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

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ABSTRACT

The purpose of this research study is to determine which approximation technique is the most successful in studying the rise in ion concentrations in forms of zinc oxide nanostructures using the Lengyel Epstein reaction model. To achieve this objective, ordinary differential equations are formulated utilizing three separate numerical methods that includes Euler, Adams Bashforth Moulton (ABM) and 4th order Runge Kutta (RK) methods. This research aims to identify the optimal approximation approach for computing concentrations of zinc ions Zn^{+2} and hydroxyl ions OH^{-} while examining the reaction kinetics of zinc oxide nanostructures. The research findings indicate 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: 4th order runge kutta method, aqueous chemical growth, adams bashforth moulton (ABM) method, euler method, lengyel epstein reaction model, zinc oxide nanostructures

1. INTRODUCTION

Due to heavy technological development new materials are discovered in order to support the growing industrial demands [1]. Zinc oxide 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 of dissolving in water. Nevertheless, it is 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,

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optical materials, polymers, plastics, batteries, 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. Zinc oxide nanoparticles may improve diabetes treatment by changing how much insulin is 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 zinc oxide are great in finding gases like hydrogen, nitrogen dioxide, carbon monoxide, and ethanol. They could swiftly interact with gases in the air since they are so tiny and have a lot of surface area. You can discover what kind of gas is in the material and how much of it there is by measuring how much electricity it can hold. When a gas touches the ZnO surface, this transformation happens. These sensors are easy to manufacture, perform well in the cold, and respond rapidly. ZnO is good for medical equipment that check breath, industrial gas leak detectors, and air pollution monitors because of these qualities.

ZnO nanoparticles have several uses, but the most important one is that they need to be made in big quantities. The aqueous chemical growth approach stands out among low temperature synthesis procedures because it works well and may be used in many different ways. The ACG method's strict control over growth conditions makes it possible to make a wide range of ZnO nanostructures, such as nanorods, nanotubes, nanowires, and nanospheres [8]. Nanostructures of zinc oxide have received a lot of attention because they have unique features. These characteristics include being cheap, safe, easy to make, highly biocompatible, having high electron transfer rates, and being 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 us figure out how much zinc ions Zn^{+2} and hydroxyl ions OH^- there are in a solution. It also helps us grasp the many processes that go 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 paper ABM method and 4th order Runge Kutta method are used to solve the differential equations of the model. The comparison of Euler's method with ABM method and the RK method

has been 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 this estimate values. That is the 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].The Lengyel Epstein reaction model has been used in recent years to investigate self organization processes that include the formation of zinc oxide (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].

EXPERIMENTAL PROCEDURE

To synthesize ZnO nanoparticles, the upkeep of a controlled environment is basic due to the characteristic helplessness of the Aqueous Chemical Growth (ACG) strategy to barometrical impacts. In this strategy, a flawless gold coated glass substrate is utilized to play down contaminants. Sometime recently commencing the method, the gold coated glass substrate is submerged in an arrangement of low concentration hydrofluoric corrosive. Hence, an intensive cleansing with acetone results, taken after by substrate drying utilizing nitrogen gas at encompassing temperature. With the basis laid, the substantive prepare unfurls, started by implies of 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 made by mixing hexamethylenetetramine and Zinc Nitrate in equal amounts in a container. When it combines this 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 zinc oxide 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 and explained in equation 2.1-2.5 [19].

$$Zn(NO_3)_2.6H_2O + 6H_2O \rightarrow Zn^{+2} + 2NO_3^- \quad (2.1)$$

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

$$(CH_2)_6N_4 + 6H_2O \rightarrow 6HCHO + 4NH_3 \quad (2.2)$$

$$NH_3 + H_2O \rightarrow NH_4 + OH^- \quad (2.3)$$

ZnO can be generated with the statement of both ions.

$$2OH^- + Zn^{+2} \rightarrow Zn(OH)_2 \quad (2.4)$$

$$Zn(OH)_2 \rightarrow ZnO\ (s)\ +\ H_2O \quad (2.5)$$

2. MATHEMATICAL MODEL

An analytical model may also be utilized to illustrate the growing rate 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 method are applied as an analytical method in this model to approximate the results in the reference [12]. The ABM method is now employed in this study to estimate the increase of zinc ion and hydroxyl ion. The subsequent equations were utilized to build the model:

$$NH_3 + H_2O \rightarrow NH_4^+ + OH^- \quad (3.1)$$

$$Zn(NO_3)_2.6H_2O + 6H_2O \rightarrow Zn^{+2} + 2NO_3^- \quad (3.2)$$

$$2OH^- + Zn^{+2} \rightarrow ZnO + H_2O \quad (3.3)$$

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.

$$\frac{dx}{dt} = f(x,y) = a_1 - x - 4\left(\frac{xy}{(1+x^2)}\right) \quad (3.4)$$

$$\frac{dy}{dt} = g(x,y) = a_2 x\left(1 - \frac{y}{(1+x^2)}\right) \quad (3.5)$$

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].

