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An Efficient Solver for Solving Chemical Kinetic Equations Using Higher Order Block Backward Differentiation Formula

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In this paper, an efficient solver known as higher order block backward differentiation formula (HOBBDF) is applied to chemical kinetic equations. In order to prove the applicability of this higher order solver, the chemical kinetic ordinary differential equations (ODEs) are numerically tested. Then, a comparison of performance between HOBBDF and two ODE solvers in MATLAB, particularly ode15s and ode23, are made. Evidently, it is proven that HOBBDF method outperforms ODE solvers in terms of accuracy. Therefore, HOBBDF method can also be applied to solve chemical kinetic equations.

Keywords: block backward differentiation formulae; initial value problem; stiff ordinary differential equations; chemical kinetic equations

I. INTRODUCTION

Air pollution is a very serious issue around the world considering its adverse effects on human health and the environment. Numerous efforts have thus been made to improve air quality and reduce air pollution, including the establishment of the air pollution forecast model to predict the atmospheric conditions. In air pollution models that describe atmospheric gas-phase chemical reactions, chemical kinetic equations play an important factor (Huang & Chang, 2001). The air pollution model is based on the Chemistry Transport Models (CTM) where the concentrations of various pollutants are described by a set of Reaction-Diffusion-Advection partial differential equations (PDEs) (Feng *et al*., 2015). Chemical kinetic equation is considered as a first order ODEs. A set of initial condition and chemical reactions can be written in the following form:

$$\frac{dC}{dt} = P - LC, \quad (1)$$
$$C(0) = C^0,$$

where $P \geq 0, \quad L \geq 0$, t is time, P and LC are the chemical production and loss rates, C is the concentration, C^0 is the initialvalue and $\frac{dC}{dt}$ represents the changes in concentration, while the actual solution depends on initial condition, P and L.

This type of equations is implied as stiff due to the extremely fast chemical reactions (Alexandrov *et al*., 1997). As implicit methods are normally used to deal with the stiffness of chemical ODE system, an appropriate chemical solver should be selected to find the solution to this problem. In the literature, there are numerous chemical solvers that are already developed for this type of equations. For atmospheric chemical kinetic, several suitable solvers are Livermore Solver for Ordinary Differential Equations, LSODE (Hindmarsh, 1980), quasi-steady-state-approximation, QSSA (Mott *et al*.,2000) and Modified backward Euler, MBE (Feng *et al*., 2015). LSODE is one of the earliest solvers for numerical solution stiff ODE. It is based on the Gear method and explicitly solves the ODE. QSSA is based on the forward Euler method while MBE is

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based on the backward Euler method.

In recent years, the study of block backward differentiation formula (BBDF) is well developed using constant and variable step size. BBDF was first introduced by (Ibrahim *et al.*, 2008) as a good solver for solving stiff ODEs since it produces better accuracy than non-block method. In addition, it is also proven effective for solving the stiff ODEs both in the lower and higher order problems (Asnor *et al.*, 2018; Zainuddin *et al.*, 2016; Yatim *et al.*, 2013). Owing to the fact that this solver is efficient, we introduce HOBBDF solver which is developed using the variable step size approach for the numerical approximations of chemical kinetic equations in (1).

This paper is organised as follows. The development of the introduced solver is summarised in Section 2 and the use of Newton's iteration in HOBBDF is briefly explained in Section 3. In Section 4, a few examples of the chemical kinetic equations from (Feng *et al.*, 2015; Hindmarsh, 1980) are numerically tested and the performance comparison of this solver with two Matlab's ODE solver will be discussed in the same section. The conclusion of this study is presented in the last section.

