5-Point Block Backward Differentiation Formulae for Solving Stiff Chemical Reaction Problems of Ordinary Differential Equations

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https://doi.org/10.56201/ijasmt.vol.12.no8.2026pg78.90

Abstract
The development and application of a 5-Point Block Backward Differentiation Formula (5PBBDF) for the numerical solution of stiff ordinary differential equations (ODEs), with an emphasis on issues related to chemical reaction kinetics, is presented in this paper. Numerical techniques with exceptional stability properties are required for stiff systems, which are frequently found in combustion modeling and reactive flow simulations. These systems are characterized by solution components that evolve on radically different timescales. By using a block formulation that concurrently computes numerical solutions at five equally spaced points, the suggested method expands upon the traditional Backward Differentiation Formula (BDF). By lowering the number of matrix factorizations needed throughout the integration interval, this block approach improves computational efficiency. A variable step-size strategy is used in its implementation to strike a balance between computational cost and local error control. The method is derived with specific coefficients optimized for both accuracy and stability. The A-stability of the 5PBBDF, which makes it especially appropriate for stiff systems, is confirmed by analyzing its stability using linear stability theory. Numerical experiments on common stiff chemical reaction problems, such as the Robertson chemical kinetics problem and a model combustion system, are used to assess the method's performance. The 5PBBDF is a reliable and effective solver for stiff ODEs in chemical engineering applications because numerical results show that it achieves better accuracy and computational efficiency than explicit methods.

Keywords: *Stiff Chemical Reaction, Linear Multistep Method, Block Method, Backward Differentiation Formulae and ODEs.*

MSC 2020 Subject Classification Number: 34A12, 65L04, 65L05, 65L06, 65L20, 80A30

1. Introduction

Stiff systems of ordinary differential equations (ODEs) frequently arise in the modeling of chemical kinetics, fluid dynamics, and control systems, where rapid changes in certain solution components co-exist with slower dynamics. Solving such systems efficiently and accurately demands numerical methods that are not only stable but also capable of achieving high-order accuracy. Among the implicit multistep methods, such as implicit Adams-Moulton that is less stable, not ideal for stiff problems, implicit Runge-Kutta very stable but too expensive

computationally, general linear methods flexible but complex, classical BDF reliable but sequential, error-prone for long steps, BBDF combines the stability of BDF, such as the parallelism of block methods, and a better cost-to-accuracy ratio, making it an attractive modern approach for stiff IVPs and as such block backward differentiation formulae (BBDF) have gained attention due to their structural advantages in solving stiff initial value problems Yunusa (2025). Collocation methods are widely considered as a way of generating numerical solution to ordinary differential equation of the form:

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

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.

A collection of numerical techniques for solving ordinary differential equations (ODEs) that are regarded as accurate and numerically stable is known as A-stable conventional block methods. These methods purposely preserve the stability for stiff problems, which are considered by quick changes in the dynamics of the system being modeled. One of the methods for realizing A-stability in block methods is through generalized backward differentiation formulae (GBDF) Yunusa, Adee and Tahir (2025). Ordinary differential equations (ODEs) can be solved using a series of implicit numerical techniques called the backward differentiation formula (BDF). Stiff ODEs are best solved using these techniques, 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 because they can be considered to have high order accuracy while maintaining stability (Atsi & Kumleng 2020). Conventional block methods are also a subclass of BDF methods that use a block structure to compute the derivative approximations. There is more freedom to choose the method's step size and sequence thanks to this block structure, making it possible to achieve higher accuracy or stability as needed. The use of A-stable conventional block methods generalized BDFs is particularly relevant for real-life problems that involve complex dynamics and are difficult to solve analytically. Furthermore, the development of A-stable conventional block methods generalized BDFs has been a significant advance in the field of numerical methods for ODEs. These methods are capable of accurately and efficiently solving stiff problems that are common in many real-world applications, making them a valuable tool for engineers, scientists, and mathematicians alike. Extended backward differentiation formula (EBDF), a class of A-stable traditional block approaches are frequently used for modeling real-world applications and numerically solving stiff problems of ordinary differential equations. GBDFs are a family of implicit methods that are widely applicable to a range of differential equations. The method's ability to compute huge systems of stiff differential equations more efficiently makes it advantageous. Backward difference approximations are used in the BGBDF method to solve the differential equation. Given its high degree, the BGBDF approach can achieve high-order accuracy (Gebregiorgis & Muleta, 2020). Similarly, stiff ordinary differential equations (ODEs), which frequently occur in scientific and engineering applications, can be effectively solved using a class of numerical techniques called A-stable hybrid block methods based on Formulas for extended backward differentiation formula (BDF). These approaches use hybrid methods to expand on the traditional backward differentiation formula (BDF) such as collocation, predictor-corrector schemes, or extrapolation, to enhance stability, accuracy and efficiency. Stiff ODEs are characterized by rapidly decaying solutions that require special numerical techniques for stability. The generalized BDF methods retain the implicit nature of BDF while allowing modifications to improve stability and accuracy (Hairer & Wanner,

