

# An efficient numerical solution of time–fractional batch reactor system

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## Abstract

Recently, an approximate solution of the time fractional chemical engineering equations by means of the homotopy perturbation method (HPM) has been presented by Khan et al. [1]. As a disadvantage of the HPM, to have reasonable solution at large values of  $t$  we should truncate HPM series with more terms, while this task is so complicated and even takes too time to complete. In this paper, we have successively applied the predictor–corrector approach on fractional chemical systems to obtain an accurate numerical solution. The numerical results are compared with obtained results by HPM. This comparison shows that predictor–corrector approach is more accurate than the HPM. As advantages of predictor-corrector over the HPM, the method reduces the computational difficulties and is easy to implement.

*Keywords:* Fractional differential equation; Volterra integral equation; Predictor–Corrector approach; Runge-Kutta method; Chemical process.

## 1. Introduction

Fractional calculus, the theory of derivatives and integrals of any arbitrary real or complex order, has an importance applications in widely diverse areas of physical mathematics and engineering sciences. Indeed, it is generalization of the idea of integer order differentiation and  $n$ -fold integration. Fractional derivatives provide powerful instrument for the description of memory and hereditary properties of various processes. In comparison with the classical integer–order derivatives, the most significant advantage of making use of

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fractional differential equations in mathematical modelling is their non-local property. It is well known that the integer order differential operator is a local operator but the fractional order differential operator is non-local. This means that the next state of a system depends not only upon its current state but also upon all of its historical states. This is more realistic and it is one reason why fractional calculus has become more and more popular in scientific and technological fields [2, 3, 4, 5]. The advantages of fractional derivatives become apparent in modeling mechanical and electrical properties of real materials, as well as in the description of properties of gases, liquids and rocks, and in many other fields (e.g., see [6, 7, 8, 9, 10]).

In this paper, we are interested into approximate solutions of time fractional chemical engineering problems via the predictor-corrector (PC) approach. This method was firstly developed for the solution of initial value problems with Caputo derivatives by Diethelm et al. [11]. The algorithm is a generalization of the classical Adams-Bashforth-Moulton integrator that is well known for the numerical solution of first-order initial problems [12, 13]. The general response expressions contain a parameter  $\alpha$  describing the order of the fractional derivative that can be varied to obtain various responses. The solutions corresponding to ordinary chemical problems, performing the same dynamics, are also determined as a special case of our general solutions. To perform a comparison, we also compare the numerical solution obtained by PC approach with the analytical solution of the homotopy perturbation method (HPM) presented by Khan et al. [1]. This comparison establish that the numerical results obtained by the PC approach are more reliable, and to the best of our knowledge, such types of numerical solutions for chemical engineering equations with fractional derivatives are presented first time.

## 2. Fractional Calculus

Fractional calculus is a field of mathematics which investigates the properties of derivative and integral operators of arbitrary orders. In this section, we review some preliminary facts of theory of the fractional calculus including notations and basic definitions which are useful in the sequel. The fractional extension of a differential equation is obtained by replacing the first time derivative by the fractional derivative  $\mathcal{D}_{*a}^\alpha$  of order  $0 < \alpha \leq 1$  and the second time derivative by the fractional derivative  $\mathcal{D}_{*a}^\alpha$  of order  $1 < \alpha \leq 2$ , where  $\mathcal{D}_{*a}^\alpha$  is the fractional differential operator in the sense of Caputo fractional derivative.

**Definition 1** ([14]). Let  $\alpha \geq 0$  and  $L_1[a, b]$  be a Lebesgue space. The operator  $\mathcal{J}_a^\alpha$  which is defined on  $L_1[a, b]$  by

$$\begin{aligned} \mathcal{J}_a^\alpha f(t) &= \frac{1}{\Gamma(\alpha)} \int_a^t (t - \tau)^{\alpha-1} f(\tau) d\tau, \quad \alpha > 0, \\ \mathcal{J}_a^0 f(t) &= f(t), \end{aligned}$$

for  $a \leq t \leq b$ , is called the Riemann-Liouville fractional integral operator of order  $\alpha$ .

**Definition 2** ([14]). Let  $\alpha > 0$  and  $n = \lceil \alpha \rceil$ . The operator  $\mathcal{D}_{*a}^\alpha$ , defined by

$$\mathcal{D}_{*a}^\alpha f(t) = J_a^{n-\alpha} D^n f(t) = J_a^{n-\alpha} f^{(n)}(t), \tag{1}$$

is called the Caputo fractional differential operator of order  $\alpha$ , whenever  $f^{(n)} \in L_1[a, b]$ .

Consider the general form of the fractional initial value problems (FIVPs):

$$\begin{aligned} \mathcal{D}_*^\alpha y(t) &= f(t, y(t)), \quad t > 0, \quad \alpha > 0, \\ y^{(k)}(0) &= d_k, \quad k = 0, \dots, n-1, \end{aligned} \tag{2}$$

where  $n$  is the smallest integer greater than or equal to  $\alpha$ ,  $y^{(k)}$  denotes the  $k$ -th derivative of  $y$ , and the real numbers  $d_k, k = 0, \dots, n-1$ , are assumed to be given. Let  $f$  be continuous and fulfill a Lipschitz condition with respect to the second variable, i.e.,

$$|f(t, y_2) - f(t, y_1)| \leq L|y_2 - y_1|$$

with some constant  $L > 0$  independent of  $t, y_1$ , and  $y_2$ , then the FIVPs (2) have an unique solution [15]. It has been known [15] that FIVP (2), if a continuous solution is admitted, is equivalent to the following Volterra integral equation:

$$y(t) = g(t) + \frac{1}{\Gamma(\alpha)} \int_0^t (t - \tau)^{\alpha-1} f(\tau, y(\tau)) d\tau, \tag{3}$$

where  $g(t) = \sum_{k=0}^{n-1} \frac{y^{(k)}(0)}{k!} t^k$  denotes the Taylor polynomial of degree  $n-1$  for the function  $y$ , centered at 0.

