

Numerical solution of stiff systems of differential equations arising from chemical reactions

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Abstract

Long time integration of large stiff systems of initial value problems, arising from chemical reactions, demands efficient methods with good accuracy and extensive absolute stability region. In this paper, we apply second derivative general linear methods to solve some stiff chemical problems such as chemical Akzo Nobel problem, HIREs problem and OREGO problem.

Keywords: General linear methods; Ordinary differential equation; Chemical reactions; Stiff systems.

1 Introduction

Chemical reaction mechanisms often include individual steps with very different reaction rates. Mathematically, this means that the corresponding ordinary differential equations (ODEs) are likely to be stiff, since the different components of the system have dramatically different time constants. Moreover, these systems are often nonlinear [4].

In the last 40 years or so, numerous works have been focusing on the development of more advanced and efficient methods for stiff problems. A potentially good numerical method for the solution of stiff systems of ODEs must have good accuracy and some reasonably wide region of absolute stabil-

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ity. A -stability requirement puts a severe limitation on the choice of suitable methods for stiff problems.

Traditional numerical methods for solving an initial value problem generally fall into two main classes: linear multistep (multistage) and Runge–Kutta (multistage) methods. In 1966, Butcher [5] introduced general linear methods (GLMs) as a unifying framework for the traditional methods to study the properties of consistency, stability and convergence, and to formulate new methods with clear advantages over these classes.

On the other hand, one of the main directions to construct methods with higher order and extensive stability region, is using higher derivatives of the solutions, and some methods have been introduced that have good properties, especially for stiff problems. See [7, 8, 9]. Although GLMs include linear multistep methods, Runge–Kutta and many other standard methods, but they were extended to second derivative general linear methods (SGLMs) to cover second derivative methods, too. These methods were introduced by Butcher and Hojjati in [6] and were studied more by Abdi and Hojjati in [1, 2, 3]. There are several interrelated aims in the use of such methods, such as high orders and stage orders, high accuracy, low error constants, satisfactory stability properties, such as A -stability or L -stability and low implementation costs. In [3], the efficiency of SGLMs are shown by comparing the accuracy versus stepsize and the number of function evaluations of SGLMs with those of SDIRK methods. These advantages of SGLMs motivate us to apply them for solving large stiff systems of initial value problems arising from chemical reactions.

The rest of the paper is organized as follows. In Section 2, we recall the basic concepts and theory of SGLMs. In Section 3, we introduce types of SGLMs and give an SGLM of order 3. In Section 4, we apply the method to solve some important initial value problems that arise from mathematical modeling of chemical reaction and give numerical results, and the paper is closed in Section 5 by concluding and giving ideas for future work.

2 A review on the SGLMs

In this section, we give a brief review of SGLMs for the numerical solution of an autonomous system of ordinary differential equation

$$y' = f(y(x)), \quad y : \mathbb{R} \rightarrow \mathbb{R}^m, \quad f : \mathbb{R}^m \rightarrow \mathbb{R}^m. \quad (1)$$

These methods are characterized by four integers: (p, q, r, s) where p and q are respectively order and stage order of the method, r is the number of input and output approximations, and s is the number of internal stages. Let $Y^{[n]} = [Y_i^{[n]}]_{i=1}^s$ be an approximation of stage order q to the vector $y(x_{n-1} + ch) = [y(x_{n-1} + c_i h)]_{i=1}^s$ and the vectors $f(Y^{[n]}) = [f(Y_i^{[n]})]_{i=1}^s$ and $g(Y^{[n]}) =$

