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Numerical Solutions of Stiff Chemical Reaction Problems using Hybrid Block Backward Differentiation Formula

Hazizah Mohd Ijam[1,*], Saufianim Jana Aksah[2], Ahmad Fadly Nurullah Rasedee[3], Norshakila Abd Rasid[4], Athraa Abdulsalam[5], Nurul Hazwani Mohd Aris[1], Fatimah Hazimi[1]

[1] School of Mathematical Sciences, College of Computing, Informatics and Mathematics, Universiti Teknologi MARA, 40450 Shah Alam, Selangor, Malaysia
[2] Centre of Foundation Studies, Universiti Teknologi MARA, Cawangan Selangor, Kampus Dengkil, 43800 Dengkil, Selangor, Malaysia
[3] Faculty of Economics and Muamalat, Universiti Sains Islam Malaysia, 71800 Nilai, Negeri Sembilan, Malaysia
[4] Mathematical Sciences Studies, College of Computing, Informatics and Mathematics, Universiti Teknologi MARA Cawangan Perak, Kampus Tapah, 35400 Tapah Road, Perak, Malaysia
[5] Department of Mathematics and Computer Applications, College of Sciences, Al-Nahrain University, Jadriya, 10072 Baghdad, Iraq

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ABSTRACT

This research paper introduces an advanced approach to address the numerical challenges associated with stiff chemical reaction problems. We propose employing a Hybrid Diagonally Implicit Block Backward Differentiation Formula coupled with strategically placed off-step points to improve the accuracy and efficiency of numerical solutions. Stiff chemical reactions, commonly encountered in various industrial processes, require advanced numerical techniques to precisely capture rapid changes in concentrations. Our hybrid formulation enhances stability and computational efficiency by building on the diagonally implicit structure of block backward differentiation formulas, offering improved performance for solving stiff chemical reaction problems. Under a specific selection of a free parameter, the method is found to possess both zero-stability and $A-$stability properties. Convergence analysis demonstrates its ability to accurately approximate exact solutions. Through rigorous experimentation and comparative analysis, this research will illustrate the effectiveness of the developed method in solving stiff ordinary differential equations. The expected outcomes include the development of the new numerical method, its validation through comprehensive numerical experiments and insights into its performance and applicability in diverse science and engineering domains.

1. Introduction

In this paper, we explore an advanced approach based on Block Backward Differentiation Formula (BBDF) in diagonally implicit structure for the numerical solutions of stiff chemical reaction problems in the form of

* *Corresponding author.*
E-mail address: hazizahijam@uitm.edu.my (Hazizah Mohd Ijam)

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$$y' = f\left(x, y\right), \quad y\left(a\right) = \mu, \quad x \in \left[a, b\right] \tag{1}$$

where $y^T = \left(y_1, y_2, \ldots, y_m\right)$, $f^T = \left(f_1, f_2, \ldots, f_m\right)$ and $\mu^T = \left(\mu_1, \mu_2, \ldots, \mu_m\right)$. The system in Eq. (1) is said to be linear with constant coefficients if $f\left(x, y\right) = Ay + \Phi\left(x\right)$, where A is an $m \times m$ constant matrix, while y, f and $\Phi\left(x\right)$ are *m*-dimensional vectors.

According to Lambert [1], Eq. (1) is classified as stiff if the eigenvalues λ_i of $\frac{\partial f}{\partial y}$ satisfy the following conditions:

i) $\text{Re}\left(\lambda_i\right) < 0,$

ii) $\max_i \left|\text{Re}\left(\lambda_i\right)\right| \gg \min_i \left|\text{Re}\left(\lambda_i\right)\right|$ where the ratio $\frac{\max_i \left|\text{Re}\left(\lambda_i\right)\right|}{\min_i \left|\text{Re}\left(\lambda_i\right)\right|}$ indicates the stiffness index.

A system is classified as stiff when the ratio of the largest to the smallest eigenvalue is extremely large, often spanning several orders of magnitude. This large ratio causes stability issues in explicit methods, necessitating the use of implicit methods for efficient and stable numerical solutions.

Chemical reactions are crucial in diverse fields such as industrial processes, environmental studies and pharmaceutical development. Precise modeling and simulation of chemical reaction systems involve solving stiff ODEs characterized by widely separated time scales. Conventional numerical methods frequently encounter difficulties in efficiently and accurately handling such systems (see [2–4]). This paper addresses this challenge by introducing an improved version of BBDF method, a novel approach designed specifically for stiff ODEs stemming from chemical reaction problems.

Over time, the Backward Differentiation Formula (BDF) has been extensively used for solving stiff ODEs. Traditionally, the BDF method approximates the solution for y_{n+1} at x_{n+1} in each integration step. However, in a prior study by Ibrahim *et al.,* [5], the BBDF approach was introduced as an alternative method to reduce the number of integration steps and processing time required by conventional numerical integrators, while still maintaining accuracy and meeting necessary stability conditions. This approach has garnered significant attention in the research community, proving to be more accurate and efficient compared to non-block methods and existing solvers (see [6–17]). Numerous efforts have been made to implement the BBDF approach in solving stiff problems, highlighting its potential to enhance computational efficiency and solution accuracy.

