RASĀYAN *J. Chem.*
Vol. 19 | No. 1 | 504-510 | January-March | 2026
ISSN: 0974-1496 | e-ISSN: 0976-0083 | CODEN: RJCABP
http://www.rasayanjournal.com
http://www.rasayanjournal.co.in

A STABLE AND HIGH ACCURACY MULTISTEP NUMERICAL DIFFERENTIATION SCHEME FOR NONLINEAR THIRD ORDER ORDINARY DIFFERENTIAL EQUATIONS ARISING IN CHEMICAL REACTION MODELING

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ABSTRACT
This investigation presents an innovative method for solving 3rd order ODEs that have predetermined beginning conditions. This method is a numerical methodology that involves multiple steps. The objective of this technique is to increase the stability and precision of numerical approximations. When it comes to systems that are complex and nonlinear, where it is difficult to find analytical solutions, this is of particular importance. When the step size parameter r is equal to 1, we provide a straightforward formula for the operation. As a result, it is simple and quick to utilise in calculations. Our process for ensuring that the technique works is to conduct numerical tests by solving a few selected 3rd order ODEs and then comparing outcomes to known precise solutions. The process of computation for this approach is more efficient since it necessitates fewer steps, and it is also more precise, which is the only advantage that this technique has, as demonstrated by the comparison. This study contributes a practical computation tool for modelling complex chemical reaction pathways and supports Sustainable Development Goal associated with industry, innovation & infrastructure by promoting reliable numerical techniques for industrial and scientific simulations. The results of the investigation show that the multistep strategy that has been recommended is a reliable and successful option for dealing with higher-order initial value problems in a variety of engineering and scientific fields.
Keywords: Numerical Techniques, Initial Value Problem, Accuracy, Chemical Kinetics, Stability, Differential Equations, Error Analysis. AMS Subject Classification: 65L05, 65L06
RASĀYAN *J. Chem.*, Vol. 19, No.1, 2026

INTRODUCTION

Ordinary differential equations play a central role in the mathematical representation of dynamic processes encountered in chemical sciences. Phenomena such as reaction kinetics, transport mechanisms, and molecular interactions are commonly expressed in terms of differential relations that describe how system variables evolve with respect to time or space. This introduction focuses on 3rd order ordinary differential equations and their application in chemistry, particularly highlighting solution techniques using multistep numerical methods. The development of numerical procedures for solving differential equations has been widely documented, with foundational contributions from Butcher, who outlined the major developments during the 20th century. Building on this groundwork, Ahmad *et al.* and Shokri advanced multistep and multiderivative methods for nonlinear ODEs and PDEs.[1-3] Krishna and collaborators focused on solution analysis, stability related to special methods for high-order equations.[4, 5] Yakusak and Owolanke & Atsi *et al.* proposed direct collocation-based techniques for 2nd order problems.[6,7] Duromola *et al.* Rama Chandra Rao and Swapna *et al.* explored hybrid and special methods.[8-10] Practical applications, such as holographic metrology, were demonstrated by Ramaiah and Gannavarpu.[11] For instance, in modelling chemical systems, the complexity increases with the involvement of multiple substances reacting with one another, requiring a system of nonlinear differential equations to accurately describe the dynamics. Such systems are sometimes represented through delay differential equations to account for time lags inherent in the chemical. Thota *et al.* proposed a robust exponential–derivative–based algorithm that achieves rapid convergence and high precision in modelling complex chemical systems.[12,13]

http://doi.org/10.31788/RJC.2026.1919552
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Usage of 3rd Order ODEs in Chemistry