$[g(Y_i^{[n]})]_{i=1}^s$ denote the stage first and second derivative values, where $g(\cdot) = f'(\cdot)f(\cdot)$. The c_i 's represent position of the internal stages within one step. The vector $c = [c_1 \ c_2 \ \dots \ c_s]^T$ is called the abscissa vector. Also, let denote by $y^{[n-1]} = [y_i^{[n-1]}]_{i=1}^r$ and $y^{[n]} = [y_i^{[n]}]_{i=1}^r$ the input and output vectors at step number n , respectively. An SGLM used for the numerical solution of (2) is given by

$$\begin{aligned} Y_i^{[n]} &= h \sum_{j=1}^s a_{ij} f(Y_j^{[n]}) + h^2 \sum_{j=1}^s \bar{a}_{ij} g(Y_j^{[n]}) + \sum_{j=1}^r u_{ij} y_j^{[n-1]}, \quad i = 1, 2, \dots, s, \\ y_i^{[n]} &= h \sum_{j=1}^s b_{ij} f(Y_j^{[n]}) + h^2 \sum_{j=1}^s \bar{b}_{ij} g(Y_j^{[n]}) + \sum_{j=1}^r v_{ij} y_j^{[n-1]}, \quad i = 1, 2, \dots, r, \end{aligned} \quad (2)$$

where $n = 1, 2, \dots, N$, $Nh = \bar{x} - x_0$ and h is the stepsize. We denote $A = [a_{ij}]$, $\bar{A} = [\bar{a}_{ij}]$, $U = [u_{ij}]$, $B = [b_{ij}]$, $\bar{B} = [\bar{b}_{ij}]$ and $V = [v_{ij}]$.

We now state the fundamental theorem on SGLMs.

Theorem 2.1 [1] *The necessary and sufficient conditions for an SGLM to be convergent are that it be consistent and zero-stable.*

The derivation of order and stage order conditions for general p and q is quite complicated. However, this analysis is quite simple for methods of stage order $q = p$. In this case, the order and stage order conditions can be expressed conveniently using the theory of functions of a complex variable. We have the following theorem on order conditions.

Theorem 2.2 [2] *The SGLM (2) with*

$$y_i^{[n-t]} = \sum_{k=0}^p h^k \alpha_{ik} y^{(k)}(x_{n-t}) + O(h^{p+1}), \quad i = 1, 2, \dots, r, \quad t = 0, 1,$$

has order p and stage order $q = p$ if and only if

$$\exp(cz) = zA \exp(cz) + z^2 \bar{A} \exp(cz) + Uw + O(z^{p+1}), \quad (3)$$

$$\exp(z)w = zB \exp(cz) + z^2 \bar{B} \exp(cz) + Vw + O(z^{p+1}), \quad (4)$$

where $e^{cz} = [e^{c_1 z}, e^{c_2 z}, \dots, e^{c_s z}]^T$ and $w = w(z) = [\sum_{k=0}^p \alpha_{ik} z^k]_{i=1}^r$.

The stability behavior of SGLMs is defined using the standard test problem of Dahlquist $y'(x) = \xi y(x)$, where ξ is a (possibly complex) number. If method (2) is applied to this problem, then the stability matrix is

$$M(z) = V + (zB + z^2 \bar{B})(I - zA - z^2 \bar{A})^{-1}U, \quad (5)$$

where $z = h\xi$. If $M(z)$ has only a single non-zero eigenvalue, $R(z)$, then the method is said to possess Runge–Kutta stability (RKS).

3 Types of SGLMs and an example

It is convenient to write coefficients of the method, that is elements of A , \bar{A} , U , B , \bar{B} and V as a partitioned $(s+r) \times (2s+r)$ matrix

$$\left[\begin{array}{c|c|c} A & \bar{A} & U \\ \hline B & \bar{B} & V \end{array} \right].$$

It is desirable to impose some restrictions on the matrices A and \bar{A} to ensure that the stages of the method can be evaluated independently and sequentially [1]. Thus these two matrices will be chosen to be of lower triangular form. Furthermore, to lower implementation costs we will assume that each of A and \bar{A} have constant diagonal elements. In [1] the authors by considering SGLMs in diagonally implicit multi-stage form, which the matrices A and \bar{A} have the lower triangular form

$$A = \begin{bmatrix} \lambda & & & \\ a_{21} & \lambda & & \\ \vdots & \vdots & \ddots & \\ a_{s1} & a_{s2} & \cdots & \lambda \end{bmatrix}, \quad \bar{A} = \begin{bmatrix} \mu & & & \\ \bar{a}_{21} & \mu & & \\ \vdots & \vdots & \ddots & \\ \bar{a}_{s1} & \bar{a}_{s2} & \cdots & \mu \end{bmatrix},$$

