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Two Numerical Approaches for Solving Fractional Model of Chemical Kinetics Problem via Chebyshev Polynomials

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Abstract: We give two new approaches for solving the order fractional model of the Chemical Kinetics (CK). The approaches (Chebyshev collocation (CC) method and the Chebyshev Galerkin (CG) method) are constituted of the Chebyshev polynomials, Galerkin method, and the collocation method where these techniques are to convert the system of differential equations into a system of algebraic equations which can be solved easily. Also, we study the error analysis for the methods. This manuscript is expected to contribute to the vast advantage of chemical science. A complete agreement is achieved between our new methods. Moreover, We also checked the stability of the proposed methods.

Keywords: Chebyshev polynomials, fractional model of chemical kinetics problems, Galerkin method, collocation method.

1 Introduction

There are many works related to mathematical modeling in chemistry, including the chemistry problem by Abbasbandy and Shirzadi [1], CK is described by a system of nonlinear differential equations in different published works such as the chemistry problem by Jawary and Raham [2], Ganji et al. [3], Dokoumetzidis et al. [4], and Matinfar et al. [5]. In recent years, fractional calculus (FC) has gained significant traction and found numerous versatile and robust applications across a range of research domains, including fluid dynamics, viscoelasticity, image processing, as well as modeling and prediction of phenomena like covid-19 (as cited in references [6] and [7]) and cancer (as cited in [8]). Several mathematicians have proposed various definitions of fractional derivatives (as mentioned in references [9] and [10]), but the two most renowned ones are the Caputo and Riemann-Liouville definitions. Many noteworthy and foundational contributions to the field of FC can be found in well-known books, such as those authored by Mainardi [11], Podlubny (in "Fractional Differential Equations" [12]), and Diethelm [13]. Additionally, the study of control theory for fractional linear systems has been explored from different angles, including research on systems with conformable fractional derivatives [14], fractal linear systems [15], and fractional linear systems in infinite-dimensional spaces [16].

In recent years, Chebyshev polynomials have gained prominence and seen extensive development in various research fields, including the physical and chemical sciences, computational sciences, image manipulation, signal analysis, data compression, and numerical analysis. They have found utility in a multitude of research applications, exemplified by works such as the solution of the non-linear one-dimensional Burgers' equation using sixth-order Chebyshev polynomials by Abd-Elhameed et al. [17], the robust spectral treatment of a class of initial value problems as presented by Youssri et al. [18], the utilization of spectral solutions for linear and nonlinear boundary value problems by Abd-Elhameed et al. [19], and the application of high-order derivatives of fifth-kind Chebyshev polynomials for solving convection-diffusion equations, again by Abd-Elhameed et al. [20], Bernstein polynomials [21], Mittag-Leffler polynomials [22] and other business [23,24,25,26,27,28]. There are other numerical methods, including Fractional BDF Methods [29], Krylov subspaces for differential matrix equation of large-scale [30,31,32], Jacobi Elliptical Function

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Method [33] and the shifted Jacobi collocation techniques [34]. It is compulsory to note that the fractional chemical kinetics problem is the first one to be solved by the CC method and CG method.

The complete paper is systematized in the following sections: An overview of basic FC is provided in section 2. The order fractional Model of both CK is provided in section 3. In sections 4 and 5, CC and CG methods are discussed and presented for both chemistry models. In Section 6, we present the estimate of the error. Numerical experiments are provided in section 7.

2 Overview of FC

In this section, we will provide essential definitions in the field of FC. It's worth noting that there exists a variety of definitions for both derivatives and integrals in the existing body of literature, as referenced by the following works: [35, 36,37,38,39].

Definition 1.*The fractional integral of order* $\nu > 0$ *of a function* Θ *can be defined as:*

$$I^{\nu}\Theta(t) = \frac{1}{\Gamma(\nu)}\int_0^t \frac{\Theta(s)}{(t-s)^{1-\nu}}ds,$$

with

$$\Gamma(\nu) = \int_0^{\infty} \mu^{\nu-1}e^{-\mu}\,d\mu, \qquad \Re(\nu) > 0.$$

Definition 2.*The Caputo fractional derivative of order* $\nu \in]0,1]$ *of a function* Θ *can be written as:*

$$D^{\nu}\Theta(t) = \frac{1}{\Gamma(1-\nu)}\int_0^t \frac{\Theta^{'}(s)}{(t-s)^{\nu}}ds.$$

3 Fractional model of CK problem

In this section, we present the order fractional model of the CK problem. Assuming that $\mathbb{D},\mathbb{E}$, and $\mathbb{H}$ represent distinct locations within a chemical process model, we proceed to describe the reactions as follows:

$$\mathbb{D} \longrightarrow \mathbb{E}, \tag{1}$$

$$\mathbb{E}+\mathbb{H} \longrightarrow \mathbb{D}+\mathbb{H}, \tag{2}$$

$$\mathbb{E}+\mathbb{E} \longrightarrow \mathbb{H}. \tag{3}$$

The concentrations within the three spaces represented by $\mathbb{D},\mathbb{E}$, and $\mathbb{H}$ are symbolized as Θ_1,Θ_2, and Θ_3, respectively. Additionally, the reaction rates for Equations (1), (2), and (3) are denoted as r_1,r_2, and r_3, respectively. We will examine an integer-order model for the chemical kinetics problem, as referenced in previous works [2,1,40,5,3].

$$\begin{cases} \frac{d\Theta_1(t)}{dt} = -r_1\Theta_1(t) + r_2\Theta_2(t)\Theta_3(t), \\ \frac{d\Theta_2(t)}{dt} = r_1\Theta_1(t) - r_2\Theta_2(t)\Theta_3(t) - r_3\Theta_2^2(t), \\ \frac{d\Theta_3(t)}{dt} = r_3\Theta_2^2(t), \end{cases} \tag{4}$$

where the initial condition $(\Theta_1(0),\Theta_2(0),\Theta_3(0)) = (1,0,0)$. The main target of this section is to convert the integer order CK problem into a fractional order CK. The order fractional model of the CK is presented as

$$\begin{cases} {}^cD_t^{\nu_1}\Theta_1(t) = -r_1\Theta_1(t) + r_2\Theta_2(t)\Theta_3(t), \\ {}^cD_t^{\nu_2}\Theta_2(t) = r_1\Theta_1(t) - r_2\Theta_2(t)\Theta_3(t) - r_3\Theta_2^2(t), \\ {}^cD_t^{\nu_3}\Theta_3(t) = r_3\Theta_2^2(t), \end{cases} \tag{5}$$

where, $D_t^{\nu_1} = \frac{d^{\nu_1}}{dt^{\nu_1}}, D_t^{\nu_2} = \frac{d^{\nu_2}}{dt^{\nu_2}}, D_t^{\nu_3} = \frac{d^{\nu_3}}{dt^{\nu_3}}$ are fractional derivative with $0 < \nu_1,\nu_2,\nu_3 \leq 1$. If $r_1 = 1, r_2 = 0$, and $r_3 = 1$ then

$$\begin{cases} {}^cD_t^{\nu_1}\Theta_1(t) = -\Theta_1(t), \\ {}^cD_t^{\nu_2}\Theta_2(t) = \Theta_1(t) - \Theta_2^2(t), \\ {}^CD_t^{\nu_3}\Theta_3(t) = \Theta_2^2(t). \end{cases} \tag{6}$$

The above system represents a nonlinear reaction that was taken from literature [1,5,3].

