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ORIGINAL PAPER

# Wavelet-based collocation method for stiff systems in process engineering

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**Abstract** Abrupt phenomena in modelling real-world systems such as chemical processes indicate the importance of investigating stiff systems. However, it is difficult to get the solution of a stiff system analytically or numerically. Two such types of stiff systems describing chemical reactions were modelled in this paper. A numerical method was proposed for solving these stiff systems, which have general nonlinear terms such as exponential function. The technique of dealing with the nonlinearity was based on the Wavelet-Collocation method, which converts differential equations into a set of algebraic equations. Accurate and convergent numerical solutions to the stiff systems were obtained. We also compared the new results to those obtained by the Euler method and 4th order Runge–Kutta method.

**Keywords** Wavelet · Collocation method · Stiff system · Numerical solution · Chemical reaction model

## 1 Introduction

Chemical reaction engineering aims at exploitation of chemical reactions on a commercial scale. Its goal is the successful design and operation of chemical reactors. Reaction engineering problems require solutions of highly nonlinear equations, which are not always amenable to analytical solution [6]. This has motivated wide applications of

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various numerical methods for the problems. The most popular numerical methods are the Euler method and fourth order Runge–Kutta method [8]. Since the considered problem of chemical reactions is a relatively stiff problem, the relative magnitude of the concentration changes quite sharply. Therefore, it is important to reduce the step size until the desired accuracy is obtained for all the numerical methods posed for solving the reaction problems. However, this will increase the computation demand significantly. This motivates the development of innovative methods for numerical computing of the systems more accurately and effectively.

Wavelet based methods are a good candidate for stiff systems. In this area, some methods have been posed recently to improve the accuracy of the numerical solutions of the nonlinear equations. Examples are the Haar-wavelet method for stiff systems [4], Wavelet-Galerkin method for population balance equations [2], and Wavelet-Collocation method for breakage equation with boundary conditions [1,5]. Generally, the Galerkin method gives better accuracy than the collocation method [7]; however, it is somewhat intractable for nonlinear problems especially for general nonlinearity such as the exponential function. The main difficulty lies on the computing of the connection coefficients [2,10]. If the Galerkin method is involved for solving the problem with the general nonlinearity, then after the wavelet transformation we can hardly get a set of neat algebraic equations.

In this paper, we will develop a Wavelet-Collocation method, which was originally developed by Bertoluzza [1] for dealing with the boundary condition problems, for numerically solving two types of mathematical models of chemical reactions. Taking advantages of the trail function from the collocation method, the developed method can handle the general nonlinearity quite easily.

The paper is organized as follows. We model two types of chemical reactions in Sect. 2. In Sect. 3, the wavelet-collocation method is briefly introduced, which was originally posed by [1] for solving the two-point boundary problem; and then a new method is developed to solve the initial condition problems mentioned in Sect. 2. Section 4 carries out numerical studies to illustrate the developed method. Finally, Sect. 5 concludes the paper.

## 2 Modelling chemical reactions

In this section we are going to briefly introduce two chemical reaction models from [8] and [9], respectively, which will be used as the test problems in Sect. 4.

### 2.1 Non-isothermal batch reactor

The nonisothermal batch reactor is operated adiabatically, which contains a liquid reaction mixture with the following reaction occurs:

$$A(l) \xrightarrow{r} P(l)$$

where $r = kC_A$ and

$$k = k_0 \exp\left(-\frac{E}{RT}\right)$$

$C_A$ is the concentration of $A$, $E$ is the activation energy for the reaction, $R$ is the gas constant, and $T$ is the absolute temperature. If the reactor is perfectly mixed, the unsteady-state mole balance for component $A$ is given by

$$\frac{dn_A}{dt} = V_R(-r) = -V_R k_0 \exp\left(-\frac{E}{RT}\right) C_A.$$

Noticing that the reactor volume, $V_R$, is constant and $C_A = n_A/V_R$, we have the following equation

