SOLVING TIME-FRACTIONAL CHEMICAL ENGINEERING EQUATIONS BY GENERALIZED DIFFERENTIAL TRANSFORM METHOD

by

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In this paper fractional differential transform method is implemented for modelling and solving system of the time fractional chemical engineering equations. In this method the solution of the chemical reaction, reactor, and concentration equations are considered as convergent series with easily computable components. Also, the obtained solutions have simplicity procedure, high accuracy and efficient.

Key words: *fractional differential equations, differential transform method, chemical reactor, reaction, concentration*

Introduction

Fractional calculus (FC) is a power tool for finding solution of non-linear problems. So, it has a tremendous use in basic sciences and engineering, see *e. g.* [1-7].

The differential transform method (DTM) gives an analytical solution if there exist in the polynomial. It has different form from the well-known series method. It is possible to find exact or approximate solution with highly accurate for differential equations by using DTM. During last two decades the DTM and its modification have been applied for a large range of problems in ODE and PDE and as well as integral equations [8-11].

Arikoglu and Ozkol [9] developed the DTM to solve linear and non-linear fractional order differential equations (FDE) which is called fractional differential transform method (FDTM). After that, Erturk *et al*. [10] by using DTM and generalized Taylor's formula introduced generalized differential transform method (GDTM) to solve FDE [11]. Later, Arikoglu and Ozkol [12] have proved that the FDTM and the GDTM have the same results. So, which name is be used for this method is not important.

There many application of these methods, The fractional order Sturm-Liouville problems of [13, 14], fractional oscillator [15], fractional Benney-Lin equation [16], fractional KdV equation [17], time-fractional telegraphic equation [18], a systems of fractional differential equations (SFDE) [19] fractional integro-differential equations (FIDE) [20], FIDE with non-local boundary conditions and fractional Klein-Gordon equation [21].

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In this work, we are looking to obtain approximate solutions of following time fractional chemical engineering problems:

$$\mathcal{D}^{\alpha_i} x_i\left(t\right) = f_i\left(t, x_1, x_2, ..., x_n\right), \quad 0 < \alpha_i \le 1, \quad i = 1, 2, \cdots, n \tag{1}$$

subject to the initial conditions:

$$x_i\left(0\right) = c_i \tag{2}$$

where $\mathcal{D}^{\alpha_i}$ is the Caputo fractional derivative of x_i. The GDTM is used to calculate the dynamics of aforementioned equation. This system contains a parameter α_i, $i = 1, 2,..., n$ indicating the order of derivative that might be varied to obtain numerous responses. It has shown that the ordinary chemical problems have same dynamics and their solution are a special case of our solutions.

The given system in eq. (1), has been solved by homotopy perturbation method (HPM), variational iteration method (VIM) and modified VIM [22-24].

Preliminaries

We review some basic definitions and properties of the FC [1-3, 6].

Definition 1. Let $x(t) \in C_\mu$, $\mu \ge -1$, the Riemann-Liouville fractional integral (J^α), of order $\alpha \ge 0$ is defined:

$$J^\alpha x\left(t\right) = \frac{1}{\Gamma\left(\alpha\right)} \int\limits_0^t \frac{x\left(s\right)}{\left(t-s\right)^{1-\alpha}}, \quad 0 < \alpha$$

For $\alpha, \beta \ge 0$ and $\gamma \ge -1$:

$$J^\alpha J^\beta x\left(t\right) = J^\beta J^\alpha x\left(t\right) = J^{\alpha+\beta} f\left(t\right)$$

$$J^\alpha t^\gamma = \frac{\Gamma\left(1+\gamma\right)}{\Gamma\left(1+\alpha+\gamma\right)} t^{\alpha+\gamma}$$

To model real-world phenomena with FDE, it is difficult to use the Riemann-Liouville derivative because of some restrictions. Therefore, researcher used the fractional derivative which is proposed by Caputo during his research on the theory of viscoelasticity [6].

Definition 2. Let $x(t) \in C_{-1}^n$, the Caputo fractional derivative is defined:

$$\mathcal{D}^\alpha x\left(t\right) = J^{n-\alpha} \mathcal{D}^n x\left(t\right) = \frac{1}{\Gamma\left(n-\alpha\right)} \int\limits_0^t \frac{f^{(n)}\left(s\right)}{\left(t-s\right)^{\alpha+1-n}} \mathrm{d}s, \quad \alpha \in \left(n-1, n\right], \quad n \in N$$

We listed two of basic properties of Caputo derivative.