4 The first approach: CC method

In this section, the Chebyshev polynomials are defined by recurrence formulae on the interval $[-1,1]$ as follows

$$CP_0(t)=1,\quad CP_1(t)=t,\quad CP_{i+1}(t)=2tCP_i(t)-CP_{i-1}(t),\quad i=1,2,3,\ldots,$$

and the collocation nodes used in this paper are the roots of Chebyshev polynomials:

$$t_i=\frac{1}{2}(1+\cos\left(\frac{(2i+1)\pi}{2N}\right)),\ i=0,1,\ldots,N-1.$$

Now, assume that the approximate solution of the Eq. (4) in the form:

$$\Theta_{j,N}(t)=\sum_{i=0}^{N}c_{j,i}CP_i(t), \tag{7}$$

For (4), we get the residuals $\Re_{j,N}(t)$, $j=\{1,2,3\}$ defined:

$$\begin{cases}\Re_{1,N}(t)={}^cD_t^{\nu_1}\Theta_{1,N}(t)+r_1\Theta_{1,N}(t)-r_2\Theta_{2,N}(t)\Theta_{3,N}(t),\\ \Re_{2,N}(t)={}^cD_t^{\nu_2}\Theta_{2,N}(t)-r_1\Theta_{1,N}(t)+r_2\Theta_{2,N}(t)\Theta_{3,N}(t)+r_3\Theta_{2,N}^2(t),\\ \Re_{3,N}(t)={}^cD_t^{\nu_3}\Theta_{3,N}(t)-r_3\Theta_{2,N}^2(t),\end{cases} \tag{8}$$

from the initial conditions, we have

$$\Theta_{1,N}(0)=1,\ \ \Theta_{2,N}(0)=0,\ \ \Theta_{3,N}(0)=0, \tag{9}$$

and by inserting the nodes into the (8) such that

$$\Re_{j,N}(t_i)=0,\quad i=1,\ldots,N. \tag{10}$$

Solving these equations (9) and (10) yields the coefficients $c_{j,0},c_{j,1},\ldots,c_{j,N}$. Thus, $\Theta_{j,N}(t)$ given in (7) are founded.

5 A second approach: CG method

In this section, we present new second approach for solving the chemistry fractional problems (4). The philosophy in applying the CG method is to find $\Theta_{j,N}$ such that

$$\int_0^1\Re_{j,N}(t)CP_i(t)\,\mathrm{d}t=0,\quad i=0,\ldots,N-1. \tag{11}$$

Eq. (11) with (9) generate $N+1$ sets of equations. Solving these equations gives the unknown coefficients $c_{j,0},c_{j,1},\ldots,c_{j,N}$. Consequently, $\Theta_{j,N}$ given in Eq. (7) can be calculated. Thus, the CG method is obtained.

6 Estimate error

In this section, we study the estimate error.

Theorem 1. *Let $\Theta_j(t)$ be the exact solution of (4) and let $\Theta_{j,N}(t)$ be the approximate solution. The error $e_{j,N}(t)=\Theta_j(t)-\Theta_{j,N}(t)$ satisfies the following equation*

$$\begin{cases}{}^cD_t^{\nu_1}e_{1,N}(t)=-r_1e_{1,N}(t)+r_2e_{2,N}(t)e_{3,N}(t)+r_2\Theta_{2,N}(t)e_{3,N}(t)+r_2\Theta_{2,N}(t)\Theta_{3,N}(t)-\Re_{1,N}(t),\\ {}^cD_t^{\nu_2}e_{2,N}(t)=r_1e_{1,N}(t)-r_2e_{2,N}(t)e_{3,N}(t)-r_2e_{2,N}(t)\Theta_{3,N}(t)-r_2\Theta_{2,N}(t)e_{3,N}(t)-r_3e_{3,N}(t)^2\\ \qquad\qquad -2r_3e_{3,N}(t)\Theta_{3,N}(t)-\Re_{2,N}(t),\\ {}^cD_t^{\nu_3}e_{3,N}(t)=r_3e_{2,N}(t)^2+2r_3e_{2,N}(t)\Theta_{2,N}(t)-\Re_{3,N}(t),\\ e_{1,N}(0)=\quad 1-\Theta_{1,N}(0),\ \ e_{2,N}(0)=-\Theta_{2,N}(0),\ \ e_{3,N}(0)=-\Theta_{3,N}(0).\end{cases} \tag{12}$$

*Proof.*We have

$$\begin{cases} \Re_{1,N}(t) = {}^cD_t^{\nu_1}\Theta_{1,N}(t) + r_1\Theta_{1,N}(t) - r_2\Theta_{2,N}(t)\Theta_{3,N}(t), \\ \Re_{2,N}(t) = {}^cD_t^{\nu_2}\Theta_{2,N}(t) - r_1\Theta_{1,N}(t) + r_2\Theta_{2,N}(t)\Theta_{3,N}(t) + r_3\Theta_{2,N}^2(t), \\ \Re_{3,N}(t) = {}^cD_t^{\nu_3}\Theta_{3,N}(t) - r_3\Theta_{2,N}^2(t), \end{cases}$$

and

$$\begin{cases} {}^cD_t^{\nu_1}\Theta_1(t) = -r_1\Theta_1(t) + r_2\Theta_2(t)\Theta_3(t), \\ {}^cD_t^{\nu_2}\Theta_2(t) = r_1\Theta_1(t) - r_2\Theta_2(t)\Theta_3(t) - r_3\Theta_2^2(t), \\ {}^cD_t^{\nu_3}\Theta_3(t) = r_3\Theta_2^2(t), \end{cases}$$