Another widely employed strategy for tackling stiff ODEs involves the use of the Runge-Kutta (RK) method. In the context of fully implicit Runge-Kutta (FIRK) methods, the necessity to assess the Jacobian matrix, denoted as *J*, and execute the lower-upper factorization at each integration stage is a prerequisite. Nevertheless, the substantial computational overhead linked with the application of FIRK methods, as outlined in [7–10,13,15,16,20,24–26], has prompted researchers to seek alternative approaches. Such alternatives are commonly referred to as diagonally implicit RK (DIRK) methods. In DIRK methods, the matrix can be rendered lower triangular with a constant value on the diagonal, streamlining the computation process. This adjustment allows for the evaluation of *J* to be conducted only once per step, mitigating the computational burden associated with FIRK methods.

In recent years, many researchers have extended conventional block methods by introducing hybrid points, also known as off-step points, to obtain numerical solutions for Eq. (1). The use of off-step points in BBDF methods has been explored in [11,15,18–20], demonstrating improved accuracy using additional data points, increased stability for stiff or oscillatory problems and greater flexibility in step size selection. These methods also enhance higher-order convergence, allowing for more precise results with fewer computational steps. A related approach using off-step points is discussed in [21–23]. In this paper, we build upon the theory from [5] and derive new stability coefficients, advancing the findings of [27].

In this study, we use a predictor-corrector (PECE) approach to enhance the accuracy and efficiency of our numerical solutions. This method reduces truncation errors and improves stability, making it particularly effective for stiff problems while allowing flexible step sizes for robust results (see [28]).

2. Methodology

This section provides an elaborate elucidation of the formulation of the proposed ρ-Hybrid Diagonally Implicit Block Backward Differentiation Formula (ρ-HDIBBDF) designed to solve Eq. (1). The general form of linear multistep method (LMM) for first order ODEs is written as

$$\sum_{j=0}^{k}\alpha_j y_{n+j} = h\sum_{j=0}^{k}\beta_j f_{n+j} \qquad k \geq 1. \tag{2}$$

where *h* is the step size. Since the interval for x is the continuous interval $[a,b]$, *h* represents the division of this continuous interval into discrete points. Consider $y_{n+j} \approx y(x_{n+j})$ and $f_{n+j} \approx f(x_{n+j}, y_{n+j})$, coefficients α_j, β_j are suitably chosen constants subject to conditions $\alpha_k = 1, |\alpha_0| + |\beta_0| \neq 0$ and *k* is defined as the order of the method employed. The method in (2) is explicit if $\beta_k = 0$ and implicit otherwise.

The formulation developed by Ijam *et al.,* [27] is extended by incorporating a hybrid block multistep method. Building upon existing BBDFs, we introduce off-step points into the formulation to create a variant with A−stability properties. The importance of employing an A−stable method lies in its ability to maintain numerical stability for stiff problems, allowing for larger step sizes without compromising accuracy. This enhancement enables more efficient computations while effectively addressing the rapid variations characteristic of stiff systems.

The two starting points, x_{n-1} and x_n with an equal step size denoted as $h = x_{n+1} - x_n$ are considered as illustrated in Figure 1. The proposed method evaluates the approximate solutions of y_{n+1} and y_{n+2} with a fixed *h*, as well as two off-step points, $y_{n+\frac{1}{2}}$ and $y_{n+\frac{3}{2}}$ with half the step size, simultaneously.

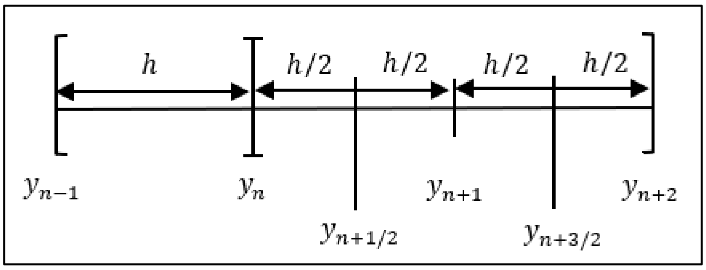

Fig. 1. Hybrid block method with two off-step points

The ρ-HDIBBDF method takes the general form of

$$\sum_{j=0}^{k+1}\alpha_{j-1,k}y_{n+j-1}=h\beta_k\left(f_{n+k}-\rho f_{n+k-\frac{1}{2}}\right) \tag{3}$$

where $k=\frac{1}{2},1,\frac{3}{2},2$. The linear difference operator, L_k associated with Eq. (3) is defined by

$$L_k\left[y(x_n);h\right]=\sum_{j=0}^{k+1}\alpha_{j-1,k}y_{n+j-1}-h\beta_k\left(f_{n+k}-\rho f_{n+k-\frac{1}{2}}\right)=C_q y^q+O\left(h^{p+1}\right)=0. \tag{4}$$

By applying the Taylor series expansion about $x=x_n$, we expand Eq. (4) to obtain