II. HIGHER ORDER BLOCK BACKWARD DIFFERENTIATION FORMULA

Three backvalues will be used to approximate two new solutions in the current block. First, find order four Lagrange polynomial and replace x with $x_{n+1} + s \cdot h$ gives the following equation

$$\sum_{j=0}^{4} P_4(x) = \sum_{j=0}^{4} y\left(x_{n+2-j}\right) \cdot L_{4,j}\left(x_{n+1} + s \cdot h\right) \qquad (2)$$

Proceed to the derivation by differentiating polynomial (2) thrice. Then, substitute s with 0 and s with 1 for obtaining the first and second point. Since this method is variable in step size, let $(x_n - x_{n-1}) = rh$, $(x_{n-1} - x_{n-2}) = rh$, $(x_{n+2} - x_{n+1}) = h$, $(x_{n+1} - x_n) = h$. Note that h is step size and r is step size ratio. Therefore, we have the updated polynomial after differentiation as follows:

First derivative :

- First point

$$\begin{aligned} &-\frac{1}{4}\frac{y_{n-2}}{r^2(2r+1)} + \frac{y_{n-1}(2r+1)}{r^2(r+1)(r+2)} + \frac{y_{n+1}}{r+1} \\ &-\frac{1}{4}\frac{y_n(2r+1)(r+1)}{r^2} + \frac{y_{n+1}}{2r+1} + \frac{1}{4}\frac{y_{n+2}(2r+1)}{r+2} \end{aligned} \qquad (3)$$

- Second point

$$\begin{aligned} &\frac{1}{2}\frac{y_{n-2}(h(r+1)+h)}{hr^2(2r+1)(r+1)} - \frac{2y_{n-1}(h(2r+1)+h)}{hr^2(r+1)(r+2)} \\ &+\frac{1}{4}\frac{y_n(h(2r+1)+h)(h(r+1)+h)}{r^2h^2} \\ &-\frac{2y_{n+1}(h(2r+1)+h)(h(r+1)+h)}{h^2(2r+1)(r+1)} \\ &+\frac{1}{2}\frac{y_{n+2}(h(r+1)+h)}{h(r+1)(r+2)} + \frac{1}{2}\frac{y_{n+2}(h(2r+1)+h)}{h(r+1)(r+2)} \\ &+\frac{3}{4}\frac{y_{n+2}(h(2r+1)+h)(h(r+1)+h)}{h^2(r+1)(r+2)} \end{aligned} \qquad (4)$$

Second derivative :

- First point

$$\begin{aligned} &\frac{1}{2}\frac{y_n(2r+1)(r+1)}{r^2} + \frac{1}{2}\frac{y_{n+2}(2r+1)}{r+2} \\ &-\frac{1}{2}\frac{y_{n-2}}{r^2(2r+1)(r+1)} + \frac{2y_{n-1}}{r^2(r+1)(r+2)} \\ &-\frac{1}{2}\frac{y_n(r+1)}{r^2} - \frac{1}{2}\frac{y_n(2r+1)}{r^2} + \frac{2y_{n+1}}{(2r+1)(r+1)} \\ &-2y_{n+1} + \frac{1}{2}\frac{y_{n+2}}{r+2} + \frac{1}{2}\frac{y_{n+2}(2r+1)}{(r+1)(r+2)} \end{aligned} \qquad (5)$$

- Second point

$$\begin{aligned} &\frac{3}{2}\frac{y_{n-2}(h(r+1)+h)}{hr^2(2r+1)(r+1)} + \frac{y_{n-2}}{r^2(2r+1)(r+1)} \\ &-\frac{2y_{n+1}(h(2r+1)+h)(h(r+1)+h)}{h^2(2r+1)(r+1)} \\ &-\frac{6y_{n-1}(h(2r+1)+h)}{hr^2(r+1)(r+2)} + \frac{3}{2}\frac{y_{n+2}(h(2r+1)+h)}{h(r+1)(r+2)} \\ &+\frac{3}{2}\frac{y_{n+2}(h(r+1)+h)}{h(r+1)(r+2)} + \frac{1}{2}\frac{y_n(h(2r+1)+h)}{r^2h} \\ &+\frac{1}{2}\frac{y_n(h(r+1)+h)}{r^2h} - \frac{4y_{n-1}}{r^2(r+1)(r+2)} \\ &-\frac{4y_{n+1}(h(r+1)+h)}{h(2r+1)(r+1)} - \frac{4y_{n+1}(h(2r+1)+h)}{h(2r+1)(r+1)} \\ &+\frac{1}{2}\frac{y_{n+2}(h(2r+1)+h)(h(r+1)+h)}{h^2(r+1)(r+2)} \\ &+\frac{y_{n+2}}{(r+1)(r+2)} + \frac{1}{2}\frac{y_{n+1}(h(2r+1)+h)(h(r+1)+h)}{r^2h^2} \end{aligned} \qquad (6)$$