Lemma 1. If $\alpha \in (n-1, n]$ and $x \in C_\mu^n$, $-1 \le \mu$ then:

$$\left(\mathcal{D}^\alpha J^\alpha\right) x\left(t\right) = x\left(t\right) \text{ and } \left(J^\alpha \mathcal{D}^\alpha\right) x\left(t\right) = x\left(t\right) - \sum_{j=0}^{n-1} x^j(0^+) \frac{t^j}{j!}, \; t > 0$$

Generalized differential transform method

Now we recall the basic idea of the GDTM and its properties. Firstly, let us define $(\mathcal{D}^\alpha)^n$:

$$\left(\mathcal{D}^\alpha\right)^n = \underbrace{\mathcal{D}^\alpha \mathcal{D}^\alpha ... \mathcal{D}^\alpha}_{n-\text{times}}$$

Theorem 1. (Generalized Taylor's Formula). Let α in (0, 1] and $(\mathcal{D}^\alpha)^k(x)t \in C(0, b)$ for $k = 0, 1,..., n + 1$ then we have [11]:

$$x(t)=\sum_{i=0}^{n}\frac{t^{i\alpha}}{\Gamma(1+i\alpha 1)}\left[\left(\mathcal{D}^\alpha\right)^i f\right](0)+\frac{\left[\left(\mathcal{D}^\alpha\right)^{n+1} f\right](\mu)}{\Gamma\left[(n+1)\alpha+1\right]}t^{(n+1)\alpha},\ 0\le\eta\le t$$

Definition 3. The generalized differential transform and the generalized differential inverse transform of an analytic function $x(t)$ are defined, respectively:

$$\mathcal{X}(k)=\frac{1}{\Gamma(\alpha k+1)}\left[\left(\mathcal{D}^\alpha\right)^k x(t)\right]_{t=0} \tag{3}$$

$$x(t)=\sum_{k=0}^{\infty}\mathcal{X}(K)t^{\alpha k} \tag{4}$$

where $0 < \alpha \le 1$, $k = 0, 1, 2,...$

It is easy to show the GDTM reduces to the DTM when $\alpha = 1$. We listed some of fundamental properties of the GDTM in the next *Theorem*.

Theorem 2. [25, 26] Let $\mathcal{X}(K)$, $\mathcal{Y}(K)$ and $\mathcal{Z}(K)$ are the generalized differential transforms of the function $x(t)$, $y(t)$, and $z(t)$, respectively:

– If

$x(t)=ay(t)\pm bz(t)$, *then* $\mathcal{X}(K)=a\mathcal{Y}(K)\pm b\mathcal{Z}(K)$ where a and b are constants.

– If

$$x(t)=y(t)z(t),\ \text{then}\ \mathcal{X}(K)=\sum_{r=0}^{k}\mathcal{Y}(r)\mathcal{Z}(K-r)$$

– If

$$x(t)=\mathcal{D}^\alpha y(t),\ \text{then}\ \mathcal{X}(K)=\frac{\Gamma\left[\alpha(k+1)+1\right]}{\Gamma(1+\alpha k)}\mathcal{Y}(k+1)$$

– If

$$x(t)=t^{n\alpha}\ \text{then}\ \mathcal{X}(K)=\delta(k-n),\ \text{where}\ \delta(k)=\begin{cases}0 & \text{if } k\ne 0\\ 1 & \text{if } k=0\end{cases}$$

Using induction and item of eq. (2) of *Theorem 2* we have:

Theorem 3. If $x(t) =(\mathcal{D}^\alpha)^n y(t)$ then :

$$\mathcal{X}(K)=\frac{\Gamma\left[\alpha(k+n)+1\right]}{\Gamma(\alpha k+1)}G(k+n) \tag{5}$$

Note: In practice to imply FDTM we need to determine α. In this order if fractional differential equation has multi order $\beta_1 \ge \beta_2 \ge ... \ge \beta_l$, then α is the greatest positive number such that $\beta_i = n_i\alpha$, $i = 1, 2,..., l$, and $n_i \in \mathbb{N}$ consequently order of fractional differential equation is $n_1\alpha$ and n_1 initial value are determined:

$$F(k)=\begin{cases}\dfrac{1}{(k\alpha)!}\left[\dfrac{\mathrm{d}^{k\alpha}f(t)}{\mathrm{d}t^{k\alpha}}\right]_{t=0}; & k\alpha\in\mathbb{N}\cup\{0\}\\ 0; & k\alpha\notin\mathbb{N}\cup\{0\}\end{cases} \tag{6}$$

where $k = 0, 1, 2, ..., n_1$.

