambda)^2}{2} + \frac{(h\lambda)^3}{4}\right)\right) \end{aligned}$$

$$= \left(1 + h\lambda + \frac{1}{2}(h\lambda)^2 + \frac{1}{6}(h\lambda)^3 + \frac{1}{24}(h\lambda)^4\right) y_n$$

For the solution to converge towards the equilibrium point, it must hold that $\left|y_{n+1}\right| < |y_n|$. Recalling that λ in Equation (12) is the dominant eigenvalue, the RK4 stability bound is obtained as:

$$\left|1 + h\lambda_{max} + \frac{1}{2}(h\lambda_{max})^2 + \frac{1}{6}(h\lambda_{max})^3 + \frac{1}{24}(h\lambda_{max})^4\right| < 1 \quad (13)$$

Inequality (13) will be solved computationally using Python to find the limit for the step size h. In addition to numerical stability, a bound for the value of h will also be sought so that the population does not take negative values, in order to maintain the biological meaning of the model (preserving population positivity). This positivity condition is fundamentally derived from the first-order approximation (evaluated at stage k_1) within the RK4 discretization scheme. This is because Inequality (13) only guarantees the convergence of the final value at the next iteration (y_{n+1}). In Inequality (13), a large step size might still produce a positive final value due to the presence of even-degree terms, even though the intermediate population values evaluated at stage k_2 or k_3 have already become negative. If these intermediate populations are negative, the RK4 algorithm stages will carry these negative numbers into the calculation of the transmission interactions, thereby destroying the validity of the iteration halfway through. Therefore, to prevent oscillations that cause population values to become negative, the value of h must be forced in such a way that the first-order approximation value remains positive, namely:

$$1 + h\lambda_{max} > 0 \quad (14)$$

The bound for the value of h obtained from Inequality (14) is predicted to be the limit at which the RK4 method produces negative populations.

3.4. Parameter Estimation and Numerical Simulation

Based on the steps previously conducted, numerical simulations are performed with parameter values obtained from other literature, varying the value of h. This study adopts basic epidemiological parameters from the study [6], which models the aggressive transmission in the early phase of an outbreak. The details of the biological parameters, and initial population proportions evaluated in this computation can be seen in Table 1.

Table 1. Parameters and Initial Values for Numerical Simulation.

Parameter	Values	References
β	0.75	[6]
σ	0.333	[6]
α	0.125	[6]
μ_1	0.006	[6]
μ	0.00006	Assumed
δ	0.001	Assumed
$s(0)$	0.99	Assumed
$e(0)$	0.009	Assumed
$i(0)$	0.001	Assumed
$r(0)$	0	Assumed

By substituting these parameters into the Jacobian matrix around the DFE point, the absolute dominant eigenvalue is obtained as $|\lambda| = 0.34$. Through Equation (13), the step size bound to keep the system computationally stable is $h < 8.19$. Meanwhile, based on the first-order approximation positivity condition in Equation (14), a much stricter tolerance limit is obtained to ensure the population maintains its biological meaning, namely $h < 2.94$.

Numerical simulations are run across several scenarios of time step size h to validate the theoretical bounds of stability and positivity. The dynamics of the population compartments respond differently to changes in the value of h, which visually demonstrates the transition of the explicit method's failure on a non-linear system. Illustrations of the conducted simulations are presented in Figures 2-4.