Third derivative :

- First point

$$-\frac{3}{2}\frac{y_n}{r^2}+\frac{3}{2}\frac{y_n(r+1)}{r^2}+\frac{3}{2}\frac{y_n(2r+1)}{r^2}+\frac{3}{2}\frac{y_{n-2}}{r^2(2r+1)}-\frac{6y_{n-1}(2r+1)}{r^2(r+1)(r+2)}-\frac{6y_{n+1}}{2r+1}-\frac{6y_{n+1}}{r+1}+\frac{3}{2}\frac{y_{n+2}}{(r+1)(r+2)}+\frac{3}{2}\frac{y_{n+2}}{r+2}+\frac{3}{2}\frac{y_{n+2}(2r+1)}{(r+1)(r+2)} \quad (7)$$

- Second point

$$\frac{9}{2}\frac{y_{n-2}}{r^2(2r+1)(r+1)}+\frac{3}{2}\frac{y_{n-2}(h(r+1)+h)}{hr^2(2r+1)(r+1)}-\frac{18y_{n-1}}{r^2(r+1)(r+2)}-\frac{6y_{n-1}(h(2r+1)+h)}{hr^2(r+1)(r+2)}+\frac{3}{2}\frac{y_n}{r^2}+\frac{3}{2}\frac{y_n(h(r+1)+h)}{r^2h}-\frac{12y_{n+1}}{(2r+1)(r+1)}+\frac{3}{2}\frac{y_n(h(2r+1)+h)}{r^2h}-\frac{6y_{n+1}(h(r+1)+h)}{h(2r+1)(r+1)}-\frac{6y_{n+1}(h(2r+1)+h)}{h(2r+1)(r+1)}+\frac{9}{2}\frac{y_{n+2}}{(r+1)(r+2)}+\frac{3}{2}\frac{y_{n+2}(h(r+1)+h)}{h(r+1)(r+2)}+\frac{3}{2}\frac{y_{n+2}(h(2r+1)+h)}{h(r+1)(r+2)} \quad (8)$$

Lastly, replace the value of *r* with 1, 2 and 10/19 into (3-8) gives the coefficients for the first point and second point as shown in the following equations.

- *Constant step size*

$$hy'_{n+1}=-\frac{1}{12}y_{n-2}+\frac{1}{2}y_{n-1}-\frac{3}{2}y_n+\frac{5}{6}y_{n+1}+\frac{1}{4}y_{n+2}$$
$$h^2y''_{n+1}=-\frac{1}{12}y_{n-2}+\frac{1}{3}y_{n-1}+\frac{1}{2}y_n-\frac{5}{3}y_{n+1}+\frac{11}{12}y_{n+2}$$
$$h^3y'''_{n+1}=-\frac{1}{2}y_{n-2}-3y_{n-1}+6y_n-5y_{n+1}+\frac{3}{2}y_{n+2}$$
$$hy'_{n+2}=\frac{1}{4}y_{n-2}-\frac{4}{3}y_{n-1}+3y_n-4y_{n+1}+\frac{25}{12}y_{n+2}$$
$$h^2y''_{n+2}=\frac{11}{12}y_{n-2}-\frac{14}{3}y_{n-1}+\frac{19}{2}y_n-\frac{26}{3}y_{n+1}+\frac{35}{12}y_{n+2}$$
$$h^3y'''_{n+2}=\frac{3}{2}y_{n-2}-7y_{n-1}+12y_n-9y_{n+1}+\frac{5}{2}y_{n+2} \quad (9)$$

