Solving Time−fractional Chemical Engineering Equations by Modified Variational Iteration Method as Fixed Point Iteration Method

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ARTICLE INFO	ABSTRACT
Article History: Received 18 May 2015 Accepted 27 October 2015 Published online 8 May 2017 Academic Editor: Ivan Gutman **Keywords:** Fractional differential equations Variational iteration method Fixed point theory Chemical reactor	The variational iteration method (VIM) was extended to find approximate solutions of fractional chemical engineering equations. The Lagrange multipliers of the VIM were not identified explicitly. In this paper we improve the VIM by using concept of fixed point iteration method. Then this method was implemented for solving system of the time fractional chemical engineering equations. The obtained approximate solutions are compared with the numerical results in the literature to show the applicability, efficiency and accuracy of the method.

1. INTRODUCTION

Fractional calculus 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. [1−8].

The VIM is one of the powerful methods within the exact and approximate analyticalsolutions for solving nonlinear equations. The method was first initiated by [9], and it was successfully used by various researchers to investigate the linear andnonlinear problems [9, 10]. We mention that Jafari et.al. applied the variational iterationmethod to the modified Camassa-Holm and Degasperis−Procesi equations andfractional Davey−Stewartson equations, [10, 11]. Momani and Odibat [12] has implementedthe variational iteration method to solve nonlinear fractional differentialequations. It was shown by several authors (see e.g. Wazwaz [13]) that this method ismore powerful than existing techniques such as the Adomian decomposition method [14, 15], perturbation

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method, etc. Besides, the VIM gives rapidly convergent successiveapproximations of the exact solution if such a solution exists. Another importantadvantage is related to the fact that the VIM is capable of greatly reducing the sizeof calculation while still maintaining high accuracy of the numerical solution.

In [16, 17], it was shown that the VIM for obtaining approximate solutions of initialvalue problems is a version of the well-established fixed point iteration methods.In this paper, we are interested into approximate solutions of time fractionalchemical engineering problems as follow:

$$
\begin{aligned}
D_*^{\alpha 1} x_1(t) &= f_1(t, x_1, ..., x_n) \\
D_*^{\alpha 2} x_2(t) &= f_2(t, x_1, ..., x_n) \\
&\vdots \\
D_*^{\alpha n} x_n(t) &= f_n(t, x_1, ..., x_n)
\end{aligned}
\tag{1}
$$

where $D_*^{\alpha i}$ is the Caputo derivative of x_i of order a_i and $0 < a_i \le 1$, subject to the initial conditions

$$
x_1(0) = c_0, x_2(0) = c_2, ..., x_n(0) = c_n.
\tag{2}
$$

The general response expressions contain a parameter α 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. The organization of this paper is as follows: In Section 2, some basic definitions and properties of the fractional calculus are given. In section 3, we introduce variational iteration method and deform it to fixed point iteration method. In Section 4, the mentioned method in Section 3 is used to seek an approximate solution of chemical Eq. (1) with the given initial conditions (2). Also, the accuracy and efficiency of the scheme is investigated with three numerical illustrations in that section. Finally, Section 5 consists of some brief conclusions.

2. PRELIMINARY

In this section, we give some definitions and properties of the fractional calculus.

Definition 2.1. A real function $f(t); t > 0$, is said to be in the space $C_\mu, \mu \in R$, if there exists a real number $p(> \mu)$, such that $f(t) = t^p f_1(t)$, where $f_1(t) \in C(0, \infty)$, and it is said to be in the space C_μ^n, if and only if $f^{(n)} \in C_\mu$, $n \in N$.