2010). The hybrid block approach further extends these properties by solving multiple points simultaneously, leading to better efficiency and reduced computational cost (Ibrahim,Mohd Noor, & Othman, 2019). The key advantage of A-stable hybrid block methods is that they preserve A-stability for higher-order schemes (i.e., they remain stable for all eigenvalues with negative real parts). Unlike conventional BDF, which loses A-stability for orders greater than two, hybridization allows higher-order stability while maintaining fast error damping (L-stability) (Butcher, 2016). Hence, in this research a class of A-stable BBDF methods with extended step numbers and higher-order accuracy, supported by rigorous theoretical foundations and validated through stiff system simulations were developed. Addressing this problem is essential to advancing the efficiency and reliability of numerical solvers for stiff initial value problems across various scientific and engineering domains.

2. Materials and Methods

Development of the Methods

Consider k- step discrete formula

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

where $\alpha_j, j = 0,1, \dots, t-1$ and $\beta_j, j = 0,1, \dots, m-1$ are the coefficients of the discrete scheme, y_{n+j} are approximations to y_{n+j} with $y_{n+j} := y(x_{n+j}), j = 0,1, \dots, k-1$ and $h := x_{n+1} - x_n$ is a non-zero constant. According to Onumanyi et al (1999), the continuous formulation of (2.1) is obtained by finding a polynomial $y(x)$ of degree $p = t + m - 1, t > 0, m > 0$ of the form

$$y(x) = \sum_{j=0}^{t-1} \alpha_j(x) \, y(x_{n+j}) + h \sum_{j=0}^{m-1} \beta_j(x) \, f(\overline{x}_{j+1}, y(\overline{x}_{n+1})) \qquad (2.2)$$

with $y(x)$ satisfying

$$y(x_{n+j}) = y_{n+j}, j \in \{0,1, \dots, t-1\}$$
$$y'(\overline{x}_j) = f\left(\overline{x}_j, y(\overline{x}_j)\right), j = 0,1, \dots, m-1$$

where $\alpha_j(x)$ and $\beta_j(x)$ are of the forms

$$\alpha_j(x) = \sum_{i=0}^{t+m-1} \alpha_{j,i+1} x^i, j \in \{0,1 \dots, t-1\} \qquad (2.3)$$

$$h\beta_j(x) = \sum_{i=0}^{t+m-1} \beta_{j,i+1} x^i, j \in \{0,1 \dots, m-1\} \qquad (2.4)$$

in (2.2) x_{n+j} are $t(0 < t \leq k)$ arbitrary chosen distinct interpolation points from $\{x_n, x_{n+1}, .., x_{n+k-1}\}$ and $\overline{x}_{j+1}$ are $m(m > 0)$ distinct collocation points belonging to $y(x)$, and are determined by using the expression for in (2.2) and the interpolation conditions (2.3) and (2.4). $\alpha_j(x)$ and $\beta_j(x)$ are subject to the following criteria:

$$\alpha_j(x_{n+i}) = \delta_{ij}, i = 0, \dots, t-1; j = 0,1 \dots, k-1 \qquad (2.5)$$
$$h\beta_j(x_{n+i}) = 0, i = 0,1, \dots, t-1; j = 0,1 \dots, m-1 \qquad (2.6)$$