$$\begin{aligned}
L_{\frac{1}{2}}\left[y(x_n);h\right]&=\alpha_{-1,\frac{1}{2}}y_{n-1}+\alpha_{0,\frac{1}{2}}y_n+\alpha_{\frac{1}{2},\frac{1}{2}}y_{n+\frac{1}{2}}-h\beta_{\frac{1}{2}}\left(f_{n+\frac{1}{2}}-\rho f_n\right)=0\\
L_1\left[y(x_n);h\right]&=\alpha_{-1,,1}y_{n-1}+\alpha_{0,1}y_n+\alpha_{\frac{1}{2},1}y_{n+\frac{1}{2}}+\alpha_{1,1}y_{n+1}-h\beta_1\left(f_{n+1}-\rho f_{n+\frac{1}{2}}\right)=0\\
L_{\frac{3}{2}}\left[y(x_n);h\right]&=\alpha_{-1,,\frac{3}{2}}y_{n-1}+\alpha_{0,\frac{3}{2}}y_n+\alpha_{\frac{1}{2},\frac{3}{2}}y_{n+\frac{1}{2}}+\alpha_{1,\frac{3}{2}}y_{n+1}+\alpha_{\frac{3}{2},\frac{3}{2}}y_{n+\frac{3}{2}}-h\beta_{\frac{3}{2}}\left(f_{n+\frac{3}{2}}-\rho f_{n+1}\right)=0\\
L_2\left[y(x_n);h\right]&=\alpha_{-1,,2}y_{n-1}+\alpha_{0,2}y_n+\alpha_{\frac{1}{2},2}y_{n+\frac{1}{2}}+\alpha_{1,2}y_{n+1}+\alpha_{\frac{3}{2},2}y_{n+\frac{3}{2}}+\alpha_{2,2}y_{n+2}-h\beta_2\left(f_{n+2}-\rho f_{n+\frac{3}{2}}\right)=0
\end{aligned} \tag{5}$$

and the terms involving the derivative of y are collected, resulting in

$$C_0y(x_n)+C_1hy'(x_n)+C_2h^2y''(x_n)+\cdots+C_qh^qy^{(q)}(x_n)=0.$$

The constant C_q in Eq. (4) are given by

$$\begin{aligned}
C_0&=\sum_{j=0}^{k+1}\alpha_{j-1,k}\\
C_1&=\sum_{j=0}^{k+1}\left[\frac{(j-1)}{1!}\alpha_{j-1,k}-\frac{k^0}{0!}\beta_k+\rho\beta_k\right]\\
&\vdots\\
C_q&=\sum_{i=0}^{k+1}\left[\frac{(j-1)^q}{q!}\alpha_{j-1,k}-\frac{k^{(q-1)}}{(q-1)!}\beta_k+\frac{(k-1)^{(q-1)}}{(q-1)!}\rho\beta_k\right],\quad q=2,3,\ldots
\end{aligned} \tag{6}$$

By setting $\alpha_{k,k}=1,\alpha_{0,1}=0$ and $\alpha_{0,2}=0$ and solving Eq. (6) simultaneously, we obtain the coefficients of $\alpha_{j-1,k}$ and β_k for the corrector formula of ρ-HDIBBDF, as listed in Eq. (7).

$$y_{n+\frac{1}{2}}=\frac{1}{4}\left(\frac{\rho+1}{\rho-2}\right)y_{n-1}+\frac{3}{4}\left(\frac{\rho-3}{\rho-2}\right)y_n+\frac{3}{4\rho-8}\rho hf_n-\frac{3}{4\rho-8}hf_{n+\frac{1}{2}},$$
$$y_{n+1}=\frac{1}{3}\left(\frac{\rho+1}{3\rho-5}\right)y_{n-1}+\frac{8}{3}\left(\frac{\rho-2}{3\rho-5}\right)y_{n+\frac{1}{2}}+\frac{2}{3\rho-5}\rho hf_{n+\frac{1}{2}}-\frac{2}{3\rho-5}hf_{n+1},$$
$$y_{n+\frac{3}{2}}=\frac{1}{2}\left(\frac{\rho+3}{8\rho-61}\right)y_{n-1}-5\left(\frac{2\rho+5}{8\rho-61}\right)y_n+5\left(\frac{8\rho+15}{8\rho-61}\right)y_{n+\frac{1}{2}}-\frac{45}{2}\left(\frac{\rho+5}{8\rho-61}\right)y_{n+1}+\frac{15}{8\rho-61}\rho hf_{n+1}-\frac{15}{8\rho-61}hf_{n+\frac{3}{2}},$$
$$y_{n+2}=\frac{1}{10}\left(\frac{\rho+3}{5\rho-36}\right)y_{n-1}-\left(\frac{5\rho+12}{5\rho-36}\right)y_{n+\frac{1}{2}}+\frac{9}{2}\left(\frac{5\rho+9}{5\rho-36}\right)y_{n+1}-\frac{9}{5}\left(\frac{7\rho+36}{5\rho-36}\right)y_{n+\frac{3}{2}}+\frac{9}{5\rho-36}\rho hf_{n+\frac{3}{2}}-\frac{9}{5\rho-36}hf_{n+2}.$$
(7)