then

$$\begin{aligned} {}^cD_t^{\nu_1}e_{1,N}(t) &= {}^cD_t^{\nu_1}(\Theta_1(t) - \Theta_{1,N}(t)) \\ &= -r_1\Theta_1(t) + r_2\Theta_2(t)\Theta_3(t) + r_1\Theta_{1,N}(t) - r_2\Theta_{2,N}(t)\Theta_{3,N}(t) - \Re_{1,N}(t) \\ &= -r_1(e_{1,N}(t) + \Theta_{1,N}(t)) + r_2(e_{2,N}(t) + \Theta_{2,N}(t))(e_{3,N}(t) + \Theta_{3,N}(t)) + r_1\Theta_{1,N}(t) \\ &\quad -r_2\Theta_{2,N}(t)\Theta_{3,N}(t) - \Re_{1,N}(t) \\ &= -r_1e_{1,N}(t) + r_2(e_{2,N}(t)e_{3,N}(t) + e_{2,N}(t)\Theta_{3,N}(t) + \Theta_{2,N}(t)e_{3,N}(t) + \Theta_{2,N}(t)\Theta_{3,N}(t)) \\ &\quad -r_2\Theta_{2,N}(t)\Theta_{3,N}(t) - \Re_{1,N}(t) \\ &= -r_1e_{1,N}(t) + r_2e_{2,N}(t)e_{3,N}(t) + r_2\Theta_{2,N}(t)e_{3,N}(t) + r_2\Theta_{2,N}(t)\Theta_{3,N}(t) - \Re_{1,N}(t). \end{aligned}$$

and

$$\begin{aligned} {}^cD_t^{\nu_2}e_{2,N}(t) &= {}^cD_t^{\nu_2}(\Theta_2(t) - \Theta_{2,N}(t)) \\ &= r_1\Theta_1(t) - r_2\Theta_2(t)\Theta_3(t) - r_3\Theta_2^2(t) - r_1\Theta_{1,N}(t) + r_2\Theta_{2,N}(t)\Theta_{3,N}(t) + r_3\Theta_{2,N}^2(t) - \Re_{2,N}(t) \\ &= r_1(e_{1,N}(t) + \Theta_{1,N}(t)) - r_2(e_{2,N}(t) + \Theta_{2,N}(t))(e_{3,N}(t) + \Theta_{3,N}(t)) - r_3(e_{3,N}(t) + \Theta_{3,N}(t))^2 \\ &\quad -r_1\Theta_{1,N}(t) + r_2\Theta_{2,N}(t)\Theta_{3,N}(t) + r_3\Theta_{2,N}^2(t) - \Re_{2,N}(t) \\ &= r_1e_{1,N}(t) - r_2(e_{2,N}(t)e_{3,N}(t) + e_{2,N}(t)\Theta_{3,N}(t) + \Theta_{2,N}(t)e_{3,N}(t) + \Theta_{2,N}(t)\Theta_{3,N}(t)) \\ &\quad -r_3(e_{3,N}(t)^2 + 2e_{3,N}(t)\Theta_{3,N}(t) + \Theta_{3,N}(t)^2) + r_2\Theta_{2,N}(t)\Theta_{3,N}(t) + r_3\Theta_{2,N}^2(t) - \Re_{2,N}(t) \\ &= r_1e_{1,N}(t) - r_2(e_{2,N}(t)e_{3,N}(t) + e_{2,N}(t)\Theta_{3,N}(t) + \Theta_{2,N}(t)e_{3,N}(t)) \\ &\quad -r_3(e_{3,N}(t)^2 + 2e_{3,N}(t)\Theta_{3,N}(t)) - \Re_{2,N}(t) \\ &= r_1e_{1,N}(t) - r_2e_{2,N}(t)e_{3,N}(t) - r_2e_{2,N}(t)\Theta_{3,N}(t) - r_2\Theta_{2,N}(t)e_{3,N}(t) \\ &\quad -r_3e_{3,N}(t)^2 - 2r_3e_{3,N}(t)\Theta_{3,N}(t) - \Re_{2,N}(t), \end{aligned}$$

and

$$\begin{aligned} {}^cD_t^{\nu_3}e_{3,N}(t) &= {}^cD_t^{\nu_3}(\Theta_3(t) - \Theta_{3,N}(t)) \\ &= r_3\Theta_2^2(t) - r_3\Theta_{2,N}^2(t) - \Re_{2,N}(t) \\ &= r_3(e_{2,N}(t) + \Theta_{2,N}(t))^2 - r_3\Theta_{2,N}^2(t) - \Re_{2,N}(t) \\ &= r_3(e_{2,N}(t)^2 + 2e_{2,N}(t)\Theta_{2,N}(t) + \Theta_{2,N}(t)^2) - r_3\Theta_{2,N}^2(t) - \Re_{2,N}(t) \\ &= r_3e_{2,N}(t)^2 + 2r_3e_{2,N}(t)\Theta_{2,N}(t) - \Re_{2,N}(t). \end{aligned}$$

By solving the Eq. (12) in the same way as Section 4 or Section 5, we get the approximation

$$e_{j,N,M}(t) = \sum_{i=0}^{M} c_{j,i}^e CP_i(t),$$

with the coefficients $c_{j,i}^e, i = 0, 1, 2, \ldots, M$ are determined by solving the error problem (12).

The importance of the theorems 1 is to use this error estimation to test the reliability of the results.

7 Numerical experiments

In this section, we showcase a series of numerical experiments aimed at elucidating the two methodologies and highlighting their effectiveness. These experiments were conducted on a laptop equipped with an Intel Core i3 processor

and 4GB of RAM, utilizing the Maple software. Our analysis is based on a fractional model of the chemical kinetics problem, with the initial condition $(\Theta_1(0),\Theta_2(0),\Theta_3(0)) = (1,0,0)$ with r_1, r_2 and r_3 are reaction rates. Let $r_1 = 0.1, r_2 = 0.02$ and $r_3 = 0.009$ as given in Aminikhah [41]. If we apply the Chebyshev Galerkin method for solving the above problem with $N = 4$, $\nu_1 = \nu_2 = \nu_3 = 1$ then the approximate solution of $\Theta_{j,4}(t)$, $j = 1,2,3$ may be written as:

$$\begin{cases} \Theta_{1,4}(t) = 0.9999999995 - 0.1000832497t + 0.005002936939t^2 - 0.00008325522424t(2t^2-1) \\ \qquad +9.96685157610^{-7}t(2t(2t^2-1)-t), \\ \Theta_{2,4}(t) = 3.13010^{-13} + 0.1000683538t - 0.005001485605t^2 + 0.00006835249296t(2t^2-1) \\ \qquad -4.90977374010^{-7}t(2t(2t^2-1)-t), \\ \Theta_{3,4}(t) = -1.10^{-16} + 0.00001489891712t - 0.000001456162535t^2 + 0.00001490516004t(2t^2-1) \\ \qquad -5.06296626610^{-7}t(2t(2t^2-1)-t). \end{cases} \tag{13}$$

If we apply the Chebyshev Collocation method for solving the above problem with $N = 4$, $\nu_1 = \nu_2 = \nu_3 = 1$, then the approximate solution of $\Theta_{j,4}(t)$, $j = 1,2,3$ may be written as:

$$\begin{cases} \Theta_{1,4}(t) = 1.000000000 - 0.1000832566t + 0.005002947148t^2 - 0.00008325926356t(2t^2-1) \\ \qquad +9.97151516810^{-7}t(2t(2t^2-1)-t), \\ \Theta_{2,4}(t) = -3.66610^{-13} + 0.1000683525t - 0.005001483687t^2 + 0.00006835179030t(2t^2-1) \\ \qquad -4.90920733210^{-7}t(2t(2t^2-1)-t), \\ \Theta_{3,4}(t) = 0.00001490419378t - 0.000001463713148t^2 + 0.00001490763382t(2t^2-1) \\ \qquad -5.06270969810^{-7}t(2t(2t^2-1)-t). \end{cases} \tag{14}$$