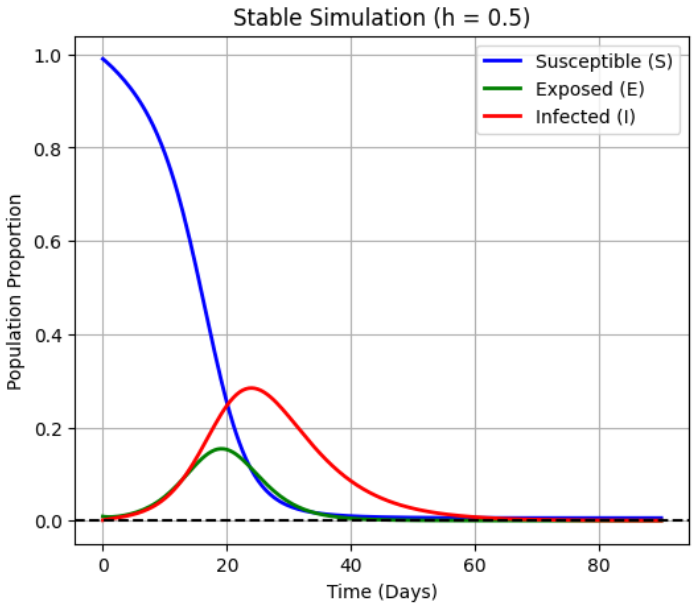

Figure 2. Graph of Population Dynamics of Susceptible, Exposed, Infected Using Step Size $h = 0.5$

In Figure 2, a simulation is performed with a step size of $h = 0.5$. This step size is chosen to be far below the analytical thresholds for both positivity and stability. The simulation curves represent a smooth and biologically meaningful transmission dynamic, where the infected (I) and exposed (E) compartments experience a rise before eventually declining towards extinction (the DFE point) without any numerical anomalies.

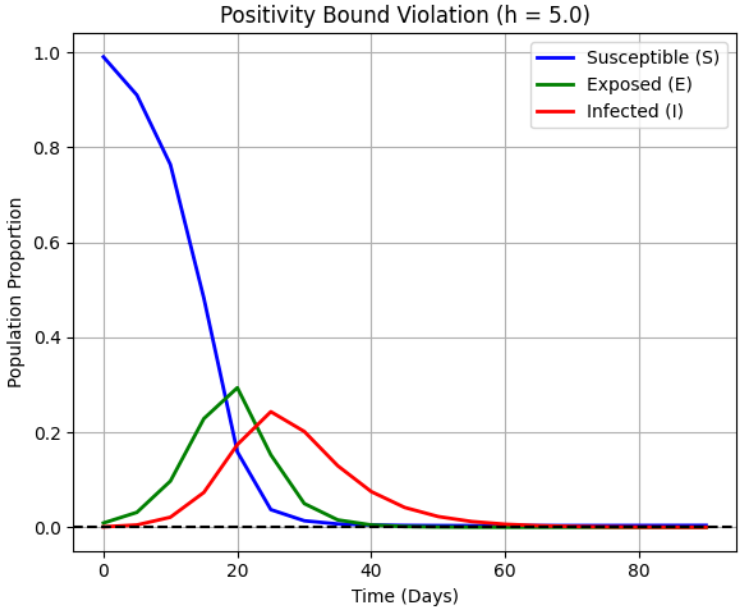

Figure 3. Graph Of Population Dynamics of Susceptible, Exposed, Infected Using Step Size $h = 5.0$

Figure 3 presents the second simulation conducted using a step size of $h = 5.0$. At this point, the step size has exceeded the first-order approximation positivity bound. Nevertheless, it can be seen that no population has yet breached the negative region.

This aligns with the analysis in the previous section, where the final solution value can still remain positive due to the presence of even-degree terms. Even though the population at the end of the iteration avoids negative values, the evaluation at the intermediate stages has experienced significant numerical deviation. The computational breakdown caused by this negative intermediate population is visible in the form of a sharp oscillation at the peak of the Exposed (E) compartment. In terms of biological meaning, this is unrealistic because the number of individuals in the incubation period that is currently rising would not suddenly drop drastically in just a few days. This indicates that the RK4 algorithm is beginning to experience difficulties in balancing the overshoot error.

