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A Class of A-Stable Hybrid Block Backward Differentiation Formulae for Solving Stiff Chemical Reaction Problems of Ordinary Differential Equations

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ABSTRACT

A major challenge in simulating chemical reaction processes is integrating the stiff systems of Ordinary Differential Equations (ODEs) describing the chemical reactions due to stiffness. Thus, it would be of interest to search systematically for stiff solvers that are close to optimal for such problems. This paper presents an implicit 2-Step and 3-Step Hybrid Block Backward Differentiation Formulae with one off-step point in (2SHBBDF) and two off-step point in (3SHBBDF) for the solutions of first-order stiff chemical reaction problems. In deriving the methods, the polynomial basis function was adopted. The paper further analyses the basic properties of the (2SHBBDF) and (3SHBBDF) which include order of accuracy, consistence, zero-stability, convergence and the stability regions of the methods was also computed. To demonstrate the accuracy of the proposed approach, some famous stiff chemical reaction problems such as Robertson problem and Stiff Chemical reactions were solved, and the results obtained were compared with those of some existing methods. The results obtained clearly show that our new methods perform better than the existing methods with which we compared our results.

1. Introduction

A class of numerical techniques used to resolve Ordinary Differential Equations (ODEs) that are thought to be both accurate and numerically stable is known as "A-stable hybrid block methods." These techniques intentionally maintain stability for stiff and real-life modeled issues, which are distinguished by rapid changes in the system's dynamics. Generalized backward differentiation formulae (GBDF) are one way to achieve A-stability in block approaches. The Backward Differentiation Formula (BDF) remains a family of implicit numerical techniques used for solving routine differential equations (ODEs). These methods are mostly effective for solving stiff ODEs, which are problems that have solutions with speedily changing behavior on different time scales. BDF methods are multi-step methods based on backward differentiation formulae, which use weighted combinations of past derivatives to approximate the solution at the current time step. BDF methods are mostly suitable for stiff problems and modeled real-life problems because they can be considered to have high order accuracy while maintaining stability (Atsi & Kumleng 2020).

Collocation methods are widely considered as a way of generating numerical solution to ordinary differential equation of the form:

$$y'(x) = f(x, y(x)),\ y(x_0) = y_0,\ x \in [x_0, x_N] \tag{1.1}$$

where $f: [x_0, x_N] \times R^n \to R^m$, $y_0 \in R^n$ is continuous and differentiable. However, it is assumed that (1.1) satisfy the existence and uniqueness theorem within the interval of integration.

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The problem appear in (1.1) is also used to study how fast bacteria grow in a colony, estimate how many people get infected with a contagious disease in a closed group over time, analyze the movement of rockets or satellites, understand fluid flow, electric circuits, simulate population growth, simple harmonic motion, the path of a particle, and chemical reactions, among other things (Ijam, Ibrahim, & Zawawi, 2024). ODEs of non-stiff systems, the challenge has always been how to find an appropriate implicit method for solving stiff ODEs that have A-stability properties. Since block methods' most significant flaw seems to be their inability to maintain stability, it is essential to develop algorithms with appropriate stability properties.

The order of interpolation points must not be greater than the order of the differential equations, which is a significant drawback of the block approach despite its many benefits (Kashkari & Syam, 2019). This setback led to the introduction of off-step spots in the block, which were dubbed the hybrid approach. Although they take longer to develop, hybrid approaches are more accurate than two traditional approaches (Runge-Kutta and linear multistep methods) and have been shown to get around the Dahlquist Zero-Stability Barrier condition by introducing function evaluation at off-step points (Kashkari & Syam, 2019).

According to Ijam, Ibrahim, and Zawawi (2024), exploratory and conceptual proof has demonstrated that adaptive step size techniques, which include the hybrid diagonally implicit BBDF, which incorporates off-step points, improves preciseness and computational performance for stiff chemical reactions, are more reliable through a greater variety in procedure dimensions than fixed step methods. Recognizing the computational effectiveness and accuracy of such methods, a modified step size form of the block backward differentiation equation (BBDE) in a diagonally implicit structure was suggested to handling stiff ordinary differential equations (ODEs), specifically for handling the problems caused by the chemical reaction problem in applied and industrial mathematics. The longitudinally implicit form, which includes a smaller triangular array and steady longitudinal inputs, provides considerable advantages for assessing the Jacobian and the below-upper decomposed. The stability qualities studied revealed that the new class is zero-stable, A zero-stable, and A-stable, ensuring steady convergence to exact solutions. Comparative studies demonstrate that the suggested method outperforms the currently available wholly implicit BBDM and ode15s in MATLAB program (Ijam *et al*., 2024).