From the Eq.(12) with $N = 4$, we construct the error equation

$$\begin{cases} {}^cD_t^{\nu_1} e_{1,4}(t) = -r_1 e_{1,4}(t) + r_2 e_{2,4}(t)e_{3,4}(t) + r_2\Theta_{2,4}(t)e_{3,4}(t) + r_2\Theta_{2,4}(t)\Theta_{3,4}(t) - \Re_{1,4}(t), \\ {}^cD_t^{\nu_2} e_{2,4}(t) = r_1 e_{1,4}(t) - r_2 e_{2,4}(t)e_{3,4}(t) - r_2 e_{2,4}(t)\Theta_{3,4}(t) - r_2\Theta_{2,4}(t)e_{3,4}(t) - r_3 e_{3,4}(t)^2 \\ \qquad -2r_3 e_{3,4}(t)\Theta_{3,4}(t) - \Re_{2,4}(t), \\ {}^cD_t^{\nu_3} e_{3,4}(t) = r_3 e_{2,4}(t)^2 + 2r_3 e_{2,4}(t)\Theta_{2,4}(t) - \Re_{3,4}(t), \\ e_{1,4}(0) = \quad 1 - \Theta_{1,4}(0), \;\; e_{2,4}(0) = -\Theta_{2,4}(0), \;\; e_{3,4}(0) = -\Theta_{3,4}(0). \end{cases} \tag{15}$$

where

$$\begin{aligned}\Re_{1,4}(t) = {} & 2.66\times10^{-9}-0.00000342851t+7.391334\times10^{-7}t^2-0.000006331623322t(2t^2-1)\\ & +9.971515168\times10^{-7}t(12t^2-3)+9.971515168\times10^{-8}t(2t(2t^2-1)-t)\\ & -0.02(-3.666000000\times10^{-13}+0.1000683525t-0.005001483687t^2\\ & +0.00006835179030t(2t^2-1)-4.909207332\times10^{(}-7)t(2t(2t^2-1)-t))\\ & (0.00001490419378t-0.000001463713148t^2+0.00001490763382t(2t^2-1)\\ & -5.062709698\times10^{(}-7)t(2t(2t^2-1)-t)),\end{aligned}$$

$$\begin{aligned}\Re_{2,4}(t) = {} & 7.10^{-10}+0.00000584921t-0.0000901839730t^2+0.000007344084890t(2t^2-1)\\ & -4.909207332\times10^{-7}t(12t^2-3)-9.971515168\times10^{-8}t(2t(2t^2-1)-t)\\ & +0.02(-3.666000000\times10^{-13}+0.1000683525t-0.005001483687t^2\\ & +0.00006835179030t(2t^2-1)-4.909207332\times10^{-7}t(2t(2t^2-1)-t))\\ & (0.00001490419378t-0.000001463713148t^2+0.00001490763382t(2t^2-1)\\ & -5.062709698\times10^{-7}t(2t(2t^2-1)-t))+0.009(-3.666000000\times10^{-13}+0.1000683525t\\ & -0.005001483687t^2+0.00006835179030t(2t^2-1)-4.90920733210^{-7}t(2t(2t^2-1)-t))^2,\end{aligned}$$

$$\begin{aligned}\Re_{3,4}(t) = {} & -3.44004\times10^{-9}-0.000002421155326t+0.00008944580292t^2\\ & -0.000001012541940t(2t^2-1)-5.062709698\times10^{(}-7)t(12t^2-3)\\ & -0.009(-3.666000000\times10^{-13}+0.1000683525t-0.005001483687t^2\\ & +0.00006835179030t(2t^2-1)-4.90920733210^{-7}t(2t(2t^2-1)-t))^2.\end{aligned}$$

We solve the Eq. (15) for the truncated limited $M=5$ by CC method and we obtain the approximation

$$\begin{aligned}e_{1,4,5}(t) = {} & -2\times10^{-17}-1.033126567\times10^{-7}t+1.775594094\times10^{-7}t^2\\ & -1.09546691510^{-7}t(2t^2-1)+4.443094862\times10^{-8}t(2t(2t^2-1)-t)\\ & -8.89253842610^{-9}t(2t(2t(2t^2-1)-t)-2t^2+1),\end{aligned}$$

$$\begin{aligned}e_{2,4,5}(t) = {} & 3.66602\times10^{-13}-2.305139230\times10^{-8}t+3.954844426\times10^{-8}t^2\\ & -2.430792251\times10^{-8}t(2t^2-1)+9.773478744\times10^{-9}t(2t(2t^2-1)-t)\\ & -1.928743091\times10^{-9}t(2t(2t(2t^2-1)-t)-2t^2+1),\end{aligned}$$

$$\begin{aligned}e_{3,4,5}(t) = {} & 3\times10^{-17}+1.262833684\times10^{-7}t-2.168598161\times10^{-7}t^2\\ & +1.336938814\times10^{-7}t(2t^2-1)-5.416416654\times10^{-8}t(2t(2t^2-1)-t)\\ & +1.082126714\times10^{-8}t(2t(2t(2t^2-1)-t)-2t^2+1).\end{aligned}$$

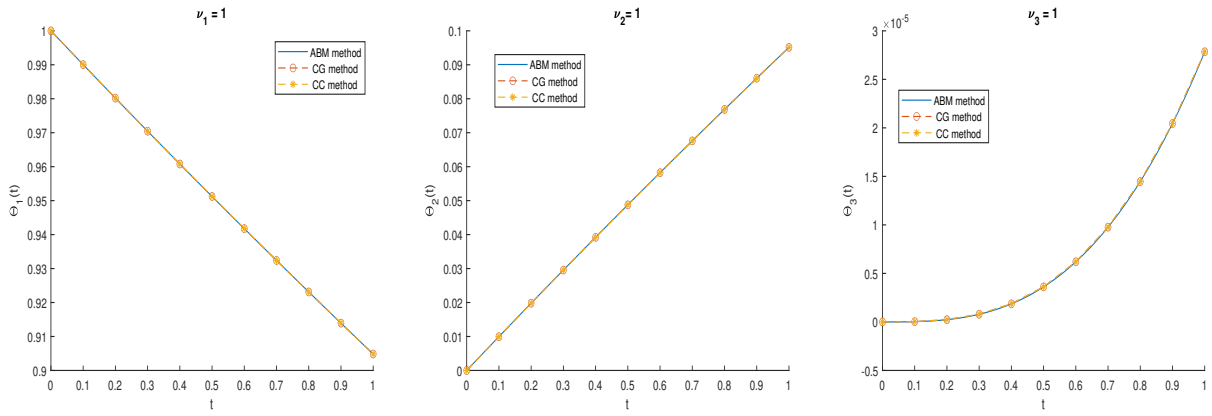

Fig. 1: Plot of comparison between CC method, CG method, and ABM solutions for $\nu_1 = \nu_2 = \nu_3 = 1$.