Eq. (7) can be rewritten in the matrix form as follows

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ -\frac{8}{3}\left(\frac{\rho-2}{3\rho-5}\right) & 1 & 0 & 0 \\ -\frac{5(8\rho+15)}{8\rho-61} & \frac{45}{2}\left(\frac{\rho+5}{8\rho-61}\right) & 1 & 0 \\ \frac{5\rho+12}{5\rho-36} & -\frac{9}{2}\left(\frac{5\rho+9}{5\rho-36}\right) & \frac{9}{5}\left(\frac{7\rho+36}{5\rho-36}\right) & 1 \end{bmatrix}\begin{bmatrix} y_{n+\frac{1}{2}} \\ y_{n+1} \\ y_{n+\frac{3}{2}} \\ y_{n+2} \end{bmatrix}$$
$$=\begin{bmatrix} 0 & \frac{1}{4}\left(\frac{\rho+1}{\rho-2}\right) & 0 & \frac{3}{4}\left(\frac{\rho-3}{\rho-2}\right) \\ 0 & \frac{1}{3}\left(\frac{\rho+1}{3\rho-5}\right) & 0 & 0 \\ 0 & \frac{1}{2}\left(\frac{\rho+3}{8\rho-61}\right) & 0 & -\frac{5(2\rho+5)}{8\rho-61} \\ 0 & \frac{1}{10}\left(\frac{\rho+3}{5\rho-36}\right) & 0 & 0 \end{bmatrix}\begin{bmatrix} y_{n-\frac{3}{2}} \\ y_{n-1} \\ y_{n-\frac{1}{2}} \\ y_n \end{bmatrix}+h\begin{bmatrix} -\frac{3}{4\rho-8} & 0 & 0 & 0 \\ \frac{2\rho}{3\rho-5} & -\frac{2}{3\rho-5} & 0 & 0 \\ 0 & \frac{15\rho}{8\rho-61} & -\frac{15}{8\rho-61} & 0 \\ 0 & 0 & \frac{9\rho}{5\rho-36} & -\frac{9}{5\rho-36} \end{bmatrix}\begin{bmatrix} f_{n+\frac{1}{2}} \\ f_{n+1} \\ f_{n+\frac{3}{2}} \\ f_{n+2} \end{bmatrix}$$
$$+h\begin{bmatrix} 0 & 0 & 0 & \frac{3\rho}{4\rho-8} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}\begin{bmatrix} f_{n-\frac{3}{2}} \\ f_{n-1} \\ f_{n-\frac{1}{2}} \\ f_n \end{bmatrix}.$$
(8)

By applying the test equation $y' = f(x,y) = \lambda y$ and assume $\lambda y = H$ into Eq. (8) yields

$$\begin{bmatrix} 1+\frac{3}{4\rho-8}H & 0 & 0 & 0 \\ -\frac{8}{3}\left(\frac{\rho-2}{3\rho-5}\right)-\frac{2\rho}{3\rho-5}H & 1+\frac{2}{3\rho-5}H & 0 & 0 \\ -\frac{5(8\rho+15)}{8\rho-61} & \frac{45}{2}\left(\frac{\rho+5}{8\rho-61}\right)-\frac{15\rho}{8\rho-61}H & 1+\frac{15}{8\rho-61}H & 0 \\ \frac{5\rho+12}{5\rho-36} & -\frac{9}{2}\left(\frac{5\rho+9}{5\rho-36}\right) & \frac{9}{5}\left(\frac{7\rho+36}{5\rho-36}\right)-\frac{9\rho}{5\rho-36}H & 1+\frac{9}{5\rho-36}H \end{bmatrix}\begin{bmatrix} y_{n+\frac{1}{2}} \\ y_{n+1} \\ y_{n+\frac{3}{2}} \\ y_{n+2} \end{bmatrix}$$

$$=\begin{bmatrix} 0 & \frac{1}{4}\left(\frac{\rho+1}{\rho-2}\right) & 0 & \frac{3}{4}\left(\frac{\rho-3}{\rho-2}\right)+\frac{3\rho}{4\rho-8}H \\ 0 & \frac{1}{3}\left(\frac{\rho+1}{3\rho-5}\right) & 0 & 0 \\ 0 & \frac{1}{2}\left(\frac{\rho+3}{8\rho-61}\right) & 0 & -\frac{5(2\rho+5)}{8\rho-61} \\ 0 & \frac{1}{10}\left(\frac{\rho+3}{5\rho-36}\right) & 0 & 0 \end{bmatrix}\begin{bmatrix} y_{n-\frac{3}{2}} \\ y_{n-1} \\ y_{n-\frac{1}{2}} \\ y_n \end{bmatrix}$$

which is equivalent to $AY_m = BY_{m-1}$.

In the next section, to ensure absolute stability, the parameter ρ is constrained to the interval (−1,1), as discussed by Ijam *et al.,* [10,13]. Specifically, we choose ρ = -3/4, a selection thoroughly justified by Ijam et al., [10]. Their extensive work demonstrates that ρ = -3/4 yields accurate numerical results with optimal stability properties.

3. Stability Analysis

3.1 Definitions

In this section, we conducted an analysis of the stability characteristics of the proposed method, with a particular focus on its order, consistency, zero stability, convergence, and A−stability. These analyses are essential for determining the method's suitability in efficiently addressing stiff ODEs. To commence, we present the widely known definitions of the method's order, consistency, zero stability, convergence and A−stability, as outlined in the numerical analysis literature in [1]:

Definition 1.

The LMM associated with the linear difference operator, L_k are said to be order p if $C_0 = C_1 = \cdots = C_p = 0, C_{p+1} \neq 0$.

Definition 2.

The LMM is said to be consistent if it has order $p \geq 1$.

Definition 3.

The method is said to be zero stable if there is no root of the first characteristic polynomial having modulus greater than one and if every root with modulus one is simple.

Definition 4.

The necessary conditions for an LMM to be convergent are that it must be consistent and zero stable.

Definition 5.

A numerical method is A−stable if its region of absolute stability covers the entire of the negative half-plane.

3.2 Order of the Method

By substituting the corresponding values of $\alpha_{j-1,k}$ and β_k into Eq. (6), which gives $C_0 = C_1 = C_2 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}, C_3 = \begin{bmatrix} -\frac{3}{22} \\ -\frac{14}{87} \\ 0 \\ 0 \end{bmatrix}$. The result indicates that $C_3 \neq 0$. Therefore, following Definition 1, it can be inferred that the derived method is of order 2.

3.3 Consistency

In accordance with Definition 2, consistency is affirmed for the ρ-HDIBBDF method, as its order exceeds one.