Test problems

Here, we solve three examples regarding to linear and non-linear chemical FDE by using the GDTM. These examples are different cases of our given system in (1).

Example 1. [23, 24]

A chemical reaction $A \rightarrow B$ takes place in two reactors. However they are well mixed but they are not at steady-state. For each stirred tank reactor, the unsteady-state mass balances are given in the form of following SFDE:

$$\begin{aligned} &\mathcal{D}^{\alpha}u(t)=\frac{1}{\tau}(CA_0-u)-\beta u,\ \mathcal{D}^{\alpha}v(t)=\frac{-1}{\tau}v-\beta u,\\ &\mathcal{D}^{\alpha}w(t)=\frac{1}{\tau}(u-w)-\beta w,\ \mathcal{D}^{\alpha}y(t)=\frac{1}{\tau}(v-y)-\beta y \end{aligned} \tag{7}$$

where τ and β are the residence time for each reactor and the rate constant for reaction of A to produce B, respectively, CA_0 and $u(=CA_1)$ are concentration of A at the inlet and the outlet of the first reactors, respectively, $w(=CA_2)$ indicates the concentration of A at the outlet of the second reactor. Also, $v(=CB_1)$ and $y(=CB_2)$ are the concentration of B at the outlet first and second reactors, respectively.

If $CA_0=10$, $\tau=5$ minute, and $\beta=0.1$ and initial conditions:

$$CA_1(0)=u(0)=0, CA_2(0)=w(0)=0, CB_1(0)=v(0)=0, CB_2(0)=y(0)=0 \tag{8}$$

Now to solve eq. (7) by the GDTM, the initial conditions are transformed by using eq. (6):

$$\mathcal{U}(0)=0,\ \mathcal{V}(0)=0,\ \mathcal{W}(0)=0,\ \mathcal{Y}(0)=0 \tag{9}$$

and inview of *Theorems 2* and *3*, the differential transformation for SFDE eq. (7) leads to the following recursive formulas:

$$\begin{aligned} \mathcal{U}(k)&=\frac{\Gamma[1+(k-1)\alpha]}{\Gamma(1+k\alpha)}\left[\frac{10\delta(k-1)-\mathcal{U}(k-1)}{5}-\frac{1}{10\mathcal{U}(k-1)}\right]\\ \mathcal{V}(k)&=\frac{\Gamma[1+(k-1)\alpha]}{\Gamma(1+k\alpha)}\left[\frac{1}{10\mathcal{U}(k-1)}-\frac{\mathcal{V}(k-1)}{5}\right]\\ \mathcal{W}(k)&=\frac{\Gamma[1+(k-1)\alpha]}{\Gamma(1+k\alpha)}\left[\frac{\mathcal{U}(k-1)-\mathcal{W}(k-1)}{5}-\frac{1}{10\mathcal{W}(k-1)}\right]\\ \mathcal{Y}(k)&=\frac{\Gamma[1+(k-1)\alpha]}{\Gamma(1+k\alpha)}\left[\frac{\mathcal{V}(k-1)-\mathcal{Y}(k-1)}{5}-\frac{1}{10\mathcal{Y}(k-1)}\right] \end{aligned} \tag{10}$$

Using eqs. (9) and (10) three terms of solution can be evaluated:

$$\mathcal{U}(1)=\frac{2}{\Gamma(1+\alpha)},\ \mathcal{V}(1)=0,\ \mathcal{W}(1)=0,\ \mathcal{Y}(1)=0 \tag{11}$$

$$\begin{aligned} &\mathcal{U}(2)=-\frac{3}{5\Gamma(1+2\alpha)},\ \mathcal{V}(2)=\frac{1}{\Gamma(1+2\alpha)},\ \mathcal{W}(2)=\frac{2}{5\Gamma(1+2\alpha)},\ \mathcal{Y}(2)=0\\ &\mathcal{U}(3)=-\frac{9}{50\Gamma(1+3\alpha)},\ \mathcal{V}(3)=\frac{-1}{10\Gamma(1+3\alpha)},\ \mathcal{W}(3)=\frac{-6}{25\Gamma(1+3\alpha)},\ \mathcal{Y}(3)=\frac{1}{25\Gamma(1+3\alpha)} \end{aligned} \tag{12}$$

