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Author (s): Kaniz Fatima[1], Basit Ali[2], Sarwat Ishaque[3], Asif Sumeer[4], and Qaiser Hafeez[5]

Affiliation (s):
[1]Department of Humanities and Social Sciences, Bahria University, Karachi Campus, Pakistan
[2]Department of Electrical Engineering, Bahria University, Karachi Campus, Pakistan
[3]Khadim Ali Shah Bukhari Institute of Technology (KASBIT), Karachi, Pakistan
[4]Shaheed Zulfiqar Ali Bhutto Institute of Science and Technology University, Gharo Campus, Karachi, Pakistan
[5]Mari Energies Limited, Islamabad, Pakistan

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Comparative Assessment of Adams-Bashforth-Moulton, 4th Order Runge-Kutta, and Euler Methods for the Synthesis of Zinc Oxide Nanostructures *via* the Lengyel Epstein Reaction Model

Kaniz Fatima[1], Basit Ali[2*], Sarwat Ishaque[3], Asif Sumeer[4], and Qaiser Hafeez[5]

[1]Department of Humanities and Social Sciences, Bahria University Karachi campus, Karachi, Pakistan
[2]Department of Electrical Engineering, Bahria University Karachi Campus, Karachi, Pakistan
[3]Department of Computer Science and Information system, KASBIT, Karachi, Pakistan
[4]Department of Management Sciences, Shaheed Zulfiqar Ali Bhutto Institute of Science and Technology University University Gharo campus, Karachi, Pakistan
[5]Mari Energies Limited, Islamabad, Pakistan

ABSTRACT

The current study aimed to determine which approximation technique is the most successful in studying the rise in ion concentrations in forms of Zinc Oxide (ZnO) nanostructures using the Lengyel Epstein Reaction Model. To achieve this objective, Ordinary Differential Equations (ODEs) were formulated utilizing three separate numerical methods. These included Euler, Adams-Bashforth-Moulton (ABM), and 4th Order Runge-Kutta (RK) methods. The current study aimed to identify the optimal approximation approach for computing concentrations of zinc ions Zn^{+2} and hydroxyl ions OH^- while examining the reaction kinetics of ZnO nanostructures. The research findings indicated that the ABM approach surpasses the Euler and RK methods, convergence speed, and reduced error relative to the Euler and RK methods. The ABM approach further verifies experimental findings about ZnO nanostructure synthesis by the aqueous chemical growth (ACG) process, that affirms its efficacy practically.

Keywords: Adams-Bashforth-Moulton (ABM) Method, aqueous chemical growth (ACG), Euler method, Lengyel Epstein Reaction Model, 4th Order Runge-Kutta (RK) method, Zinc Oxide nanostructures (ZnO)

Highlights

- The study formulates and solves the Lengyel–Epstein reaction model for ZnO nanostructure synthesis using three numerical schemes (Euler, 4th order Runge–Kutta, and Adams–Bashforth–Moulton) to track Zn^{2+} and OH^- concentration dynamics.

*Corresponding Author: Basitali.bukc@bahria.edu.pk

- Quantitative error analysis against reference solutions shows that the multistep Adams–Bashforth–Moulton method achieves the lowest absolute percentage errors and fastest convergence, outperforming both Euler and 4th order Runge–Kutta for this nonlinear kinetic system.
- By linking numerical performance to experimentally observed aqueous chemical growth behavior, the work establishes Adams–Bashforth–Moulton as the most reliable computational tool for accurately modeling ZnO nanostructure growth kinetics.

1. INTRODUCTION

Due to heavy technological development, new materials are discovered in order to support the growing industrial demands [1]. Zinc oxide (ZnO) is one of the fundamental chemicals which is remarkably beneficial in a variety of technologies, thereby cementing its place in the contemporary world. ZnO is distinguished by its white granular form, which is incapable to be dissolved in water. Nevertheless, it can be readily dissolved in mild acids and bases. ZnO nanoparticles exhibit superior physical and chemical properties in comparison to other metal oxides due to their small dimension of less than 100 nm. ZnO is a critical component of numerous industries, such as glass and paint, optical materials, polymers, plastics, batteries, as well as coatings and cosmetics due to its distinctive quality [2].