Definition 2.2. The Riemann–Liouville fractional integral operator (J^α), of order $\alpha > 0$, of a function $f \in C_\mu, \mu \geq -1$, is defined as

$$J^\alpha f(t) = \frac{1}{\Gamma(\alpha)} \int_0^t (t-s)^{\alpha-1} f(s)ds, \quad \alpha > 0,$$

$$J^\alpha f(t) = f(t), \quad \alpha = 0.$$

The main properties of the operator (J^α) can be found in [18, 19], we mention only the following: For $f \in C_\mu, \mu \geq -1, \alpha, \beta \geq 0$ and $\gamma > -1$:

1. $J^\alpha J^\beta f(t) = J^{\alpha+\beta} f(t)$

2. $J^\alpha J^\beta f(t) = J^\beta J^\alpha f(t)$

3. $J^\alpha t^\gamma = \dfrac{\Gamma(\gamma+1)}{\Gamma(\alpha+\gamma+1)} t^{\alpha+\gamma}$

The Riemann–Liouville derivative has certain disadvantages when trying to model real-world phenomena with fractional differential equations. Therefore, we shall introduce a modified fractional differential operator D^α proposed by Caputo in his work on the theory of viscoelasticity [20].

Definition 2.3. The fractional derivative of $f(t)$ in the Caputo sense is defined as

$$D^\alpha f(t) = J^{n-\alpha} D^n f(t) = \frac{1}{\Gamma(n-\alpha)} \int_0^t (t-s)^{n-\alpha-1} f^{(n)}(s)ds$$

Also, we need here two of it's basic properties.

Lemma 2.1. If $n-1 < \alpha \leq n, n \in N$ and $f \in C_\mu^n, \mu \geq -1$ then $(D^\alpha J^\alpha)f(t) = f(t)$ and

$$(J^\alpha D^\alpha)f(t) = f(t) - \sum_{k=0}^{n-1} f^{(k)}(0^+)\frac{t^k}{k!}, t > 0.$$

3. THE VIM AND FIXED POINT ITERATION METHOD

To illustrate the basic concepts of the VIM we consider the following general nonlinear system:

$$L_i(u_i(t)) + N(u_1(t),...,u_m(t)) = g_i(t); \ i = 1,2,...,m, \tag{3}$$

where L_i is the linear operator and N_i is the nonlinear operator, and $g_i(t)$ is the inhomogeneous term. In the VIM correction function for Eq. (3) can be written as [9]:

$$u_{i,n+1}(t) = u_{i,n}(t) + \int_0^t \lambda_i(t-\tau)(L_i(u_{i,n}(\tau)) + N_i(\tilde{u}_1(\tau),...,\tilde{u}_m(\tau)) - g_i(\tau))d\tau; \ i = 1,2,...,m. \tag{4}$$

It is obvious that the successive approximation $u_{i,n}; n \geq 0$ can be established by determining λ_i, a general Lagrange multiplier, which can be identified optimally via the variational theory [21]. The function $\tilde{u}_{i,n}$ is a restricted variation, which means $\delta\tilde{u}_{i,n} = 0$. Therefore, we first determine the Lagrange multiplier λ_i that will be identified via integration by parts. The successive approximations $u_{i,n}(t), n > 0$ of the solution $u_i(t)$ will be readily obtained upon using the obtained Lagrange multiplier and by using any selective function $u_{i,0}$ as zeroth approximation which satisfy in given initial condition. Consequently, the exact solution may be procured by using,

$$u_i(t) = \lim_{n \to \infty} u_{i,n}(t) \tag{5}$$

Obviously, identification of the Lagrange multipliers is crucial to derive a variational iteration formula. Now, if we change our attitude and consider the VIM as special case of fixed point iteration [16, 17] we can find a simple and straight manner to determine Lagrange multipliers. In this order from (3) if L^{-1} exist then we have:

$$u_i(t) = \phi_i(t) + L_i^{-1}[g_i(t) - N_i(u_1(t),...,u_m(t))]; \ i = 1,2,...,m, \tag{6}$$

where $\phi_i(t)$ is $Ker(L_i)$ which determined by initial condition. In fact, we get Lagrange multipliers automatically while calculating inverse of operator L_i. Applying simple fixed point iteration method on (6) we get

$$u_{i,n+1}(t) = \phi_i(t) + L_i^{-1}[g_i(t) - N_i(u_{1,n}(t),...,u_{m,n}(t))]; \ i = 1,2,...,m. \tag{7}$$