have divided SGLMs into four types, depending on the nature of the differential system to be solved and the computer architecture that is used to implement these methods. Types 1 and 2 are those with arbitrary a_{ij} and \bar{a}_{ij} where $\lambda = \mu = 0$ and $\lambda > 0$, $\mu < 0$, respectively. Such methods are appropriate respectively for nonstiff and stiff differential systems in a sequential computing environment. For type 3 or 4 methods, $A = \lambda I$ and $\bar{A} = \mu I$, where $\lambda = \mu = 0$ or $\lambda > 0$, $\mu < 0$, respectively. Such methods are appropriate for nonstiff or stiff differential systems in a parallel computing environment.

Second derivative diagonally implicit multistage integration methods (SDIMSIMs) as a subclass of SGLMs have been introduced in [2]. They are characterized by the following properties:

- Coefficients matrices A and \bar{A} are lower triangular with the same parameters λ and μ on the diagonal respectively.
- Coefficients matrix V is a rank 1 matrix with nonzero eigenvalue equal to 1 to guarantee preconsistency.
- Order p , stage order q , number of external stages r , and the number of internal stages s are all approximately equal.

SDIMSIS can be divided into four types according to the above classification of SGLMs [1]. These four types, together with their intended applications and architectures, are shown in Table 1.

Table 1: Types of SDIMSIS with their intended applications and architectures

Type 1	A strictly lower triangular	\bar{A} strictly lower triangular	nonstiff	sequential
Type 2	$A - \lambda I$ strictly lower triangular	$\bar{A} - \mu I$ strictly lower triangular	stiff	sequential
Type 3	$A = \mathbf{0}$	$\bar{A} = \mathbf{0}$	nonstiff	parallel
Type 4	$A = \lambda I$	$\bar{A} = \mu I$	stiff	parallel

An SDIMSIS with $p = q = 3$ and $r = s = 2$

We consider an SDIMSIS with $p = q = 3$, $r = s = 2$, $U = I$ and $V = ev^T$ for which $ve^T = 1$. This method which has been introduced in [2], is A - and L -stable. The abscissa vector of the method is $c = [0 \ 1]^T$ and its coefficients are given by the partitioned matrix

$$\left[\begin{array}{cc|cc|cc} \frac{2}{5} & 0 & -\frac{1}{12} & 0 & 1 & 0 \\ \frac{55}{27} & \frac{2}{5} & -\frac{7}{27} & -\frac{1}{12} & 0 & 1 \\ \frac{2737}{2700} & \frac{9}{100} & -\frac{7}{270} & 0 & \frac{9}{10} & \frac{1}{10} \\ \hline \frac{217}{2700} & -\frac{37}{2700} & -\frac{293}{540} & -\frac{31}{540} & \frac{9}{10} & \frac{1}{10} \end{array} \right]. \quad (6)$$

We apply this method to solve some important initial value problems which exhibit stiffness and arise from mathematical modeling of chemical reactions. Other efficient methods in this class can be found in [1, 2, 3].

4 Numerical solution of stiff chemical problems

In this section, we apply the method (6) on some famous chemical problems to show its efficiency.

4.1 Chemical Akzo Nobel problem

General information

This initial value problem is a stiff system of 6 non-linear differential equations. It has been taken from [10].

Mathematical description of the problem

The problem is of the form

$$\frac{dy}{dt} = f(y), \quad y(0) = y_0, \quad (7)$$

with

$$y \in \mathbb{R}^6, \quad 0 \leq t \leq 180. \quad (8)$$

The function f is defined by

$$f(y) = \begin{pmatrix} -2r_1 + r_2 - r_3 - r_4 \\ -\frac{1}{2}r_1 - r_4 - \frac{1}{2}r_5 + F_{in} \\ r_1 - r_2 + r_3 \\ -r_2 + r_3 - 2r_4 \\ r_2 - r_3 + r_5 \\ -r_5 \end{pmatrix},$$