Third-order differential equations naturally appear in chemical modelling when system dynamics exhibits higher- order temporal or spatial effects that cannot be sufficiently represented using lower-order formulations. Such situations occur when the governing dynamics involve higher-order temporal or spatial effects, often linked to complex transport, diffusion or delayed response mechanisms. In reaction–diffusion processes, for instance, the interaction between concentration gradients and reaction kinetics may lead to higher-order formulations after suitable reductions. Similarly, chemical systems exhibiting inertial effects, relaxation behaviour, or memory-dependent responses, such as those encountered in viscoelastic media, naturally give rise to third-order differential models. The relevance of third-order equations in chemical research stems from their ability to capture features that are frequently overlooked by first- or second-order descriptions. Lower-order models may fail to represent experimental observations accurately, particularly when multiple interacting processes evolve on different time scales. With the growing interest in advanced chemical systems, including nanoscale reactors, non-equilibrium catalytic processes, and complex biochemical pathways, the need for mathematically richer models has become increasingly evident. 3rd order ordinary differential equations offer a suitable framework for representing such phenomena with greater fidelity. Obtaining analytical solutions for 3rd order ordinary differential equations is generally challenging, especially in the presence of nonlinear terms, variable coefficients, or coupling between multiple reactive species. Closed-form solutions are typically limited to idealised cases and are rarely available for chemically realistic models. As a consequence, numerical methods play a crucial role in the practical analysis of these equations, providing approximate solutions that balance accuracy with computational efficiency. Among the available numerical approaches, multistep methods are mostly effective for solving third-order equations. These methods make use of previously computed solution values to advance the numerical approximation, which often leads to improved accuracy and stability over extended integration intervals. Their structure allows flexibility in accommodating the specific characteristics of chemical systems, such as stiffness, smooth solution behaviour, or oscillatory dynamics. In contemporary computational chemistry, multistep schemes are often combined with adaptive step-size strategies and error monitoring techniques. This adaptability is especially important for chemical processes in which reaction rates vary significantly over time or where different stages of the reaction demand different levels of temporal resolution. Thus, multistep numerical methods have become an essential component in the numerical treatment of 3rd order ODEs arising in chemical modelling and simulation. The present computational framework for modelling complex chemical reaction pathways supports SDG, which is related to industry, innovation & infrastructure, through enhancing the reliability of computational tools used in industrial and scientific applications.

EXPERIMENTAL

The proposed multistep numerical differentiation scheme is derived using polynomial interpolation over equidistant grid points. Coefficients are derived systematically to obtain an explicit formulation for 3rd order ordinary differential equations under the condition r = 1. The method is structured to minimise computational complexity while preserving numerical stability. Numerical values are reported in tabular form to ensure reproducibility. Graphical illustrations are included to provide qualitative insight into the numerical convergence behaviour.

General Procedure of Multistep Methods

The linear multistep method of k-step for solving $w' = q(v, w)$ is:

$$w_{n+l} = \sum_{l=0}^{k-1} c_l w_{n+l} + h \sum_{l=0}^{k} d_l q_{n+l}$$

Where c_l and d_l are multipliers/coefficients, and h being step length, and q_{n+l} is estimated at v_{n+l}.

Equations of 3rd order are generally of the type.

$$w''' = q(v, w, w', w''),$$

To ensure a unique solution, the initial values of w, w' and w'' at v=0 are specified as:

$$w''(0) = w_0'', \quad w'(0) = w_0' \quad \text{and} \quad w(0) = w_0 \qquad (1)$$

Numerical methods for solving ordinary differential equations sometimes use a multistep approach. This method estimates solutions at numerous locations by merging answers from previous points. The solution by the method of (1) is:

$$w_{n+1} = \sum_{l=1}^{k} c_l w_{n+1-l} + h^3 \sum_{l=0}^{k} d_l w''_{n+1-l}$$

Here, the step size is represented by the variable 'h'.

The Method Derivation

The (k+1) abscissas v_{n+1}, v_n, - - -, v_{n-k+1}, the interpolating polynomial for the function w(u) is R(u).

$$R(u) = \sum_{m=0}^{k} (-1)^m \binom{-p}{m} \nabla^m w_{n+1}, \quad \text{Where } p = \frac{v - v_{n+1}}{h}$$

(2)

After three times differentiating (2) about u, we get:

$$R'''(v) = \left(\frac{1}{h^3}\right) \sum_{m=0}^{k} \frac{d^3}{dp^3} \left[(-1^m) \binom{-p}{m} \right] \nabla^m w_{n+1}.$$