And

$$\alpha_j'(\overline{x}_i) = 0, i = 1, \dots, t-1; j = 0,1 \dots, k-1 \qquad (2.7)$$
$$h\beta_j'(\overline{x}_i) =, i = \delta_{ij}, 1, \dots, t-1; j = 0,1 \dots, m-1 \qquad (2.8)$$

In matrix form, $(2.5) - (2.6)$ and $(3.9) - (3.10)$ give's

$$DC = I$$

I is the identity matrix with dimensions

$$D = \begin{pmatrix} 1 & x_n & x_n^2 & \cdots & \cdots & x_n^{t+m-1} \\ 1 & x_{n+1} & x_{n+1}^2 & \cdots & \cdots & x_{n+1}^{t+m-1} \\ \vdots & \vdots & \vdots & \cdots & \ddots & \vdots \\ 1 & x_{n+t-1} & x_{n+t-1}^2 & \cdots & \cdots & x_{n+t-1}^{t+m-1} \\ 0 & 1 & 2\overline{x}_0 & \cdots & (t+m-1) & \overline{x}_0^{t+m-2} \\ \vdots & \vdots & \vdots & \cdots & \ddots & \vdots \\ 0 & 1 & 2\overline{x}_{m-1} & \cdots & (t+m-1) & \overline{x}_{m-1}^{t+m-2} \end{pmatrix} \quad (2.9)$$

and

$$C = \begin{pmatrix} \alpha_{01} & \alpha_{11} & \cdots & \alpha_{t-1,1} & h\beta_{01} & \cdots & h\beta_{m-1,1} \\ \alpha_{02} & \alpha_{12} & \cdots & \alpha_{t-1,2} & h\beta_{02} & \cdots & h\beta_{m-1,2} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ \alpha_{0,t+m} & \alpha_{1,t+m} & \cdots & \alpha_{t-1,t-m} & h\beta_{0,t+m} & \cdots & h\beta_{m-1,t-m} \end{pmatrix}$$

Each of the square matrices C and D has the dimension $(t+m)\times(t+m)$. The columns of $C = D^{-1}$, which yield the continuous coefficients $\alpha_j(x)$ and $\beta_j(x)$ in (2.2), are obtained by inverting matrix D.

3. Derivation of Conventional Block Method

The BGBDF for step number $k = 5$ were constructed from GBDF with the aid of a code in MAPLE 18 software. The derivation procedure was presented for $k = 5$, and the techniques were derived using the same approach.

3.1 Derivation of 5PBBDF

Adee (2013) used (3.2) to find his collocation points v, in the form

$$\sum_{i=0}^{k} \alpha_j \, y_{n+i} = hf_{n+v} \quad (3.1)$$

Where

$$j = v \equiv \begin{cases} \frac{k+1}{2}, \text{ when k is odd} \\ \frac{k+2}{2}, \text{ when k is even} \end{cases} \quad (3.2)$$

and for reasons of numerical stability, (3.1) is written as

$$\sum_{i=-v}^{k-v} \alpha_j \, y_{n+i} = hf_n, n = v, \cdots, N-1 \quad (3.3)$$

Equation (3.1) is usually referred to as the main GBDF method. From equation (3.2), our $j = v$ is in the form of

$$j = v \equiv \begin{cases} \frac{k-1}{2}, \text{ when k is odd} \\ \frac{k-2}{2}, \text{ when k is even} \end{cases} \quad (3.4)$$

when $k = 5, v = 2,$ the continuous formulation of GBDF (3.1) becomes

$$y(x) = \sum_{j=0}^{4} \alpha_j(x) \, y_{n+j} + h\beta_2(x) f_{n+2} \quad (3.5)$$

Expressing (3.5) accordingly gives

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

Using MAPLE 18 software code or Gaussian elimination method, the continuous coefficients $\alpha_0(\xi), \alpha_1(\xi), \alpha_2(\xi), \alpha_3(\xi), \alpha_4(\xi)$ and $\beta_2(\xi)$ derived and substituted into (3.1) giving the continuous formulation of GBDF for $k = 5$ (CGBDF5).

$$\begin{pmatrix} y(\xi) = \alpha_0(\xi)y_n + \alpha_1(\xi)y_{n+1} \\ +\alpha_2(\xi)y_{n+2} + \alpha_3(\xi)y_{n+3} + \alpha_4(\xi)y_{n+4} + h\beta_2(\xi)f_{n+2} \end{pmatrix} \quad (3.6)$$

where

$\alpha_0(\xi) = -\frac{1}{48}(\xi^5 - 12\xi^4 + 55\xi^3 - 120\xi^2 + 124\xi - 48)$

