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A semi-analytical iterative technique for solving chemistry problems

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Abstract The main aim and contribution of the current paper is to implement a semi-analytical iterative method suggested by Temimi and Ansari in 2011 namely (TAM) to solve two chemical problems. An approximate solution obtained by the TAM provides fast convergence. The current chemical problems are the absorption of carbon dioxide into phenyl glycidyl ether and the other system is a chemical kinetics problem. These problems are represented by systems of nonlinear ordinary differential equations that contain boundary conditions and initial conditions. Error analysis of the approximate solutions is studied using the error remainder and the maximal error remainder. Exponential rate for the convergence is observed. For both problems the results of the TAM are compared with other results obtained by previous methods available in the literature. The results demonstrate that the method has many merits such as being derivative-free, and overcoming the difficulty arising in calculating Adomian polynomials to handle the non-linear terms in Adomian Decomposition Method (ADM). It does not require to calculate Lagrange multiplier in Variational Iteration Method (VIM) in which the terms of the sequence become complex after several iterations, thus, analytical evaluation of terms becomes very difficult or impossible in VIM. No need to construct a homotopy in Homotopy Perturbation Method (HPM) and solve the corresponding algebraic equations. The MATHEMATICA® 9 software was used to evaluate terms in the iterative process.

1. Introduction

In practical life, there are many phenomena in Chemistry, Mechanics, Biology, Physics and Fluid Dynamics can be represented by either linear or nonlinear differential equations. In Chemistry for example, the condensations of carbon dioxide and phenyl glycidyl ether and chemical kinetics problem are represented by systems of nonlinear ordinary differential equations (ODEs).

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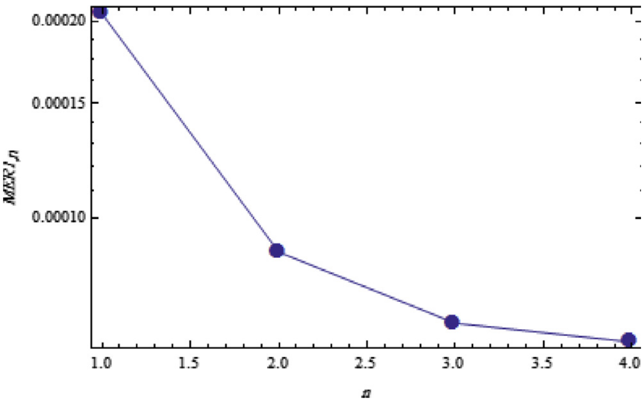

Figure 1 Logarithmic plots of $MER_{1,n}$ against n is 1 through 4 and $m = 1$.

Carbon dioxide (CO_2) is used in many fields such as plant photosynthesis, fire extinguishers, and removing caffeine from coffee. Carbon dioxide is generally a beneficial gas which consists of one carbon atom and two oxygen atoms (Duan et al., 2015; AL-Jawary and Radhi, 2015; Muthukaruppan et al., 2012). On the other hand the chemical kinetics system introduced by Robertson in 1966 is a nonlinear model (Aminikhah, 2011; Ganji et al., 2007).

Many types of ODEs are solved either analytically or numerically for examples: the Variational Iteration Method (VIM) is used to solve the nonlinear settling particle equation of Motion (Ganji, 2012). The He's Homotopy Perturbation Method (HPM), which does not need small parameter in the equation is implemented for solving the nonlinear Hirota–Satsuma coupled KdV partial differential equation (Ganji and Rafei, 2006). Deniz and Bildik (2014) have implemented the comparison of Adomian Decomposition Method (ADM) and Taylor matrix method for solving different kinds of partial differential equations. Also, Bildik and Deniz (2015a) have used both Taylor collocation and ADM for solving systems of ordinary differential equations. Moreover, Bildik and Deniz (2015b) have successfully implemented taylor collocation method, lambert w function and VIM for solving systems of delay differential equations. Wazwaz (2005) has used the ADM for solving the Bratu-type equations.

Several methods have been used to solve the system of condensations of carbon dioxide and phenyl glycidyl ether and obtained analytical approximate solutions such as, Adomian Decomposition Method (ADM) was applied to simple steady-state condensations of CO_2 and PGE (Duan et al., 2015; Muthukaruppan et al., 2012), the VIM (AL-Jawary and Radhi, 2015) and the iterative method (DJM) (AL-Jawary et al., 2016).

On the other hand, the chemical kinetics problem is solved by many methods and the solution is obtained as approximate solutions. Ganji et al. (2007) have successfully implemented both the VIM and HPM for the system. Khader (2013) has used the so-called Picard–Pade technique to solve the system. Also, Aminikhah (2011) has used (HPM) to solve the system. Moreover, Matinfar et al. (2014) have applied the homotopy analysis method (HAM) and the solutions obtained by HAM have high accuracy in comparison with HPM and VIM introduced in Ganji et al. (2007).

Furthermore, some analytic and approximate methods have recently been used and implemented to solve different chemical and physics problems and other sciences for examples: Differential Transform Method (DTM) has been used to solve fourth order singularly perturbed two-point boundary value problems which occur in chemical reactor theory (El-Zahar, 2013). Matinfar et al. (2015) have found that the interaction of electromagnetic wave with electron is solved by VIM. In Vazquez-Leal et al. (2015) the authors present a comparison of Homotopy Perturbation Method (HPM), Nonlinearities Distribution Homotopy Perturbation Method (NDHPM), Picard, and Picard–Padé methods to solve Michaelis–Menten equation. Also, Cá zares-Ramírez and Espinosa-Paredes (2016) the authors studied the behavior of heat and mass transfer during hydrogen generation in the core of the boiling water reactor (BWR). Makinde (2007a,b) has implemented the ADM to compute an approximation to the solution of the non-linear system of differential equations governing the SIR epidemic model and the ratio-dependent predator–prey system with constant effort harvesting. In addition, Makinde (2009) has successfully applied the ADM coupled with Padé approximation technique and VIM to approximate the solution of the governing non-linear systems of a mathematical model that describes the dynamics of re-infection under the assumption that the vaccine induced immune protection may wane over time.

Recently, Temimi and Ansari (2011a) have introduced the semi-analytical iterative technique in 2011 for solving nonlinear problems. The TAM is used for solving many differential equations, such as nonlinear second order multi-point boundary value problems (Temimi and Ansari, 2011b), nonlinear ordinary differential equations (Temimi and Ansari, 2015), korteweg–de vries equations (Ehsani et al., 2013) and the results obtained from the method indicate that the TAM is accurate, fast, appropriate, time saver and has a higher convergence.

In this paper, the TAM will be applied to solve two chemical problems. The first problem is a nonlinear system of the concentrations of carbon dioxide and phenyl glycidyl ether. The other is a chemical kinetics problem which is also represented by a nonlinear system of ODEs. Special discussion is given for the study of the convergence based on Temimi and Ansari (2015), the error analysis of the method (TAM), the error remainders and the convergence of the TAM will be discussed.

This paper has been organized as follows: In Section 2, the steady-state of the chemical problems will be introduced. In Section 3, the basic idea of TAM is presented and discussed. In Section 4, solving the chemical problems by the TAM will be given. In Section 5, the convergence and error analysis are introduced and discussed. In Section 7, the numerical simulation will be illustrated and discussed. Finally, the conclusion in Section 8 will be given.

2. Steady-state of the chemical problems

2.1. Condensations of carbon dioxide and phenyl glycidyl ether

The mathematical formulation of the concentrations of Carbon dioxide and phenyl glycidyl ether can be shown as follows (Muthukaruppan et al., 2012):