**Remark 1.** For simplicity in notations, we show  $\mathcal{J}_0^\alpha$  and  $\mathcal{D}_{*0}^\alpha$  by  $\mathcal{J}^\alpha$  and  $\mathcal{D}_*^\alpha$ , respectively.

### 3. A brief investigation of the predictor-corrector approach

In order to motivate the construction of the predictor-corrector method and obtain a numerical solution on  $[0, T]$ , assume that we are working on a uniform grid  $\{t_n = nh : n = 0, 1, \dots, N\}$  with some integer  $N$  and  $h = T/N$ . The basic idea is as follow: assuming that we have already calculated approximations  $y_n \approx y(t_n)$  ( $n = 1, 2, \dots, N - 1$ ), then we try to obtain the approximation  $y_{n+1}$  by means of Eq. (3) calculated at  $t = t_{n+1}$ :

$$y(t_{n+1}) = g(t_{n+1}) + \frac{1}{\Gamma(\alpha)} \int_0^{t_{n+1}} (t_{n+1} - \tau)^{\alpha-1} f(\tau, y(\tau)) d\tau.$$

The corrector formula (i.e., the fractional variant of the one-step Adams–Moulton method) is given as

$$y_{n+1} = g(t_{n+1}) + \frac{h^\alpha}{\Gamma(\alpha + 2)} \sum_{j=0}^n a_{j,n+1} f(t_j, y_j) + \frac{h^\alpha}{\Gamma(\alpha + 2)} f(t_{n+1}, y_{n+1}^P), \quad (4)$$

where

$$a_{j,n+1} = \begin{cases} n^{\alpha+1} - (n - \alpha)(n + 1)^\alpha, & j = 0, \\ (n - j + 2)^{\alpha+1} + (n - j)^{\alpha+1} - 2(n - j + 1)^{\alpha+1}, & 1 \leq j \leq n, \\ 1, & j = n + 1. \end{cases} \quad (5)$$

Furthermore, the predicted value  $y_{n+1}^P$  is determined by the fractional Adams–Bashforth method as follows

$$y_{n+1}^P = g(t_{n+1}) + \frac{1}{\Gamma(\alpha)} \sum_{j=0}^n b_{j,n+1} f(t_j, y_j),$$

where

$$b_{j,n+1} = \frac{h^\alpha}{\alpha} ((n + 1 - j)^\alpha - (n - j)^\alpha). \quad (6)$$

The mathematical analysis of the predictor-corrector method in [16] shows that one may expect the following behavior from error statement

$$\max_{j=0,1,\dots,N} |y(t_j) - y_j| = \mathcal{O}(h^p)$$

where  $p = \max\{1 + \alpha, 2\}$  and the quantities  $h$  and  $N$  are related according to  $h = T/N$ , and  $T$  is the upper bound of the interval on which we are looking for the solution.

## 4. Chemical Engineering Applications

In this section, in order to show the efficiency and accuracy of the predictor–corrector method, we extend this method to apply on some systems of fractional differential equations which are arising in chemical reactors and reactions. For  $\alpha = 1$ , these systems are ordinary cases and one may use the well-known Runge-Kutta method to obtain their numerical solutions. So, we first apply the predictor–corrector procedure to solve the integer-order case and compare the numerical results with the solutions which have obtained by Runge-Kutta method. Then, numerical solutions for other values of  $\alpha$  will be presented.

### 4.1. Chemical Reactor

A reaction  $A \rightarrow B$  takes place in two reactors in series. The reactors are well mixed but are not at steady-state. The unsteady-state mass balance for each stirred tank reactor gives the following differential equations [17]:

$$\frac{d CA_1}{dt} = \frac{1}{\tau} (CA_0 - CA_1) - k CA_1, \quad (7)$$

$$\frac{d CB_1}{dt} = \frac{1}{\tau} CB_1 + k CA_1, \quad (8)$$

$$\frac{d CA_2}{dt} = \frac{1}{\tau} (CA_1 - CA_2) - k CA_2, \quad (9)$$

$$\frac{d CB_2}{dt} = \frac{1}{\tau} (CB_1 - CB_2) - k CB_2, \quad (10)$$

where

- $CA_0$  is the concentration of  $A$  at the inlet of the first reactor,
- $CA_1$  is the concentration of  $A$  at the outlet of the first reactor (and inlet of the second),
- $CA_2$  is the concentration of  $A$  at the outlet of the second reactor,
- $CB_1$  is the concentration of  $B$  at the outlet of the first reactor (and inlet of the second),
- $CB_2$  is the concentration of  $B$  in the second reactor,
- $\tau$  is the residence time for each reactor,

- $k$  is the rate constant for reaction of  $A$  to produce  $B$ .