$\alpha_1(\xi) = \frac{1}{6}(\xi^5 - 11\xi^4 + 44\xi^3 - 76\xi^2 + 48\xi)$

$\alpha_2(\xi) = \frac{1}{4}(\xi^4 - 8\xi^3 + 19\xi^2 - 12\xi)$

$\alpha_3(\xi) = -\frac{1}{6}(\xi^5 - 9\xi^4 + 28\xi^3 - 36\xi^2 + 16\xi)$

$\alpha_4(\xi) = \frac{1}{48}(\xi^5 - 8\xi^4 + 23\xi^3 - 28\xi^2 + 12\xi)$

$\beta_2(\xi) = \frac{1}{4}(\xi^5 - 10\xi^4 + 35\xi^3 - 50\xi^2 + 24\xi)$

and $\xi = x - x_n, \quad 0 \le \xi \le 5h$

Evaluating (3.6) at $\xi = 5h$ and its first derivative at $\xi = 0, h, 3h, 4h, 5h$. After collecting the terms and putting it in a block form gives five-point conventional block method (5PCBM) in the form of

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} y_{n+1} \\ y_{n+2} \\ y_{n+3} \\ y_{n+4} \\ y_{n+5} \end{pmatrix} =$$

$$\begin{pmatrix} 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} y_{n-1} \\ y_{n-2} \\ y_{n-3} \\ y_{n-4} \\ y_n \end{pmatrix} + h \begin{pmatrix} 0 & 0 & 0 & 0 & \frac{251}{720} \\ 0 & 0 & 0 & 0 & \frac{29}{90} \\ 0 & 0 & 0 & 0 & \frac{27}{80} \\ 0 & 0 & 0 & 0 & \frac{14}{45} \\ 0 & 0 & 0 & 0 & \frac{95}{144} \end{pmatrix} \begin{pmatrix} f_{n-1} \\ f_{n-2} \\ f_{n-3} \\ f_{n-4} \\ f_n \end{pmatrix}$$

$$+h\begin{pmatrix} \frac{323}{360} & -\frac{11}{30} & \frac{53}{360} & -\frac{19}{720} & 0 \\ \frac{62}{45} & \frac{4}{15} & \frac{2}{45} & -\frac{1}{90} & 0 \\ \frac{51}{40} & \frac{9}{10} & \frac{21}{40} & -\frac{3}{80} & 0 \\ \frac{64}{45} & \frac{8}{15} & \frac{64}{45} & \frac{14}{45} & 0 \\ -\frac{25}{72} & \frac{25}{6} & -\frac{175}{72} & \frac{425}{144} & 0 \end{pmatrix}\begin{pmatrix} f_{n+1} \\ f_{n+2} \\ f_{n+3} \\ f_{n+4} \\ f_{n+5} \end{pmatrix} \tag{3.7}$$

where

$$A^1 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}, A^0 = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix},$$

$$B^1 = \begin{pmatrix} \frac{323}{360} & -\frac{11}{30} & \frac{53}{360} & -\frac{19}{720} & 0 \\ \frac{62}{45} & \frac{4}{15} & \frac{2}{45} & -\frac{1}{90} & 0 \\ \frac{51}{40} & \frac{9}{10} & \frac{21}{40} & -\frac{3}{80} & 0 \\ \frac{64}{45} & \frac{8}{15} & \frac{64}{45} & \frac{14}{45} & 0 \\ -\frac{25}{72} & \frac{25}{6} & -\frac{175}{72} & \frac{425}{144} & 0 \end{pmatrix}, B^0 = \begin{pmatrix} 0 & 0 & 0 & 0 & \frac{251}{720} \\ 0 & 0 & 0 & 0 & \frac{29}{90} \\ 0 & 0 & 0 & 0 & \frac{27}{80} \\ 0 & 0 & 0 & 0 & \frac{14}{45} \\ 0 & 0 & 0 & 0 & \frac{95}{144} \end{pmatrix}$$