ZnO nanoparticles are becoming more and more important in medicine, especially in the quickly growing areas of cancer and antimicrobial therapies. Its unique capacity to produce reactive oxygen species (ROS) and release zinc ions indicates that it may be an effective therapeutic agent. ZnO nanoparticles may improve diabetes treatment by changing insulin level in the body [3, 4]. ZnO has several unique qualities since it is a natural semiconductor. It can conduct electricity, detect chemicals, make piezoelectricity, and be photosensitive. No matter what the temperature is around them, ZnO nanoparticles give forth a glowing light. They have a band gap of 3.4 to 3.7 eV and a large excitonic binding energy [5]. The band gap renders ZnO an effective UV absorber, making it a valuable component in sunscreens, skin creams, and wound-healing ointments. ZnO nanoparticles have several medicinal advantages and may potentially serve as medication carriers due to their exceptional biocompatibility, as validated by the US Food and Medication Administration [6, 7].

Nanostructures made of ZnO are considerably helpful in finding gases,

such as hydrogen, nitrogen dioxide, carbon monoxide, and ethanol. They could swiftly interact with gases in the air since they are tiny and have a lot of surface area. Moreover, it can be discovered that what kind of gas is present in the material along with its quantity by measuring how much electricity it can hold. This transformation happens when a gas touches the ZnO surface. These sensors are easy to manufacture, perform well in the cold, as well as respond rapidly. ZnO is good for medical equipment that checks breath, industrial gas leak detectors, and air pollution monitors due to these qualities.

ZnO nanoparticles have several uses. Furthermore, they need to be made in large quantity. The aqueous chemical growth (ACG) approach stands out among low temperature synthesis procedures. This is because it works well and may be used in many different ways. The ACG method's strict control over growth conditions renders it possible to make a wide range of ZnO nanostructures, such as nanorods, nanotubes, nanowires, and nanospheres [8]. Nanostructures of ZnO have received considerable attention due to their unique features. These are cheaper, safer, easy to make, highly-biocompatible, have high electron transfer rates, and are able to do better analysis [9]. By optimizing the growing conditions, many morphologies of ZnO may be produced [10, 11].

Mathematical analysis of the Lengyel Epstein reaction model may also be used to look at the making of ZnO nanostructures. This model helps figure out how much zinc ions Zn^{+2} and hydroxyl ions OH^{-} are there in a solution. Moreover, it also helps grasp the many processes that are followed into making ZnO nanostructures in practical math modeling [12]. The differential equations used in this model can be solved by using different numerical techniques. Euler's method has been consistently used to predict the concentrations of ions in this model. The other numerical techniques can also be used in Lengyel Epstein reaction model to determine the concentration of zinc ions Zn^{2+} and hydroxyl ions OH^{-}.

In this study, ABM method and 4th Order Runge-Kutta method were used to solve the differential equations of the model. The comparison of Euler's method with ABM method and the RK method was carried out. This combination of methodologies is designed to not only enhance the accuracy and durability of the modeling process but also to identify the complex forces that are causing the absorptions of Zn ions and hydroxyl ions to change over time. This novel approach aims to enhance the understanding

of the development of ZnO nanoparticles, thereby establishing a connection between theoretical concepts and practical observations.

The ABM method is used to attain efficiency and accuracy of higher level. This method includes the predictor and the corrector steps. In the predictor step, it estimates the solution by using previous values and the corrector step refines the estimated values. Due to this reason, this method provides more stability and accuracy in the model. This method is widely used in the modeling of non-linear dynamic systems [13]. In recent years, the Lengyel Epstein reaction model has been used to investigate the self-organization processes that include the formation of ZnO nanostructures that go beyond chemical oscillations. It helps in explaining how the size, shape, and arrangement of ZnO nanostructures during synthesis are influenced by reaction diffusion interactions between ions. The model offers a simple but effective mathematical method to understand how chemical reactions and diffusion work together to regulate the production and structuring of nanomaterial [14, 15].

1.1. Experimental Procedure

To synthesize ZnO nanoparticles, the upkeep of a controlled environment is basic due to the characteristic helplessness of the ACG strategy to barometrical impacts. In this strategy, a flawless gold-coated glass substrate is utilized to play down contaminants. The gold-coated glass substrate is submerged in an arrangement of low concentration hydrofluoric corrosive. As a result, the substrate is first subjected to an intensive acetone cleaning process and subsequently dried with nitrogen gas at ambient temperature. With the basis laid, the substantive preparation unfurls, starting by implying the spin coating strategy. Utilizing rotational speeds of 4500 revolutions per minute, a mixture of Zinc acetate is added to the substrate through numerous cycles of spin coating. Post-application, the substrate is subjected to a temperature of 70°C, advancing the stabilization of the solution [12].