By replacing $w'''(v)$ with its approximation $R'''(v)$ in equation (2) and evaluating at v = v_{n+1-r} with (p = -r), the following relation is obtained.

$$\sum_{m=0}^{k} \xi_{r,\ m} \nabla^m w_{n+1} = h^2 q_{n+1-r} \tag{3}$$

here $\xi_{r,m} = \frac{d^2}{ds^2} [(-1)^m \binom{-p}{m}]$ (4)

Derivation of the Generating Function

The generating function is defined as: $F_{r,v} = \sum_{m=0}^{\infty} \xi_{r,m} s^m$ (5)

Substituting the expression for $\xi_{r,m}$ from equation (4) into equation (5) yields:

$$F_{r,s} = \sum_{m=0}^{\infty} \xi_{r,m} s^m = -(1-s)^r [\log(1-s)]^3 at\ p = -r$$

(6)

Details of the Explicit Method

In (3), if r =1, A class of techniques will be represented as:

$$\sum_{m=0}^{k} \xi_{1,\ m} \nabla^m w_{n+1} = h^3 q_{n+1} \tag{7}$$

From equation (7) it follows that $\xi_{1,\ m}$ represents the factor of v^m, obtained from the series expansion and $-(1-s)^1[\log(1-s)]^3$ is expressed using 't'. The multipliers of $\xi_{1,\ m}$ are shown in Table-1. Functional values are used for displaying deviations in (7).

Thus, equation (7) reduces to: $\sum_{l=0}^{k} c_l w_{n+1-l} = h^3 q_n$ (8)

Equation (8) represents a general explicit multistep framework derived from the proposed numerical differentiation approach. The structure of this formulation allows flexibility in selecting the step parameter. k, which directly controls the accuracy order of the resulting method. By appropriately choosing k Higher-order schemes can be systematically constructed without altering the underlying derivation process. This property makes the proposed framework adaptable for problems requiring varying precision levels.

The local truncation error associated with equation (8) is given by:

$$LTE = \xi_{1,\ k+1} h^{k+1} w^{k+1}(\eta)$$

To illustrate the applicability of the derived formulation, explicit multistep schemes of different accuracy orders are constructed. These schemes are obtained by selecting successive values of the parameter. k in

equation (8). Each resulting method utilises previously computed solution values to achieve higher accuracy while maintaining computational efficiency.

Table-1: Numerical Values of the Coefficient $\xi_{1,m}$ for m = 0,1, 2, ….,7 used in the Multistep Scheme

M	0	1	2	3	4	5	6	7	8
$\xi_{1,m}$	0	0	0	-1	$\frac{-1}{2}$	$\frac{-1}{4}$	$\frac{-1}{8}$	$\frac{-7}{120}$	$\frac{-1}{48}$

Table-2: Coefficient Values c_l Corresponding to different Step Parameters k in the Derived Multistep Formulation

k	l								
	0	1	2	3	4	5	6	7	8
3	-1	3	-3	1					
4	$\frac{-3}{2}$	5	-6	3	$\frac{-1}{2}$				
5	$\frac{-7}{4}$	$\frac{25}{4}$	$\frac{-17}{2}$	$\frac{11}{2}$	$\frac{-7}{4}$	$\frac{1}{4}$			
6	$\frac{-15}{8}$	7	$\frac{-83}{8}$	8	$\frac{-29}{8}$	1	$\frac{-1}{8}$		
7	$\frac{-29}{15}$	$\frac{889}{120}$	$\frac{-58}{5}$	$\frac{241}{24}$	$\frac{-17}{3}$	$\frac{89}{40}$	$\frac{-8}{15}$	$\frac{7}{120}$	
8	$\frac{-469}{240}$	$\frac{303}{40}$	$\frac{-731}{60}$	$\frac{269}{24}$	$\frac{-57}{8}$	$\frac{407}{120}$	$\frac{-67}{60}$	$\frac{9}{40}$	$\frac{-1}{48}$

The following formulations demonstrate the systematic progression from third-order to higher-order accuracy. The simplest nontrivial implementation of the proposed framework corresponds to the third-order case. For the 3rd order, taking k = 4 in equation (8), this leads to the following explicit multistep scheme.