Let assume that the initial conditions of all the dependent variables are zero, i.e.:

$$CA_1(0) = 0, \quad CA_2(0) = 0, \quad CB_1(0) = 0, \quad CB_2(0) = 0. \quad (11)$$

For brevity, we introduce the following notation to denote the dependent variables:

$$u(t) = CA_1, \quad v(t) = CB_1, \quad w(t) = CA_2, \quad y(t) = CB_2. \quad (12)$$

Now, writing the equation in more general form and using the notation (12), equations (7)–(10) transform to

$$\mathcal{D}_*^\alpha u(t) = \frac{1}{\tau} (CA_0 - u(t)) - ku(t), \quad (13)$$

$$\mathcal{D}_*^\alpha v(t) = \frac{1}{\tau} v(t) + ku(t), \quad (14)$$

$$\mathcal{D}_*^\alpha w(t) = \frac{1}{\tau} (u(t) - w(t)) - kw(t), \quad (15)$$

$$\mathcal{D}_*^\alpha y(t) = \frac{1}{\tau} (v(t) - y(t)) - ky(t), \quad (16)$$

subject to the following initial conditions

$$u(0) = CA_1(0) = 0, \quad (17)$$

$$v(0) = CB_1(0) = 0, \quad (18)$$

$$w(0) = CA_2(0) = 0, \quad (19)$$

$$y(0) = CB_2(0) = 0. \quad (20)$$

We seek for the concentrations of  $A$  and  $B$  in both reactors during their first  $T$  minutes of operation. To this aim suppose that  $CA_0$  is equal to 10,  $k = 0.1 \text{ min}^{-1}$  and  $\tau = 5 \text{ min}$ .

Let us consider equations (13) and (17) together. These two equations form an FIVP which is equivalent to the following Volterra integral equation:

$$u(t) = \frac{1}{\Gamma(\alpha)} \int_0^t (t - \eta)^{\alpha-1} \left( \frac{1}{\tau} (CA_0 - u(\eta)) - ku(\eta) \right) d\eta. \quad (21)$$

In the same way, by considering equations (14), (15) and (16) corresponding with the initial conditions (18), (19) and (20) follows that:

$$v(t) = \frac{1}{\Gamma(\alpha)} \int_0^t (t - \eta)^{\alpha-1} \left( \frac{1}{\tau} v(\eta) + ku(\eta) \right) d\eta, \tag{22}$$

$$w(t) = \frac{1}{\Gamma(\alpha)} \int_0^t (t - \eta)^{\alpha-1} \left( \frac{1}{\tau} (u(\eta) - w(\eta)) - kw(\eta) \right) d\eta, \tag{23}$$

$$y(t) = \frac{1}{\Gamma(\alpha)} \int_0^t (t - \eta)^{\alpha-1} \left( \frac{1}{\tau} (v(\eta) - y(\eta)) - ky(\eta) \right) d\eta. \tag{24}$$

Assume that we are working on a uniform grid  $\{t_n = nh : n = 0, 1, \dots, N\}$  with some integer  $N$  and  $h := T/N$ . The basic idea is, assuming that we have already for  $j = 1, 2, \dots, n$  calculated approximations

$$u_j \approx u(t_j), \quad v_j \approx v(t_j), \quad w_j \approx w(t_j), \quad y_j \approx y(t_j),$$

then we try to obtain the approximations of  $u_{n+1}, v_{n+1}, w_{n+1}$  and  $y_{n+1}$  by means of the following equations

$$u(t_{n+1}) = \frac{1}{\Gamma(\alpha)} \int_0^{t_{n+1}} (t_{n+1} - \eta)^{\alpha-1} \left( \frac{1}{\tau} (CA_0 - u(\eta)) - ku(\eta) \right) d\eta,$$

$$v(t_{n+1}) = \frac{1}{\Gamma(\alpha)} \int_0^{t_{n+1}} (t_{n+1} - \eta)^{\alpha-1} \left( \frac{1}{\tau} v(\eta) + ku(\eta) \right) d\eta,$$

$$w(t_{n+1}) = \frac{1}{\Gamma(\alpha)} \int_0^{t_{n+1}} (t_{n+1} - \eta)^{\alpha-1} \left( \frac{1}{\tau} (u(\eta) - w(\eta)) - kw(\eta) \right) d\eta,$$

$$y(t_{n+1}) = \frac{1}{\Gamma(\alpha)} \int_0^{t_{n+1}} (t_{n+1} - \eta)^{\alpha-1} \left( \frac{1}{\tau} (v(\eta) - y(\eta)) - ky(\eta) \right) d\eta.$$

According to equation (4), the corrector formulas are obtained as:

$$u_{n+1} = \frac{h^\alpha}{\Gamma(\alpha + 2)} \sum_{j=0}^n a_{j,n+1} \left( \frac{1}{\tau} (CA_0 - u_j) - ku_j \right) + \frac{h^\alpha}{\Gamma(\alpha + 2)} \left( \frac{1}{\tau} (CA_0 - u_{n+1}^P) - ku_{n+1}^P \right) \quad (25)$$

$$v_{n+1} = \frac{h^\alpha}{\Gamma(\alpha + 2)} \sum_{j=0}^n a_{j,n+1} \left( \frac{1}{\tau} v_j + ku_j \right) + \frac{h^\alpha}{\Gamma(\alpha + 2)} \left( \frac{1}{\tau} v_{n+1}^P + ku_{n+1}^P \right), \quad (26)$$

$$w_{n+1} = \frac{h^\alpha}{\Gamma(\alpha + 2)} \sum_{j=0}^n a_{j,n+1} \left( \frac{1}{\tau} (u_j - w_j) - kw_j \right) + \frac{h^\alpha}{\Gamma(\alpha + 2)} \left( \frac{1}{\tau} (u_{n+1}^P - w_{n+1}^P) - kw_{n+1}^P \right), \quad (27)$$

$$y_{n+1} = \frac{h^\alpha}{\Gamma(\alpha + 2)} \sum_{j=0}^n a_{j,n+1} \left( \frac{1}{\tau} (v_j - y_j) - ky_j \right) + \frac{h^\alpha}{\Gamma(\alpha + 2)} \left( \frac{1}{\tau} (v_{n+1}^P - y_{n+1}^P) - ky_{n+1}^P \right). \quad (28)$$