then the inverse transform of the series solutions are given:

$$u(t) = -\frac{3t^{2\alpha}}{5\Gamma(1+2\alpha)} + \frac{9t^{3\alpha}}{50\Gamma(3\alpha+1)} + \frac{2t^{\alpha}}{\Gamma(1+\alpha)} + \dots$$

$$v(t) = \frac{t^{2\alpha}}{5\Gamma(1+2\alpha)} - \frac{t^{3\alpha}}{10\Gamma(1+3\alpha)} + \dots$$

$$w(t) = \frac{2t^{2\alpha}}{5\Gamma(2\alpha+1)} - \frac{6t^{3\alpha}}{25\Gamma(3\alpha+1)} + \dots$$

$$y(t) = \frac{t^{3\alpha}}{25\Gamma(3\alpha+1)} + \dots$$

If we continue this process all components of the exact solution can be obtained:

$$u(t) = \frac{20}{3}\left[1 - E_\alpha\left(\frac{-20}{3}t^\alpha\right)\right]$$

$$v(t) = \frac{10}{3}\left[1 - 3E_\alpha\left(\frac{-1}{5}t^\alpha\right) + 2E_\alpha\left(\frac{-3}{10}t^\alpha\right)\right]$$

$$w(t) = \frac{40}{9}\left[1 - \sum_{m=0}^{\infty}\frac{(1-m)\left(\frac{-3}{10}\right)^m}{\Gamma(m\alpha+1)}t^{m\alpha}\right]$$

$$y(t) = \frac{20}{9}\left[1 - 9E_\alpha\left(\frac{-1}{5}t^\alpha\right) + \sum_{m=0}^{\infty}\frac{(8-2m)\left(\frac{-3}{10}\right)^m}{\Gamma(m\alpha+1)}t^{m\alpha}\right]$$

Example 2. Consider following SFDE which is the concentrations of three reactants [23, 24]:

$$\mathcal{D}^\alpha u(t) = -\kappa_1 u + \kappa_2 vw,\ \mathcal{D}^\alpha v(t) = -\kappa_3 u - k_4 vw - \kappa_5 v^2,\ \mathcal{D}^\alpha w(t) = \kappa_6 v^2 \tag{13}$$

where κ_i, $i = 1, 2,..., 6$ are constants with ($\kappa_1 = 0.04$, $\kappa_2 = 0.01$, $\kappa_3 = 400$, $\kappa_4 = 100$, $\kappa_5 = 30000$, and $\kappa_6 = 30$).

The initial conditions:

$$u(0) = 1,\ v(0) = w(0) = 0 \tag{14}$$

the initial conditions are transformed by using eq. (6):

$$\mathcal{U}(0) = 1,\ \mathcal{V}(0) = \mathcal{W}(0) = 0 \tag{15}$$

and the differential transform method formula for concentration equations:

$$\mathcal{U}(k)=\frac{\Gamma\left[1+(\kappa-1)\alpha\right]}{\Gamma(\kappa\alpha+1)}\left[\kappa_2\sum_{i=0}^{\kappa-1}\mathcal{W}(i)\mathcal{V}(\kappa-1-i)-\kappa_1\mathcal{U}(\kappa-1)\right]$$

$$\mathcal{V}(\kappa)=\frac{\Gamma\left[1+(\kappa-1)\alpha\right]}{\Gamma(\kappa\alpha+1)}\left[-\kappa_4\sum_{i=0}^{\kappa-1}\mathcal{W}(i)\mathcal{V}(\kappa-1-i)-\kappa_5\sum_{i=0}^{\kappa-1}\mathcal{V}(i)\mathcal{V}(\kappa-1-i)+\kappa_3\mathcal{U}(\kappa-1)\right] \tag{16}$$

$$\mathcal{W}(\kappa)=\frac{\Gamma\left[1+(\kappa-1)\alpha\right]}{\Gamma(o\alpha+1)}\left[\kappa_6\sum_{i=0}^{\kappa-1}\mathcal{V}(i)\mathcal{V}(\kappa-1-i)\right]$$