When utilizing a computer to solve ordinary differential equations, many methods exist to provide approximate solutions at distinct time intervals. It examine the efficacy of three prevalent methodologies that includes Euler's method, RK method, and ABM method that concentrate on their efficacy in examining the growth kinetics of zinc oxide ZnO nanostructures.

2.1. Euler's method:

It is a fundamental numerical approach for approximating the solution of ordinary differential equations 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 give 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 estimation of the next point. These methods ultimate for solving ordinary differential equations 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 ordinary differential equations by integrating a system of equations across discrete time steps. The ABM method is used deliberately in this study to improve the computational efficiency of the Lengyel reaction model for the growth kinetics of Zinc oxide 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 ordinary differential equations, 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 time step. The predictor formula for 'x' is given by:

$$x_{pred} = x_i + \frac{\Delta t}{24}(55f_i - 59f_{i-1} + 37f_{i-2} - 9f_{i-3}) \quad (3.6)$$

The predictor formula for 'y' is given by:

$$y_{pred} = y_i + \frac{\Delta t}{24}(55g_i - 59g_{i-1} + 37g_{i-2} - 9g_{i-3}) \quad (3.7)$$

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:

$$x_{i+1} = x_i + \frac{\Delta t}{24}\left(9f_{pred} + 19f_i - 5f_{i-1} + f_{i-2}\right) \quad (3.8)$$

$$y_{i+1} = y_i + \frac{\Delta t}{24}\left(9g_{pred} + 19g_i - 5g_{i-1} + g_{i-2}\right) \quad (3.9)$$

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 ABM, RK, and Euler's method compare to each other. This table has important comments on 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
4^{th} 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 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 Multistep method but high accuracy and efficient for long time integration but it requires initial values.

3. RESULTS AND DISCUSSION

This study analyzes how well different numerical approaches can simulate the amounts of hydroxide ions OH^- and zinc ions Zn^{+2} over time. It wants to know not only 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 numbers are used as a reference to compare other approaches against.

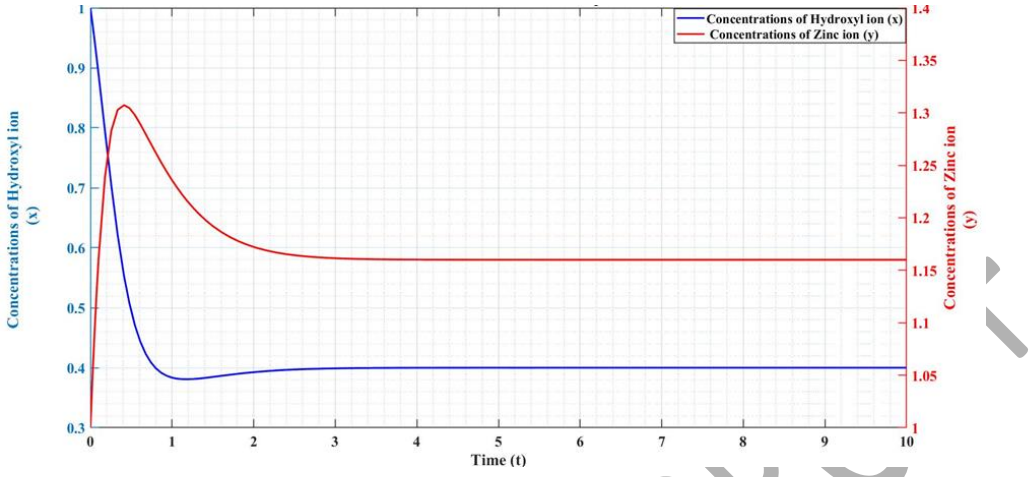

Figure 1: Reference numerical solution for concentrations of Zn^{+2} and OH^{-}.