Furthermore, the predicted values  $u_{n+1}^P$ ,  $v_{n+1}^P$ ,  $w_{n+1}^P$  and  $y_{n+1}^P$  are determined by

$$u_{n+1}^P = \frac{1}{\Gamma(\alpha)} \sum_{j=0}^n b_{j,n+1} \left( \frac{1}{\tau} (CA_0 - u_j) - ku_j \right), \quad (29)$$

$$v_{n+1}^P = \frac{1}{\Gamma(\alpha)} \sum_{j=0}^n b_{j,n+1} \left( \frac{1}{\tau} v_j + ku_j \right), \quad (30)$$

$$w_{n+1}^P = \frac{1}{\Gamma(\alpha)} \sum_{j=0}^n b_{j,n+1} \left( \frac{1}{\tau} (u_j - w_j) - kw_j \right), \quad (31)$$

$$y_{n+1}^P = \frac{1}{\Gamma(\alpha)} \sum_{j=0}^n b_{j,n+1} \left( \frac{1}{\tau} (v_j - y_j) - ky_j \right), \quad (32)$$

where  $a_{j,n+1}$  and  $b_{j,n+1}$  are defined by equations (5) and (6).



Let us consider equations (13)-(16) subject to the initial conditions (17)-(20). For  $\alpha = 1$ , we deal with a system of ordinary differential equations. So one may use the well-known Runge-Kutta (RK) method to obtain numerical solutions. To apply the RK method, we can use builtin command ode45 in MATLAB software. This command is based on an explicit RK formula. It is a one-step solver, which needs only the solution at the immediately preceding time point. In general, ode45 is the best function to apply as a first try for most problems [18]. Table 1, represents the obtained numerical solutions of chemical reactor system by RK method for  $\alpha = 1$  which the step size  $h$  is chosen equal to  $h = 1/10$ .

$t_j$	Numerical approximations of			
	$u(t_j)$	$v(t_j)$	$w(t_j)$	$y(t_j)$
0.0	0.0000	0.0000	0.0000	0.0000
0.5	0.9286	0.0230	0.0453	0.0008
1.0	1.7279	0.0848	0.1642	0.0055
1.5	2.4158	0.1760	0.3353	0.0167
2.0	3.0079	0.2889	0.5418	0.0360
2.5	3.5176	0.4171	0.7705	0.0638
3.0	3.9562	0.5557	1.0112	0.1002
3.5	4.3337	0.7004	1.2561	0.1447
4.0	4.6587	0.8480	1.4994	0.1966
4.5	4.9384	0.9959	1.7368	0.2550
5.0	5.1791	1.1421	1.9652	0.3189
5.5	5.3863	1.2850	2.1825	0.3874
6.0	5.5647	1.4234	2.3874	0.4594
6.5	5.7182	1.5565	2.5791	0.5339
7.0	5.8503	1.6837	2.7573	0.6102
7.5	5.9640	1.8047	2.9220	0.6874
8.0	6.0619	1.9192	3.0736	0.7647
8.5	6.1461	2.0270	3.2125	0.8416
9.0	6.2186	2.1284	3.3393	0.9175
9.5	6.2810	2.2233	3.4547	0.9919
10.0	6.3348	2.3119	3.5593	1.0644

Table 1: Numerical solutions of chemical reactor system for  $\alpha = 1$ .

To apply the predictor-corrector approach, first we set  $h = 1/10$ , then at each iteration, according to the predictor formulas which are established in equations (29)-(32), values of  $u_{n+1}^P$ ,  $v_{n+1}^P$ ,  $w_{n+1}^P$ ,  $y_{n+1}^P$  for  $n = 0, 1, \dots, N-1$  are calculated. After predicting the unknown values, using equations (25)-(28), predicted values will correct and the numerical solution of the system will be obtain. This procedure is routine and can be implemented easily. As an adviser, to decrease the running time, it highly recommend that all of coefficients  $a_{j,n+1}$  and  $b_{j,n+1}$  for  $j = 0, 1, \dots, n$ ,  $n = 0, 1, \dots, N-1$ , should be calculated at beginning of any implementation code. This action is so effective and can decrease calculation the computation time.

There are also some methods which can be applied to solve fractional differential equations. Among these methods, some of them present numerical and some of them present analytical solutions. One of the analytical methods, which widely used to solve initial fractional differential equations, is the homotopy perturbation method (HPM) [19, 20]. Unlike predictor-corrector (PC) and RK, which are numerical methods, HPM presents an analytical solution. HPM can also apply on the chemical system of fractional differential equations [1, 21]. For example, the chemical reactor system for  $0 < \alpha \leq 1$  is solved in [1], and the first four components of the HPM series are reported as follow:

$$\begin{aligned}\tilde{u}(t) &= \frac{6t^\alpha}{\Gamma(\alpha + 1)} - \frac{1.2t^{2\alpha}}{\Gamma(2\alpha + 1)} + \frac{0.18t^{3\alpha}}{\Gamma(3\alpha + 1)}, \\ \tilde{v}(t) &= \frac{0.4t^{2\alpha}}{\Gamma(2\alpha + 1)} - \frac{0.46t^{3\alpha}}{\Gamma(3\alpha + 1)}, \\ \tilde{w}(t) &= \frac{0.8t^{2\alpha}}{\Gamma(2\alpha + 1)} - \frac{0.24t^{3\alpha}}{\Gamma(3\alpha + 1)}, \\ \tilde{y}(t) &= \frac{0.04t^{3\alpha}}{\Gamma(3\alpha + 1)}.\end{aligned}$$