In a similar vein, Ijam, *et al.* (2024) proposed an enhanced method for addressing the computational challenges related to stiff chemical reactions. They proposed using a mixture of the Cross-wise Implicitly Block Reverse Differentiation Algorithm in conjunction with strategically selected off-step locations to increase the preciseness and effectiveness of numerical approaches. Stiff chemical reactions, which are ubiquitous in many industrial processes, necessitate complex numerical approaches to accurately record rapid changes in concentration. Our hybrid formulation improves stability as well as computational speed by extending the longitudinally implicit framework of block reverse differentiation algorithms, resulting in better performance when addressing stiff chemical reactions questions. When a specific free parameter was chosen, the approach was discovered to have both zero-stability and A-stability features. Convergence analysis proved its capacity to accurately estimate exact answers. Through thorough experimentation and comparative analysis, this study demonstrated the efficiency of the established method in analyzing complex standard differential equations. The expected objectives include the creation of a new numerical method, validation through extensive numerical experiments, and insights into its performance and applicability in a variety of science and engineering disciplines.

Motivated by the literatures mentioned above, the goal of this study is to use polynomial basis functions to build a 2-step and 3-step Hybrid Block Backward Differentiation Formula with one off-step point (2SHBBDF) and (3SHBBDF) for solving chemical reaction problems that include stiff first-order ODEs. The approach will be used to solve issues involving stiff chemical reactions of the form (1.1). It was determined that choosing the spots where the step is halved will result in zero-stable formulas after a number of points were investigated for the selection of off-step positions. The suggested approaches have an advantage over those created by Khalsaraei and Molayi (2020) in that they provide improved precision and concurrent approximations of the solutions with off-step locations.

2. Method

Two-Step Hybrid Block Backward Differentiation Formulae

Consider k- step discrete formula

$$y(x_{n+k}) = \sum_{j=0}^{k-1} \alpha_j y_{n+j} + h\sum_{j=0}^{k-1} \beta_j f\left(\overline{x}_j, y(\overline{x})\right) \tag{2.1}$$

from equation 2.1. The continuous formulation of GBDF becomes

$$y(x) = \sum_{j=0}^{k-1} \alpha_j(x) y_{n+j} + h\beta_v(x) f_{n+v} \tag{2.2}$$

we consider $j = v$ in the form of

$$j = v \equiv \begin{cases} \frac{k-1}{2}, \text{when k is odd} \\ \frac{k-2}{2}, \text{when k is even} \end{cases} \tag{2.3}$$

to develop two step hybrid method when $k = 2$, then $v = 0$, according to equation 2.1. The continuous formulation of GBDF becomes

$$y(x) = \sum_{j=0}^{k-1} \alpha_j(x) y_{n+j} + h\beta_0(x) f_n \tag{2.4}$$

$$y(x) = \alpha_0(x) y_n + \alpha_{\frac{1}{2}}(x) y_{n+\frac{1}{2}} + \alpha_1(x) y_{n+1} + h\beta_0(x) f_n \tag{2.5}$$

Putting (2.5) in matrix form we have

$$D = \begin{pmatrix} 1 & x_n & x_n{}^2 & x_n{}^3 \\ 1 & x_{n+\frac{1}{2}} & x_{n+\frac{1}{2}}{}^2 & x_{n+\frac{1}{2}}{}^3 \\ 1 & x_{n+1} & x_{n+1}{}^2 & x_{n+1}{}^3 \\ 0 & 1 & x_n & x_n{}^2 \end{pmatrix} \tag{2.6}$$

Using Gaussian elimination method, the continuous coefficients $\alpha_0(x), +\alpha_{\frac{1}{2}}(x), +\alpha_1(x)$ and $\beta_0(x)$ are derived and substituted giving the continuous formulation of two step hybrid method for $k = 2$ (2SHBDF) in the form

$$y(\xi) = \alpha_0(\xi) y_n + \alpha_{\frac{1}{2}}(\xi) y_{n+\frac{1}{2}} + \alpha_1(\xi) y_{n+1} + h\beta_0(\xi) f_n \tag{2.7}$$

where

$$\alpha_0(x) = 6\xi^3 - 7\xi^2 + 1, \alpha_{\frac{1}{2}}(x) = 8\xi^2 - 8\xi^3, \alpha_1(x) = 2\xi^3 - \xi^2, \beta_0(x) = 2\xi^3 - 3\xi^2 + \xi,$$

$$\xi = x - x_n, 0 \le \xi \le 2h$$

Evaluating (2.7) at $\xi = 2h, \frac{3}{2}h$and its first derivative at $\xi = 2h, \frac{3}{2}h$. After collecting the terms and putting it in block form we obtained