In the interim, a solution is carefully prepared by mixing hexamethylenetetramine and Zinc Nitrate in equal amounts in a container. When it is combined with 250 ml of deionized water, it gets a ready-to-use solution. Then, using a specific holder, the pre-coated substrate is introduced to the combined solution. After being immersed, the container is put in an oven that has been warmed to 100°C and left there for 7 hours.

After the synthesis phase, the oven is switched off for 30 minutes to cool down. At the completion of this process, the substrate is no longer attached to the holder. The final result is a coating of ZnO nanorods [16–18].

A transformational evolution happens when the pH of the solution is regulated by the addition of 25% ammonia solution. This pH manipulation causes the formation of ZnO nanowires, which broadens and diversifies the scope and variety of the synthesized nanostructures. Two ions are required for the production of ZnO. The first is zinc ion (Zn^{+2}), whereas the second is hydroxyl ion (OH^-). After the disintegration of zinc nitrate, Zn^{+2} may be produced from metal salt as explained in equation 1-5 [19].

$$Zn(NO_3)_2.6H_2O + 6H_2O \rightarrow Zn^{+2} + 2NO_3^- \quad (1)$$

Afterwards, the hydrothermal division of HMT, OH^- may occur.

$$(CH_2)_6N_4 + 6H_2O \rightarrow 6HCHO + 4NH_3 \quad (2)$$

$$NH_3 + H_2O \rightarrow NH_4 + OH^- \quad (3)$$

ZnO can be generated with the statement of both ions.

$$2OH^- + Zn^{+2} \rightarrow Zn(OH)_2 \quad (4)$$

$$Zn(OH)_2 \rightarrow ZnO\ (s) + H_2O \quad (5)$$

2.MATHEMATICAL MODEL

An analytical model may also be utilized to illustrate the growing rate of the Zn^{+2} and OH^- concentrations that are desirable for the synthesis of ZnO [5]. The Lengyel reaction model is applied for this analytical model. Euler's and RK methods are applied as analytical methods in this model to approximate the results in the reference [12]. The ABM method was employed in this study to estimate the increase of zinc ion and hydroxyl ion. The subsequent equations were utilized to build the model:

$$NH_3 + H_2O \rightarrow NH_4^+ + OH^- \quad (6)$$

$$Zn(NO_3)_2.6H_2O + 6H_2O \rightarrow Zn^{+2} + 2NO_3^- \quad (7)$$

$$2OH^- + Zn^{+2} \rightarrow ZnO + H_2O \quad (8)$$

The differential equations derived in [11] using the Lengyel Epstein reaction model are as follows: where x and y indicate the concentrations of $OH^-$and Zn^{+2}, respectively.

$$\frac{dx}{dt} = f(x, y) = a_1 - x - 4\left(\frac{xy}{(1+x^2)}\right) \tag{9}$$

$$\frac{dy}{dt} = g(x, y) = a_2 x\left(1 - \frac{y}{(1+x^2)}\right) \tag{10}$$

The suggested differential equations were built using the theory presented by Carmen Chicone in [20]. The differential equations above are affected by the values of a_1 and a_2. To calculate the steady-state concentrations, use $a_2 > \frac{3a_1}{5} - \frac{25}{a_1}$. The experimental development of ZnO was observed to end at a given time period and to exhibit linear behavior [21, 22].

While utilizing a computer to solve ODEs, many methods exist to provide approximate solutions at distinct time intervals. It examines the efficacy of three prevalent methodologies including Euler's method, RK method, and ABM method that concentrate on their efficacy in examining the growth kinetics of ZnO nanostructures.

2.1.Euler's Method

It is a fundamental numerical approach for approximating the solution of ODEs by linearly extrapolating from the present position using the derivative. Despite its apparent simplicity, Euler's approach can result in severe inaccuracies, particularly when working with stiff equations or complex dynamics. Euler's approach may provide basic insights in the context of ZnO nanostructure formation. However, it is restricted in precision and accuracy.