To compare accuracy of PC and HPM, we applied PC on the chemical reactor system for  $\alpha = 1$  and obtained numerical solutions. Table 2 shows a comparison between the results of HPM and PC algorithms. In this table we report the absolute different between the results of these algorithms and Runge-Kutta scheme. As we can see from Table 2, the values of  $|\text{PC} - \text{RK}|$  are much less than the values of  $|\text{HPM} - \text{RK}|$ , therefore the results of PC are very better than the HPM's results. In addition, for large values of  $t$ , the latter is

$t_j$	$u$		$v$		$w$		$y$	
	RK - PC	RK - HPM	RK - PC	RK - HPM	RK - PC	RK - HPM	RK - PC	RK - HPM
0.5	0.00013	1.92514	0.00007	0.01740	0.00017	0.04973	0.00002	0.00008
1.0	0.00023	3.70213	0.00012	0.03852	0.00026	0.19584	0.00003	0.00120
1.5	0.00029	5.33544	0.00014	0.01524	0.00031	0.42971	0.00002	0.00577
2.0	0.00034	6.83207	0.00016	0.10221	0.00033	0.73822	0.00001	0.01736
2.5	0.00036	8.20119	0.00016	0.36505	0.00031	1.10452	0.00001	0.04037
3.0	0.00038	9.45379	0.00015	0.82568	0.00029	1.50882	0.00002	0.07982
3.5	0.00038	10.6025	0.00014	1.53748	0.00024	1.92888	0.00004	0.14116
4.0	0.00037	11.6612	0.00013	2.55467	0.00021	2.34057	0.00005	0.23009
4.5	0.00036	12.6453	0.00011	3.93216	0.00016	2.71817	0.00006	0.35251
5.0	0.00034	13.5708	0.00009	5.72541	0.00012	3.03478	0.00007	0.51441

Table 2: Comparison of the results obtained by PC and HPM with RK for chemical reactor system in case of  $\alpha = 1$ .

very large, hence the results of HPM cannot be trustworthy in general. As a matter of fact, the accuracy of obtained results by PC in comparison with HPM, is in a good agreement with results of RK. It must be noted that, to have an accurate solution for large values of  $t$  by HPM, we should truncate HPM series with more terms. This action is so complicated and even too time consuming. But, the PC approach is very easy to implement and is fast to obtain numerical solutions. Table 3 presents a comparison in time between RK and PC for various choices of  $h$  and  $T$ .

Method	$T = 1, h = 0.1$	$T = 1, h = 0.01$	$T = 10, h = 0.1$	$T = 10, h = 0.01$
RK	0.101216	0.145065	0.192890	0.318806
PC	0.007715	0.054452	0.153416	0.291095

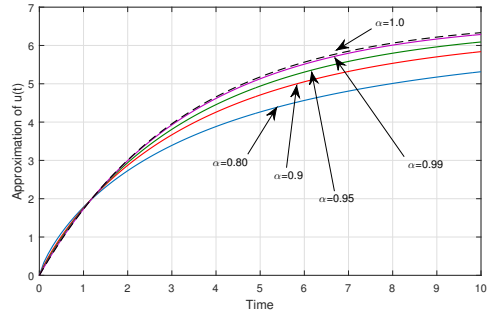
Table 3: Comparison of running time of RK and PC (in second) for chemical reactor system in case of  $\alpha = 1$ .

Now, in the case  $0 < \alpha < 1$  we intend to present an approximate solution for the chemical reactor system. Since obtained solutions by PC for  $\alpha = 1$  was more accurate than HPM, so it is expected that this method can also be efficient for  $0 < \alpha < 1$  and numerical results be close to exact solution.

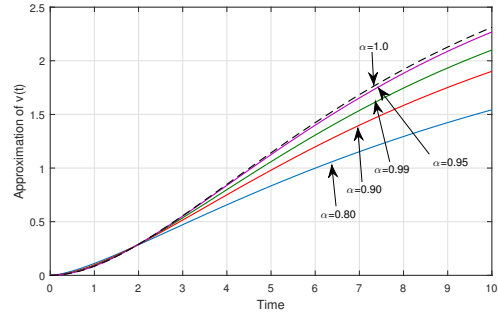
Table 4 represents numerical solutions of the chemical reactor system for  $\alpha = 0.5$  and  $\alpha = 0.75$  which are obtained by PC. Further in Figure 1, numerical solutions of the chemical reactor system for various choices of  $\alpha$  are plotted. From these plots, one can see as  $\alpha$  approaches to 1, numerical solutions approaches to RK results (dashed black lines) too, i.e., in limit sense, solution of the system of fractional differential equations approaches to that of the integer-order system of ordinary differential equations.