and by the CG method, we obtain the approximation

$$\begin{aligned} e_{1,4,5}(t) = & -2\times 10^{-17} - 1.033126567\times 10^{-7}t + 1.775594094\times 10^{-7}t^2 \\ & -1.095466915\times 10^{-7}t(2t^2-1) + 4.443094862\times 10^{-8}t(2t(2t^2-1)-t) \\ & -8.892538426\times 10^{-9}t(2t(2t(2t^2-1)-t)-2t^2+1), \end{aligned}$$

$$\begin{aligned} e_{2,4,5}(t) = & \ 3.66602\times 10^{-13} - 2.305139230\times 10^{-8}t + 3.954844426\times 10^{-8}t^2 \\ & -2.430792251\times 10^{-8}t(2t^2-1) + 9.773478744\times 10^{-9}t(2t(2t^2-1)-t) \\ & -1.928743091\times 10^{-9}t(2t(2t(2t^2-1)-t)-2t^2+1), \end{aligned}$$

$$\begin{aligned} e_{3,4,5}(t) = & \ 3\times 10^{-17} + 1.262833684\times 10^{-7}t - 2.168598161\times 10^{-7}t^2 \\ & +1.336938814\times 10^{-7}t(2t^2-1) - 5.416416654\times 10^{-8}t(2t(2t^2-1)-t) \\ & +1.082126714\times 10^{-8}t(2t(2t(2t^2-1)-t)-2t^2+1). \end{aligned}$$

Figure 1, Plot of comparison between Chebyshev Galerkin method, Chebyshev Collocation method, and ABM [42] for $\nu_1 = \nu_2 = \nu_3 = 1$. We have depicted a comparison between numerically obtained solutions using by Chebyshev Galerkin method, Chebyshev Collocation method, and ABM schemes for the values of $N = 4$. It is clear from all figures that both obtained solutions by our methods and ABM are identical. Figure 2, the absolute error and estimation of absolute error. Table 1 compares the obtained approximate solution at $\nu_1 = \nu_2 = \nu_3 = 1$ where $N = 4$ and the method in [43] with $N = 64$. Figure 3, Plot of comparison between Chebyshev Galerkin method, Chebyshev Collocation method, and ABM solutions for $\nu_1 = \nu_2 = \nu_3 = \{0.89, 0.9\}1$ for the values of $N = 4$. It is clear from all figures that both obtained solutions by our methods and ABM are identical. Table 2 compares the obtained approximate solution at $\nu_1 = \nu_2 = \nu_3 = 0.89$ where $N = 4$ with ABM. Table 3 compares the obtained approximate solution at $\nu_1 = \nu_2 = \nu_3 = 0.9$ where $N = 4$ with ABM. Figure 4, Plot of comparison between Chebyshev Galerkin method and Chebyshev Collocation method for $\nu_1 = 0.7, \nu_2 = 0.8, \nu_3 = 0.9$. We have depicted a comparison between numerical obtained solutions using by Chebyshev Galerkin method, and the Chebyshev Collocation method for the values of $N = 4$. Figure 5, Plot of comparison between Chebyshev Galerkin method and Chebyshev Collocation method for $\nu_1 = 0.7, \nu_2 = 0.8, \nu_3 = 0.9$. We have depicted a comparison between numerical obtained solutions using by Chebyshev Galerkin method, and the Chebyshev Collocation method for the values of $N = 6$.

*Remark.*To check the stability of the proposed two methods, we introduce the small perturbation $\Theta_j^p(t) = (1-\varepsilon)\Theta_j(t)$ and impose it upon problems Eq. (4) with $\nu_1 = \nu_2 = \nu_3 = \{0.89, 0.9, 1\}$ and $N = 4$. Then, the resulting perturbed problems are solved using the proposed two methods to evaluate the perturbation solution $\Theta_{j,N}^p(t)$. In Table 4, we list the max absolute errors of the perturbed problems defined by

$$\max_{0\le t\le 1} |\Theta_j^{ABM}(t) - \Theta_{j,N}^p(t)|,$$

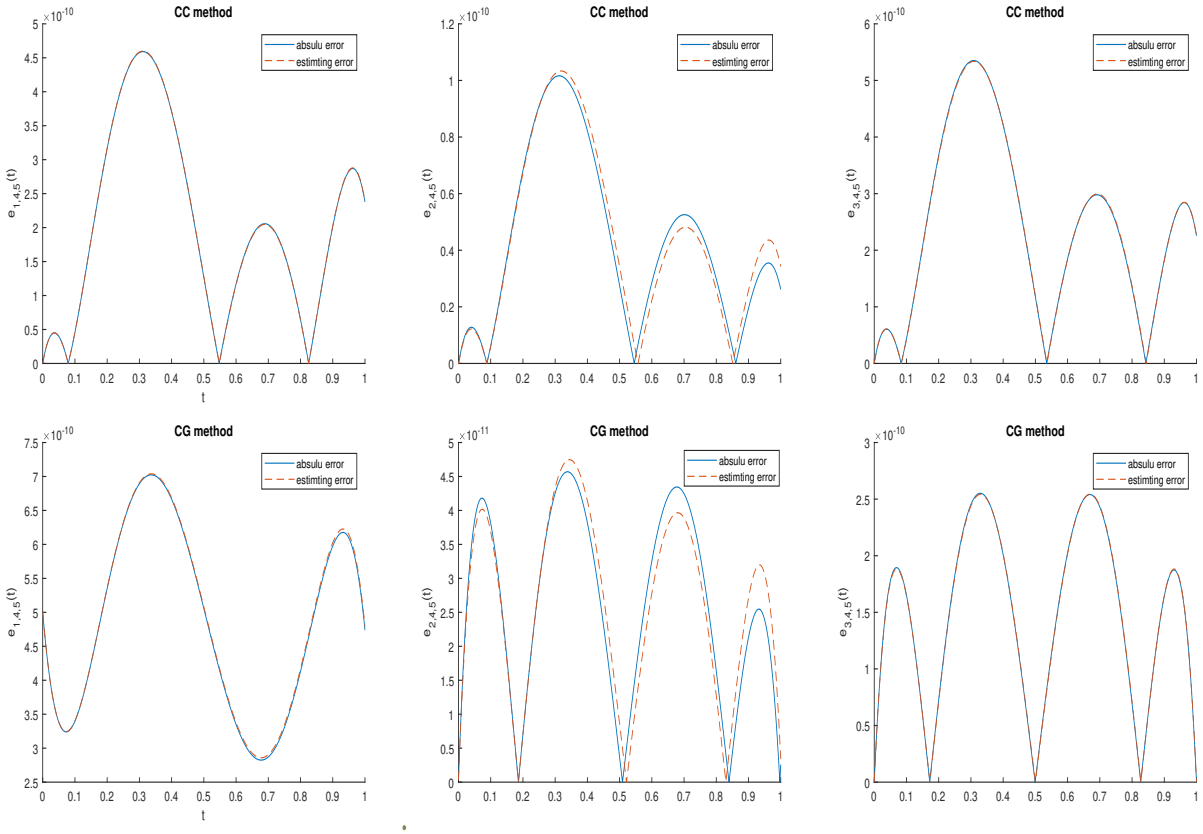

Fig. 2: The absolute error and estimation of absolute error for $(N,M) = (4,5)$.