2.2.4th Order Runge-Kutta Method

This method is a commonly-used numerical integration method that is better than Euler's method in terms of accuracy. Four intermediary steps are required to estimate the next point. These methods are ultimate for solving ODEs with moderate to complicated problems. RK gives a more accurate depiction of the behavior of the system than Euler's method when applied to the growth kinetics of ZnO nanostructures.

2.3.Adams-Bashforth-Moulton Method

This method is a numerical approach for solving ODEs by integrating a system of equations across discrete time steps. The ABM method was used deliberately in this study to improve the computational efficiency of the

Lengyel reaction model for the growth kinetics of ZnO nanostructures. Using the ABM method, the following processes can be used to determine the growth rate of ZnO at each time step. When utilizing a computer to solve ODEs, many methods exist to provide approximate solutions at distinct temporal points.

The predictor step employs a fourth-order-ABM method to predict the values of x and y at the next step. The predictor formula for 'x' is given by:

$$x_{pred} = x_i + \frac{\Delta t}{24}(55f_i - 59f_{i-1} + 37f_{i-2} - 9f_{i-3}) \tag{11}$$

The predictor formula for 'y' is given by:

$$y_{pred} = y_i + \frac{\Delta t}{24}(55g_i - 59g_{i-1} + 37g_{i-2} - 9g_{i-3}) \tag{12}$$

Here, f_i and g_i depicts the evaluated results of the equations rate at time t_i.

Using the predicted values x_{pred} and y_{pred} from the predictor step, a corrected estimate for **x** and **y** is obtained using the ABM corrector formula:

$$x_{i+1} = x_i + \frac{\Delta t}{24}\left(9f_{pred} + 19f_i - 5f_{i-1} + f_{i-2}\right) \tag{13}$$

$$y_{i+1} = y_i + \frac{\Delta t}{24}\left(9g_{pred} + 19g_i - 5g_{i-1} + g_{i-2}\right) \tag{14}$$

The combination process continues over the specified period of time, that refines the values of x and y using the estimated and corrected predictions.

Table 1 shows how the three numerical approaches used in this study, that is ABM, RK, and Euler's method were compared to each other. This table shows how well each method works, how accurate they are, and novel formulas, especially when coupled with the Lengyel Epstein reaction model to show how ZnO is made.

Table 1. Comparison of Numerical Methods with their Formulas and Order of Accuracy

Method	Formula	Order of Accuracy	Remarks
Euler's Method	$y_{n+1} = y_n + h\,f(t_n, y_n)$	1st order	It is simple and fast but has less accuracy.

Method	Formula	Order of Accuracy	Remarks
4th Order Runge-Kutta Method	$y_{n+1} = y_n + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)$ $k_1 = h\,f(x_n, y_n)$ $k_2 = h\,f\left(x_n + \frac{h}{2},\ y_n + \frac{k_1}{2}\right)$ $k_3 = h\,f\left(x_n + \frac{h}{2},\ y_n + \frac{k_2}{2}\right)$ $k_4 = h\,f(x_n + h,\ y_n + k_3)$	4th order	It is a multi-step method but very accurate and widely used in nonlinear systems.
Adams-Bashforth-Moulton Method	Predictor formula: $y_{n+1}^{p} = y_n + \frac{\Delta t}{24}(55f_n - 59f_{n-1} + 37f_{n-2} - 9f_{n-3})$ Corrector formula: $y_{n+1}^{C} = y_n + \frac{\Delta t}{24}(9f_{n+1}^{p} + 19f_n - 5f_{n-1} + f_{n-2})$	4th order	It is a multistep method, has high accuracy, and is efficient for long time integration. However, it requires initial values.

3.RESULTS

This study analyzed how well different numerical approaches can simulate the amounts of hydroxide ions OH^- and zinc ions Zn^{+2} over time. The study not only aimed to determine how accurate each approach is but also how effectively they show the main dynamics of the chemical system. Figure 1 shows the reference numerical solution, which may be used as a point of reference. This answer says that the lowest amount of OH^- is 0.3808 at about 1.19 hours, while the maximum amount of Zn^{+2} is 1.30732 at around 0.41 hours. These figures are used as benchmark references against which other approaches are evaluated.