$t$	$\alpha = 0.5$				$\alpha = 0.75$			
	$u$	$v$	$w$	$y$	$u$	$v$	$w$	$y$
0	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
2	2.2887	0.2459	0.4494	0.0424	2.6581	0.2809	0.5186	0.0431
4	2.8811	0.4110	0.7292	0.0928	3.7042	0.6124	1.0800	0.1449
6	3.2494	0.5415	0.9417	0.1414	4.3308	0.9093	1.5484	0.2702
8	3.5144	0.6505	1.1139	0.1870	4.7494	1.1645	1.9280	0.4010
10	3.7197	0.7442	1.2586	0.2298	5.0471	1.3819	2.2354	0.5284
12	3.8859	0.8265	1.3832	0.2698	5.2685	1.5671	2.4861	0.6481
14	4.0246	0.8998	1.4924	0.3073	5.4385	1.7254	2.6923	0.7586
16	4.1429	0.9660	1.5894	0.3425	5.5726	1.8616	2.8637	0.8594
18	4.2458	1.0261	1.6765	0.3757	5.6806	1.9792	3.0075	0.9509
20	4.3362	1.0812	1.7553	0.4071	5.7693	2.0815	3.1292	1.0337
22	4.4168	1.1320	1.8273	0.4368	5.8433	2.1709	3.2333	1.1086
24	4.4891	1.1791	1.8933	0.4649	5.9057	2.2496	3.3229	1.1762
26	4.5546	1.2230	1.9543	0.4917	5.9592	2.3191	3.4007	1.2374
28	4.6143	1.2640	2.0108	0.5172	6.0053	2.3808	3.4686	1.2929
30	4.6691	1.3024	2.0634	0.5415	6.0455	2.4359	3.5285	1.3433
32	4.7195	1.3386	2.1125	0.5647	6.0809	2.4853	3.5815	1.3891
34	4.7662	1.3727	2.1586	0.5869	6.1122	2.5297	3.6286	1.4308
36	4.8095	1.4050	2.2019	0.6082	6.1402	2.5699	3.6709	1.4690
38	4.8500	1.4357	2.2427	0.6286	6.1652	2.6064	3.7089	1.5039
40	4.8878	1.4648	2.2813	0.6482	6.1878	2.6396	3.7432	1.5360
42	4.9234	1.4925	2.3179	0.6671	6.2083	2.6699	3.7744	1.5654
44	4.9568	1.5189	2.3526	0.6853	6.2269	2.6977	3.8028	1.5926
46	4.9883	1.5442	2.3856	0.7028	6.2440	2.7233	3.8288	1.6178
48	5.0182	1.5683	2.4170	0.7197	6.2597	2.7469	3.8527	1.6411
50	5.0464	1.5915	2.4470	0.7360	6.2741	2.7687	3.8747	1.6627

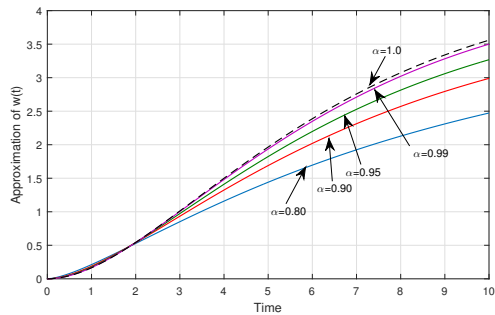
Table 4: Approximate solutions of the chemical reactor system for  $\alpha = 0.5$  and  $0.75$  at specific times in second.



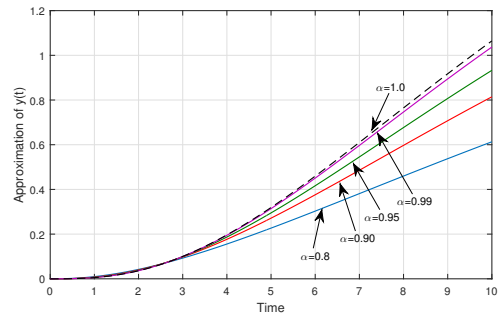
(a) Approximations of  $u(t)$ .



(b) Approximations of  $v(t)$ .



(c) Approximations of  $w(t)$ .



(d) Approximations of  $y(t)$ .

Figure 1: Approximate solutions of  $u(t)$ ,  $v(t)$ ,  $y(t)$  and  $w(t)$  of the chemical reactor system for various choices of  $\alpha$ .

#### 4.2. Chemical Reaction

The nonlinear reaction chemical system of fractional differential equations, has the following form [1],

$$\mathcal{D}_*^\alpha u(t) = -u(t), \tag{33}$$

$$\mathcal{D}_*^\alpha v(t) = u(t) - v^2(t), \tag{34}$$

$$\mathcal{D}_*^\alpha w(t) = v^2(t), \tag{35}$$

and initial conditions are given by

$$u(0) = 1, \quad v(0) = 0, \quad w(0) = 0. \tag{36}$$

To solve the problem using the PC method, first we apply same procedure in the previous problem, and obtain the following Volterra integral equations:

$$u(t) = 1 - \frac{1}{\Gamma(\alpha)} \int_0^t (t - \eta)^{\alpha-1} u(\eta) d\eta, \tag{37}$$

$$v(t) = \frac{1}{\Gamma(\alpha)} \int_0^t (t - \eta)^{\alpha-1} (u(\eta) - v^2(\eta)) d\eta, \tag{38}$$

$$w(t) = \frac{1}{\Gamma(\alpha)} \int_0^t (t - \eta)^{\alpha-1} v^2(\eta) d\eta. \tag{39}$$

Similarly, we are working on a uniform grid  $\{t_n = nh : n = 0, 1, \dots, N\}$  for some integer  $N$  and  $h := T/N$ , and try to obtain the approximations  $u_{n+1}, v_{n+1}$  and  $w_{n+1}$  by means of the following equations

$$u(t_{n+1}) = 1 - \frac{1}{\Gamma(\alpha)} \int_0^{t_{n+1}} (t_{n+1} - \eta)^{\alpha-1} u(\eta) d\eta,$$

$$v(t_{n+1}) = \frac{1}{\Gamma(\alpha)} \int_0^{t_{n+1}} (t_{n+1} - \eta)^{\alpha-1} (u(\eta) - v^2(\eta)) d\eta,$$

$$w(t_{n+1}) = \frac{1}{\Gamma(\alpha)} \int_0^{t_{n+1}} (t_{n+1} - \eta)^{\alpha-1} v^2(\eta) d\eta.$$

According to equation (4), the predictor and corrector formulas are obtained as follow:

(a) **Predictor formulas:**

$$u_{n+1}^P = 1 - \frac{1}{\Gamma(\alpha)} \sum_{j=0}^n b_{j,n+1} u_j,$$

$$v_{n+1}^P = \frac{1}{\Gamma(\alpha)} \sum_{j=0}^n b_{j,n+1} (u_j - v_j^2),$$

$$w_{n+1}^P = \frac{1}{\Gamma(\alpha)} \sum_{j=0}^n b_{j,n+1} v_j^2,$$

where  $a_{j,n+1}$  and  $b_{j,n+1}$  are defined by Eqs. (5) and (6).