where the r_i and F_{in} are auxiliary variables, given by

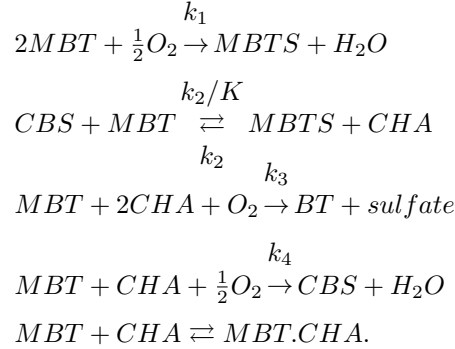
$$\begin{aligned} r_1 &= k_1 \cdot y_1^4 \cdot y_2^{\frac{1}{2}}, & k_1 &= 18.7, \\ r_2 &= k_2 \cdot y_3 \cdot y_4, & k_2 &= 0.58, \\ r_3 &= \frac{k_2}{K} \cdot y_1 \cdot y_5, & K &= 34.4, \\ r_4 &= k_3 \cdot y_1 \cdot y_4^2, & k_3 &= 0.09, \\ r_5 &= k_4 \cdot y_6^2 \cdot y_2^{\frac{1}{2}}, & k_4 &= 0.42, \\ F_{in} &= klA \cdot \left(\frac{p(O_2)}{H} - y_2 \right), & klA &= 3.3, \\ p(O_2) &= 0.9, & H &= 737. \end{aligned} \quad (9)$$

Finally, the initial vector y_0 is given by

$$y_0 = (0.437, 0.00123, 0, 0, 0, 0.367)^T.$$

Origin of the problem

The problem originates from Akzo Nobel Central Research in Arnhem, The Netherlands. It describes a chemical process, in which 2 species, *MBT* and *CHA*, are mixed, while oxygen is continuously added. The resulting species of importance is *CBS*. The reaction equations, as given by Akzo Nobel, are



The last equation describes an equilibrium

$$Ks^1 = \frac{[MBT.CHA]}{[MBT] \cdot [CHA]},$$

while the others describe reactions, whose velocities are given by

$$\begin{aligned}
 r_1 &= k_1 \cdot [MBT]^4 \cdot [O_2]^{\frac{1}{2}}, \\
 r_2 &= k_2 \cdot [MBTS] \cdot [CHA], \\
 r_3 &= \frac{k_2}{K} \cdot [MBT] \cdot [CBS], \\
 r_4 &= k_3 \cdot [MBT] \cdot [CHA]^2, \\
 r_5 &= k_4 \cdot [MBT.CHA]^2 \cdot [O_2]^{\frac{1}{2}},
 \end{aligned}$$

respectively. Here the square brackets '['] denote concentrations. The inflow of oxygen per volume unit is denoted by F_{in} , and satisfies

$$F_{in} = kLA \cdot \left(\frac{p(O_2)}{H} - [O_2] \right),$$

where kLA is the mass transfer coefficient, H is the Henry constant and $p(O_2)$ is the partial oxygen pressure. $p(O_2)$ is assumed to be independent of $[O_2]$. The parameters k_1 , k_2 , k_3 , k_4 , K , kLA , H and $p(O_2)$ are given constants. The process is started by mixing 0.437 mol/liter $[MBT]$ with 0.367 mol/liter $[MBT.CHA]$. The concentration of oxygen at the beginning