$$-\left(\frac{3}{2}\right) w_{n+1} + 5w_n - 6w_{n-1} + 3w_{n-2} - \left(\frac{1}{2}\right) w_{n-3} = h^3 q_n$$

$$w_{n+1} = \left(\frac{2}{3}\right)\left(5w_n - 6w_{n-1} + 3w_{n-2} - \frac{1}{2} w_{n-3} - h^3 q_n\right)$$

$$w_{n+1} = \left(\frac{10}{3}\right) w_n - 4w_{n-1} + 2w_{n-2} - \frac{1}{3} w_{n-3} - \frac{2}{3} h^3 q_n$$

As the parameter k increases, additional previous solution values are included in the scheme, which results in a higher - order approximation.

4th order: By choosing k = 5 in equation (8), a fourth-order explicit multistep scheme is obtained, which is written as

$$-\left(\frac{7}{4}\right) w_{n+1} + \left(\frac{25}{4}\right) w_n - \left(\frac{17}{2}\right) w_{n-1} + \left(\frac{11}{2}\right) w_{n-2} - \left(\frac{7}{4}\right) w_{n-3} + \left(\frac{1}{4}\right) w_{n-4} = h^3 q_n$$

$$w_{n+1} = \frac{4}{7}\left(\frac{25}{4} w_n - \frac{17}{2} w_{n-1} + \frac{11}{2} w_{n-2} - \frac{7}{4} w_{n-3} + \frac{1}{4} w_{n-4} - h^3 q_n\right)$$

$$w_{n+1} = \frac{25}{7} w_n - \frac{34}{7} w_{n-1} + \frac{22}{7} w_{n-2} - w_{n-3} + \frac{1}{7} w_{n-4} - \frac{4}{7} h^3 q_n$$

5th order: Setting k = 6 in equation (8) yields a fifth-order explicit multistep formulation, given by

$$-\left(\frac{15}{8}\right) w_{n+1} + 7w_n - \left(\frac{83}{8}\right) w_{n-1} + 8w_{n-2} - \left(\frac{29}{8}\right) w_{n-3} + w_{n-4} - \left(\frac{1}{8}\right) w_{n-5} = h^3 q_n$$

$$w_{n+1} = \frac{8}{15}\left(7w_n - \frac{83}{8} w_{n-1} + 8w_{n-2} - \frac{29}{8} w_{n-3} + w_{n-4} - \frac{1}{8} w_{n-5} - h^3 q_n\right)$$

$$w_{n+1} = \left(\frac{56}{15}\right) w_n - \left(\frac{83}{15}\right) w_{n-1} + \left(\frac{64}{15}\right) w_{n-2} - \left(\frac{29}{15}\right) w_{n-3} + \left(\frac{8}{15}\right) w_{n-4} - \left(\frac{1}{15}\right) w_{n-5} - \left(\frac{8}{15}\right) h^3 q_n$$

6th order: When k = 7 is substituted into equation (8), the resulting scheme attains sixth-order accuracy and is expressed as

$$\frac{-29}{15} w_{n+1} + \frac{889}{120} w_n - \frac{58}{5} w_{n-1} + \frac{241}{24} w_{n-2} - \frac{17}{3} w_{n-3} + \frac{89}{40} w_{n-4} - \frac{8}{15} w_{n-5} + \frac{7}{120} w_{n-6} = h^3 q_n$$

$$w_{n+1} = \frac{15}{29}\left(\frac{889}{120}w_n - \frac{58}{5}w_{n-1} + \frac{241}{24}w_{n-2} - \frac{17}{3}w_{n-3} + \frac{89}{40}w_{n-4} - \frac{8}{15}w_{n-5} + \frac{7}{120}w_{n-6} - h^3 q_n\right)$$

$$w_{n+1} = \frac{889}{145}w_n - 6w_{n-1} + \frac{1205}{232}w_{n-2} - \frac{85}{29}w_{n-3} + \frac{267}{232}w_{n-4} - \frac{8}{29}w_{n-5} + \frac{7}{232}w_{n-6} - \frac{15}{29}h^3 q_n$$

RESULTS AND DISCUSSION

To assess the effectiveness of the proposed multistep numerical differentiation approach, several benchmark third-order initial value problems are considered. These test problems are selected due to the availability of exact analytical solutions, which allows a direct evaluation of numerical accuracy. Error behaviour, convergence characteristics, and stability trends are examined to demonstrate the practical reliability of the developed schemes.