$$\frac{dC_A}{dt} = -k_0 C_A \exp\left(-\frac{E}{RT}\right). \tag{1}$$

The unsteady-state energy balance equation is given by

$$\rho V_R C_p \frac{dT}{dt} = -\Delta H_{RXN} r V_R, \tag{2}$$

where $\rho$ is the density of the reaction mixture, $C_p$ is the average heat capacity of the reaction mixture, and $\Delta H_{RXN}$ is the heat of reaction, which is a function of temperature. Let $K_1 = -k_0$, $K_2 = \frac{-\Delta H_{RXN} k_0}{\rho C_p}$. Then Eqs. 1 and 2 read as the following

$$\frac{dC_A}{dt} = K_1 C_A \exp\left(-\frac{E}{RT}\right), \tag{3}$$

$$\frac{dT}{dt} = K_2 C_A \exp\left(-\frac{E}{RT}\right) \tag{4}$$

where $T = T_0$ and $C_A = C_{A0}$ initially.

### 2.2 The Robert problem

The Robert problem describes the kinetics of an autocatalytic reaction, which was first proposed by Robertson [9]. If the mass action law is applied for the rate functions, the following mathematical model can be set up

$$\begin{aligned} y_1' &= -k_1 y_1 + k_3 y_2 y_3 \\ y_2' &= k_1 y_1 - k_2 y_2^2 - k_3 y_2 y_3 \,, \\ y_3' &= k_2 y_2^2 \end{aligned} \tag{5}$$

where $k_i, i = 1, 2, 3$ are the rate constants, and $y_i, i = 1, 2, 3$ are the concentrations of three chemical species involved. This problem is very popular in numerical studies and often is used as a test problem for the stiff integrators comparisons.

## 3 Wavelet-Collocation method

### 3.1 Collocation method

The collocation method is also called the residual method. It is a widely used method for numerical solutions of ordinary and partial differential equations although it is not as accurate as the Galerkin method.

Consider the following problem

$$\mathbb{L}u(x) = f(x,t)$$

where $\mathbb{L}$ is a differential operator. Let us define the residual $R$ as the following

$$R = \mathbb{L}u - f$$

Now approximate the $u(x)$ as the sum of trial functions $w_k$

$$u(x) = \sum_{k=1}^{n} u_k w_k$$

and substitute this approximation into the equation of the residual $R$ above. Then we try to adjust the coefficients $u_k$ to make $R = 0$. Generally speaking, it is not realistic to get this point for all the values of $x$. However, we might be able to choose $n$ collocation points where we have $R(x_k) = 0, k = 1, \ldots, n$.

Normally, we define the trial functions as the Dirac delta function

$$w_k = \delta(x - x_k) = \begin{cases} 1, & x = x_k, \\ 0, & \text{otherwise} \end{cases} \tag{6}$$

### 3.2 Wavelet-based collocation method

The wavelet-based collocation method was initially posed by Bertoluzza [1] to deal with the Dirichlet boundary value problem

$$\begin{aligned} \mathbb{L}u &= f \in (0,1), \\ u(0) &= a, \\ u(1) &= b, \end{aligned}$$

where the authors defined the following trial function

$$\theta(n) = \int_{-\infty}^{\infty} \phi(x)\phi(x-n)dx, n \in \mathbb{Z},$$

by the integral of the product of two scaling functions, $\phi(\cdot)$, constructed by Daubechies [3]. $\phi(\cdot)$ has a compact support $[0, L-1]$. Considering the boundary conditions, they

approximated the unknown function $u(x)$ by $j$ level wavelet series expansion as the following form

$$u_j(x) = u(0)\sum_{k=-\infty}^{k=0}\theta(2^j x - k) + \sum_{k=1}^{2^j-1} u_j(x_k)\theta(2^j x - k) + u(1)\sum_{k=2^j}^{\infty}\theta(2^j x - k),$$

which verifies $u_j(0) = a, u_j(1) = b$, and $Au_j(x_n) = f(x_n), n = 1, \ldots, 2^j - 1$. This method is stable and convergent according to [1].

### 3.3 Wavelet Collocation method for the initial value problem in [0, 1]

Now, let us switch the focus to the initial value problem (IVP) in the finite interval $[0, D]$ with $D = 1$. We have the following scheme for numerically solving the IVP based on Bertoluzza's method.