and its normalized discrete Scheme, called five-point conventional normalized discrete scheme (5PCNDS) as

$$y_{n+1} = y_n + h\left[\frac{251}{720}f_n + \frac{323}{360}f_{n+1} - \frac{11}{30}f_{n+2} + \frac{53}{360}f_{n+3} - \frac{19}{720}f_{n+4}\right] \tag{3.8}$$

$$y_{n+2} = y_n + h\left[\frac{29}{90}f_n + \frac{62}{45}f_{n+1} + \frac{4}{15}f_{n+2} + \frac{2}{45}f_{n+3} - \frac{1}{90}f_{n+4}\right] \tag{3.9}$$

$$y_{n+3} = y_n + h\left[\frac{27}{80}f_n + \frac{51}{40}f_{n+1} + \frac{9}{10}f_{n+2} + \frac{21}{40}f_{n+3} - \frac{3}{80}f_{n+4}\right] \tag{3.10}$$

$$y_{n+4} = y_n + h\left[\frac{14}{45}f_n + \frac{64}{45}f_{n+1} + \frac{8}{15}f_{n+2} + \frac{64}{45}f_{n+3} + \frac{14}{45}f_{n+4}\right] \tag{3.11}$$

$$y_{n+5} = y_n + h\left[\frac{95}{144}f_n - \frac{25}{72}f_{n+1} + \frac{25}{6}f_{n+2} - \frac{175}{72}f_{n+3} + \frac{425}{144}f_{n+4}\right] \tag{3.12}$$

2. Analysis of Basic Properties of *5PBBDF*

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 of 5PBBDF

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. Using tailor's series expansion on (3.8), (3.9),

(3.10), (3.11) and (3.12), shows the order and error constant of the new method in the table below.

Table 3.1 : Order and Error Constant of 5PCBGBDF

Equation	Order	Error Constant
y_{n+1}	5	$\frac{3}{160}$
y_{n+2}	5	$\frac{1}{90}$
y_{n+3}	5	$\frac{3}{160}$
y_{n+4}	6	$-\frac{8}{945}$
y_{n+5}	5	$\frac{95}{288}$

3.2 Convergence of 5PBBDF

The convergence of the BGBDF was determined using Fantula's (1991) methodology. Consequently, used the form of a single r-point multistep approach to describe the block method.

$$A^{(0)}Y_M = \sum_{i=0}^{k} A^{(i)}Y_{m-i} + h\sum_{i=0}^{k} B^{(i)}F_{m-i} \quad (3.13)$$

Where h is a fixed mesh size within a block, $A^{(i)}$ and $B^{(i)}, i = 0, 1, \dots, k$ are $(r \times r)$ matrices respectively with elements $a_{ij}^{(i)}$ and $b_{ij}^{(i)}, j = 0, 1, \dots, r$. Specifically, $A^{(0)}$ is an $(r \times r)$ identity matrx. $Y_m, Y_{m-i}, F_m,$ and F_{m-i} are vectors of numerical estimates as described thus. With the r-vector, Y_m, F_m (for $n = mr, m = 0, 1 \dots$) specified as $Y_m = [y_{n+1}, y_{n+2}, \dots, y_{n+r}]^T, Y_{m-i} = [y_{n-r}, \dots, y_{n-r}, y_n]^T, F_m = [f_{n+1}, f_{n+2}, \dots, f_{n+r}]^T, F_{m-i} = [f_{n-r}, \dots, f_{n-r}, f_n]^T$ for $n = mr$ for some integer $m \geq 0$. Using (3.7), when $k = 5$, the first charateristics polynomial $\rho(\lambda)$ of the 5PCBGBDF is given by $\rho(\lambda) = [\lambda.A^{(0)} - A^{(1)}] = \lambda^5 - \lambda^4 = \lambda^4(\lambda - 1) = 0.$ Now, $\rho(\lambda) = 0 \Leftrightarrow \lambda = 0, 0, 0, 0, 1.$ Accordingly, the 5SCBGBDF is zero-stable. Table 3.1 indicates that the block is of order $p = 5$ with the indicated error constants, therefore consistent and by (3.7) the 5PCBGBDF is convergent.