Here recursive formula (7) are constructed for two special case of linear fractional differential equation as follow

$$\begin{cases} if \ L(u) = D^\alpha u \quad then \quad L^{-1}(f) = \int_0^t \frac{(t-\tau)^{\alpha-1}}{\Gamma(\alpha)} f(\tau)\, d\tau \quad and \\ \\ u_{n+1}(t) = \phi(t) + \int_0^t \frac{(t-\tau)^{\alpha-1}}{\Gamma(\alpha)} (g(\tau) - N(u_n(\tau)))\, d\tau, \end{cases} \tag{8}$$

$$\begin{cases} \text{if } L(u) = D^{\alpha}u + \omega u \text{ then } L^{-1}(f) = \int_0^t (t-\tau)^{\alpha-1} E_{\alpha,\alpha}(-\omega(t-\tau)^{\alpha}) f(\tau) d\tau \text{ and} \\ u_{n+1}(t) = \phi(t) + \int_0^t (t-\tau)^{\alpha-1} E_{\alpha,\alpha}(-\omega(t-\tau)^{\alpha})[g(\tau) - N(u_n(\tau))] d\tau. \end{cases} \quad (9)$$

4. TEST PROBLEMS

In this section, we present three examples to illustrate the applicability of new method to solve linear and nonlinear chemical fractional differential equations.

Example 4.1. *Chemical Reactor.* A reaction $A \to B$ 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 are given in the form of system of fractional differential equations are

$$D^{\alpha}u(t) = \frac{1}{\tau}(CA_0 - u) - \beta u$$

$$D^{\alpha}v(t) = \frac{-1}{\tau}v - \beta u$$

$$D^{\alpha}w(t) = \frac{1}{\tau}(u - w) - \beta w \quad (10)$$

$$D^{\alpha}y(t) = \frac{1}{\tau}(v - y) - \beta y$$

where CA_0 is the concentration of A at the inlet of first reactor. $CA_1 (= u)$ is the concentration of A at the outlet of the first reactor (and inlet of the second). $CA_2 (= w)$ is the concentration of A at the outlet of the second reactor. $CB_1 (= v)$ is the concentration of B at the outlet of the first reactor (and inlet of the second). $CB_2 (= y)$ is the concentration of B in the second reactor. τ is the residence time for each reactor, and β is the rate constant for reaction of A to produce B. Consider CA_0 is equal to 10, $\beta = 0.1$ and $\tau = 5$. Initial conditions

$$CA_1(0) = u(0) = 0, CA_2(0) = w(0) = 0, CB_1(0) = v(0) = 0, CB_2(0) = y(0) = 0 \quad (11)$$

By setting L_1, L_2, L_3 and L_4 for this system

$$L_1(u(t)) = D^\alpha u(t) + \frac{3}{10} u(t)$$

$$L_2(v(t)) = D^\alpha v(t) + \frac{1}{5} v(t)$$

$$L_3(w(t)) = D^\alpha w(t) + \frac{3}{10} w(t)$$ (12)

$$L_4(y(t)) = D^\alpha y(t) + \frac{3}{10} y(t)$$

and using (9), the transform of Eq. (10) with initial conditions (11) leads to the following recurrence relations:

$$u_{n+1}(t) = \int_0^t (t-\tau)^{\alpha-1} E_{\alpha,\alpha}(-\frac{3}{10}(t-\tau)^\alpha)(2)\,d\tau$$ (13)

$$v_{n+1}(t) = \int_0^t (t-\tau)^{\alpha-1} E_{\alpha,\alpha}(-\frac{1}{5}(t-\tau)^\alpha)[\frac{1}{10}u_n(\tau)]\,d\tau$$ (14)

$$w_{n+1}(t) = \int_0^t (t-\tau)^{\alpha-1} E_{\alpha,\alpha}(-\frac{3}{10}(t-\tau)^\alpha)[\frac{1}{5}u_n(\tau)]\,d\tau$$ (15)

$$y_{n+1}(t) = \int_0^t (t-\tau)^{\alpha-1} E_{\alpha,\alpha}(-\frac{3}{10}(t-\tau)^\alpha)[\frac{1}{5}v_n(\tau)]\,d\tau$$ (16)