3.4 Zero Stability

The stability polynomial $R(t,H)$ for the proposed method in Eq. (3) is determined based on the root locations obtained by solving the characteristic equation, represented by $\det(At - B) = 0$, resulting in

$$\begin{aligned} R(t,H) = {} & t^4 - \frac{160315}{156244}t^3 + \frac{277131}{18124304}t^2 H + \frac{19935}{9062152}t^2 H^2 + \frac{1215}{18124304}t^2 H^3 - \frac{1131506}{1132769}t^4 H \\ & + \frac{422469}{1132769}t^4 H^2 - \frac{906759}{18124304}t^3 H^3 - \frac{69876}{1132769}t^4 H^3 + \frac{4320}{1132769}t^4 H^4 - \frac{17477171}{18124304}t^3 H \\ & - \frac{451875}{1132769}t^3 H^2 - \frac{10935}{9062152}H^4 t^3 + \frac{4071}{156244}t^2. \end{aligned} \tag{9}$$

According to [1], when *H* = 0, the roots *r* coincides with the zeros ξ of the first characteristic polynomial $\rho(\xi)$, which by zero stability, all roots lie in or on the unit circle. When substituted $H = 0$ into Eq. (9), it yields

$$R(t,H) = t^4 - \frac{160315}{156244}t^3 + \frac{4071}{156244}t^2 \tag{10}$$

and solving Eq. (10) for t , gives $t = 0, 0, 1, 0.02606$. Since the roots of the stability polynomial in Eq. (9) align with the criteria set forth in Definition 3, it can be asserted that the method is zero-stable.

3.5 Convergence

With demonstrated consistency and zero stability, as presented in Subsections 3.3 and 3.4, respectively, it can be inferred by Definition 4 that this method has converged.

3.6 A−stability

In this subsection, the absolute stability regions are provided to offer insights into the stability properties of the methods. The boundary of the stability regions for the proposed method is established by substituting $t = e^{i\theta}$ into Eq. (9) and solving $R(t,H)$ for t. The plots in Figure 2 illustrate the complex *H*-plane for a range of $\theta \in [0, 2\pi]$, where $|t| < 1$.

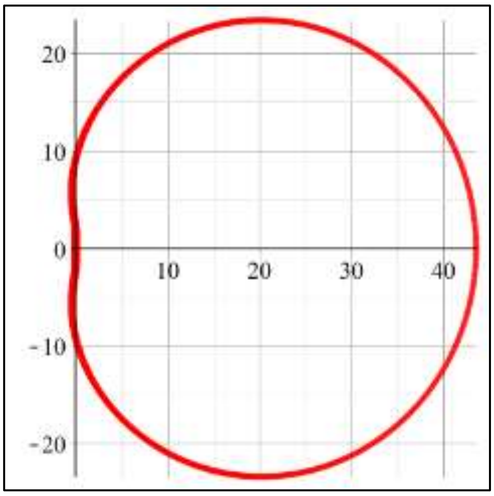

Fig. 2. Stability region for *ρ*-HDIBBDF

Illustrated in Figure 2, the absolute stability region for *ρ*-HDIBBDF is situated beyond the closed contour of the graph, with the unstable region contained within. In accordance with Definition 5, the method is deemed A−stable, as the absolute stability region covers the entire half-plane. Consequently, the proposed method is well-suited for the efficient solution of stiff ODEs.

4. Numerical Results

In this section, numerical solutions for three stiff chemical reaction problems are obtained using the proposed method, *ρ*-HDIBBDF and will be compared with two existing methods of the same order. The tested problems will be solved with varying step sizes, specifically, $H = 10^{-2}, 10^{-4}, 10^{-6}$.

Test Problem 1: Nonlinear stiff chemical reaction problem (the Kaps problem) in [19]

$$y_1' = -\left(\varepsilon^{-1} + 2\right) y_1 + \varepsilon^{-1} y_2^2 \qquad y_1(0) = 1 \qquad x \in [0, 20]$$
$$y_2' = y_1 - y_2\left(1 + y_2\right) \qquad y_2(0) = 1 \qquad \varepsilon = 10^{-3}$$

Exact solutions: $y_1(x) = e^{-2x}, \quad y_2(x) = e^{-x}$

Test Problem 2: Modified nonlinear stiff chemical reaction problem of Robertson in [27]

$$y_1' = -0.04 y_1 + 10^4 y_2 y_3 - 0.96 e^{-x} \qquad y_1(0) = 1 \qquad x \in [0, 1]$$
$$y_2' = 0.04 y_1 - 10^4 y_2 y_3 - \left(3 \times 10^7\right) y_2^2 - 0.04 e^{-x} \qquad y_2(0) = 0$$
$$y_3' = \left(3 \times 10^7\right) y_2^2 + e^{-x} \qquad y_3(0) = 0$$

Exact solutions: $y_1(x) = e^{-x}, \quad y_2(x) = 0, \quad y_3(x) = 1 - e^{-x}$

Origin of the problem: The ROBER problem, as defined by Robertson, H., represents the kinetics of an autocatalytic reaction (see [19]). The composition of the reactions is as follows:

$$A \xrightarrow{k_1} B$$
$$B + B \xrightarrow{k_2} C + B$$
$$B + C \xrightarrow{k_3} A + C$$

Chemical species *A*, *B* and *C* are involved in the reactions, and the rate constants for these reactions are denoted as k_1, k_2 and k_3, respectively. y_1, y_2 and y_3 are refer to the concentrations of *A*, *B* and *C*, respectively and $y_1(0), y_2(0)$ and $y_3(0)$ are the concentrations at time $t = 0$.