Consider the following system

$$\begin{aligned} \mathbb{L}u &= f \in [0, 1], \\ u(0) &= a \end{aligned} \tag{7}$$

where $\mathbb{L}$ is a differential operator and $f$ is a nonlinear function in the interval [0, 1]. Redefine the functions as the following for $k = 1, \ldots, 2^j - 1$

$$\tilde{\theta}_{j,k}(x) = \theta_{j,k}(x), \tilde{\theta}_{j,0}(x) = \sum_{l=-\infty}^{0}\theta_{j,l}(x), \tilde{\theta}_{j,2^j}(x) = \sum_{l=2^j}^{\infty}\theta_{j,l}(x), \tag{8}$$

with $\theta_{j,l} = \theta(2^j x - l)$, where the new function $\tilde{\theta}_{j,k}$ still have the similar properties to that of $\theta_{j,k}$. Noticing that the compact support of the trial function, $\theta(x)$, is $[1 - L, L - 1]$, the last two functions of Eq. 8 have the following form

$$\tilde{\theta}_{j,0}(x) = \sum_{l=1-L}^{0}\theta_{j,l}(x), \tilde{\theta}_{j,2^j}(x) = \sum_{l=2^j}^{2^j+L-1}\theta_{j,l}(x). \tag{9}$$

By the definition of Eqs. 8 and 12, we can approximate the solution of the initial value problem (7) by

$$u_j(x) = a\tilde{\theta}_{j,0}(x) + \sum_{k=1}^{2^j} u_{j,k}\tilde{\theta}_{j,k}(x), \tag{10}$$

where $u_{j,k}$ are the coefficients to be determined. Let $\theta^{(n)}(x) = \frac{d^n\theta(x)}{dx^n}$ be the $n$th derivative of function $\theta(x)$. Then from Eq. 10, we have

$$u_j^{(n)}(x) = 2^{nj}\left(a\tilde{\theta}_{j,0}^{(n)}(x) + \sum_{k=1}^{2^j} u_{j,k}\tilde{\theta}_{j,k}^{(n)}(x)\right). \tag{11}$$

Substituting Eqs. 10 and 11 into Eq. 7, and the collocation discretization scheme give a set of algebraic equations

$$\mathbb{L}u_j(x_l) = f(x_l, u_j(x_l)), l = 1, \ldots, 2^j$$

which determine the values of the coefficients $u_{j,k}$.

### 3.4 Wavelet Collocation method for the initial value problem in [0, $D$]

If $D > 1$ and is an integer, there are two schemes for the initial value problem. Consider system (7) again, and here we use the interval [0, $D$] instead of the original one [0, 1].

The first scheme is based on the one we mentioned in Sect. 3.3. The only thing to be done here is to transfer the interval, [0, $D$] into a unit interval, [0, 1], by scaling transformation. And then we can apply the method mentioned in Sect. 3.3. This is an easy way for us to apply, where we approximate the unknowns by a higher level wavelet series expansion in the interval we consider after a scaling transformation. In this case, we need to make some modifications to the original equations; actually, it is to multiply a constant from the scaling transformation, to one side of the equation. However, this may increase the stiffness in the problem we are considering.

In order to overcome this shortcoming, we would like to work out the following scheme for solving the IVP. Since $D$ is an integer, we can divide the entire interval into $D$ sub-unit intervals. In each subinterval, we approximate the unknowns by a wavelet series expansion of some level. Generally, we can get the similar accuracy solutions by a lower level wavelet expansion in this scheme. Precisely, we define the following trial functions for the second scheme for $k = 1, \ldots, 2^j D - 1$ under $j$ level wavelet approximation

$$\tilde{\theta}_{j,k}(x) = \theta_{j,k}(x), \tilde{\theta}_{j,0}(x) = \sum_{l=1-L}^{0} \theta_{j,l}(x), \tilde{\theta}_{j,2^j D}(x) = \sum_{l=2^j D}^{2^j D+L-1} \theta_{j,l}(x). \tag{12}$$

instead of that defined in Eq. 8.

If $D > 1$ is not an integer, we may convert it into an integer first by a scaling transformation, or use the the first scheme mentioned above.

In the following section, we are going to apply both schemes to the nonlinear systems we modelled in Sect. 2.