Figure 2 illustrates that which Euler's method found. 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 isn't surprising given that individuals know that Euler's method is simple but not particularly accurate. It's a fast method to get an estimate, but it's not the ideal solution if you need it to be really accurate.

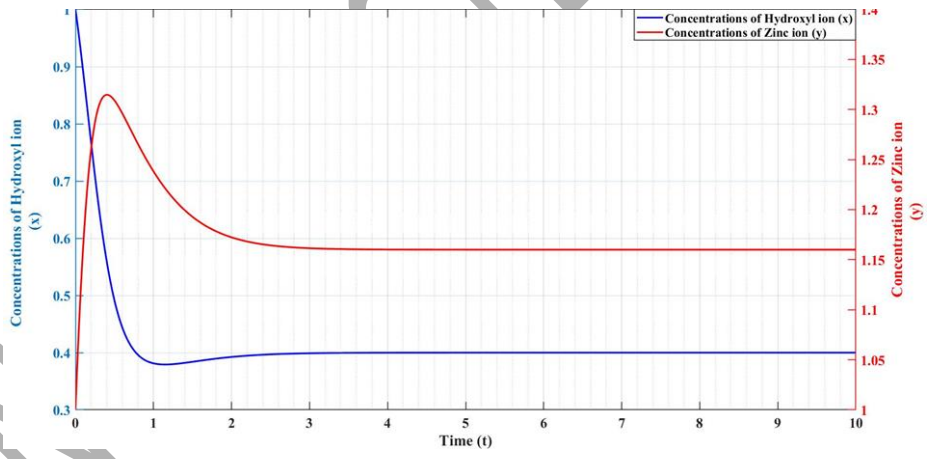

Figure 2: Euler's method concentrations of Zn^{+2} and OH^{-}.

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.

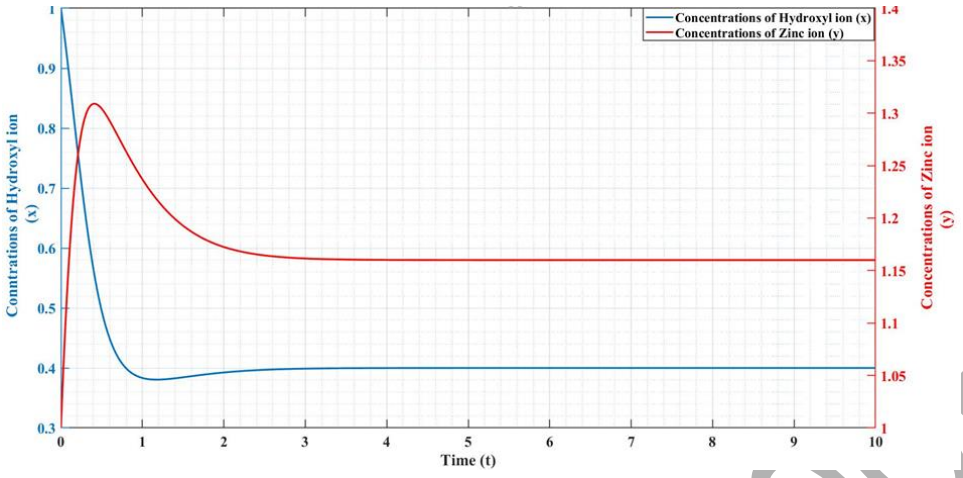

Figure 3: RK method concentrations of Zn^{+2} and OH^{-}.

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.