Using eqs. (20) and (16) three terms of solution can be evaluated:

$$\mathcal{U}(1)=-\frac{0.04}{\Gamma(1+\alpha)},\ \mathcal{V}(1)=\frac{400}{\Gamma(1+\alpha)},\ \mathcal{W}(1)=0$$

$$\mathcal{U}(2)=\frac{0.0016}{\Gamma(1+2\alpha)},\ \mathcal{V}(2)=-\frac{16}{\Gamma(1+2\alpha)},\ \mathcal{W}(2)=0, \tag{17}$$

$$\mathcal{U}(3)=-\frac{0.000064}{\Gamma(1+3\alpha)},\ \mathcal{V}(3)=\frac{\left[0.64-\dfrac{4800000000\Gamma(1+2\alpha)}{\Gamma(\alpha+1)^2}\right]}{\Gamma(3\alpha+1)},\ \mathcal{W}(3)=\frac{4800000\Gamma(1+2\alpha)}{\Gamma(1+\alpha)^2\Gamma(1+3\alpha)}$$

The first four components of the series for $\alpha = 1$ are given:

$$u(t) = 1 - 0.04t + 0.0008t^2 - 0.0000106667t^3$$

$$v(t) = 400t - 8t^2 - 1.6\cdot 10^9 t^3,\ w(t) = 1600000t^3$$

and it is the same of solution in [22].

Example 3. The chemical reaction of two reactors might be presented in the form of SFDES [23, 24]:

$$\mathcal{D}^\alpha u(t)=-u,\quad u(0)=1,\ \mathcal{D}^\alpha v(t)=u-v^2,\quad v(0)=0,\ \mathcal{D}^\alpha w(t)=v^2,\ w(0)=0 \tag{18}$$

The Differential transform method formula for this reaction equation:

$$\mathcal{U}(k)=\frac{\Gamma\left[1+(\kappa-1)\alpha\right]}{\Gamma(\kappa\alpha+1)}\left[\mathcal{U}(\kappa-1)\right]$$

$$\mathcal{V}(\kappa)=\frac{\Gamma\left[1+(\kappa-1)\alpha\right]}{\Gamma(\kappa\alpha+1)}\left[\mathcal{U}(\kappa-1)-\sum_{i=0}^{\kappa-1}\mathcal{V}(i)\mathcal{V}(\kappa-1-i)\right] \tag{19}$$

$$\mathcal{W}(\kappa)=\frac{\Gamma\left[1+(\kappa-1)\alpha\right]}{\Gamma(\kappa\alpha+1)}\left[\sum_{i=0}^{\kappa-1}\mathcal{V}(i)\mathcal{V}(\kappa-1-i)\right]$$

$$\mathcal{U}(0)=1,\ \mathcal{V}(0)=\mathcal{W}(0)=0 \tag{20}$$

By using recurrence relation (19) and initial conditions (20) three terms of solutions are obtained:

$$\mathcal{U}(1)=-\frac{1}{\Gamma(1+\alpha)},\ \mathcal{V}(1)=\frac{1}{\Gamma(1+\alpha)},\ \mathcal{W}(1)=0$$
$$\mathcal{U}(2)=\frac{1}{\Gamma(1+2\alpha)},\ \mathcal{V}(2)=-\frac{1}{\Gamma(1+2\alpha)},\ \mathcal{W}(2)=0 \tag{21}$$
$$\mathcal{U}(3)=-\frac{1}{\Gamma(1+3\alpha)},\ \mathcal{V}(3)=\frac{\left[\Gamma(1+\alpha)^2-\Gamma(1+2\alpha)\right]}{\Gamma(1+\alpha)^2\Gamma(3\alpha+1)},\ \mathcal{W}(3)=\frac{\Gamma(2\alpha+1)}{\Gamma(\alpha+1)^2\Gamma(1+3\alpha)}$$

In view of eq. (4):

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

Which is the same of solution in [23, 24].

Conclusion

In this work, we applied the GDTM to obtain analytical and as well as approximate solution of the chemical reaction, reactor, and concentration equations. The obtained results using the GDTM agree well with the given numerical results by HPM and VIM and MVIM. Also it has been shown that the GDTM is very convenient and effective for solving SFDE.

Numerical computations in this paper has been done by using the MATHEMATICA.

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