## 4 Numerical studies

### 4.1 Application to the nonisothermal batch reactor

Consider the initial value problem described by Eqs. 3 and 4 with the time interval [0, 1]. Let us set the values of the model parameters as the following for the nonisothermal batch reactor

$$\begin{aligned} &C_{A0} = 1.0,\ T_0 = 300^\circ\mathrm{K},\ E/R = 300^\circ\mathrm{K} \\ &K_1 = -0.1\,\mathrm{s}^{-1},\ K_2 = \frac{1.0^\circ\mathrm{K}}{\mathrm{gmole}-\mathrm{s}}, \end{aligned} \tag{13}$$

and take $L = 6$ and $j = 8$, then we have the numerical solutions obtained by the wavelet-collocation method (WCM) posed in Sect. 3.3, Euler method (EM) and 4th order Runge–Kutta method (RKM). The results are plotted in Fig. 1 for comparisons with the exact solution.

### 4.2 Application to the Robertson problem

In this section, we will apply the wavelet-based collocation method for numerical solving the Robertson problem. For numerical computing purpose, we set the parameters as the following values:

$$k_1 = 0.04,\ k_2 = 10^4,\ k_3 = 3 \times 10^7$$

and the initial conditions as $y_1(0) = 1,\ y_2(0) = y_3(0) = 0$.

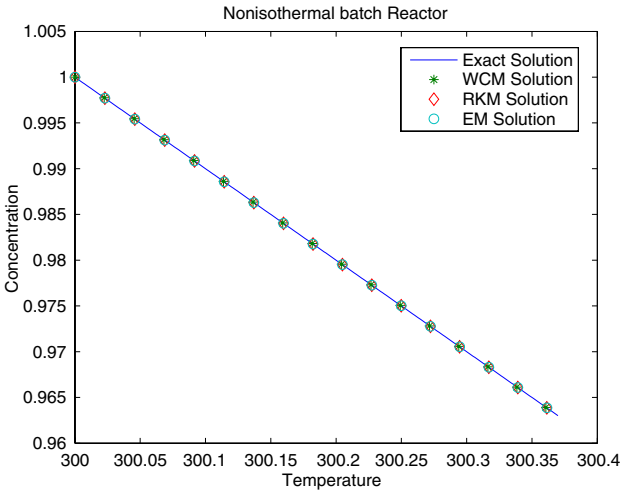


**Fig. 1** Comparisons of solutions obtained by EM, RKM and WCM

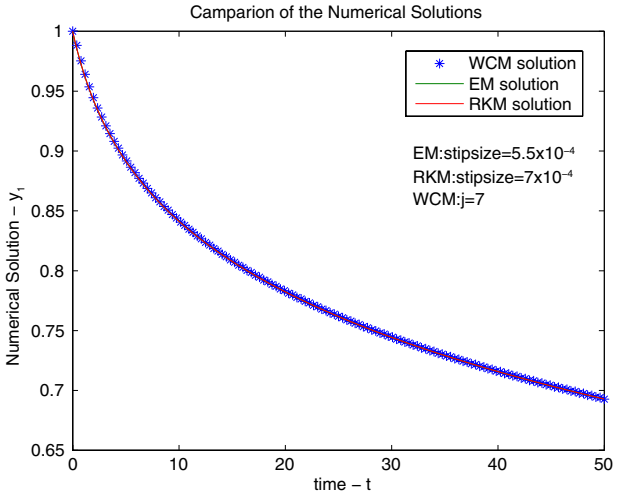


**Fig. 2** Comparison of solution $y_1$ obtained by EM, RKM and WCM

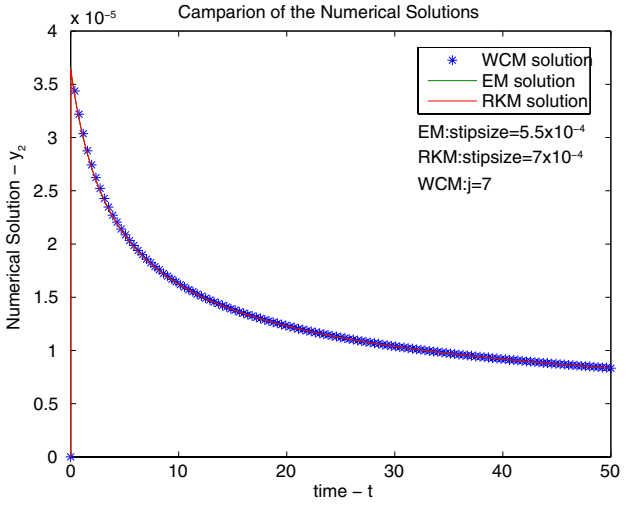


**Fig. 3** Comparison of solution $y_2$ obtained by EM, RKM and WCM

Comparisons between the Eular method (EM), Runge–Kutta method (RKM) and wavelet-collocation method (WCM) are shown in Figs. 2–4, respectively. The step-size and computing time, which is execution on a 1.80 GHz Pentium IV running Windows 2002 Professional, are shown in Table 1.