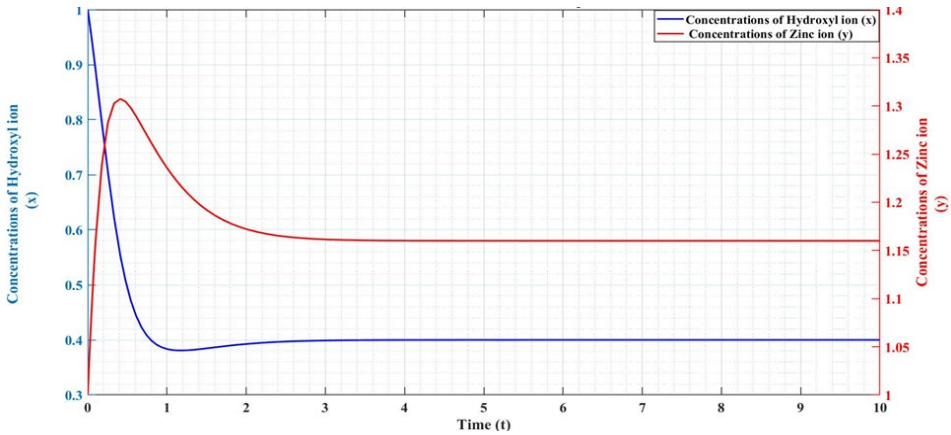

Figure 1. Reference Numerical Solution for Concentrations of Zn^{+2} and OH^{-}

Figure 2 illustrates the findings of Euler's method. It gets the timing of these events right but it greatly underestimates the concentration of OH^{-} (0.379341) and overestimates the concentration of Zn^{2+} (1.314709). This is not surprising given that individuals know that Euler's method is simple but not particularly accurate. It is a fast method to get an estimate but it is not an ideal solution if accuracy needs to be achieved.

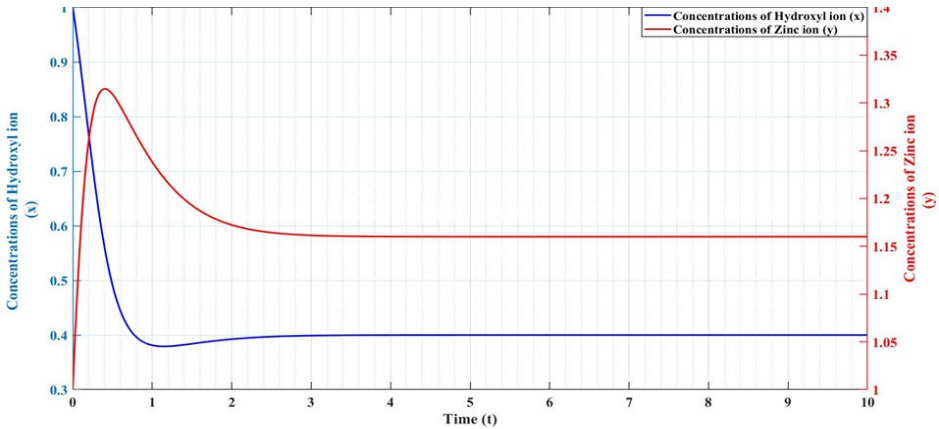

Figure 2. Euler's Method Concentrations of Zn^{+2} and OH^{-}

On the other hand, the RK method, presented in Figure 3, performs significantly better. The results it produces 0.380547 for OH^{-} and 1.309011 for Zn^{2+} are very close to the values of the reference numerical solution. This method strikes a great balance between accuracy and computational effort, making it a strong choice for problems like this where detail matters.