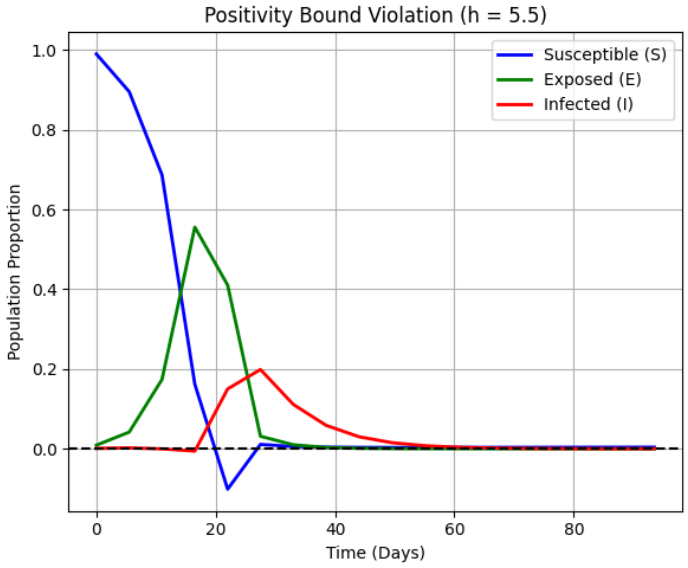

Figure 4. Graph Of Population Dynamics of Susceptible, Exposed, Infected Using Step Size $h = 5.5$

The fatal violation of the positivity bound is empirically confirmed in the third simulation using $h = 5.5$, which is presented in Figure 4. At this step size, the Susceptible (S) curve plunges sharply, crossing the zero axis into the negative domain right during the peak of the outbreak infection. This condition proves the occurrence of a loss of positivity in the population. Although the RK4 algorithm can still continue the population calculation using Equation (5), in the real world, a negative population is impossible, and thus the obtained model solution loses its interpretation.

Based on all the experiments conducted, conclusions can be drawn regarding the use of the RK4 method in solving epidemiological models. Merely satisfying the stability bound is apparently not enough to ensure that the obtained solution holds biological meaning. There are other criteria that are more crucial and have stricter bounds, namely requiring the system to maintain population positivity. The positivity condition in Inequality (14) mathematically only acts as a necessary condition to guarantee the positivity of the final solution. This means that a violation of this bound does not immediately produce a negative population value, even though the intermediate stages of the RK4 algorithm have experienced numerical deviations, as seen in the second simulation. When the RK4 algorithm fails to maintain this bound, the negative numbers will also become part of the calculation in the disease transmission interaction in the subsequent iteration. Given that the model requires a positive population from the start, the generated solution will no longer make sense.

This computational anomaly will eventually cause the solutions of other compartments to suffer the same impact. Therefore, in designing simulations for diseases with aggressive transmission rates, determining the computational time step size must be prioritized to prevent the emergence of negative values from the very beginning of the calculation.

4. CONCLUSIONS

This research has proven that, in solving the system of non-linear ordinary differential equations (ODEs) in the SEIR epidemiological model, satisfying the stability bound of the Fourth-Order Runge-Kutta (RK4) method is not sufficient to guarantee the validity of the biological meaning of a simulation. Through Jacobian matrix linearization and numerical simulations using aggressive outbreak transmission parameters, it is shown that the step size bound h required to satisfy the positivity condition is stricter than its stability bound. The algorithm's failure to maintain this positivity not only results in anomalies in the form of negative populations, which are biologically impossible, but also triggers a flaw in the solution because the negative numbers become part of the disease transmission rate calculation in the subsequent iteration. Thus, preserving population positivity becomes a necessary condition that must be established so that the solution generated from the simulation holds biological meaning.

AI Disclosure Statement

During the preparation of this manuscript, the authors utilized Google Gemini tools to assist in the development and writing of the programming code used for the numerical simulation. The authors have directly verified, thoroughly tested all generated code, and take full legal and ethical responsibility for the accuracy, integrity, and originality of the simulation results and the overall manuscript.

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