3.3 Regions of Absolute Stability of 5PBBDF

The classic backward differentiation formula (BDF), which is well-known for its robust stability characteristics for stiff equations, serves as the foundation for the BGBDF approach. For a k-step BGBDF, the stability function is derived from

$$\sum_{j=0}^{k} A_j Y_{n+j} = h\sum_{j=0}^{k} B_j F_{n+j} \quad (3.14)$$

for the test equation $y' = \lambda y$, this gives a rational function:

$$R(z) = \frac{P(z)}{Q(z)}$$

where $Q(z) \neq 0, z = h\lambda$: nondimensional number combining step size $h$and problem eigenvalue λ. $P(z)$ comes from the coefficients on the right-hand side of the scheme (the part involving past derivatives). $Q(z)$ comes from the coefficients on the left-hand side (the part involving present and past solution values). Thus, the pair $P(z)$, $Q(z)$ encodes the numerical method. $R(z)$ is the stability function that dictates amplification/decay per step. The linear stability analysis of the new method was studied and is done by plotting the absolute stability regions of the main discrete GBDF methods and the new convention block GBDF methods for $k = 5$.

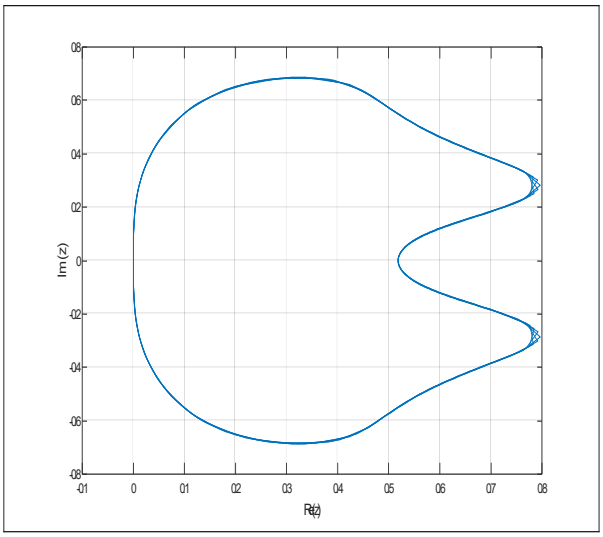

Figure 1: Region of Absolute Stability (RAS) of *5PBBDF* is A-Stable

4. Numerical Problems

Numerical results are produced by applying the suggested 5PCBGBDF method to various well-known chemical reaction situations in order to assess their reliability. Providing comparisons with alternative multistep techniques by using MATLAB R2015a to code and implement the new methods derived.

Problem 1: (*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 method and compared the results with forth order Two step hybrid method with one off-step point Khalsaraei, Shokri, Molayi (2020). The new class of multistep multiderivative hybrid methods for the numerical solution of chemical stiff systems of first order IVPs. 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 4.1. Shows the Absolute Error of Problem 1

X	y_i	***5PBBDF***	**Soomro et al** (2023)	**Khalsaraei et al** (2020)
	y_1	8.45E-25	7.38E-24	7.14E – 21
50	y_2	2.63E-25	4.83E-25	3.34E – 19

Problem 2: (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 $y_3 = 1, 0 \le x \le 2.$

This problem is solved using h = 10-5 for 5PCBGDF. Table 4.2 shows the integration results for

this problem at x = 2. Compared with the formulas of two-step hybrid method by Khalsaraei et al (2020) of order five and Soomro et al (2023), the 5PCBGDF method provides more accurate results in terms of Absolute error.

Table 4.3: Absolute Errors of Problem 2

X	y_i	***5PBBDF***	**Soomro et al** (2023)	**Khalsaraei et al** (2020)
	y_1	3.46E-19	1.1E-17	0.61E - 16
2.0	y_2	5.34E-18	2.29E-11	0.53E - 10
	y_3	6.69E-17	4.39E-11	0.74E - 10

Problem 3: *(Robertson Problem)*

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

$$f_1 = -0.04y_1 + 10^4 y_2 y_3$$
$$f_2 = 0.04y_1 - 10^4 y_2 y_3 - 3 \times 10^{7y_2^2},$$
$$f_3 = 3 \times 10^7 y_2^2$$

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

$$A \xrightarrow{K_1} B$$
$$A + B \xrightarrow{K_1} C + B$$
$$B + C \xrightarrow{K_1} A + C$$

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 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, $k_1 = 0.04, k_2 = 3 \times 107$ and $k_3 = 104$ 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.