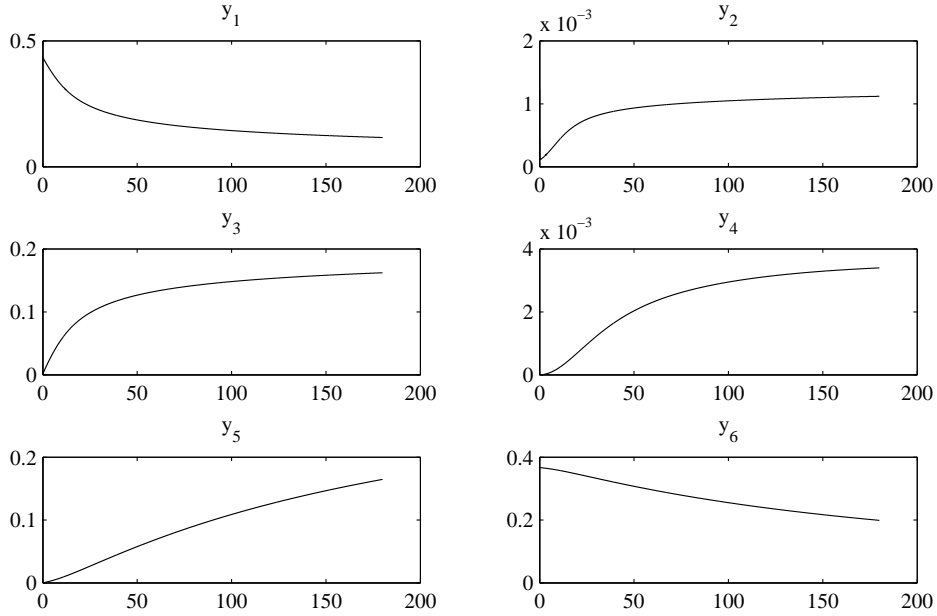


Figure 1: Chemical Akzo Nobel problem: numerical solution obtained by SDIMSIM of order $p = q = 3$ and $r = s = 2$

is 0.00123 mol/liter. Initially, no other species are present. The simulation is performed on the time interval $[0, 180 \text{ minutes}]$.

Identifying the concentrations $[MBT]$, $[O_2]$, $[MBTS]$, $[CHA]$, $[CBS]$, $[MBT.CHA]$ with y_1, \dots, y_6 respectively, one easily arrives at the mathematical formulation of the preceding subsection. Solution of this problem at $t = 180$ using method (6) is reported in Table 2. Behavior of the solution components is shown in Figure 1.

Table 2: Results of the Chemical Akzo Nobel problem at $t = 180$

y_i	Solution at $t = 180$
y_1	0.116160227121356
y_2	0.001119418167053
y_3	0.162126172160781
y_4	0.003396981306527
y_5	0.164618511821187
y_6	0.198953326600100

4.2 Problem HIRES

General information

This initial value problem is a stiff system of 8 non-linear differential equations. It was proposed by Schäfer in 1975. The name HIRES was given by Hairer and Wanner [13]. It refers to “High Irradiance Response”, which is described by this IVP ODE.

Mathematical description of the problem

The problem is of the form

$$\frac{dy}{dt} = f(y), \quad y(0) = y_0,$$

with

$$y \in \mathbb{R}^8, \quad 0 \leq t \leq 321.8122.$$

The function f is defined by

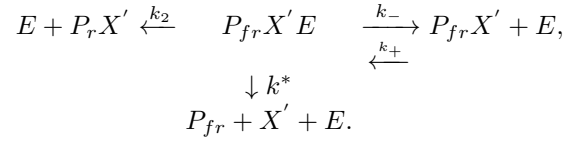
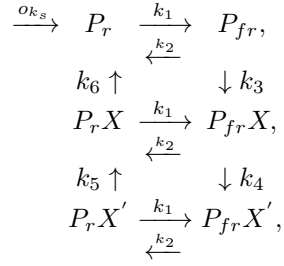
$$f(y) = \begin{pmatrix} -1.71y_1 + 0.43y_2 + 8.32y_3 + 0.0007 \\ 1.71y_1 - 8.75y_2 \\ -10.03y_3 + 0.43y_4 + 0.035y_5 \\ 8.32y_2 + 1.71y_3 - 1.12y_4 \\ -1.745y_5 + 0.43y_6 + 0.43y_7 \\ -280y_6y_8 + 0.69y_4 + 1.71y_5 - 0.43y_6 + 0.69y_7 \\ 280y_6y_8 - 1.81y_7 \\ -280y_6y_8 + 1.81y_7 \end{pmatrix}. \quad (10)$$

The initial vector y_0 is given by

$$y_0 = (1, 0, 0, 0, 0, 0, 0, 0.0057)^T.$$

Origin of the problem

The problem originates from plant physiology and is described in [14]. It explains the ‘High Irradiance Response’ (HIRES) of Photomorphogenesis on the basis of Phytochrome, by means of a chemical reaction involving 8 reactants. The reaction scheme is given below.