- *Half of the step size*

$$hy'_{n+1}=-\frac{1}{80}y_{n-2}+\frac{5}{48}y_{n-1}-\frac{15}{16}y_n+\frac{8}{15}y_{n+1}+\frac{5}{16}y_{n+2}$$
$$h^2y''_{n+1}=-\frac{1}{120}y_{n-2}+\frac{1}{24}y_{n-1}+\frac{7}{8}y_n-\frac{28}{15}y_{n+1}+\frac{23}{24}y_{n+2}$$
$$h^3y'''_{n+1}=\frac{3}{40}y_{n-2}-\frac{5}{8}y_{n-1}+\frac{21}{8}y_n-\frac{16}{5}y_{n+1}+\frac{9}{8}y_{n+2}$$
$$hy'_{n+2}=\frac{1}{30}y_{n-2}-\frac{1}{4}y_{n-1}+\frac{3}{2}y_n-\frac{16}{5}y_{n+1}+\frac{23}{12}y_{n+2}$$
$$h^2y''_{n+2}=\frac{7}{60}y_{n-2}-\frac{5}{6}y_{n-1}+\frac{17}{4}y_n-\frac{88}{15}y_{n+1}+\frac{7}{3}y_{n+2}$$
$$h^3y'''_{n+2}=\frac{7}{40}y_{n-2}-\frac{9}{8}y_{n-1}+\frac{33}{8}y_n-\frac{24}{5}y_{n+1}+\frac{13}{8}y_{n+2} \quad (10)$$

- *Increment of the step size to a factor 1.9*

$$hy'_{n+1}=-\frac{6859}{15600}y_{n-2}+\frac{89167}{46400}y_{n-1}-\frac{1131}{400}y_n+\frac{1292}{1131}y_{n+1}+\frac{13}{64}y_{n+2}$$
$$h^2y''_{n+1}=-\frac{130321}{226200}y_{n-2}+\frac{130321}{69600}y_{n-1}-\frac{161}{200}y_n-\frac{1540}{1131}y_{n+1}+\frac{2423}{2784}y_{n+2}$$
$$h^3y'''_{n+1}=\frac{6859}{2600}y_{n-2}-\frac{267501}{23200}y_{n-1}+\frac{2793}{200}y_n-\frac{2584}{377}y_{n+1}+\frac{57}{32}y_{n+2}$$
$$hy'_{n+2}=\frac{13718}{9425}y_{n-2}-\frac{6859}{1200}y_{n-1}+\frac{174}{25}y_n-\frac{64}{13}y_{n+1}+\frac{3095}{1392}y_{n+2}$$
$$h^2y''_{n+2}=\frac{48013}{8700}y_{n-2}-\frac{363527}{17400}y_{n-1}+\frac{2399}{100}y_n-\frac{1048}{87}y_{n+1}+\frac{2387}{696}y_{n+2}$$
$$h^3y'''_{n+2}=\frac{144039}{15080}y_{n-2}-\frac{157757}{4640}y_{n-1}+\frac{285}{8}y_n-\frac{5472}{377}y_{n+1}+\frac{3097}{928}y_{n+2} \quad (11)$$

III. IMPLEMENTATION OF HOBBDF METHOD

We used Newton's iteration to implement the method. The formulae in the previous section are written in Newton's iteration form which require the solution of linear systems at each iteration with an approximate Jacobian matrix. Rearranging the equation will produce the system of linear equations that will be solved later. Therefore, the system of

linear equations is as follows.