Table 4.3: The Absolute Errors of Problem 3.

X	y_i	*5PBBDF*	Soomro et al (2023)	Khalsaraei et al (2020)
0.4	y_1	5.30E-08	7.183E-08	9.851E - 01
	y_2	3.52E-08	1.227E-11	3.386E - 05
40	y_1	4.09E-08	1.040E-04	7.158E - 01
	y_2	3.91E-08	4.010E-09	9.185E - 06
4000	y_1	3.97E-08	8.395E-05	1.832E - 01
	y_2	3.95E-08	5.251E-10	9.942E - 07

5. Discussion

Based on the table 4.1, the comparison focuses on the magnitude of the computed values (likely absolute errors or residuals) for y_1 and y_2 at $x = 50$. 5PBBDF and Soomro et al. (2023) methods yield very small errors of similar order five, but 5PBBDF is consistently more accurate. Khalsaraei's errors are substantially higher, suggesting a less accurate method, different test problem, or possibly a different error norm. Therefore, 5PBBDF performs best (smallest errors), closely followed by Soomro et al. (2023). Khalsaraei et al. (2020) is significantly less accurate for this test case. Based on table 4.2, 5PBBDF (smallest errors) is vastly superior and Errors increase slightly from y_1 to y_3 but remain below 10^{-16}. This indicates excellent accuracy and likely a high-order method. Soomro et al. (2023) (moderate errors) For $y_2$and y_3,errors jump dramatically y_1 ($\sim 10^{-11}$ and $10^{-18} - 10^{-17}$), suggesting possible instability or reduced accuracy for stiff components**.** The large discrepancy in y_2, y_3 suggests the problem may be stiff or sensitive, and only 5PBBDF maintains high precision across all solution components.

Similarly, table 4.3 indicate 5PBBDF maintains remarkably consistent errors across all x and both components. This indicates excellent stability and uniform accuracy regardless of step size or integration range. Soomro et al. (2023) shows variable performance. This suggests component-dependent accuracy and possibly some instability or error growth in y_1 over longer intervals. Khalsaraei et al. (2020) gives very large errors for $y_1$and moderate errors for y_2. The huge y_1 error at y_2 $x = 0.4(0.9851)$ is alarming, indicating poor accuracy or method failure for one component even at small x . 5PBBDF is the most robust and accurate overall (consistent 10^{-8} errors across all cases). Soomro et al. is excellent for y_2 but loses accuracy for y_1 at larger x. Khalsaraei et al. is unreliable for y_1 (errors up to ~100%) and only moderately accurate for y_2. The proposed 5PBBDF method demonstrates the best performance among the methods considered. It consistently produces the smallest errors, maintains high accuracy and stability across different step sizes and solution components, and shows little or no error growth over longer integration intervals. This indicates that 5PBBDF is more reliable, robust, and suitable for solving stiff problems than the methods of Soomro et al. (2023) and Khalsaraei et al. (2020).

6. Conclusion

For the numerical solution of stiff systems of first-order IVPs resulting from chemical reactions, such as the Robertson problem and stiff chemical issues, an implicit 5PBBDF approach has been developed in this study. The method is based on the block BDF, which instantly generates three approximation solutions at each stage of the integration. The 5PBBDF is convergent since the approach is consistent and zero-stable according to stability analysis. The approach is deemed appropriate for solving stiff ODEs since it possesses an A-stability characteristic. Applying the 5PBBDF approach improves the accuracy of the numerical solutions in terms of absolute error at

specific sites, as demonstrated by the numerical results acquired through the method and compared to Soomro et al. (2023) and Khalsaraei et al. (2020). Because of their greater stability region and high order accuracy, the suggested technique can therefore be effectively used to stiff systems produced by chemical reactions. Consequently, it can be said that the 5PBBDF might be a suitable alternative solver for stiff ODEs. It would be advantageous to use variable step sizes for solving ODEs in order to increase efficiency.

5PBBDF is a promising and efficient solver for stiff ODEs, although future work could improve its efficiency further by incorporating variable step-size strategies.

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