We start with initial approximations $u_0(t) = 0, v_0(t) = 0, w_0(t) = 0, y_0(t) = 0$, which satisfy in Eqs. (11). In right hand said of Eq.(13) there isn't u_n so its exact solution will obtain at first iteration . In the second iteration we get exact solutions of $v(t)$ and $w(t)$ by using the exact solution of $u(t) = u_1(t)$ in right hand said of Eqs. (14) and (15). Finally, in the third iteration all exact solutions can be obtain as follow

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

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

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

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

Example 4.2. *Concentration of Reactants.* The concentrations of three reactants are in the form of a system of nonlinear FDEs as

$$D^\alpha u(t) = -k_1 u + k_2 v\, w$$
$$D^\alpha v(t) = -k_3 u - k_4 v\, w - k_5 v^2 \tag{17}$$
$$D^\alpha w(t) = k_6 v^2$$

where k_1, k_2, k_3, k_4, k_5 and k_6 are constant parameters ($k_1 = 0.04$, $k_2 = 0.01$, $k_3 = 400$, $k_4 = 100$, $k_5 = 30000$, $k_6 = 30$). The initial conditions are given by

$$u(0) = 1, \quad v(0) = 0, \quad w(0) = 0. \tag{18}$$

By setting $L = D^\alpha$ as a linear operator for every equation in (17) and using (8), we get the recursive formula for concentration equations as follow

$$u_{n+1}(t) = -\int_0^t \lambda(t-\tau)(-k_1 u_n(\tau) + k_2 v_n(\tau) w_n(\tau))\, d\tau$$

$$v_{n+1}(t) = -\int_0^t \lambda(t-\tau)(-k_3 u_n(\tau) + k_4 v_n(\tau) w_n(\tau) + k_5 v_n^2(\tau))\, d\tau \tag{19}$$

$$w_{n+1}(t) = \int_0^t \lambda(t-\tau)(k_6 v_n^2(\tau))\, d\tau$$

where

$$\lambda(t,\tau) = \frac{(t-\tau)^{\alpha-1}}{\Gamma(\alpha)}$$

By starting with an initial approximation $u_0(t) = 1$, $v_0(t) = 0$ and $w_0(t) = 0$ given by Eq. (18) and using the above iteration formulae (19) we can directly obtain the other components. The first four components of the series are given by

$$u(t) = 1 - \frac{t^\alpha}{25\Gamma(1+\alpha)} + \frac{t^{2\alpha}}{625\Gamma(1+2\alpha)} - \frac{t^{3\alpha}}{15625\Gamma(1+3\alpha)}$$

$$v(t) = -\frac{400 t^\alpha}{\Gamma(1+\alpha)} + \frac{16 t^{2\alpha}}{\Gamma(1+2\alpha)} - \frac{4800000000 t^{3\alpha}}{\Gamma(1+\alpha)^2 \Gamma(1+3\alpha)} \tag{20}$$

$$w(t) = \frac{4800000 t^{3\alpha}}{\Gamma(1+\alpha)^2 \Gamma(1+3\alpha)}$$

For $\alpha = 1$ we have

$$u(t) = 1 - 0.04t + 0.0008 t^2 - 0.000106667 t^3$$

$$v(t) = 400t - 8t^2 - 1.6 \times 10^9 t^3$$

$$w(t) = 1600000 t^3$$

which is the same of solution in [22].