For Test Problem 3, the exact solutions are unknown, therefore the approximation values are obtained to be compared with MATLAB stiff solver, ode15s.

Test Problem 3: Nonlinear oregonator chemical reaction problem in Hairer and Wanner [29]

$$y_1' = 77.27\left(y_2 - y_1 y_2 + y_1 - 8.375 \times 10^{-6} y_1^2\right) \qquad y_1(0) = 1 \qquad x \in [0, 400]$$
$$y_2' = \frac{1}{77.27}\left(y_3 - y_2 + y_1 y_2\right) \qquad y_2(0) = 2$$
$$y_3' = 0.161\left(y_1 - y_3\right) \qquad y_3(0) = 3$$

Origin of the problem: The OREGO problem stems from the well-known Belousov-Zhabotinsky reaction. When chemicals like bromous acid, bromide ions and cerium ions are mixed, they undergo a chemical reaction that oscillates in structure and colour (red to blue and back) after an initial inactive phase. The Oregonator mechanism follows this pattern

$$A + Y \rightarrow X + P$$
$$X + Y \rightarrow 2P$$
$$A + X \rightarrow 2X + 2Z$$
$$2X \rightarrow A + P$$
$$B + Z \rightarrow \frac{1}{2} fY$$

with standard notations for the assignments and effective concentrations:

hypobromous acid	$\left[HBrO2\right] = X$	5.025×10^{-11}
Bromide	$\left[Br^{-}\right] = Y$	3.0×10^{-7}
Cerium – 4	$\left[CE\left(IV\right)\right] = Z$	2.412×10^{-8}
Bromate	$\left[BrO_3^{-}\right] = A$	
all oxidizable organic species	$\left[Org\right] = B$	
	$\left[HOBr\right] = P$	

where y_1, y_2 and y_3 are refer to the concentrations of *X*, *Y* and *Z*, respectively.

The abbreviations utilized in numerical results are listed below in Table 1.

Table 1
Description of the abbreviations used

Notation	Description
H	Step size
TS	Total steps
MAXE	Maximum error
TIME	Computational time in Microsecond
ρ-HDIBBDF	The derived method
ρ-DIBBDF	*ρ*-Diagonally Implicit Block Backward Differentiation Formula derived in Ijam *et al.,* [27]
NDIBBDF	Diagonally Implicit Block Backward Differentiation Formula by Babangida *et al.,* [30]
ode15s	Variable step, variable order solver based on numerical differentiation formula in MATLAB

The numerical results for Test Problems 1–3 are presented in Tables 2–4. The results are obtained using the C programming language and the methods are compared based on accuracy, total steps taken and computational time.

Tables 2–4 display the numerical outcomes of *ρ*-HDIBBDF for three test problems, highlighting its accuracy. A thorough review of the tabulated results across test problems 1 and 2 reveals that as the step size decreases, MAXE improves, signifying heightened accuracy. To visually depict the performance of the methods, graphs of $\log_{10} MAXE$ against $\log_{10} TIME$ were generated, as illustrated in Figures 3–4.

Table 2
Numerical results for Test Problem 1

H	Method	ρ	TS	MAXE	TIME
10^{-2}	ρ-HDIBBDF	-3/4	1000	2.63600e-04	1.70046e-05
	ρ-DIBBDF	-3/4	1000	5.28528e-04	3.73354e-05
	NDIBBDF	1/5	1000	5.99388e-04	4.84041e-05
10^{-4}	ρ-HDIBBDF	-3/4	100000	3.05335e-08	1.14600e-03
	ρ-DIBBDF	-3/4	100000	6.16862e-08	1.25609e-03
	NDIBBDF	1/5	100000	7.19977e-08	3.94726e-03
10^{-6}	ρ-HDIBBDF	-3/4	10000000	1.67696e-11	8.44418e-02
	ρ-DIBBDF	-3/4	10000000	1.13746e-11	9.37730e-02
	NDIBBDF	1/5	10000000	3.37188e-11	1.34732e-01

Table 3
Numerical results for Test Problem 2

H	Method	ρ	TS	MAXE	TIME
10^{-2}	ρ-HDIBBDF	-3/4	50	7.66634e-05	3.77463e-06
	ρ-DIBBDF	-3/4	50	1.60447e-04	1.52997e-05
	NDIBBDF	1/5	50	1.95517e-04	2.15107e-05
10^{-4}	ρ-HDIBBDF	-3/4	5000	7.77988e-09	3.56956e-04
	ρ-DIBBDF	-3/4	5000	1.62943e-08	5.77681e-04
	NDIBBDF	1/5	5000	1.99133e-08	3.12601e-03
10^{-6}	ρ-HDIBBDF	-3/4	500000	2.76684e-11	1.96184e-03
	ρ-DIBBDF	-3/4	500000	1.82327e-11	2.92248e-02
	NDIBBDF	1/5	500000	5.82263e-11	3.98782e-01