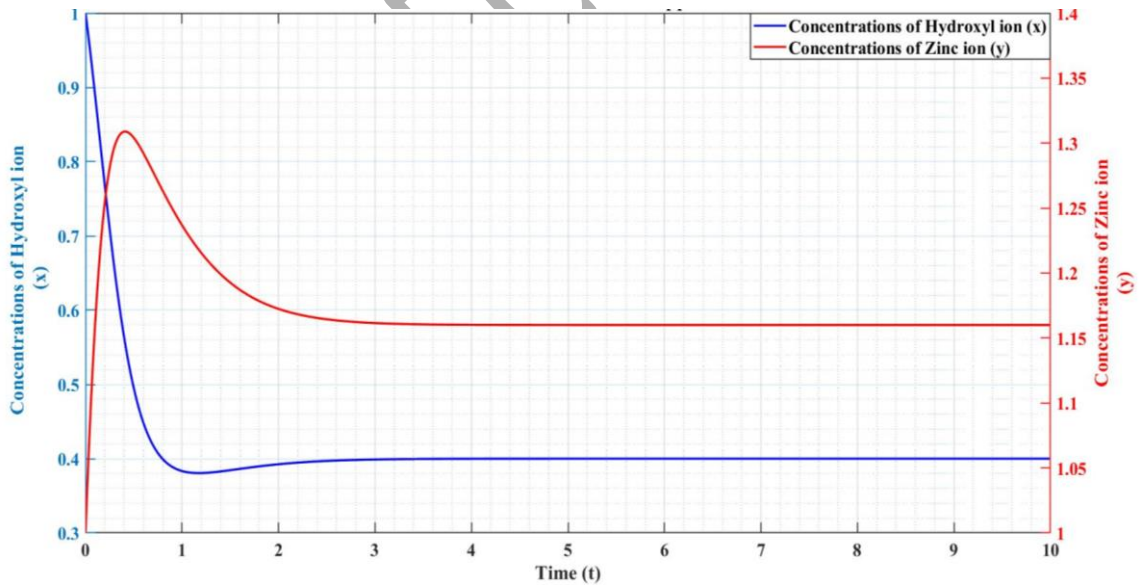

Figure 4: ABM method concentrations of Zn^{+2} and OH^{-}.

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 says 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 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 us all we need to know about how precise and different each method is for figuring out different chemical concentrations, which helps us figure out how well they operate on their own. Figure 5 demonstrates how wrong each of the three numerical techniques was.

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, best suited for accurate modeling of synthesis of ZnO

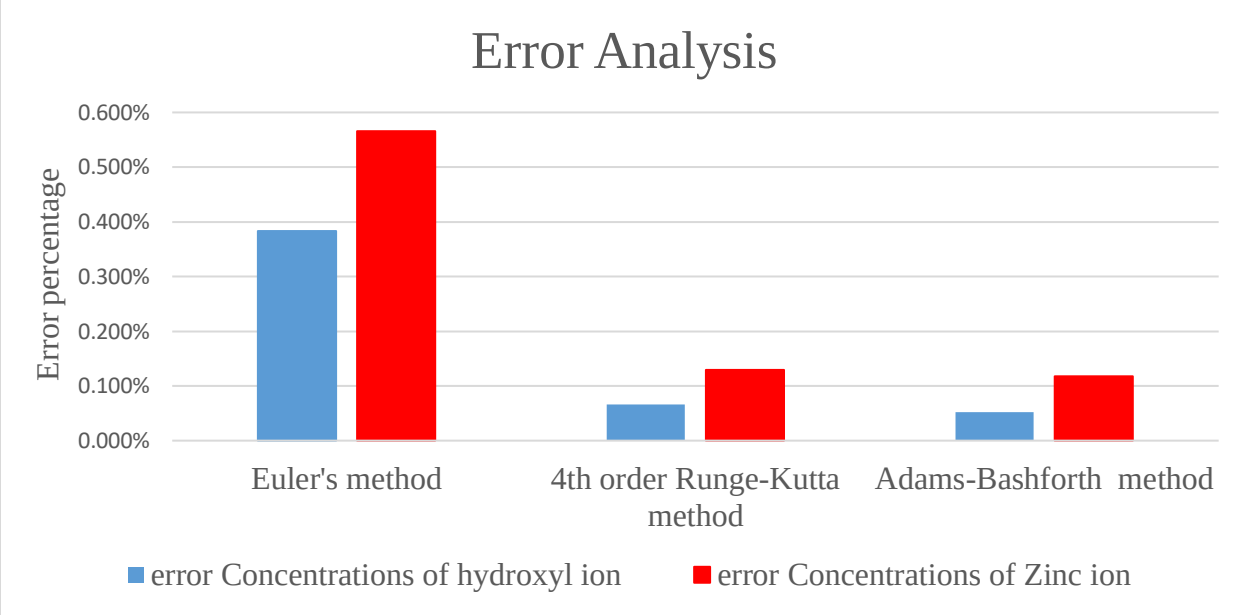

Figure 5: Error of OH^- and Zn^{+2} concentrations for numerical techniques.

Conclusion:

In this research study three different numerical methods have been compared and based on their error comparison the authenticity of the model has been checked. When it comes to numerically solving ordinary differential equations (ODEs), the approach it chooses relies on how accurate, fast, stable, and complicated the system is. Euler's approach is easy to use but not very accurate, thus it's good for tasks that don't 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 like 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.

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