The values of the parameters were taken from [13].

$$\begin{aligned}
k_1 &= 1.71, k_2 = 0.43, k_3 = 8.32, k_4 = 0.69, k_5 = 0.035, \\
k_6 &= 8.32, k_+ = 280, k_- = 0.69, k^* = 0.69, o_{k_s} = 0.0007.
\end{aligned}$$

Identifying $P_r, P_{fr}, P_r X, P_{fr} X, P_r X', P_{fr} X', P_{fr} X' E$ and E with $y_i, i = 1, 2, \dots, 8$, respectively, the differential equations mentioned in (10) easily follow. The obtained solution of this problem at the end of time interval is reported in Table 3. Plots in the Figure 2 show the behavior of $P_r, P_{fr}, P_r X, P_{fr} X, P_r X'$, and $P_{fr} X'$, computed using the method (6).

Table 3: Results of the problem HIRES at $t = 321.8122$

y_i	Solution at $t = 321.8122$
y_1	$0.73714105836 \times 10^{-3}$
y_2	$0.14425050468 \times 10^{-3}$
y_3	$0.58889121959 \times 10^{-4}$
y_4	$0.11756696043 \times 10^{-2}$
y_5	$0.23866504368 \times 10^{-2}$
y_6	$0.62398915376 \times 10^{-2}$
y_7	$0.28502050925 \times 10^{-2}$
y_8	$0.28497949075 \times 10^{-2}$

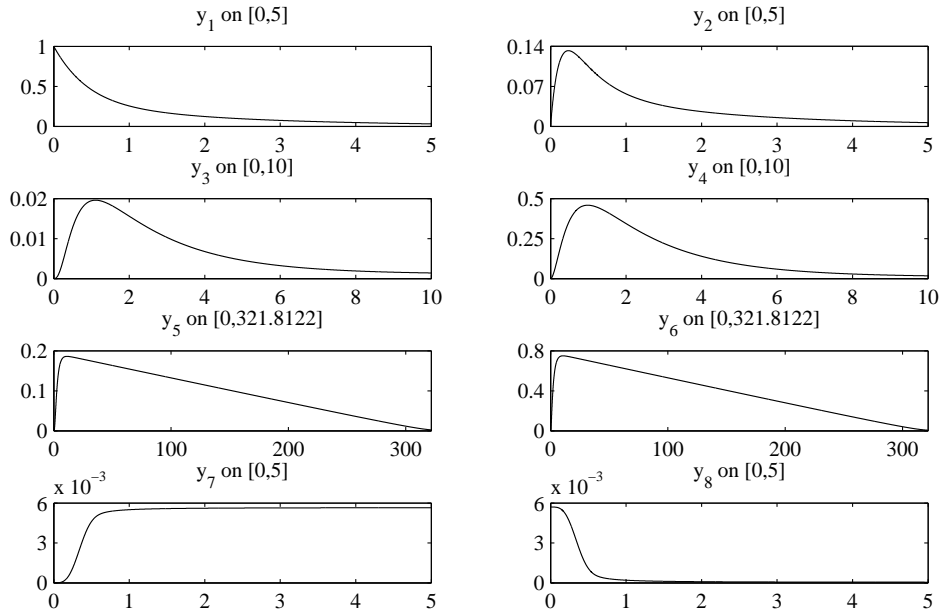


Figure 2: Problem HIREs: numerical solution obtained by SDIMSIM of order $p = q = 3$ and $r = s = 2$

4.3 Problem OREGO

General information

The problem consists of a stiff system of 3 non-linear ordinary differential equations. The name Orego was given by Hairer and Wanner [13] and refers to the Oregonator model which is described by this ODE. The Oregonator model takes its name from the University of Oregon where in the 1972 Field, Körös and Noyes [11] proposed this model for the Belousov–Zhabotinskii reaction.