Example 4.3. Chemical Reaction there is the system of nonlinear FDE equation which representing a nonlinear reaction,

$$D^{\alpha}u(t) = -u$$

$$D^{\alpha}v(t) = u - v^2 \quad (21)$$

$$D^{\alpha}w(t) = v^2$$

with the initial conditions are given by

$$u(0) = 1, \ v(0) = 1, \ w(0) = 0. \tag{22}$$

By setting $L = D^{\alpha}$ as a linear operator for every equation in (21) and using (8), the recursive formula for reaction equation (21) is

$$u_{n+1}(t) = 1 - \int_0^t \lambda(t-\tau)u_n(\tau)d\tau$$

$$v_{n+1}(t) = -\int_0^t \lambda(t-\tau)(-u_n(\tau)v_n^2(\tau))\,d\tau \quad (23)$$

$$w_{n+1}(t) = \int_0^t \lambda(t-\tau)v_n^2(\tau)\,d\tau$$

where

$$\lambda(t,\tau) = \frac{(t-\tau)^{\alpha-1}}{\Gamma(\alpha)}.$$

By using recurrence relation (23) and initial approximation $u_0(t) = 1, v_0(t) = 0$ and $w_0(t) = 0$ given by Eq. (22) three Iteration terms of solutions are obtained as follow:

$$\begin{cases} u_1(t) = 1 - \dfrac{t^{\alpha}}{\Gamma(1+\alpha)}, \\[2mm] v_1(t) = \dfrac{t^{\alpha}}{\Gamma(1+\alpha)}, \\[2mm] w_1(t) = 0, \end{cases} \tag{24}$$

$$\begin{cases} u_2(t) = 1 - \dfrac{t^{\alpha}}{\Gamma(1+\alpha)} + \dfrac{t^{2\alpha}}{\Gamma(1+2\alpha)}, \\[3mm] v_2(t) = \dfrac{t^{\alpha}}{\Gamma(1+\alpha)} - \dfrac{t^{2\alpha}}{\Gamma(1+2\alpha)} - \dfrac{t^{3\alpha}\Gamma(1+2\alpha)}{\Gamma(1+\alpha)^2\Gamma(1+3\alpha)}, \\[3mm] w_2(t) = \dfrac{t^{3\alpha}\Gamma(1+2\alpha)}{\Gamma(1+\alpha)^2\Gamma(1+3\alpha)}, \end{cases} \tag{25}$$

$$
\begin{cases}
u_3(t) = 1 - \dfrac{t^{\alpha}}{\Gamma(1+\alpha)} + \dfrac{t^{2\alpha}}{\Gamma(1+2\alpha)} - \dfrac{t^{3\alpha}}{\Gamma(1+3\alpha)}, \\[3ex]
v_3(t) = \dfrac{t^{\alpha}}{\Gamma(1+\alpha)} - \dfrac{t^{2\alpha}}{\Gamma(1+2\alpha)} - \left(\dfrac{1}{\Gamma(1+3\alpha)} - \dfrac{\Gamma(1+2\alpha)}{\Gamma(1+\alpha)^2\Gamma(1+3\alpha)}\right)t^{3\alpha}, \\[3ex]
w_3(t) = \dfrac{t^{3\alpha}\Gamma(1+2\alpha)}{\Gamma(1+\alpha)^2\Gamma(1+3\alpha)}.
\end{cases}
\tag{26}
$$

In the third iteration the first four components of the series solution are expressed and we have the following approximate solution

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

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

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

which is the same of solution in [23].

5. CONCLUSION

For illustration purposes, we considered three examples. Results obtained using the scheme presented here agree well with the numerical results presented elsewhere. Results also show that the numerical scheme is very effective and convenient for solving nonlinear partial differential equations of fractional order. The numerical computations associated with the three examples discussed above were performed by using the Computer Algebra System Mathematica.

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