Noted that

$\begin{bmatrix} e_{n+1} \\ e_{n+2} \end{bmatrix}^{(i+1)}$: Difference between $y_{n+1,n+2}{}^{(i+1)}$ and $y_{n+1,n+2}{}^{(i)}$

$\begin{bmatrix} B_1 \\ B_2 \end{bmatrix}$: Backvalues of the new two points

$W = \left(\frac{\partial f_{n+1,n+2}}{\partial y_{n+1,n+2}} \right)$, $Y = \left(\frac{\partial f_{n+1,n+2}}{\partial y'_{n+1,n+2}} \right)$ and

$Z = \left(\frac{\partial f_{n+1,n+2}}{\partial y''_{n+1,n+2}} \right)$: Jacobian matrix

The general form of linear systems, $\hat{E} = \hat{M}^{-1}\hat{N}$ is shown below.

$$\hat{E} = \begin{bmatrix} e_{n+1} \\ e_{n+2} \end{bmatrix}^{(i+1)},$$

$$\hat{M} = \begin{bmatrix} a & b \\ c & d \end{bmatrix},$$

$$\hat{N} = \left(\begin{bmatrix} -1 & \theta_1 \\ \theta_2 & -1 \end{bmatrix} \begin{bmatrix} y_{n+1} \\ y_{n+2} \end{bmatrix} + h^3 \begin{bmatrix} \alpha_1 & 0 \\ 0 & \alpha_2 \end{bmatrix} \begin{bmatrix} F_1 \\ F_2 \end{bmatrix} + \begin{bmatrix} B_1 \\ B_2 \end{bmatrix} \right),$$

$$a = 1 - Wh^3\alpha_1 - Yh^2\alpha_1\beta_1 - Zh\alpha_1\gamma_1,$$
$$b = -\theta_1 - Yh^2\alpha_1\beta_2 - Zh\alpha_1\gamma_2,$$
$$c = -\theta_2 - Yh^2\alpha_2\hat{\beta}_1 - Zh\alpha_2\hat{\gamma}_1,$$
$$d = 1 - Wh^3\alpha_2 - Yh^2\alpha_2\hat{\beta}_2 - Zh\alpha_2\hat{\gamma}_2,$$

$$F_1 = f\left(y_{n+1}, y'_{n+1}, y''_{n+1}\right),$$
$$F_2 = f\left(y_{n+2}, y'_{n+2}, y''_{n+2}\right)$$

IV. NUMERICAL EXPERIMENTS

Numerical experiments are conducted on the chemical kinetic equations taken from (Feng *et al.*, 2015) and (Feng *et al.*, 2017). Results of the performance for the three solvers are presented in this section. All the results are presented in Tables 1-3 and Figure 1-12. The general form of the model is described earlier in equation (1):

Model 1

P=30, L=1,
$C(t) = 30 - 10e^{-t}$, $C(0) = 20$,
$t \in [0,5]$

Model 2

P=5, L=1,
$C(t) = 35 + 15e^{-t}$, $C(0) = 20$,
$t \in [0,5]$

Model 3

P=60, L=1,
$C(t) = 60 - 10e^{-t}$, $C(0) = 50$,
$t \in [0,5]$

The notations used in the tables and figures are listed as follows.

The numerical results are illustrated in the following tables and figures.

MR	Maximum error
AR	Average error
TL	Tolerance limit
HOBBDF	Higher order block backward differentiation formula
ode15s and ode23s	MATLAB's ODE solvers

Table 1. Performance of all the methods for Model 1

Method	TL	MR	AR
HOBBDF	10^{-2}	5.0258e-004	7.8750e-006
	10^{-3}	9.4945e-005	2.9670e-006
	10^{-4}	4.8851e-005	1.0177e-006
	10^{-5}	1.1892e-005	1.2388e-007
ode15s	10^{-2}	1.4221e-001	3.6458e-002
	10^{-3}	2.0884e-002	8.7366e-003
	10^{-4}	2.5744e-003	1.5591e-003
	10^{-5}	3.7705e-004	1.6426e-004
ode23s	10^{-2}	3.2447e-002	1.4571e-002
	10^{-3}	1.9854e-002	9.7256e-003
	10^{-4}	4.7127e-003	3.1245e-003
	10^{-5}	1.0651e-003	7.4249e-004