	$\Theta_1(t)$				$\Theta_2(t)$			
t	ABM	Method [43]	CC	CG	ABM	Method [43]	CC	CG
0.1	0.9900	0.9901	0.9900	0.9900	0.0100	0.0100	0.0100	0.0100
0.2	0.9802	0.9802	0.9802	0.9802	0.0198	0.0198	0.0198	0.0198
0.3	0.9704	0.9704	0.9704	0.9704	0.0296	0.0296	0.0296	0.0296
0.4	0.9608	0.9608	0.9608	0.9608	0.0392	0.0393	0.0392	0.0392
0.5	0.9512	0.9512	0.9512	0.9512	0.0488	0.0489	0.0488	0.0488
0.6	0.9418	0.9418	0.9418	0.9418	0.0582	0.0585	0.0582	0.0582
0.7	0.9324	0.9324	0.9324	0.9324	0.0676	0.0680	0.0676	0.0676
0.8	0.9231	0.9231	0.9231	0.9231	0.0769	0.0775	0.0769	0.0769
0.9	0.9139	0.9139	0.9139	0.9139	0.0860	0.0869	0.0860	0.0860
1.0	0.9048	0.9048	0.9048	0.9048	0.0951	0.0963	0.0951	0.0951

	$\Theta_3(t)$			
t	ABM	Method [43]	CC	CG
0.1	$2.9776e-08$	$3.0e-8$	$2.9820e-08$	$2.9611e-08$
0.2	$2.3643e-07$	$2.4e-7$	$2.3680e-07$	$2.3650e-07$
0.3	$7.9200e-07$	$7.9e-7$	$7.9254e-07$	$7.9225e-07$
0.4	$1.8634e-06$	$1.8e-6$	$1.8638e-06$	$1.8636e-06$
0.5	$3.6123e-06$	$3.6e-6$	$3.6124e-06$	$3.6123e-06$
0.6	$6.1956e-06$	$6.2e-6$	$6.1954e-06$	$6.1954e-06$
0.7	$9.7653e-06$	$9.8e-6$	$9.7650e-06$	$9.7651e-06$
0.8	$1.4469e-05$	$1.5e-5$	$1.4468e-05$	$1.4469e-05$
0.9	$2.0448e-05$	$2.0e-5$	$2.0448e-05$	$2.0448e-05$
1.0	$2.7842e-05$	$2.8e-5$	$2.7842e-05$	$2.7842e-05$

Table 1: Comparison of the approximate solutions using the two proposed methods versus the method in [43] with $\nu_1 = \nu_2 = \nu_3 = 1$.

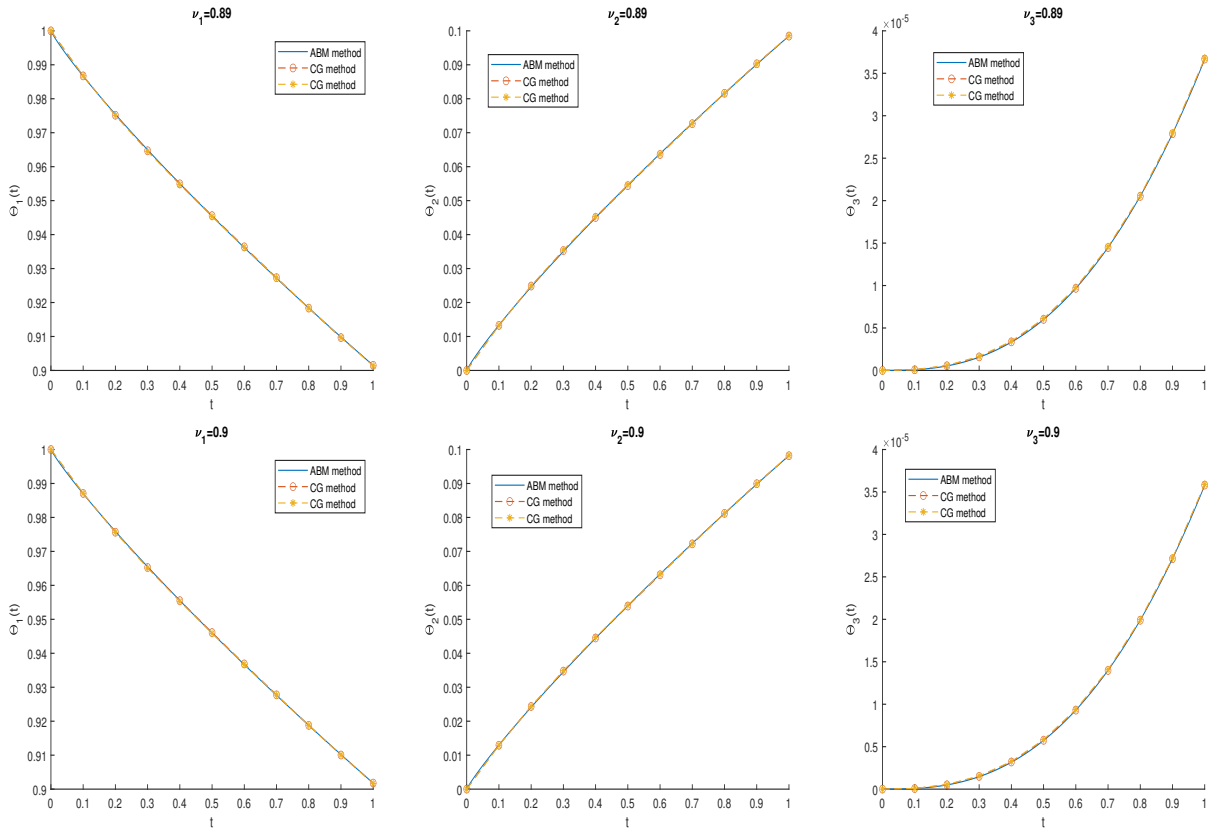

Fig. 3: Plot of comparison between CC method, CG method, and ABM solutions for $\nu_1 = \nu_2 = \nu_3$.