(b) **Corrector formulas:**

$$u_{n+1} = 1 - \frac{h^\alpha}{\Gamma(\alpha + 2)} \sum_{j=0}^n a_{j,n+1} u_j - \frac{h^\alpha}{\Gamma(\alpha + 2)} u_{n+1}^P,$$

$$v_{n+1} = \frac{h^\alpha}{\Gamma(\alpha + 2)} \sum_{j=0}^n a_{j,n+1} (u_j - v_j^2) + \frac{h^\alpha}{\Gamma(\alpha + 2)} (u_{n+1}^P - (v_{n+1}^P)^2),$$

$$w_{n+1} = \frac{h^\alpha}{\Gamma(\alpha + 2)} \sum_{j=0}^n a_{j,n+1} v_j^2 + \frac{h^\alpha}{\Gamma(\alpha + 2)} (v_{n+1}^P)^2.$$

This problem is also solved by HPM [1] where the first four components of the HPM series are given by:

$$\tilde{u}(t) = 1 - \frac{t^\alpha}{\Gamma(\alpha + 1)} + \frac{t^{2\alpha}}{\Gamma(2\alpha + 1)} - \frac{t^{3\alpha}}{\Gamma(3\alpha + 1)},$$

$$\tilde{v}(t) = \frac{t^\alpha}{\Gamma(\alpha + 1)} + \frac{t^{2\alpha}}{\Gamma(2\alpha + 1)} - \frac{t^{3\alpha}}{\Gamma(3\alpha + 1)} \left( 1 - \frac{\Gamma(2\alpha + 1)}{(\Gamma(\alpha + 1))^2} \right),$$

$$\tilde{w}(t) = \frac{t^{3\alpha}}{\Gamma(3\alpha + 1)} \left( \frac{\Gamma(2\alpha + 1)}{(\Gamma(\alpha + 1))^2} \right).$$

For  $\alpha = 1$ , the chemical reaction system is an ordinary system. So we apply the RK method to solve it numerically. In order to compare accuracy of PC and HPM, obtained solutions in case  $\alpha = 1$  by these methods are compared with RK results. Table 5 shows this comparison.

$t_j$	$u$		$v$		$w$	
	RK - PC	RK - HPM	RK - PC	RK - HPM	RK - PC	RK - HPM
0.5	0.00055	0.00236	0.00168	0.27915	0.00113	0.01487
1.0	0.00066	0.03455	0.00216	1.16330	0.00149	0.20457
1.5	0.00060	0.16063	0.00158	2.67234	0.00097	0.86328
2.0	0.00048	0.46867	0.00079	4.85488	0.00030	2.28045
2.5	0.00037	1.06125	0.00018	7.80055	0.00018	4.71902
3.0	0.00027	2.04979	0.00022	11.6206	0.00048	8.42912
3.5	0.00019	3.55103	0.00045	16.4356	0.00064	13.6570
4.0	0.00013	5.68498	0.00059	22.3694	0.00071	20.6488
4.5	0.00009	8.57361	0.00065	29.5475	0.00074	29.6510
5.0	0.00006	12.3400	0.00068	38.0955	0.00074	40.9112

Table 5: Comparison of the results of PC and HPM with RK.



For  $0 < \alpha < 1$ , Figure 2 shows analytical and numerical solutions which are obtained by HPM and PC, respectively, for some various choices of  $\alpha$  close to 1. Further, for  $\alpha = 1$  the approximate numerical solution of the chemical reaction system which is obtained by RK is plotted.