$$\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&1\end{pmatrix}\begin{pmatrix}y_{n+\frac{1}{2}}\\y_{n+1}\\y_{n+\frac{3}{2}}\\y_{n+2}\end{pmatrix}=\begin{pmatrix}0&0&0&1\\0&0&0&1\\0&0&0&1\\0&0&0&0\end{pmatrix}\begin{pmatrix}y_{n-\frac{1}{2}}\\y_{n-1}\\y_{n-\frac{3}{2}}\\y_n\end{pmatrix}+h\begin{pmatrix}0&0&0&\frac{53}{144}\\0&0&0&\frac{19}{36}\\0&0&0&\frac{9}{16}\\0&0&0&\frac{5}{9}\end{pmatrix}\begin{pmatrix}f_{n-\frac{1}{2}}\\f_{n-1}\\f_{n-\frac{3}{2}}\\f_n\end{pmatrix}+$$

$$h\begin{pmatrix}0&0&\frac{5}{18}&-\frac{7}{48}\\0&0&\frac{8}{9}&-\frac{5}{12}\\0&0&\frac{3}{2}&-\frac{9}{16}\\0&0&\frac{16}{9}&-\frac{1}{3}\end{pmatrix}\begin{pmatrix}f_{n+\frac{1}{2}}\\f_{n+1}\\f_{n+\frac{3}{2}}\\f_{n+2}\end{pmatrix} \tag{2.8}$$

After matrix multiplication, we obtain the normalized scheme in the form of

$$y_{n+\frac{1}{2}}=y_n+h\left[\frac{53}{144}f_n+\frac{5}{18}f_{n+\frac{3}{2}}-\frac{7}{48}f_{n+2}\right], y_{n+1}=y_n+h\left[\frac{19}{36}f_n+\frac{8}{9}f_{n+\frac{3}{2}}-\frac{5}{12}f_{n+2}\right]$$

$$y_{n+\frac{3}{2}}=y_n+h\left[\frac{9}{16}f_n+\frac{3}{2}f_{n+\frac{3}{2}}-\frac{9}{16}f_{n+2}\right], y_{n+2}=y_n+h\left[\frac{5}{9}f_n+\frac{16}{9}f_{n+\frac{3}{2}}-\frac{1}{3}f_{n+2}\right] \tag{2.9}$$

Three-Step Hybrid Block Backward Differentiation Formulae

From equation (2.3), when $k=3, v=1$, the continuous formulation of 3SHBGBDF becomes

$$y(x)=\sum_{j=0}^{2}\alpha_j(x)\,y_{n+j}+h\beta_1 f_{n+1} \tag{2.10}$$

Expressing (2.10) accordingly gives

$$D=\begin{pmatrix}1&x_n&x_n^2&x_n^3&x_n^4&x_n^5\\1&x_{n\frac{1}{2}}&x_{n+\frac{1}{2}}^2&x_{n+\frac{1}{2}}^3&x_{n+\frac{1}{2}}^4&x_{n+\frac{1}{2}}^5\\1&x_{n+1}&x_{n+1}^2&x_{n+1}^3&x_{n+1}^4&x_{n+1}^5\\1&x_{n+\frac{3}{2}}&x_{n+\frac{3}{2}}^2&x_{n+\frac{3}{2}}^3&x_{n+\frac{3}{2}}^4&x_{n+\frac{3}{2}}^5\\1&x_{n+2}&x_{n+2}^2&x_{n+2}^3&x_{n+2}^4&x_{n+2}^5\\0&1&x_{n+1}&x_{n+1}^2&x_{n+1}^3&x_{n+1}^4\end{pmatrix} \tag{2.11}$$

Using Maple software, the continuous coefficients $\alpha_0(x), \alpha_{\frac{1}{2}}(x), \alpha_1(x), \alpha_{\frac{3}{2}}(x), \alpha_2(x)$ and $\beta_1(x)$ are derived and substituted accordingly gives the continuous formulation of GBDF for $k=3$ in the form of

$$y(\xi)=\alpha_0(x)y_n+\alpha_{\frac{1}{2}}(x)y_{n+\frac{1}{2}}+\alpha_1(x)y_{n+1}+\alpha_{\frac{3}{2}}(x)y_{n+\frac{3}{2}}+\alpha_2(x)y_{n+2}+h\beta_1(x)f_{n+1} \tag{2.12}$$

where

$$\alpha_0=-\frac{2}{3}\xi^5+4\xi^4-\frac{55}{6}\xi^3+10\xi^2-\frac{31}{6}\xi+1, \alpha_{\frac{1}{2}}=\frac{16}{3}\xi^5-\frac{88}{3}\xi^4+\frac{176}{3}\xi^3-\frac{152}{3}\xi^2+16\xi,$$