Mathematical description of the problem

The problem is of the form

$$\frac{dy}{dt} = f(y), \quad y(0) = y_0,$$

with

$$y \in \mathbb{R}^3, \quad 0 \leq t \leq 360.$$

The function f is defined by

$$f(y) = \begin{pmatrix} s(y_2 - y_1 y_2 + y_1 - q y_1^2) \\ \frac{1}{s}(-y_2 - y_1 y_2 + y_3) \\ w(y_1 - y_3) \end{pmatrix}.$$

The values of the parameters s , q and w are

$$s = 77.27, \quad w = 0.161, \quad q = 8.375 \times 10^{-6}.$$

The initial vector y_0 is given by $(1, 2, 3)^T$.

Origin of the problem

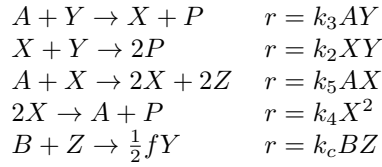
The OREGO problem originates from the celebrated Belousov–Zhabotinskii (BZ) reaction. When certain reactions, like bromous acid, bromide ion and cerium ion, are combined, they exhibit a chemical reaction which, after an induction period of inactivity, oscillates with change in structure and in color, from red to blue and viceversa.

The color changes are caused by alternating oxidation–reductions in which the cerium switches its oxidation state from $Ce(III)$ to $Ce(IV)$.

Field, Körös and Noyes formulated the following model for the most important parts of the kinetic mechanism that gives rise to oscillation in the BZ reaction. This mechanism can be summarized as three concurrent processes [12]:

- the reduction of Bromate (BrO_3^-) to Bromine (Br) via the reducing agent bromide (Br^-). Bromomalonic acid ($BrMA$) is produced;
- the increase of hypobromous acid ($HBrO_2$) at an accelerating rate and the production of $Ce(IV)$. Here we have a sudden change in color from red to blue;
- the reduction of Cerium catalyst $Ce(IV)$ to $Ce(III)$. Here we have a gradual change in color from blue to red.

Then, from this mechanism the following Oregonator scheme is obtained



Here, using the conventional notation the assignments and the effective concentration are

hypobromous acid	$[HBrO_2] = X$	5.025×10^{-11}
Bromide	$[Br^-] = Y$	3.0×10^{-7}
Cerium - 4	$[CE(IV)] = Z$	2.412×10^{-8}
Bromate	$[BrO_3^-] = A$	
all oxidizable organic species	$[Org] = B$	
	$[HOBr] = P$	

The reaction rate equations for the intermediate species X, Y, and Z are

$$\begin{aligned}
\frac{dX}{dt} &= s(Y - XY + X - qX^2), \\
\frac{dY}{dt} &= \frac{1}{s}(-Y - XY + fZ), \\
\frac{dZ}{dt} &= w(X - Z),
\end{aligned}$$

with $f = 1$, and s , w , and q as in the previous subsection.

Solution of this problem at $t = 360$ using method (6) is reported in Table 4. Behavior of the solution components is shown in Figure 3.

Table 4: Results of the OREGO problem at $t = 360$

y_i	Solution at $t = 360$
y_1	$0.1000814868842 \times 10^1$
y_2	$0.1228180744895 \times 10^4$
y_3	$0.1320568339839 \times 10^3$

5 Conclusion

For stiff systems, because of the stability condition, the time step restriction becomes severe, specially when they have to be integrated over long periods of time. High order accuracy, good stability properties and low implementation