Table 2. Performance of all the methods for Model 2

Method	TL	MR	AR
HOBBDF	10^{-2}	1.2373e-003	2.8019e-005
	10^{-3}	3.3781e-004	1.0557e-005
	10^{-4}	8.3498e-005	1.4910e-006
	10^{-5}	2.5054e-005	2.3636e-007
ode15s	10^{-2}	1.5746e-001	3.8563e-002
	10^{-3}	2.1590e-002	6.3368e-003
	10^{-4}	3.1403e-003	6.3397e-004
	10^{-5}	3.8742e-004	1.7889e-004
ode23s	10^{-2}	4.8578e-002	2.1378e-002
	10^{-3}	1.6555e-002	9.6202e-003
	10^{-4}	3.5750e-003	2.3225e-003
	10^{-5}	7.6955e-004	5.1699e-004

Table 3. Performance of all the methods for Model

Method	TL	MR	AR
HOBBDF	10^{-2}	2.0700e-002	5.4845e-003
	10^{-3}	8.3437e-003	1.9041e-003
	10^{-4}	2.3445e-003	5.3644e-004
	10^{-5}	7.7423e-004	2.2145e-004
ode15s	10^{-2}	2.5892e-001	6.9056e-002
	10^{-3}	4.7026e-002	1.3441e-002
	10^{-4}	9.5387e-003	3.2398e-003
	10^{-5}	8.9294e-004	3.6767e-004
ode23s	10^{-2}	3.9526e-002	1.8409e-002
	10^{-3}	2.9072e-002	1.3174e-002
	10^{-4}	7.6836e-003	4.8750e-003
	10^{-5}	1.7573e-003	1.2258e-003