$$\alpha_1=4\xi^4-16\xi^3+19\xi^2-6\xi, \alpha_{\frac{3}{2}}=-\frac{16}{3}\xi^5+24\xi^4-\frac{112}{3}\xi^3+24\xi^2-\frac{16}{3}\xi,$$

$$\alpha_2=\frac{2}{3}\xi^5-\frac{8}{3}\xi^4+\frac{23}{6}\xi^3-\frac{7}{3}\xi^2+\frac{1}{2}\xi,\beta_1=4\xi^5-20\xi^4+35\xi^3-25\xi^2+6\xi$$

where $\xi=x-x_n, 0\le\xi\le 3h$

Evaluating (2.12) at $\xi=\frac{5}{2}h, 3h$ and its first derivative at $\xi=x_n, 2h, \frac{5}{2}h, 3h$. After collecting the terms and putting it in a block form we obtain three step hybrid block method (3SHBM) in the form

$$\begin{pmatrix}1&0&0&0&0&0\\0&1&0&0&0&0\\0&0&1&0&0&0\\0&0&0&1&0&0\\0&0&0&0&1&0\\0&0&0&0&0&1\end{pmatrix}\begin{pmatrix}y_{n+\frac{1}{2}}\\y_{n+1}\\y_{n+\frac{3}{2}}\\y_{n+2}\\y_{n+\frac{5}{2}}\\y_{n+3}\end{pmatrix}=$$

$$\begin{pmatrix}0&0&0&0&0&1\\0&0&0&0&0&1\\0&0&0&0&0&1\\0&0&0&0&0&1\\0&0&0&0&0&1\\0&0&0&0&0&1\end{pmatrix}\begin{pmatrix}y_{n-\frac{1}{2}}\\y_{n-1}\\y_{n-\frac{3}{2}}\\y_{n-2}\\y_{n-\frac{5}{2}}\\y_{n}\end{pmatrix}+h\begin{pmatrix}0&0&0&0&0&\frac{8197}{28800}\\0&0&0&0&0&\frac{599}{1800}\\0&0&0&0&0&\frac{1029}{3200}\\0&0&0&0&0&\frac{71}{225}\\0&0&0&0&0&\frac{365}{1152}\\0&0&0&0&0&\frac{63}{200}\end{pmatrix}\begin{pmatrix}f_{n-\frac{1}{2}}\\f_{n-1}\\f_{n-\frac{3}{2}}\\f_{n-2}\\f_{n-\frac{5}{2}}\\f_{n}\end{pmatrix}$$

$$+h\begin{pmatrix}0&\frac{2333}{5760}&0&-\frac{943}{1920}&\frac{91}{225}&-\frac{593}{5760}\\0&\frac{361}{360}&0&-\frac{101}{120}&\frac{152}{225}&-\frac{61}{360}\\0&\frac{861}{640}&0&-\frac{333}{640}&\frac{12}{25}&-\frac{81}{640}\\0&\frac{64}{45}&0&\frac{1}{15}&\frac{64}{225}&-\frac{4}{45}\\0&\frac{1625}{1152}&0&\frac{125}{384}&\frac{5}{9}&-\frac{125}{1152}\\0&\frac{57}{40}&0&\frac{9}{40}&\frac{24}{25}&\frac{3}{40}\end{pmatrix}\begin{pmatrix}f_{n+\frac{1}{2}}\\f_{n+1}\\f_{n+\frac{3}{2}}\\f_{n+2}\\f_{n+\frac{5}{2}}\\f_{n+3}\end{pmatrix} \tag{2.13}$$

and the normalized discrete Scheme, three step hybrids normalized discrete scheme (3SHNDS) as

$$y_{n+\frac{1}{2}}=y_n+h\left[\frac{8197}{28800}f_n+\frac{2333}{5760}f_{n+1}-\frac{943}{1920}f_{n+2}+\frac{91}{225}f_{n+\frac{5}{2}}-\frac{593}{5760}f_{n+3}\right]$$

$$y_{n+1}=y_n+h\left[\frac{599}{1800}f_n+\frac{361}{360}f_{n+1}-\frac{101}{120}f_{n+2}+\frac{152}{225}f_{n+\frac{5}{2}}-\frac{61}{360}f_{n+3}\right]$$

$$y_{n+\frac{3}{2}}=y_n+h\left[\frac{1029}{3200}f_n+\frac{861}{640}f_{n+1}-\frac{333}{640}f_{n+2}+\frac{12}{25}f_{n+\frac{5}{2}}-\frac{81}{640}f_{n+3}\right]$$