If we increase the step-sizes for Eular method or 4th Runge–Kutta method, the computing time will decrease. However, the numerical solutions will be unstable, see Figs. 5–7.

If the numerical solutions are computed based on the second scheme proposed in Sect. 3.4, we will see that the results are almost similar to those obtained by the

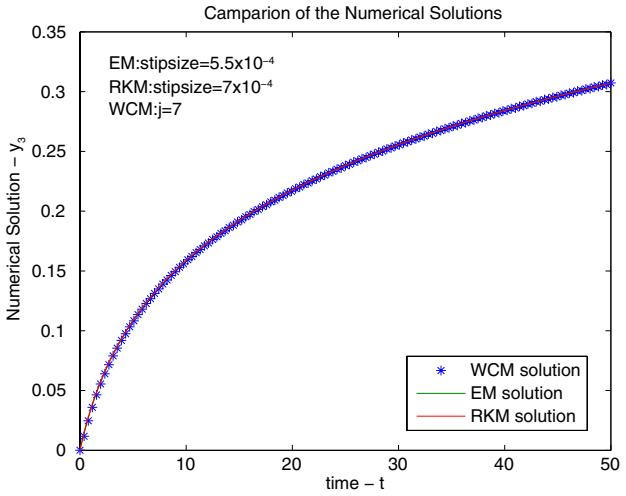


**Fig. 4** Comparison of solution $y_3$ obtained by EM, RKM and WCM

**Table 1** Comparisons of CPU time and step-size

| Method | Stepsize or level of wavelet | CUP time (s) | Results |
|---|---|---|---|
| EM | 5.5000e-04 | 460.241 | Good |
| EM | 5.7000e-04 (EM) | 461.393 | Bad |
| RKM | 7.0000e-04 (RKM) | 1634.150 | Good |
| RKM | 8.0000e-04 (RKM) | 1153.365 | Bad |
| WCM1 | $j = 7$ | 199.036 | Good |
| WCM2 | $j = 2$ | 647.161 | Good |