Figure 1. Solutions for Model 1 at tolerance 10^{-2}

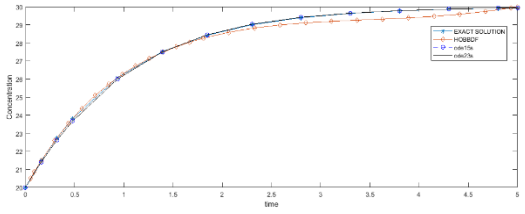


Figure 2. Solutions for Model 1 at tolerance 10^{-3}

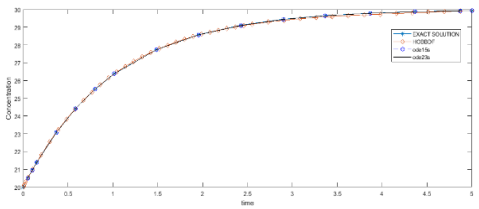


Figure 3. Solutions for Model 1 at tolerance 10^{-4}

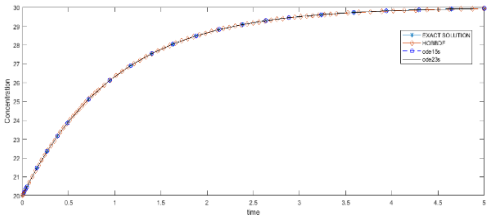


Figure 4. Solutions for Model 2 at tolerance 10

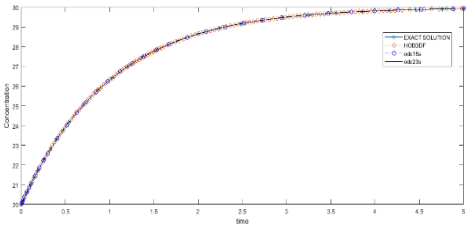


Figure 5. Solutions for Model 2 at tolerance 10^{-2}

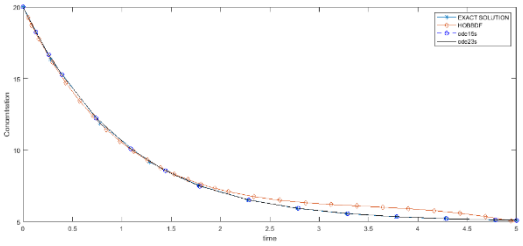


Figure 6. Solutions for Model 2 at tolerance 10^{-3}

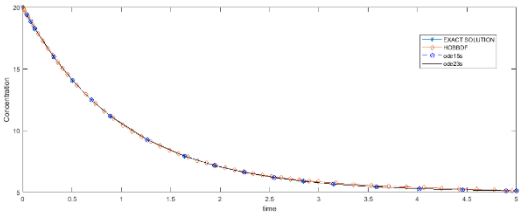


Figure 7. Solutions for Model 2 at tolerance 10^{-4}

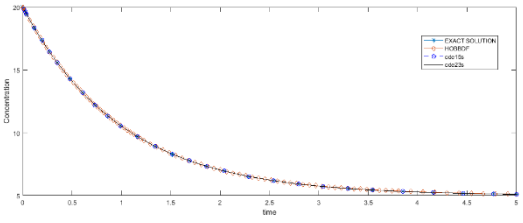


Figure 8. Solutions for Model 2 at tolerance 10^{-5}

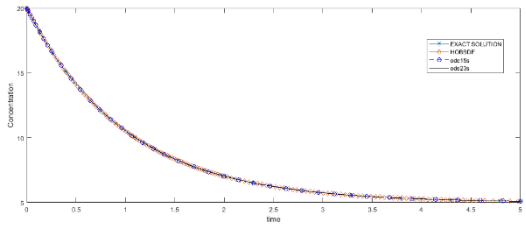


Figure 9. Solutions for Model 3 at tolerance 10^{-}

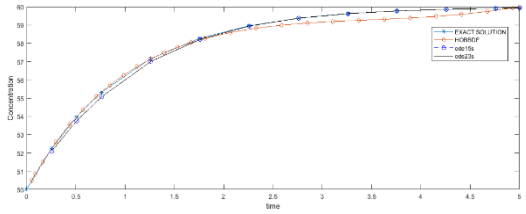


Figure 10. Solutions for Model 3 at tolerance 10^{-3}

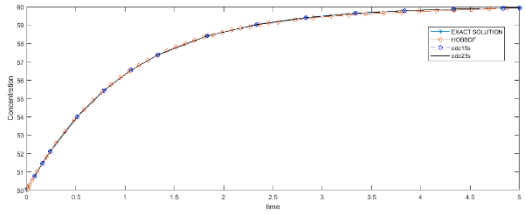


Figure 11Solutions for Model 3 at tolerance 10^{-4}

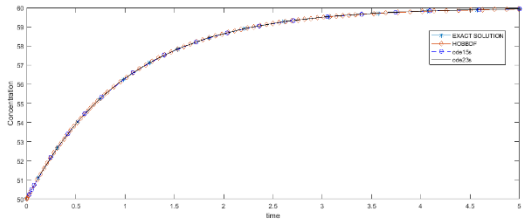
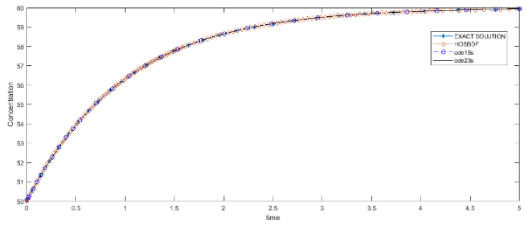


Figure 12Solutions for Model 3 at tolerance 10^{-5}



Tables 1-3 show that the accuracies of the approximate solution are improved when the problems are solved using HOBBDF method as compared to ode15s and ode23s. The errors are also reduced as the tolerance values decrease. As the accuracy is improved, the approximate solutions are converged to the actual solution as presented in Figures 1-12.

V. CONCLUSIONS

An efficient solver was employed to solve the chemical kinetic equations. The numerical results show the accuracy of HOBBDF method. This solver is found to produce more accurate results than ode15s and ode23s since it converges to the exact solution when the tolerance value is reduced. In conclusion, HOBBDF method can be applied to solve the chemical kinetic equations.

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