	$\Theta_1(t)$			$\Theta_2(t)$			$\Theta_3(t)$		
t	ABM	CC	CG	ABM	CC	CG	ABM	CC	CG
0.1	0.9867	0.9868	0.9895	0.0133	0.0132	0.0105	$8.4760e-08$	$8.8754e-08$	$3.4552e-08$
0.2	0.9754	0.9751	0.9794	0.0246	0.0249	0.0206	$5.3412e-07$	$5.8432e-07$	$2.7686e-07$
0.3	0.9650	0.9645	0.9695	0.0350	0.0355	0.0305	$1.5622e-06$	$1.6518e-06$	$9.0257e-07$
0.4	0.9550	0.9547	0.9598	0.0450	0.0453	0.0402	$3.3375e-06$	$3.4458e-06$	$2.0805e-06$
0.5	0.9454	0.9453	0.9502	0.0546	0.0547	0.0498	$6.0032e-06$	$6.1100e-06$	$3.9725e-06$
0.6	0.9362	0.9362	0.9408	0.0638	0.0638	0.0592	$9.6848e-06$	$9.7776e-06$	$6.7339e-06$
0.7	0.9272	0.9272	0.9314	0.0728	0.0727	0.0685	$1.4495e-05$	$1.4571e-05$	$1.0513e-05$
0.8	0.9184	0.9184	0.9222	0.0816	0.0816	0.0778	$2.0534e-05$	$2.0603e-05$	$1.5451e-05$
0.9	0.9098	0.9097	0.9131	0.0901	0.0903	0.0869	$2.7896e-05$	$2.7973e-05$	$2.1683e-05$
1.0	0.9015	0.9014	0.9042	0.0985	0.0986	0.0958	$3.6664e-05$	$3.6773e-05$	$2.9336e-05$

Table 2: Comparison of the approximate solutions using the proposed methods versus the method ABM with $\nu_1 = \nu_2 = \nu_3 = 0.89$.

with $N = 4$ for problems Eq.(4). The numerical results listed in Table 4 show that there are no total changes in the final results and that our proposed two approaches are stable.

8 Conclusion

In this work, two numerical approaches are proposed to solve fractional chemical kinetics numerically. Our presented tabular and graphical outcomes clearly demonstrate that by increasing the number of collocation points, denoted as a larger value of "N," the quality of the solution improves significantly. The key benefit of employing both the Chebyshev

	$\Theta_1(t)$			$\Theta_2(t)$			$\Theta_3(t)$		
t	ABM	CC	CG	ABM	CC	CG	ABM	CC	CG
0.1	0.9870	0.9871	0.9871	0.0130	0.0129	0.0129	$7.7169e-08$	$8.0568e-08$	$7.0945e-08$
0.2	0.9759	0.9756	0.9756	0.0241	0.0244	0.0244	$4.9661e-07$	$5.4024e-07$	$5.1211e-07$
0.3	0.9655	0.9651	0.9653	0.0345	0.0349	0.0347	$1.4706e-06$	$1.5481e-06$	$1.4991e-06$
0.4	0.9555	0.9553	0.9555	0.0445	0.0447	0.0445	$3.1694e-06$	$3.2625e-06$	$3.1949e-06$
0.5	0.9460	0.9459	0.9461	0.0540	0.0541	0.0539	$5.7397e-06$	$5.8309e-06$	$5.7501e-06$
0.6	0.9367	0.9367	0.9369	0.0633	0.0633	0.0631	$9.3114e-06$	$9.3903e-06$	$9.3029e-06$
0.7	0.9276	0.9277	0.9278	0.0724	0.0723	0.0722	$1.4002e-05$	$1.4067e-05$	$1.3979e-05$
0.8	0.9188	0.9188	0.9188	0.0812	0.0812	0.0812	$1.9916e-05$	$1.9975e-05$	$1.9890e-05$
0.9	0.9102	0.9101	0.9100	0.0898	0.0899	0.0899	$2.7154e-05$	$2.7221e-05$	$2.7139e-05$
1.0	0.9018	0.9016	0.9018	0.0982	0.0983	0.0982	$3.5803e-05$	$3.5897e-05$	$3.5812e-05$

Table 3: Comparison of the approximate solutions using the proposed method versus the method ABM with $\nu_1 = \nu_2 = \nu_3 = 0.9$.

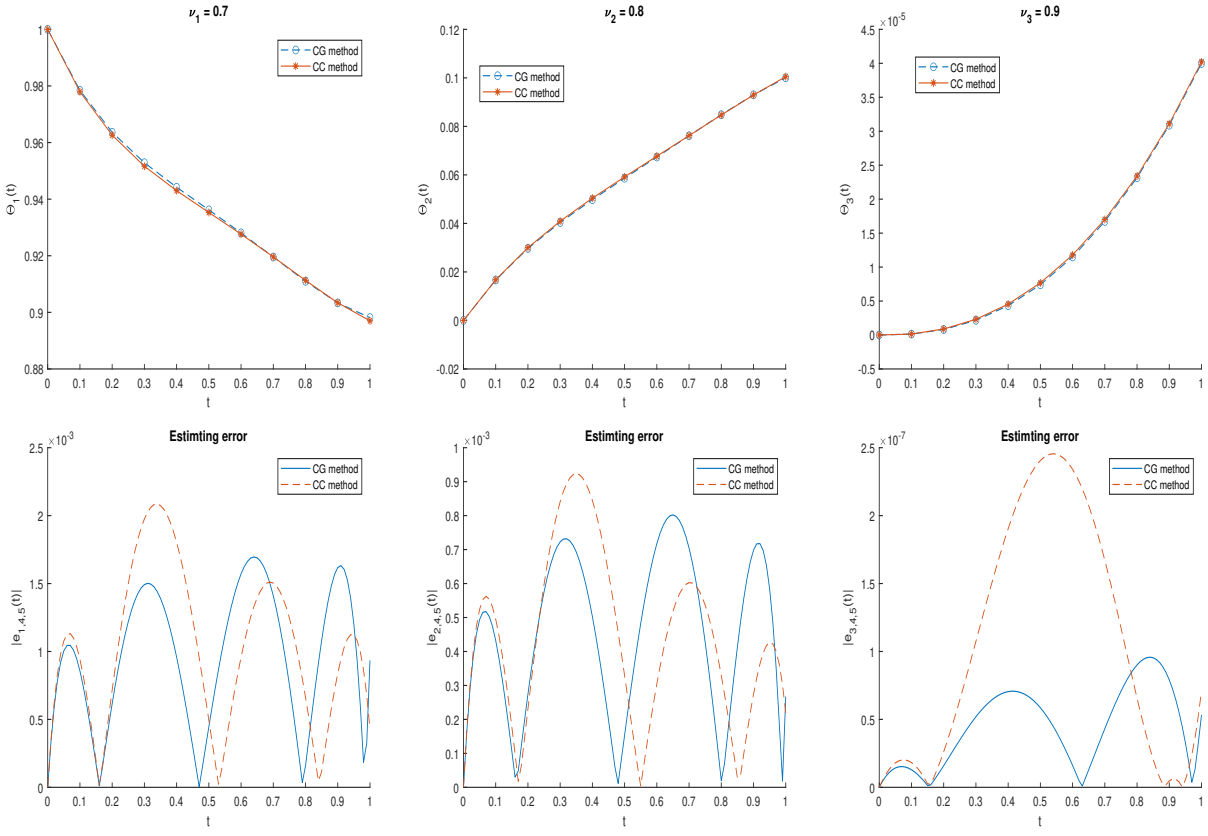

Fig. 4: Plot of comparison between CC method, CG method, and ABM solutions for $\nu_1 = 0.7, \nu_2 = 0.8, \nu_3 = 0.9$ with $(N,M) = (4,5)$.