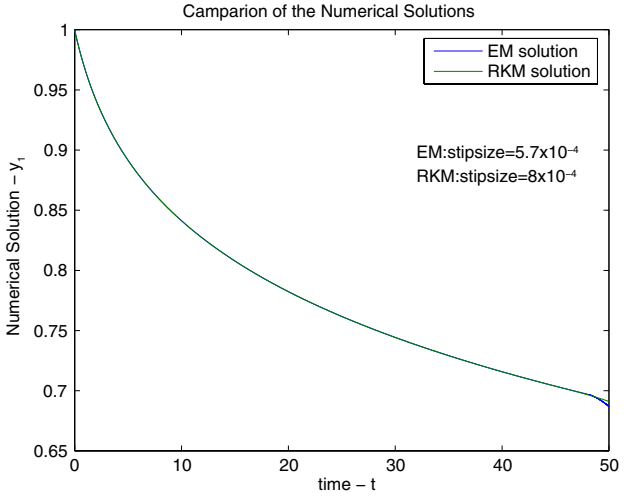


**Fig. 5** Comparison of solution $y_1$ obtained by EM and RKM

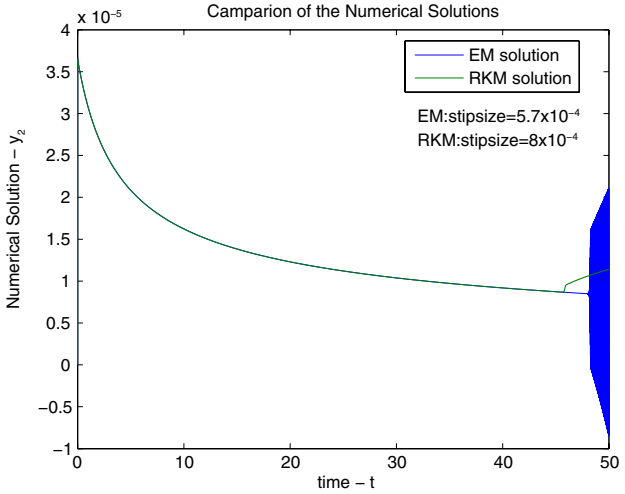


**Fig. 6** Comparison of solution $y_2$ obtained by EM and RKM

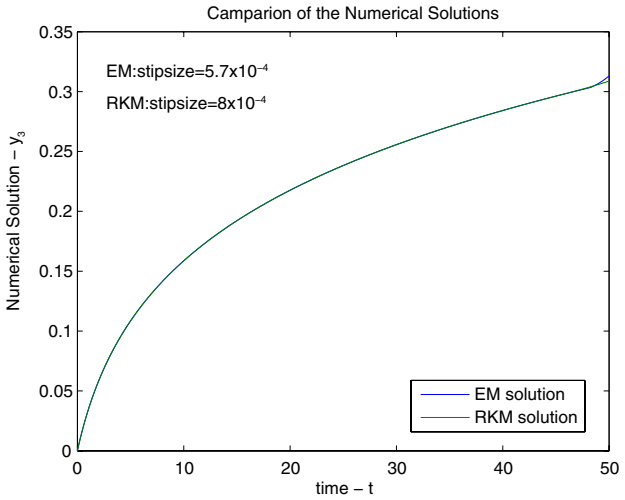


**Fig. 7** Comparison of solution $y_3$ obtained by EM and RKM

method posed in Sect. 3.3 (see Figs. 8–10), but there is a need for longer computing time (Table 1). However, the solution near the stiff part is better than the first method, see Fig. 9.

## 5 Conclusion

The main task of this paper is to develop a wavelet-based method for numerical solving the processes from the chemical engineering, which involve in the multi-equation

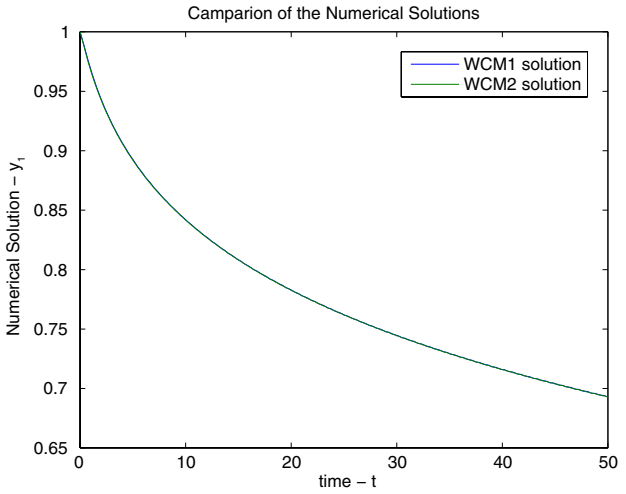


**Fig. 8** Comparison of solution $y_1$ obtained by WCM1 and WCM2

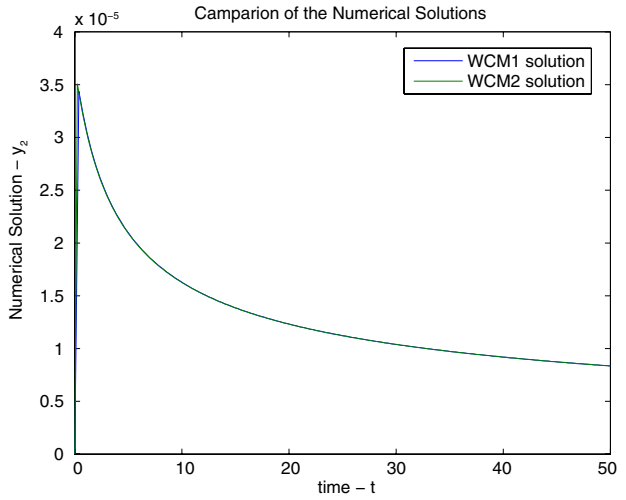


**Fig. 9** Comparison of solution $y_2$ obtained by WCM1 and WCM2

nonlinear problem with the general nonlinearity. Stable and accurate numerical results are obtained as shown from the given figures.