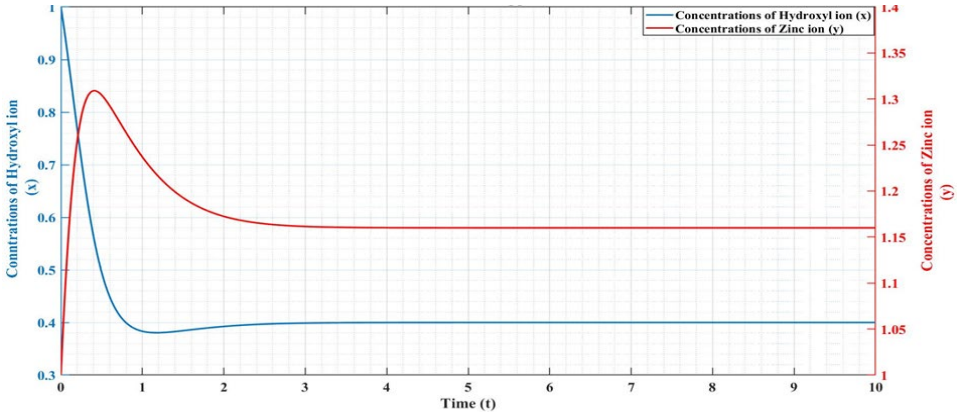

Figure 3. RK Method Concentrations of Zn^{+2} and OH^{-}

Similarly, the ABM method, shown in Figure 4, also delivers impressive accuracy. The minimum OH^{-} concentration is estimated at 0.3806, whereas the highest Zn^{+2} concentration is 1.30886, closely aligning with the precise solution. This multi-step technique leverages knowledge from preceding phases to enhance its predictions. It estimates the minimum OH^{-} concentration as 0.3806 and the maximum Zn^{+2} concentration as 1.30886, virtually matching the reference numerical solution. As a multi-step approach, it benefits from using information from earlier steps to improve its predictions.

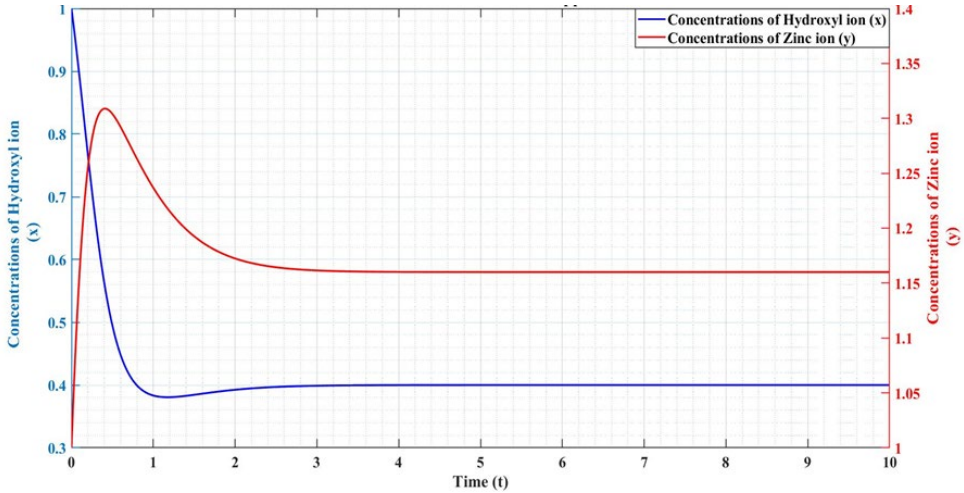

Figure 4. ABM Method Concentrations of Zn^{+2} and OH^{-}

The ABM approach, depicted in Figure 4, also works quite effectively.

The lowest concentration of OH^- is thought to be 0.3806, while the greatest concentration of Zn^{+2} is 1.30886, which is quite near to the exact solution. This multi-step method uses information from earlier steps to make its predictions better. It shows that the lowest OH^- concentration is 0.3806 and the highest Zn^{+2} concentration is 1.30886, which is almost the same as the reference numerical solution. It is a multi-step process that uses information gathered from preceding phases to make better predictions.

Table 2. Numerical Method Concentrations for Zn^{+2} and OH^-

Numerical Technique	OH^- Concentrations	Zn^{+2} Concentrations
	Time(t) = 1.18658	Time(t) =0.41048
Euler's Method	0.379341	1.314709
4th Order Runge-Kutta Method	0.380547	1.309011
Adams-Bashforth-Moulton Method	0.3806	1.30886

By comparing the numerical results with the known reference numerical solutions, the error of the mathematical methods employed to solve the differential equations of the Lengyel Epstein reaction model was determined. The following formula was used to determine the absolute percentage error:

$$\text{Error (\%)} = \left|\frac{\text{Numerical} - \text{reference numerical}}{\text{reference numerical}}\right| \times 100$$