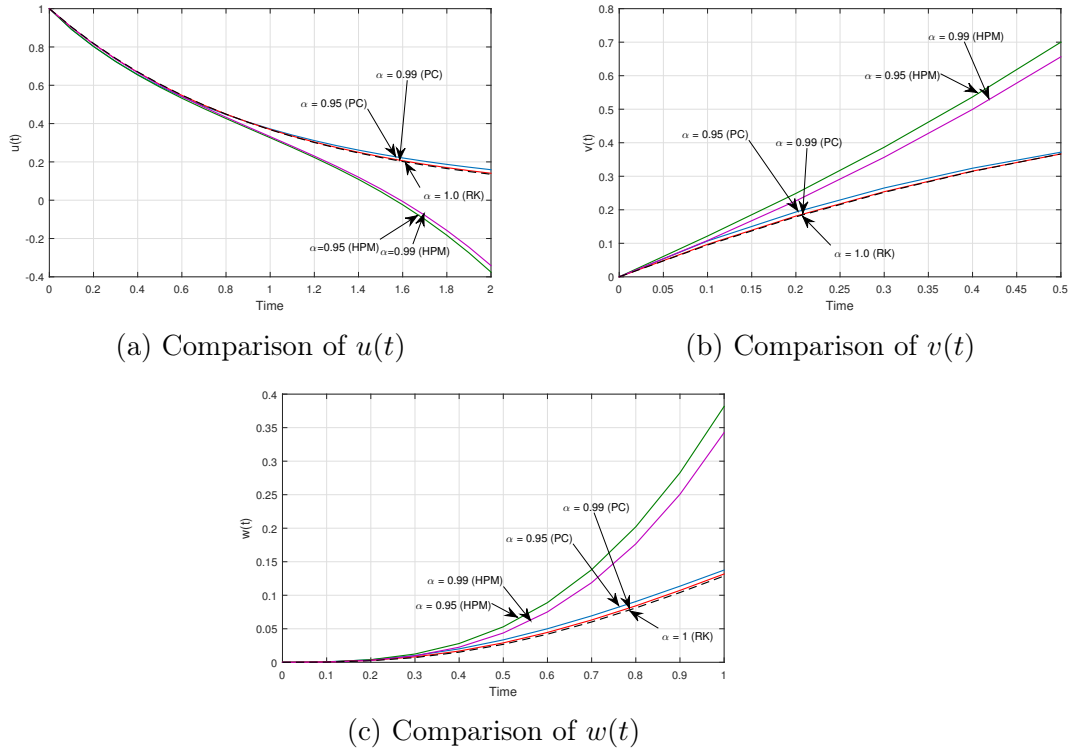


Figure 2: Approximate solutions of  $u(t), v(t), w(t)$  of the chemical reactor system for various choices of  $\alpha$ .

It is known [22] as  $\alpha$  approaches to 1, the exact solution of the chemical reaction system should also approach to the corresponding solution of system in the case  $\alpha = 1$ . For  $\alpha = 1$ , we have not any information about the exact solutions, but a reliable approximations of those exist (numerical solutions obtained by RK). As we conclude from Figure 2, analytical solutions obtained by HPM do not approach to RK solutions, therefore HPM can not be accepted as a valuable method for the chemical reaction system. Finally in Table 4 we have presented the numerical solutions obtained by PC approach of the chemical reaction system for  $\alpha = 0.25, \alpha = 0.5$  and  $\alpha = 0.75$ .

$t$	$\alpha = 0.25$			$\alpha = 0.5$			$\alpha = 0.75$		
	$u(t)$	$v(t)$	$w(t)$	$u(t)$	$v(t)$	$w(t)$	$u(t)$	$v(t)$	$w(t)$
0	1.0000	0.0000	0.0000	1.0000	0.0000	0.0000	1.0000	0.0000	0.0000
5	0.3645	0.3874	0.2481	0.2327	0.3813	0.3860	0.1106	0.3386	0.5508
10	0.3241	0.3842	0.2916	0.1707	0.3461	0.4832	0.0592	0.2561	0.6848
15	0.3017	0.3804	0.3178	0.1413	0.3230	0.5357	0.0416	0.2154	0.7430
20	0.2864	0.3770	0.3366	0.1233	0.3063	0.5704	0.0326	0.1905	0.7769
25	0.2748	0.3740	0.3512	0.1107	0.2933	0.5959	0.0271	0.1733	0.7996
30	0.2656	0.3713	0.3631	0.1014	0.2829	0.6157	0.0234	0.1605	0.8162
35	0.2580	0.3689	0.3731	0.0941	0.2741	0.6318	0.0206	0.1504	0.8289
40	0.2515	0.3667	0.3818	0.0882	0.2666	0.6452	0.0185	0.1423	0.8392
45	0.2458	0.3647	0.3895	0.0832	0.2601	0.6567	0.0169	0.1355	0.8476
50	0.2409	0.3628	0.3963	0.0790	0.2544	0.6666	0.0155	0.1298	0.8547
55	0.2364	0.3611	0.4025	0.0754	0.2492	0.6754	0.0144	0.1248	0.8608
60	0.2324	0.3595	0.4081	0.0723	0.2446	0.6831	0.0134	0.1205	0.8661
65	0.2288	0.3580	0.4132	0.0695	0.2404	0.6901	0.0126	0.1166	0.8708
70	0.2255	0.3565	0.4180	0.0670	0.2365	0.6965	0.0119	0.1132	0.8749
75	0.2224	0.3552	0.4224	0.0647	0.2330	0.7023	0.0113	0.1100	0.8787
80	0.2196	0.3539	0.4265	0.0627	0.2297	0.7076	0.0107	0.1072	0.8821
85	0.2169	0.3527	0.4304	0.0608	0.2266	0.7125	0.0102	0.1046	0.8851
90	0.2145	0.3516	0.4340	0.0592	0.2238	0.7171	0.0098	0.1023	0.8880
95	0.2121	0.3505	0.4374	0.0576	0.2211	0.7213	0.0094	0.1001	0.8906
100	0.2100	0.3494	0.4406	0.0561	0.2186	0.7252	0.0090	0.0980	0.8930

Table 6: Approximate solutions of the chemical reaction system for various choices of  $\alpha$  at specific times in second.

### 5. Concluding remarks

In this paper, the fractional predictor–corrector approach has been successfully applied to find the numerical solutions of the system of reactor and reaction equations with fractional orders. These solutions will be very useful in many areas of science and engineering, where these equations are seen, especially in chemical engineering. These solutions will also be useful in practical scientific research in future investigations. Although the exact solutions of the mentioned systems of equations for  $0 < \alpha \leq 1$  are not known, but with aim of Runge-Kutta method we can find a good approximation of the solutions in the case  $\alpha = 1$  which we consider them as the exact solution. Therefore, to make a comparison between predictor–corrector approach and HPM, we calculated absolute errors at various times. This comparison established that in contrast with the HPM, the predictor-corrector provides

more accurate solution. In the case  $0 < \alpha < 1$  we also showed that as  $\alpha$  approaches to 1, the numerical solutions of the chemical systems obtained by current method converge to the corresponding solution of systems in the case  $\alpha = 1$ , while this fact did not happen in HPM. As an advantage of predictor-corrector over the HPM, the method reduces the computational difficulties and has very easy to implementation.

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