Table 4
(a) Approximate solutions of $y_1(x)$ for Test Problem 3

x	ρ-HDIBBDF	ode15s
0	1	1
20	2.7592375213e+1	2.7694042443e+1
40	1.0005765914e+0	1.0005772292e+0
60	1.0008746230e+0	1.0008746638e+0
80	1.0014591409e+0	1.0014595860e+0
100	1.0024499598e+0	1.0024450131e+0
120	1.0041180119e+0	1.0041180876e+0
140	1.0069297957e+0	1.0069245946e+0
160	1.0116838451e+0	1.0117673390e+0
180	1.0197634207e+0	1.0197676067e+0
200	1.0336162966e+0	1.0336284516e+0
220	1.0577314841e+0	1.0577878013e+0
240	1.1008487863e+0	1.1007820164e+0
260	1.1817948736e+0	1.1817371633e+0
280	1.3490005510e+0	1.3487884271e+0
300	1.7797210611e+0	1.7790787590e+0
320	4.9477305937e+0	4.9334847095e+0
340	1.0005659549e+0	1.0005658773e+0
360	1.0008148683e+0	1.0008146706e+0
380	1.0013552502e+0	1.0013503921e+0
400	1.0022749000e+0	1.0022735383e+0

(b) Approximate solutions of $y_2(x)$ for Test Problem 3

x	ρ-HDIBBDF	ode15s
0	2	2
20	9.9276220727e-1	9.9243562629e-1
40	1.7353155305e+3	1.7351633542e+3
60	1.1443398044e+3	1.1442337819e+3
80	6.8632865835e+2	6.8626388443e+2
100	4.0916618099e+2	4.0912758031e+2
120	2.4383323413e+2	2.4381016155e+2
140	1.4530283410e+2	1.4529223198e+2
160	8.6587189289e+1	8.6597107500e+1
180	5.1597745733e+1	5.1607395094e+1
200	3.0746864251e+1	3.0752834605e+1
220	1.8321054294e+1	1.8327286047e+1
240	1.0915366103e+1	1.0920157298e+1
260	6.5002441155e+0	6.5032084339e+0
280	3.8648259901e+0	3.8666303360e+0
300	2.2818584576e+0	2.2829182517e+0
320	1.2505049722e+0	1.2514306841e+0
340	1.7679103532e+3	1.7678823620e+3
360	1.2281814830e+3	1.2285953262e+3
380	7.3886459915e+2	7.3912761146e+2
400	4.4057572429e+2	4.4073323966e+2

(c) Approximate solutions of $y_3(x)$ for Test Problem 3

x	ρ-HDIBBDF	ode15s
0	3	3
20	5.5001802191e+0	5.5045727499e+0
40	2.0713781977e+3	2.0710642864e+3
60	8.3722824261e+1	8.3695537494e+1
80	4.3064229668e+0	4.3068524784e+0
100	1.1341682283e+0	1.1340537885e+0
120	1.0088222993e+0	1.0088077233e+0
140	1.0061758163e+0	1.0061807790e+0
160	1.0100597843e+0	1.0100705523e+0
180	1.0169857345e+0	1.0169385773e+0
200	1.0288426840e+0	1.0288443878e+0
220	1.0493895754e+0	1.0493198273e+0
240	1.0858317299e+0	1.0858650265e+0
260	1.1532442646e+0	1.1531883210e+0
280	1.2885003491e+0	1.2883373853e+0
300	1.6137513726e+0	1.6133147535e+0
320	3.2075955743e+0	3.2031167190e+0
340	3.2811073640e+3	3.2891749322e+3
360	1.3205757622e+2	1.3236993576e+2
380	6.2375537437e+0	6.2525364944e+0
400	1.2111795585e+0	1.2116215558e+0

The efficiency curves depicted in Figures 3–4 demonstrate a significant improvement in the performance of the proposed method across all step sizes when compared to the other two methods, ρ-DIBBDF and NDIBBDF. This underscores the method's exceptional accuracy and efficiency, emphasizing its superior performance over alternative approaches. In cases where theoretical solutions are unavailable for Test Problem 3, the solution curves presented in Figure 5 exhibit a notable agreement with the MATLAB stiff solver, ode15s.