$$y_{n+2}=y_n+h\left[\frac{71}{225}f_n+\frac{64}{45}f_{n+1}+\frac{1}{15}f_{n+2}+\frac{64}{225}f_{n+\frac{5}{2}}-\frac{4}{45}f_{n+3}\right]$$

$$y_{n+\frac{5}{2}} = y_n + h\left[\frac{365}{1152}f_n + \frac{1625}{1152}f_{n+1} + \frac{125}{384}f_{n+2} + \frac{5}{9}f_{n+\frac{5}{2}} - \frac{125}{1152}f_{n+3}\right]$$

$$y_{n+3} = y_n + h\left[\frac{63}{200}f_n + \frac{57}{40}f_{n+1} + \frac{9}{40}f_{n+2} + \frac{24}{25}f_{n+\frac{5}{2}} + \frac{3}{40}f_{n+3}\right] \quad (2.14)$$

3. Stability Properties of the Methods

The following section comprises the analysis of basic properties of the proposed method. These properties include order, consistency, zero-stability and convergence. The region of absolute stability of the method shall also be determined.

3.1 Order and Error Constant Hybrid Methods

Definition 3.1 (*Order and Error Constant*). The LMM (2.1) associated with the linear difference operator is said to be of order p if $C_1 = C_2 = \cdots = C_p = 0$ and $C_{p+1} \neq 0$. The term $C_{p+1} \neq 0$ is called the error constant of the method. By using tailor's series expansion on (2.9) and (3.4) the order and error constant of the hybrid block generalized backward differentiation formulae (HBGBDF) are presented in table 3.1 below

Table 3.1: Order and Error Constants of 2SHBGBDF and 3SHBGBDF

Methods	Order	Error Constant
Method (2.9)	$(i)\ y_{n+\frac{1}{2}},\quad p=3$	$\frac{47}{1152}$
	$(ii)\ y_{n+1},\quad p=3$	$\frac{7}{72}$
	$(iii)\ y_{n+\frac{3}{2}},\quad p=3$	$\frac{15}{128}$
	$(iv)\ y_{n+2},\quad p=3$	$\frac{1}{9}$
Method (2.14)	$(i)\ y_{n+\frac{1}{2}},\quad p=5$	$\frac{1603}{230400}$
	$(ii)\ y_{n+1},\quad p=5$	$\frac{13}{1200}$
	$(iii)\ y_{n+\frac{3}{2}},\quad p=5$	$\frac{231}{25600}$
	$(iv)\ y_{n+2},\quad p=5$	$\frac{7}{900}$
	$(v)\ y_{n+\frac{5}{2}},\quad p=5$	$\frac{25}{3072}$
	$(vi)\ y_{n+3},\quad p=5$	$\frac{3}{400}$

Therefore, this can be demonstrated that the proposed methods are of order three and five.

3.2 Consistency of the Hybrid Methods

Definition 3.2 (*Consistency*)

The LMM (2.1) is said to be consistent if it is of order $p \geq 1$. It is therefore clear that the 2SHBBDF and 3SHBBDF are consistent since it has order $p = 3$, and $p = 5$ respectively which satisfies Definition (3.2)

Zero Stability Analysis of the Hybrid Methods

Definition 3.3 (*Zero-stable*)

If no root of the characteristic polynomial has a modulus greater than one and every root with modulus one is simple, then LMM (2.2) is said to be zero-stable.

$$\lambda\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&1\end{pmatrix}-\begin{pmatrix}0&0&0&1\\0&0&0&1\\0&0&0&1\\0&0&0&1\end{pmatrix}=\begin{pmatrix}\lambda&0&0&-1\\0&\lambda&0&-1\\0&0&\lambda&-1\\0&0&0&\lambda-1\end{pmatrix}$$

determinant: $\lambda^4 - \lambda^3 = \lambda^3(\lambda - 1) = 0, \lambda_1 = \lambda_2 = \lambda_3 = 0$ and $\lambda = 1$

Since all the roots lie within $\lambda \leq 1$ described in Definition 4.1; hence, it is concluded that the methods 2SHBBDF and 3SHBBDF are zero-stable.

Convergence of the Hybrid Methods

Definition 3.4 (*Convergence*): Consistency and zero-stability are required conditions for the LMM (2.1) to be convergent. Therefore, we conclude that the newly derived 2SHBBDF and 3SHBBDF are convergent since it is consistent and zero-stable.

3.3 Stability Region of the Hybrid Methods

Definition 3.5 (*A-stable*); The term "A-stable" refers to a method that is stable for all λ in the left-half plane ($Re(z) \leq 0$). The stability region for A-stable method covers up the complete negative left-half plane.