collocation method and the Chebyshev Galerkin method lies in their ability to transform complex problems into a set of algebraic equations, whether linear or nonlinear. This approach greatly simplifies the computational process and aligns it with computer-based techniques. This new comparative study between the Chebyshev collocation method and the Chebyshev Galerkin method for fractional chemical kinetics that both approaches can be applied successfully to the chemistry problems of chemistry science.

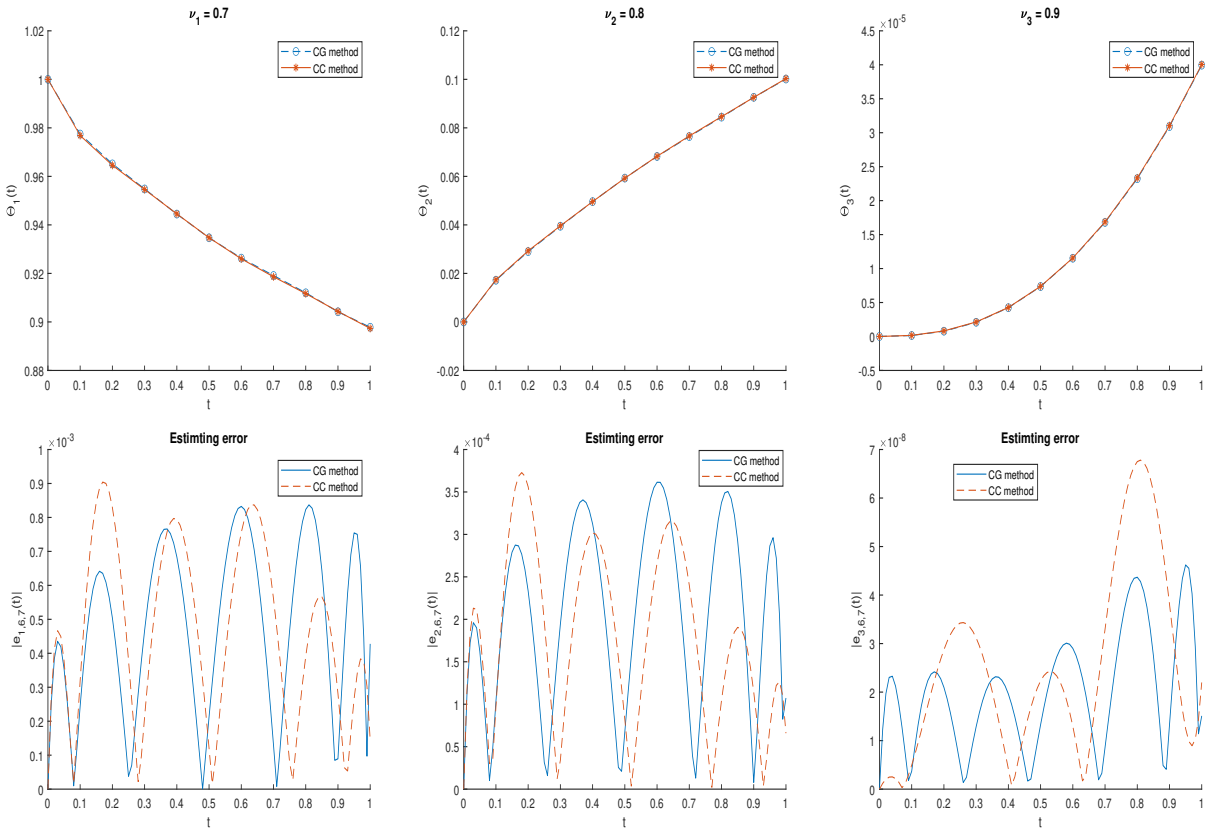

Fig. 5: Plot of comparison between CC method, CG method, and ABM solutions for $\nu_1 = 0.7, \nu_2 = 0.8, \nu_3 = 0.9$ with $(N,M) = (6,7)$.

	$\nu_1 = 1$					
	CG method			CC method		
ε	Θ_1	Θ_2	Θ_3	Θ_1	Θ_2	Θ_3
10^{-1}	1.98×10^{-9}	2.78×10^{-6}	2.78×10^{-6}	2.64×10^{-9}	2.78×10^{-6}	2.78×10^{-6}
10^{-4}	6.11×10^{-10}	2.82×10^{-9}	2.78×10^{-9}	4.42×10^{-10}	2.78×10^{-9}	2.55×10^{-9}
10^{-8}	7.59×10^{-10}	4.24×10^{-11}	2.55×10^{-10}	4.46×10^{-10}	9.80×10^{-11}	5.35×10^{-10}
	$\nu_1 = 0.89$					
	CG method			CC method		
ε	Θ_1	Θ_2	Θ_3	Θ_1	Θ_2	Θ_3
10^{-1}	3.97×10^{-4}	3.97×10^{-4}	3.65×10^{-6}	4.39×10^{-4}	4.39×10^{-4}	3.56×10^{-6}
10^{-4}	3.97×10^{-4}	3.97×10^{-4}	3.30×10^{-8}	4.39×10^{-4}	4.39×10^{-4}	1.09×10^{-7}
10^{-8}	3.97×10^{-4}	3.97×10^{-4}	3.32×10^{-8}	4.39×10^{-4}	4.39×10^{-4}	1.09×10^{-7}
	$\nu_1 = 0.9$					
	CG method			CC method		
ε	Θ_1	Θ_2	Θ_3	Θ_1	Θ_2	Θ_3
10^{-1}	3.49×10^{-4}	3.49×10^{-4}	3.57×10^{-6}	3.79×10^{-4}	3.80×10^{-4}	3.49×10^{-6}
10^{-4}	3.49×10^{-4}	3.49×10^{-4}	2.90×10^{-8}	3.79×10^{-4}	3.79×10^{-4}	9.37×10^{-8}
10^{-8}	3.49×10^{-4}	3.49×10^{-4}	2.92×10^{-8}	3.79×10^{-4}	3.79×10^{-4}	9.41×10^{-8}

Table 4: Max absolute errors of perturbed problems for (4) with $\nu_1 = \nu_2 = \nu_3 = \{0.89, 0.9, 1\}$ and $N = 4$.

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