When finding out the concentrations of OH^- and Zn^{+2} at various periods, the three numerical methods, that is Euler, RK, and ABM give substantially-distinct results. At t=1.18658, the highest errors for Euler's method are 0.383% for OH^- and 0.565% for Zn^{+2}. This means that it is not particularly accurate. The RK method and the ABM technique both cut down on errors by a lot at their own times. The error rates for OH^- and Zn^{+2} are 0.129% and 0.118%, respectively. This study demonstrates the trade-off between the simplicity and accuracy of a numerical approach, since ABM's concentration estimations have decreased error rates. Using the Euler methodology, the RK method of fourth order, and the ABM approach, Table 3 illustrates the error check for the concentrations of OH^- and Zn^{+2}. This table also indicates how well each method works for calculating chemical kinetics in ZnO synthesis by showing how accurate and beneficial they are. It tells about how precise and different each method is for figuring out

different chemical concentrations, which helps figure out how well they operate on their own. Figure 5 demonstrates how wrong each of the three numerical techniques were.

Table 3. Error-based Computational Efficiency Comparison of Numerical Techniques

Numerical Technique	Error of OH^- Concentrations	Error of Zn^{+2} Concentrations	Relative Efficiency (R.E)
	Time(t) = 1.18658 hr	Time(t) =0.41048 hr	
Euler's Method	0.383%	0.565%	R.E is low due to high error rates; method is simple but less accurate. So, this is not suitable for synthesis of ZnO.
4th Order Runge-Kutta Method	0.066%	0.129%	R.E is moderate, good balance of accuracy, and computational effort. It is better than Euler so, it can be widely used for synthesis of ZnO
Adams-Bashforth-Moulton Method	0.053%	0.118%	R.E is high because it has lowest error values and is best suited for accurate modeling of synthesis of ZnO

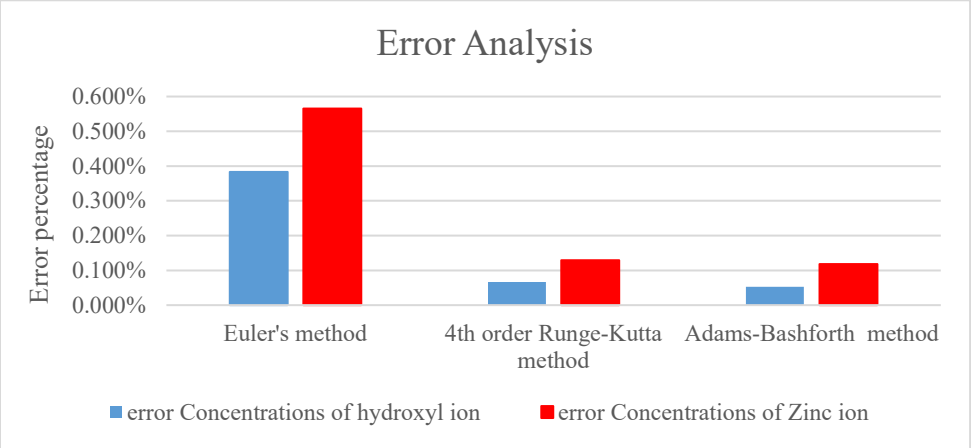

Figure 5. Error of OH^- and Zn^{+2} Concentrations for Numerical Techniques

4. CONCLUSION

In the current study, three different numerical methods were compared and based on their error comparison, the authenticity of the model was checked. When it comes to numerically solving ODEs, the approach chosen relies on how accurate, fast, stable, and complicated the system is. Euler's approach is easy to use but not very accurate. Thus, it is good for tasks that do not need a lot of processing. On the other hand, RK and ABM are more accurate, and ABM is usually the most accurate since it includes processes for predicting and correcting. When working with complicated systems, such as the growth kinetics of ZnO nanostructures, where indirect interactions are important, both RK and ABM methods are better than Euler's method. ABM is especially good at capturing complex behaviors while still being reasonably fast.

Author Contributions

Kaniz Fatima: methodology, conceptualization. **Basit Ali:** data curation, software, formal analysis. **Sarwat Ishaque:** supervision, validation. **Asif Sumeer:** investigation, visualization. **Qaiser Hafeez:** writing – review & editing.

Conflict of Interest

The authors of the manuscript have no financial or non-financial conflict of interest in the subject matter or materials discussed in this manuscript.

Data Availability Statement

The data associated with the study may be provided by the corresponding author if requested/

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Generative AI Disclosure Statement

The authors did not used any type of generative artificial intelligence software for this research.

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