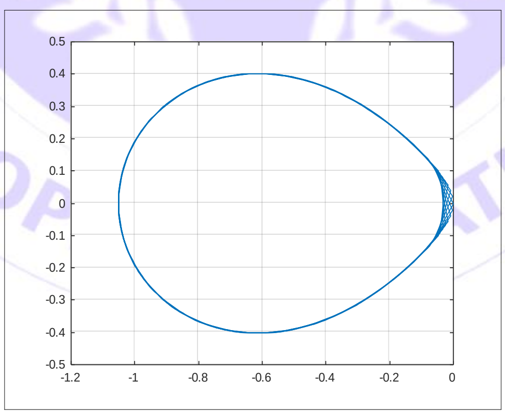

Figure 3.1: Region of Absolute Stability (RAS) of 2SHBBDF

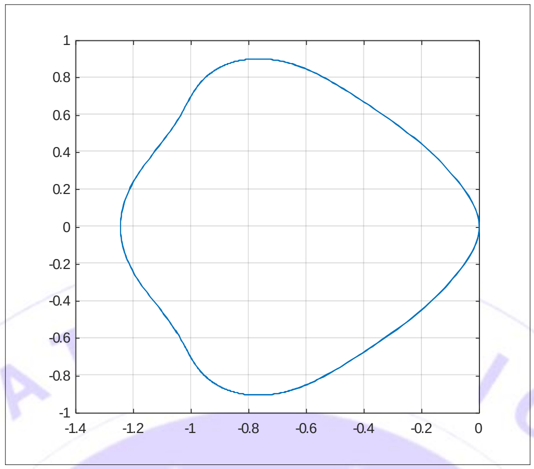

Figure 3.2: Region of Absolute Stability (RAS) of 3SHBBDF

Definition: A numerical method is said to be A-stable if the whole of the left-half plane $\{Z\ :\ Re(Z) \leq 0\}$ is contained in the region. $\{Z\ :\ Re(Z) \leq 1\}$ Where $R(Z)$ is called the stability polynomial of the method. (Lambert, 1973). The region of absolute stability of the newly constructed hybrid block methods are plotted with the help of MATLAB $R2015a$. This absolute stability regions are A-Stable since it consists of the set of points in the complex plane outside the enclosed figure

4. Results

To test the reliability of the proposed 2SHBBDF and 3SHBBDF method, some numerical results are obtained by applying the methods on some well-known chemical reaction problems. Comparison is done with other multistep methods. The 2SHBBDF and 3SHBBDF methods has been coded and implemented with MATLAB $R2015a$.

Problem 4.1: (*Stiff Chemical Reaction Problem*)

A chemistry problem with a stiff system is considered below

$$y_1' = -0.013y_2 - 1000y_1y_2 - 2500y_1y_2,$$

$$y_2' = -0.013y_2 - 1000y_1y_2,$$

$$y_3' = -2500y_1y_2$$

with initial value $y_1 = 0, y_2 = 1$ and $y_3 = 1,\ 0 \leq x \leq 2.$

This problem is solved using $h = 10^{-5}$ for Soomro *et al.* (2023). Table 4.1 shows the integration results for this problem at $x = 2$. Our methods were Compared with the formulas of two-step hybrid method by Khalsaraei and Molayi (2020) and three-step hybrid method with order five by Soomro *et al.* (2023). The 2SHBGBDF and 3SHBGBDF methods provides more accurate results in terms of Absolute error.

Table 4.1. Results Comparison of problem 4.1

x	y_i	2SHBBDF	3SHBBDF	Khalsaraei *et al.* (2020)	Soomro *et al.* (2023)
2.0	y_1	$9.77E-17$	$1.26E-20$	$0.61E-16$	$1.1E-17$
	y_2	$4.41E-16$	$1.43E-19$	$0.53E-10$	$2.29E-11$
	y_3	$2.96E-16$	$3.96E-19$	$0.74E-10$	$4.39E-11$

Problem 4.2: (*Robertson Problem*)

A stiff system of three non-linear ODEs is involved in the Robertson problem. In 1966, Robertson proposed it in (1967). Wanner (1996) came up with the name ROBER. The file rober contained the software part of the problem which can be found in Mazzia and Cash (2012). The problem is described mathematically in the form.

$\frac{dy}{df} = F(y), y(0) = y_0$

with $y \in R^3, x \in [0, X]$ and the function $F$is specified by $(f_1, f_2, f_3)^T$where,

$f_1 = -0.04y_1 + 10^4 y_2 y_3$

$f_2 = 0.04y_1 - 10^4 y_2 y_3 - 3 \times 10^7 y_2^2$

$f_3 = 3 \times 10^7 y_2^2$

with the initial value $y_1 = 1, y_2 = 0$ and $y_3 = 0$.