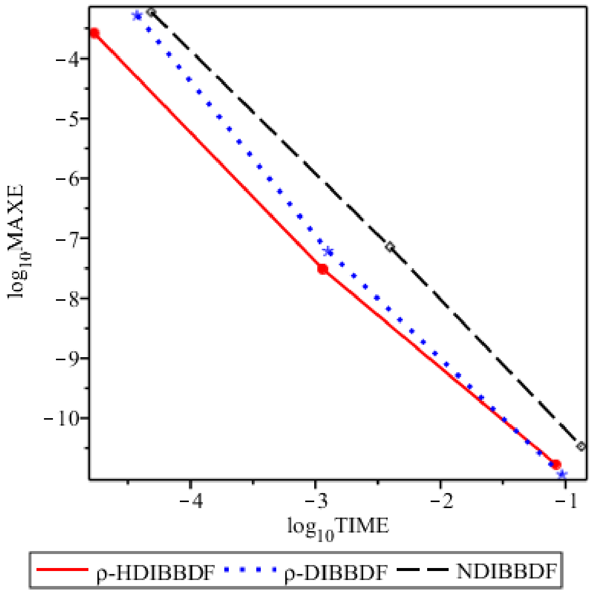

Fig. 3. Efficiency curves for Test Problem 1

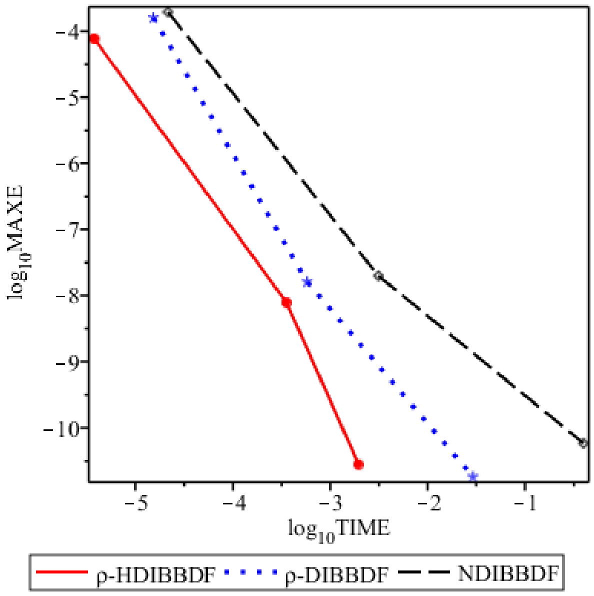

Fig. 4. Efficiency curves for Test Problem 2

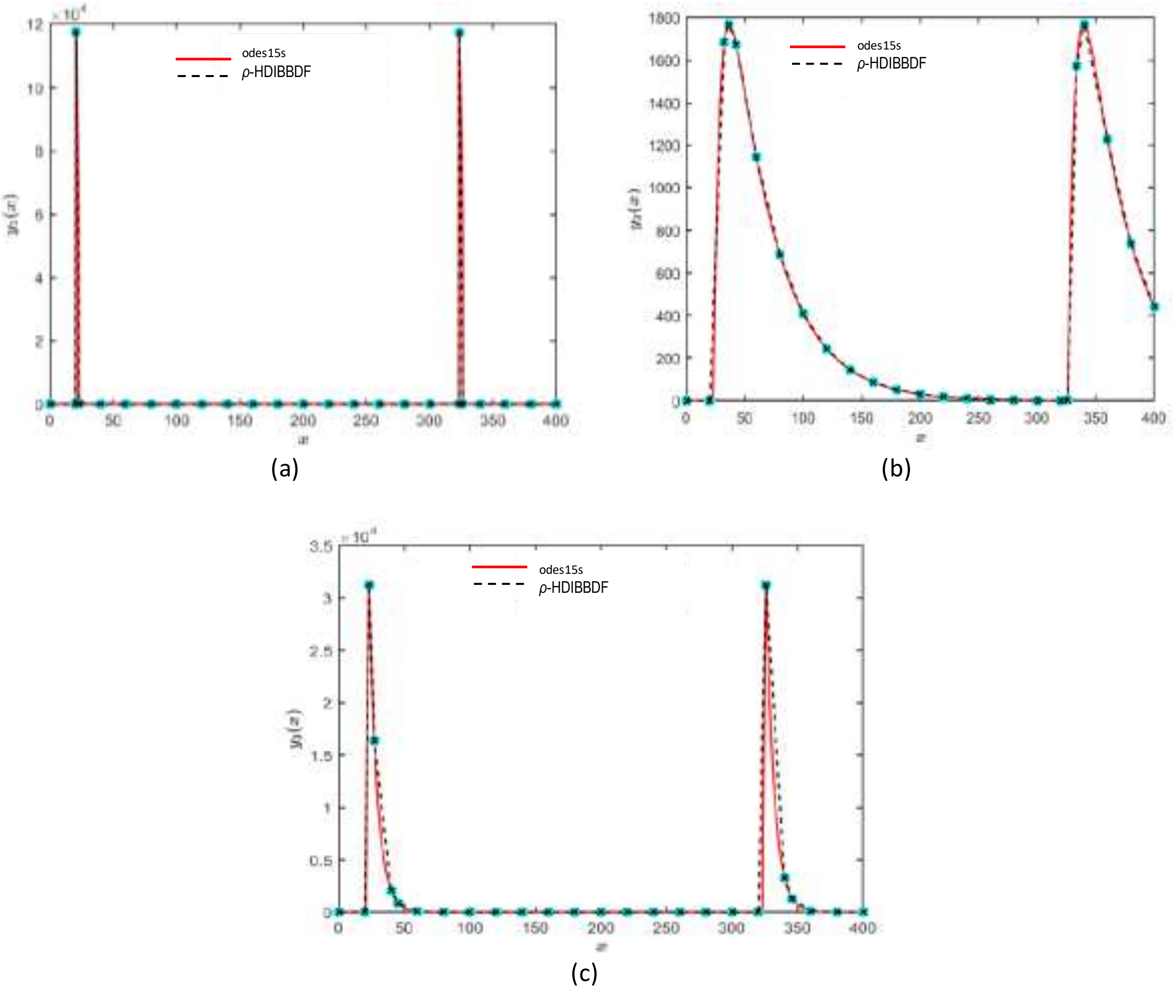

Fig. 5. Solution curves of ρ-HDIBBDF and ode15s for Test Problem 3, (a) $y_1(x)$, (b) $y_2(x)$, (c) $y_3(x)$

5. Conclusions

In summary, the newly introduced method, ρ-HDIBBDF, exhibits second-order accuracy, possesses both consistency and zero stability, thereby demonstrating convergence. Across all comparison metrics, including total steps, computational time and maximum error, the proposed method has proven to be more efficient than the methods it was compared against. Future research may focus on exploring adaptive strategies to further enhance the efficiency and applicability of this method. Consequently, the proposed method showcases successful applicability to stiff systems arising from chemical reactions, attributed to its high-order accuracy and broader stability region. Furthermore, the proposed method holds potential applications in a diverse array of fields, contributing to our understanding of natural processes, industrial applications, and environmental phenomena.

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