Problem-1: We examine a third-order initial value problem defined by the following differential equation, subject to prescribed initial conditions $\frac{d^3w}{dv^3} + \frac{3}{(1+v)}\left(\frac{dw}{dv}\right)^2 = e^{3w}$ with w(0) = 1, w′(0) = 0 and w″(0) = 1.

Problems of this type often arise in chemical kinetics, thermodynamics, and information theory.The analytical solution is given by $w(v) = -\log(1+v)$ which is a nonlinear logarithmic function.

The numerical differentiation (ND) approach of the 5th order is:

$$w_{n+1} = \frac{56}{15}w_n - \frac{83}{15}w_{n-1} + \frac{64}{15}w_{n-2} - \frac{29}{15}w_{n-3} + \frac{8}{15}w_{n-4} - \frac{1}{15}w_{n-5} - \frac{8}{15}h^3 q_n$$

Here $q(v,w) = e^{3w} - \frac{3}{(1+v)^3}$

The numerical values presented in Table-3 are generated using the derived fifth-order multistep formulation and are compared with corresponding closed-form reference solutions for accuracy.

Table-3: Numerical Accuracy of the Derived k = 6 Multistep ND Scheme

V	Analytical Solution	k=6 multistep ND scheme	Abs. error
0	0.00000000000000000	0.00000064515367328	0.000000645153673280
0.1	0.04139268515822510	0.04139296623288310	0.000000281074658048
0.2	0.07918124604762480	0.07918125161229540	0.000000005564670572
0.3	0.11394335230683700	0.11394313868120200	0.000000213625635237
0.4	0.14612803567823800	0.14612763986461000	0.000000395813627957
0.5	0.17609125905568100	0.17609070601268300	0.000000553042998286
0.6	0.20411998265592500	0.20411928957437300	0.000000693081552094
0.7	0.23044892137827400	0.23044810029138400	0.000000821086890229
0.8	0.25527250510330600	0.25527156453282900	0.000000940570477503
0.9	0.27875360095282900	0.27875254697710700	0.000001053975722642
1	0.30102999566398100	0.30102883262843600	0.000001163035544705

The consistently small magnitude of the absolute deviation confirms the high accuracy and computational reliability of the proposed numerical scheme. To visually examine the numerical performance of the scheme, the absolute deviation is plotted against the independent variable, as shown in Fig.-1.

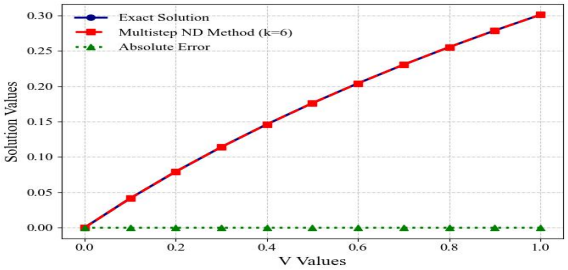

Fig.-1: Error Convergence Behaviour of the Proposed ND Approach for Problem1

Accurate numerical simulation of chemical processes supports sustainable industrial modelling, consistent with SDG-9.

Problem 2: As a second test case, a classical exponential- type growth problem is considered to further validate the effectiveness of the proposed formulation.

$\frac{d^3w}{dv^3} + \left(1 + \frac{2}{v}\right)\frac{d^2w}{dv^2} = \left[\left(2 + \frac{2}{v}\right)e^v - v\right] + \log\ w$, with w (0) = w′ (0) = w" (0) = 1, which is fundamental in modelling population dynamics, radioactive decay and chemical reactions.