Robertson (1967) defined the ROBER problem as the kinetics of an autocatalytic reaction. The composition of the reactions is as follows:

$$A \overset{K_1}{\rightarrow} B$$

$$B + B \overset{K_2}{\rightarrow} C + B$$

$$B + C \overset{K_3}{\rightarrow} A + C$$

A, B, and C are the chemical species and k_1, k_2 and k_3 are the rate constants. The following mathematical model, consisting of a set of three ODEs, can be put up under some ideal conditions Aiken (1985) and the assumption that the mass action law is implemented to the rate functions.

$$\begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} = \begin{pmatrix} -k_1 y_1 + k_3 y_2 y_3 \\ k_1 y_1 - k_2 y_2^2 - k_3 y_2 y_3 \\ k_2 y_2^2 \end{pmatrix}$$

with $(y_1(0), y_2(0), y_3(0))^T = (y_{01}, y_{02}, y_{03})^T$, where$y_1, y_2$ and y_3 refers to the concentrations of A, B, and C respectively, and y_{01}, y_{02} and y_{03} are concentrations at time $t = 0$. In the test problem, $k_1 = 0.04, k_2 = 3 \times 10^7$ and $k_3 = 10^4$ are the numerical values of rate constants with the initial concentrations $y_{01} = 1, y_{02} = 0$ and $y_{03} = 0$. The cause for stiffness is the substantial variation in reaction rate constants. This system features a modest, very rapid initial transient phase for problems arising from chemical kinetics. This is followed by a highly smooth fluctuation of the components, which would be acceptable for a numerical technique with a large step-size. For $x \in [0, 4000]$, the ODE system is integrated. The numerical results by proposed methods at the points $x = 0.4, 40, 4000$ are shown in Table 4.2 below

Table 4.2. Results Comparison of problem 4.2

x	y_i	2SHBBDF	3SHBBDF	Khalsaraei *et al.* (2020)	Soomro *et al.* (2023)
	y_1	1.15E-10	5.68E-11	9.851E-01	7.183E-08
0.4	y_2	1.08E-09	2.64E-10	3.386E-05	1.227E-11
	y_1	1.02E-08	3.91E-09	7.158E-01	1.040E-04
40	y_2	1.02E-07	1.10E-08	9.185E-06	4.010E-09
	y_1	3.97E-06	2.48E-07	1.832E-01	8.395E-05
4000	y_2	1.39E-05	3.90E-06	9.942E-07	5.251E-10

Problem 4.3

(*Stiff Chemical Reaction Problem*)

Consider the stiff system IVPs

$y_1' = -1002y_1 + 1000y_2^2$

$y_2' = y_1 - y_2(1 - y_2)$

with the initial conditions as $y_1(0) = 1$ and $y_2(0) = 1$ having exact solution as

$y_1 = exp(-2x), \;\; y_2 = exp(-x)$

This problem is solved at $x = 50$by the new methods and compared the results with both Khalsaraei and Molayi $(2020)$and three-step hybrid method with order five by Soomro *et al.* (2023). Here the step-size $h = 0.05$ is used for compared and proposed methods. The smaller step-size can also be used to get more accurate results.

Table 4.3. Results Comparison of problem 4.3

x	y_i	2SHBBDF	3SHBBDF	Khalsaraei *et al.* (2020)	Soomro *et al.* (2023)
	y_1	1.03E-28	8.62E-26	7.14E-21	7.38E-24
50	y_2	3.27E-19	6.83E-25	3.34E-19	4.83E-25

Problem 4.4. We consider another stiff system of equation

$y' = -y_1 - 30y_2 + 30e^{-t} \;\; y_1(0) = 1.$

$y' = 30y_1 - y_2 - 30e^{-t}, \; y_2(0) = 1.$

The stiffness ratio of this problem is 1:200 and the exact solution is

$y_1(t) = e^{-t}, \quad y_2(t) = e^{-t}$

Table 4.4. Results Comparison of problem 4.4

x	y_i	2SHBBDF	3SHBBDF	Yakubu (2018)
	y_1	4.08E-08	2.38E-13	6.44E-4
5	y_2	1.51E-08	2.59E-13	2.60E-4
	y_1	4.54E-10	8.98E-15	4.07E-5
50	y_2	2.02E-10	6.73E-15	1.53E-5
	y_1	2.06E-14	2.11E-17	1.87E-9
150	y_2	9.17E-15	2.39E-18	1.32E-9
	y_1	9.36E-19	3.82E-20	7.14E-14
250	y_2	4.16E-19	9.92E-21	8.47E-14
	y_1	1.30E-29	5.43E-27	7.08E-26
500	y_2	5.78E-30	2.24E-27	1.35E-24

Problem 4.5 Consider the highly stiff ODE

$y' = -10(y-1)^2, \quad y(0) = 2$

with exact solution $y(t) = 1 + \frac{1}{1+10t}$

Some block numerical schemes for solving initial value problems in ODEs. This problem was earlier discussed by (Yau, 2011), he showed that many predictor-corrector and block methods become unstable with this problem, including the hybrid methods. however, the newly derived block method is used for the integration of this problem within the interval $0 \leq t \leq 0.1$. The authors James *et al.* (2013) solved this stiff problem by adopting a new 3-point block method with step size ratio at $r = 1$ and of order five. we present the result for problem using the newly derived method in the table below with also order five.