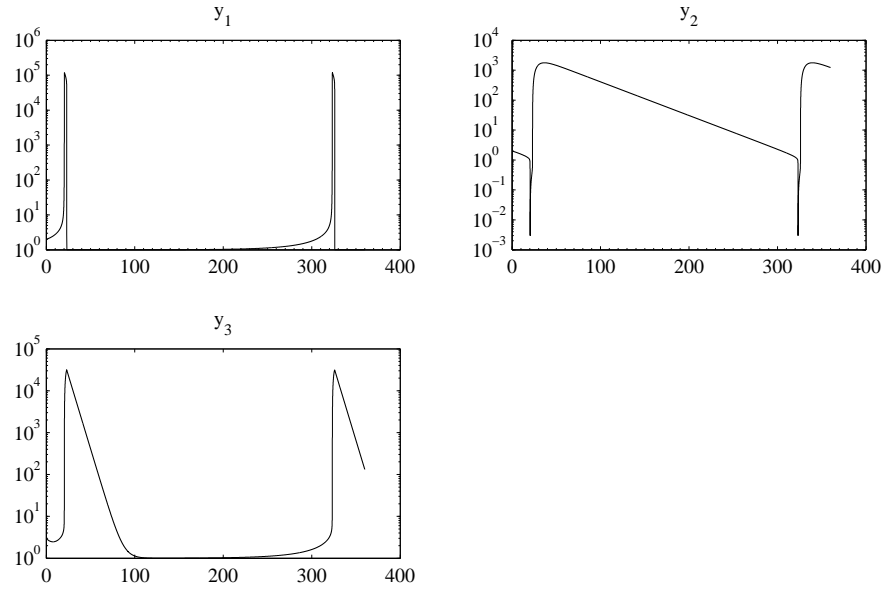


Figure 3: Chemical OREGO problem: numerical solution obtained by SDIMSIM of order $p = q = 3$ and $r = s = 2$

cost of the SGLMs make them to be successful in applying on large stiff systems of initial value problems arising from chemical reactions. Although the SGLMs are capable in giving accurate and stable results, as reported in the numerical experiments, but in can be equipped by a strategy for adjusting stepsize when the integration proceeds. It is the subject of our future works.

References

1. Abdi, A. and Hojjati, G. *An extension of general linear methods*, Numer. Algor., 57 (2011), 149–167.
2. Abdi, A. and Hojjati, G. *Maximal order for second derivative general linear methods with Runge-Kutta stability*, Appl. Numer. Math., 61 (2011), 1046–1058.
3. Abdi, A., Braš, M. and Hojjati, G. *On the construction of second derivative diagonally implicit multistage integration methods*, Appl. Numer. Math., 76 (2014), 1–18.

4. Burg, K.V. *Statistical Models in Applied Science*, J. Wiley, New York, 1975.
5. Butcher, J. C. *On the convergence of numerical solutions to ordinary differential equations*, Math. Comp., 20 (1966), 1–10.
6. Butcher, J. C. and Hojjati, G. *Second derivative methods with RK stability*, Numer. Algor., 40 (2005), 415–429.
7. Cash, J. R. *Second derivative extended backward differentiation formula for the numerical integration of stiff systems*, SIAM J. Numer. Anal., 18 (1981), 21–36.
8. Enright, W. H. *Second derivative multistep methods for stiff ordinary differential equations*, SIAM J. Numer. Anal., 11 (1974), 321–331.
9. Hojjati, G., Rahimi Ardabili, M.Y. and Hosseini, S.M. *New second derivative multistep methods for stiff systems*, Appl. Math. Model., 30 (2006), 466–476.
10. Eriksson, K., Johnson, C. and Logg, A. *Explicit time-stepping for stiff ODEs*, SIAM J. Sci. Comput., 25 (2003), 11–42.
11. Field, R. J., Körös, E. and Noyes, R. M. *Oscillation in chemical systems, part. 2. thorough analysis of temporal oscillations in the bromate–cerium–malonic acid system*. *Journal of the American Society*, 94 (1972), 8649–8664.
12. Gray, C. *An analysis of the Belousov–Zhabotinskii reaction*. *Rose-Hulman Undergraduate Mathematics Journal*, 3(1), 2002. <http://www.rose-hulman.edu/mathjournal/>.
13. Hairer, E. and Wanner, G. *Solving Ordinary Differential Equations II: Stiff and Differential-algebraic Problems*, Springer-Verlag, 1991.
14. Schäfer, E. *A new approach to explain the ‘high irradiance responses’ of photomorphogenesis on the basis of phytochrome*, J. of Math. Biology, 2 (1975), 41–56.