As mentioned in the previous sections, the Galerkin method has a better accuracy for numerically solving the differential equations. However, it is hard to be developed to deal with the nonlinear problems, especially for the problems with general nonlinearities such as the exponential function. On the contrary, it is so easy for the wavelet-based collocation method to do so.

Both the Euler method and 4th order Runge–Kutta method are the good choice for numerically solving the nonlinear system mentioned in the previous section, however,

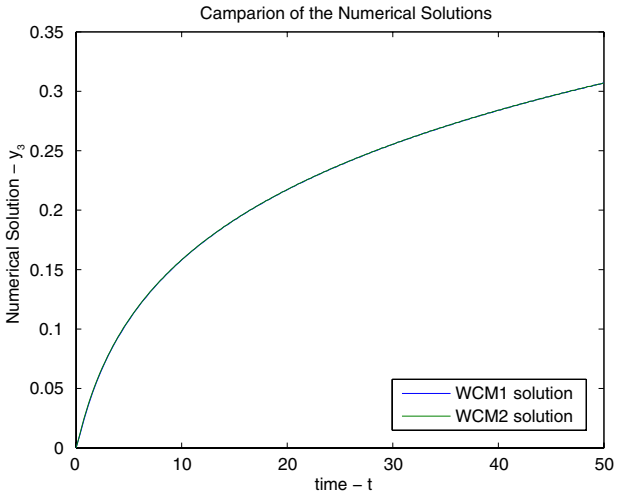


**Fig. 10** Comparison of solution $y_3$ obtained by WCM1 and WCM2

it is very necessary to reduce the step size to 0.02 s in order to get the desired accurate results since the concentration $C_A$ changes quickly during the 100 s reaction in the nonisothermal batch reactor model. In the Robert problem, the step size must be reduced to less than $5.5 \times 10^{-4}$ for Euler method and $7 \times 10^{-4}$ for Runge–Kutta method, which results in a longer computing time.

We have noticed that we can get better numerical solutions for the stiff systems. However, benefits have not been observed for using wavelet-based method for regular systems.

We have also noticed that there is a possibility to improve the accuracy of the numerical solutions by increasing the value of $j$.

Further work is continuing to demonstrate more achievements of wavelet methods for solving problems encountered in chemical/process engineering systems.

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## References

1. S. Bertoluzza, G. Naldi, A wavelet collocation method for the numerical solution of partial differential equations, Appl. Comput. Harm. Anal. **3**, 1–9 (1996)
2. M. Chen, C. Hwang, Y. Shih, The computation of wavelet-galerkin approximation on a bounded interval, Int. J. Numer. Methods Eng. **39**, 2921–2944 (1996)
3. I. Daubechies, *Ten Lectures on Wavelets* (SIAM, Philadelphia, 1992)
4. C.H. Hsiao, Haar wavelet approach to linear stiff systems, Math. Comput. Simu. **64**, 561–567 (2004)
5. Y. Liu, M.O. Tadé, New wavelet-based adaptive method for the breakage equation, Powder Technol. **139**, 61–68 (2004)
6. S.W. Ravindra, S.M. Arun, Optimal non-isothermal reactor network for Van de Vusse reaction, Int. J. Chem. React. Eng. **3**, 1–18 (2005) (http://www.bepress.com/ijcre/vol3/A3)
7. R.G. Rice, D.D. Do, Appl. Math. & Model. Chem. Eng. (John Wiley & Sons, Inc., New York, 1994)

8. J.B. Riggs, *An Introduction to Numerical Methods for Chemical Engineerings*, 2nd edn. (Texas Tech University Press, USA, 1994)
9. H.H. Robertson, *The Solution of a Set of Reaction Rate Equations* (Academic Press, 1966), pp. 178–182
10. T. Zhang, Y.-C. Tian, M.O. Tadé, J. Utomo, Comments on "The Computation of Wavelet-Galerkin Approximation on a Bounded Interval", Int. J. Numer. Meth. Eng. **72**, 244–251 (2007)