The Analytical Solution is Given by w(v)= e^v

The numerical differentiation (ND) approach of the 5th order is

$$w_{n+1} = \frac{56}{15}w_n - \frac{83}{15}w_{n-1} + \frac{64}{15}w_{n-2} - \frac{29}{15}w_{n-3} + \frac{8}{15}w_{n-4} - \frac{1}{15}w_{n-5} - \frac{8}{15}h^3q_n$$

Here $q(v,w)=e^v - v + \log w$

Table-4: Numerical Accuracy of the Derived k = 6 Multistep ND Scheme

V	Analytical Solution	k=6 multistep ND scheme	Abs. error
0	1.00000000000000000	0.99999893629727400	0.00000106370272557
0.1	1.10517091807565000	1.10516981980255000	0.000001098273100464
0.2	1.22140275816017000	1.22140161363577000	0.000001144524396368
0.3	1.34985880757600000	1.34985760389090000	0.000001203685107143
0.4	1.49182469764127000	1.49182342052834000	0.000001277112926523
0.5	1.64872127070013000	1.64871990439179000	0.000001366308342465
0.6	1.82211880039051000	1.82211732746086000	0.000001472929645807
0.7	2.01375270747048000	2.01375110866095000	0.000001598809531433
0.8	2.22554092849247000	2.22553918251903000	0.000001745973442713
0.9	2.45960311115695000	2.45960119449711000	0.000001916659846835
1	2.71828182845905000	2.71827971511643000	0.000002113342612464

The close agreement between numerical and reference solutions across the computational interval demonstrates the robustness of the multistep numerical differentiation approach.

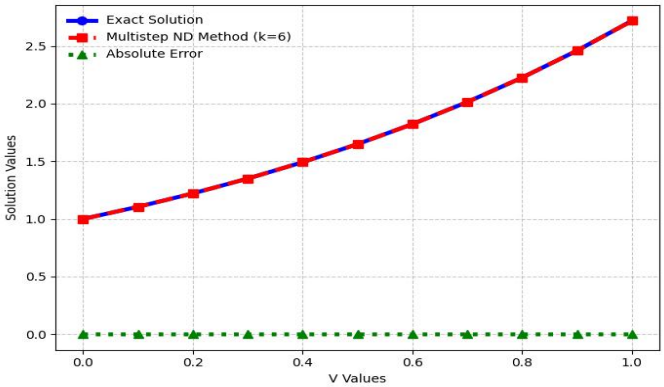

Fig.-2: Error Convergence Behaviour of the Proposed ND Approach for Problem 2.
All Tables and Figures Presented in this Study are Generated Exclusively from Independently Performed Numerical Computations Using the Derived Multistep Formulation

CONCLUSION

In this research, a multistep numerical differentiation (ND) approach has been successfully developed and applied to resolve 3rd order ODEs with given initial conditions. The method, specifically formulated for the case r = 1, provides an explicit solution framework that is both efficient and easy to implement. Through numerical comparisons with exact solutions, it is seen that the projected approach yields extremely precise results with minimal computational error. The accuracy of the obtained solutions

confirms the method's reliability and effectiveness. The reduced error and close agreement with the actual values highlight the strength of the multistep approach, making it a valuable tool for answering high-order ODEs in practical situations. This study supports the development of reliable numerical tools that promote innovation and practical applicability. Future research may focus on adaptive step-size strategies and hybrid formulations for stiff systems.

ACKNOWLEDGMENTS

The authors would like to express their gratitude to the authorities of their Institutions for providing the basic facilities for this research.

CONFLICT OF INTERESTS

The authors confirm that this research was conducted without trade / commercial/monetary dealings that may possibly be interpreted as a potential/possible conflict of interest.

AUTHOR CONTRIBUTIONS

This present work is related to *SDG-9: Industry, Innovation & Infrastructure.* All the authors contributed significantly to this manuscript, participated in reviewing/editing and approved the final draft for publication. The research profile of the authors can be verified from their ORCID ids, given below:

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Cite this article as: Swapna Ch *et al.*, *Rasayan J. Chem.*, 19(1), 504-510(2026), https://doi.org/10.31788/RJC.2026.1919552.

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