TABLE 4.5: Numerical Result of 3SHBGBDF

X	Exact Solution	Computed Result	3SHBBDF	EOK
0.1	1.9090909091	1.9093653765	9.26E-07	1.07E-04
0.2	1.8333333333	1.8337548972	9.90E-07	2.38E-04
0.3	1.7692307692	1.7697268394	8.87E-07	4.51E-04
0.4	1.7142857143	1.7148140868	6.98E-07	6.20E-04

0.5	1.6666666667	1.6672025713	8.17E-07	8.84E-04
0.6	1.6250000000	1.6255289393	4.67E-07	1.03E-03
0.7	1.5882352941	1.5887489480	7.29E-07	1.27E-03
0.8	1.5555555556	1.5560493726	2.89E-07	1.53E-03
0.9	1.5263157895	1.5267875368	6.35E-07	1.75E-03
1.0	1.5000000000	1.5004488731	1.55E-07	1.81E-03

4. Discussion

The results generated by the developed 2SHBGBDF and 3SHBGBDF methods are displayed in Tables 4.1, 4.2, 4.3, 4.4 and 4.5. In Table 4.1, comparison on the basis of absolute error was made using the 2SHBGBDF and 3SHBGBDF of order 3 and 5 at the point $x = 2,\ \ x = 3$ respectively with the methods of Soomro *et al.* (2023) and Khalsaraei and Molayi (2020) at the step-size $h = 10^{-5}$. Table 4.2 shows that our new methods 2SHBBDF and 3SHBBDF are more accurate and performs relatively better than the methods of Soomro *et al.* (2023) and Khalsaraei and Molayi (2020) and significantly better than their methods. Table 4.3 shows the numerical integration results for the problem 4.3 at $x = 0.4{,}40$ and 4000 using the proposed 2SHBBDF and 3SHBBDF approach in comparison to that of Soomro *et al.* (2023) and Khalsaraei and Molayi (2020) at $h = 0.001$. The comparison of the absolute errors in Table 4.3 for different points of x demonstrates the dominancy of our methods over the methods given in Soomro *et al*. (2023) and Khalsaraei and Molayi (2020) in terms of accuracy at $h = 0.05$. According to Table 4.3 also, it is observed that the 2SHBGBDF method of order 3 is more effective than the two-step hybrid method of forth order with one off-step point Khalsaraei and Molayi (2020). It can be seen that the 2SHBBDF and 3SHBBDF methods of order 3 and 5 respectively performs better than the fourth order Two step hybrid method with one off-step point Khalsaraei and Molayi (2020) and Soomro et al. (2023) three step hybrid method of fifth order, as shown by tables (4.1-4.3), 2SHBBDF and 3SHBBDF are well suited to nonlinear chemical reaction problems of a stiff nature. According to Table 4.4, our new methods 2SHBBDF and 3SHBBDF performed accurately and better than that of Yakubu (2018), also in Table 4.5 shows that our methods out class that of Okunuga *et al.* (2013) and James *et al.* (2013).

5. Conclusion

In this paper, an implicit 2SHBBDF and 3SHBBDF methods has been derived for the numerical solution of stiff systems of first-order IVPs arising from chemical reactions such as Robertson problem and stiff chemical problems. The approach is based on the block BDF. Based on stability analysis of the new methods 2SHBBDF and 3SHBBDF, the methods are consistent and stable; thus, the methods are convergent. Since it has an A-stability property, the method is declared suitable for solving stiff ODEs. The numerical results obtained through the 2SHBBDF and 3SHBBDF and compared to Soomro *et al.* (2023), Khalsaraei and Molayi (2020), Yakubu (2018) and Okunuga *et al.* (2013) evidenced that by applying the new methods, the accuracy of the numerical solutions in terms of absolute error at specific points is improved. Hence, the proposed methods can be successfully applied on stiff systems generated from chemical reactions because of their high order accuracy and wider stability region. Therefore, it can be concluded that the 2SHBBDF and 3SHBBDF could be an appropriate substitute solver for stiff ODEs.

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