

Review

Akbari-Ganji's method "AGM" to chemical reactor design for non-isothermal and non-adiabatic of mixed flow reactors

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In this paper, the chemical reactor with the energy changing (non-isotherm) and non-monotonic reactions in a mixed flow is investigated and also the sets of complex nonlinear differential equations obtained from the reaction behavior in these systems are solved by a new method. The set of differential equations are consisted of the mass equilibrium and energy (temperature) changing at concentration governing the reactors. Our purpose is to enhance the ability of solving the mentioned nonlinear differential equation with a simple and innovative approach which entitled "Akbari-Ganji's Method" or "AGM". Comparisons are made between AGM and numerical method (Runge- Kutta45). The results show that this method is very effective and simple and can be applied for other nonlinear problems.

Key words: New method, Akbari-Ganji's method (AGM), nonlinear differential equation, mixed flow, non-monotonic reactions, non-adiabatic, reactor design.

INTRODUCTION

In this study, a mixed flow reactor is investigated through resolving a set of nonlinear differential equations governing its chemical reactions by a new analytical method. The interaction of chemical reactions in chemical reactors attracted the attention of many researchers according to the complexity of the reaction kinetics since the knowledge of real performance of reactions in reactors is helpful in the analysis and design process of reactors and are of great importance for researchers in the fields of

mechanical and chemical engineering. In the context of designing a reactor, the reaction properties of chemical reactants especially in the presence of catalyst are very important since most of these reactions are complex and completely nonlinear which makes the designing process to be critical. In fact, analytical resolution of nonlinear differential equations governing these processes is a very difficult task which requires a precise and convenient analytical method. Therefore, in this paper, a new analytical

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method capable of solving nonlinear differential equations governing the design of chemical reactors has been presented entitled AGM (Akbari-Ganji's method) which can be applied in all of the fields of engineering and basic sciences because of its high precision and convergence in dealing with problems with high nonlinearity. Consequently, many new techniques have been presented in the literature namely Homotopy Perturbation Method (HPM) (Ganji, et al. 2009a; Ganji, et al. 2009b), the Elliptic Lindstedt-Poincare method (LP) (Masdemont* 2005; Navarro 2008), Adomian Decomposition Method (Abbasbandy 2007; Adomian 1994), EXP-function Method (Chang, 2011; He and Wu, 2006) and variational Iteration Method (Ganji, et al. 2007; He 1999). For instance, the classical Blasius' equation was solved using VIM and also this method was utilized to give approximate solutions for some well-known non-linear problems. Another analytical method called the He's Amplitude Frequency Formulation method (Akbari, et al. 2014c) which was first presented by Ji-Huan He. This method rapidly gives convergent successive approximations of the exact solution. Other methods do not have this ability to precisely and accurately solve the problems, so nonlinear differential equations such as the problem presented in this case study should be solved by utilizing new approaches like AGM (Akbari, et al. 2014a; Akbari, et al. 2014b; Akbari, et al. 2014d).

The analytical method [Akbari-Ganji's Method (AGM)]

Boundary conditions and initial conditions are required for the calculation procedure used in analytical methods for each linear and nonlinear differential equation. In order to comprehend the given method, two differential equations governing engineering processes will be solved in this new manner. In accordance with the given boundary conditions, the methodology of AGM can be presented in the following form:

$$p_k : f(u, u', u'', \dots, u^{(m)}) = 0 \quad ; \quad u = u(x) \quad (1)$$

Boundary conditions:

$$\begin{cases} u(x) = u_0, u'(x) = u_1, \dots, u^{(m-1)}(x) = u_{m-1} & \text{at } x = 0 \\ u(x) = u_{L_0}, u'(x) = u_{L_1}, \dots, u^{(m-1)}(x) = u_{L_{m-1}} & \text{at } x = L \end{cases} \quad (2)$$

To solve the first differential equation in respect to the boundary conditions in $x=L$ in Equation 2, the series of letters in the n th order with constant coefficients which is the answer of the first differential equation is considered as follows:

$$u(x) = \sum_{i=0}^n a_i x^i = a_0 + a_1 x^1 + a_2 x^2 + \dots + a_n x^n \quad (3)$$

With more precise answer from Equation 1, the more we have choice of series sentences from Equation 3. Approximately five or six sentences from the series are enough to solve nonlinear differential equations. In the answer of Equation 3 regarding the series from degree (n), there are ($n+1$) unknown coefficients that need ($n+1$) equations to be specified. The boundary conditions of Equation 2 are used to solve a set of equations which consisting of ($n+1$) ones.

The boundary conditions are applied on the functions as follows:

a) The application of the boundary conditions for the answer of differential Equation 2 is presented in the following form:

If $x = 0$:

$$\begin{cases} u(0) = a_0 = u_0 \\ u'(0) = a_1 = u_1 \\ u''(0) = a_2 = u_2 \\ \vdots \quad \quad \quad \vdots \quad \quad \quad \vdots \end{cases} \quad (4)$$

And when $x = L$:

$$\begin{cases} u(L) = a_0 + a_1 L + a_2 L^2 + \dots + a_n L^n = u_{L_0} \\ u'(L) = a_1 + 2a_2 L + 3a_3 L^2 + \dots + n a_n L^{n-1} = u_{L_1} \\ u''(L) = 2a_2 + 6a_3 L + 12a_4 L^2 + \dots + n(n-1)a_n L^{n-2} = u_{L_{m-1}} \\ \vdots \quad \quad \quad \vdots \quad \quad \quad \vdots \quad \quad \quad \vdots \quad \quad \quad \vdots \end{cases} \quad (5)$$

b) After substituting Equation 3 into Equation 1, the application of the boundary conditions on differential Equation 1 is done according to the following procedure:

$$\begin{matrix} p_0 : f(u(0), u'(0), u''(0), \dots, u^{(m)}(0)) \\ p_1 : f(u(L), u'(L), u''(L), \dots, u^{(m)}(L)) \\ \vdots \quad \quad \quad \vdots \quad \quad \quad \vdots \quad \quad \quad \vdots \quad \quad \quad \vdots \end{matrix} \quad (6)$$

With regard to the choice of n ; ($n < m$) sentences from Equation 3 and in order to make a set of equations consisting of ($n+1$) equations and ($n+1$) the unknown, we confronted a number of additional unknowns which are indeed the coefficients of Equation 3. Therefore, to resolve this problem, we should derive m times from Equation 1 according to the additional unknowns in the aforementioned set of differential equations and then this is the time to apply the boundary conditions of Equation 2

as follows.

$$\begin{aligned} P'_k &: f(u', u'', u''', \dots, u^{(m+1)}) \\ P''_k &: f(u'', u''', u^{(IV)}, \dots, u^{(m+2)}) \\ &\vdots \\ &\vdots \\ &\vdots \end{aligned} \quad (7)$$

c) Application of the boundary conditions on the derivatives of the differential equation P_k in Equation 7 is done in the form of:

$$P'_k : \begin{cases} f(u'(0), u''(0), u'''(0), \dots, u^{(m+1)}(0)) \\ f(u'(L), u''(L), u'''(L), \dots, u^{(m+1)}(L)) \end{cases} \quad (8)$$

$$P''_k : \begin{cases} f(u''(0), u'''(0), \dots, u^{(m+2)}(0)) \\ f(u''(L), u'''(L), \dots, u^{(m+2)}(L)) \end{cases} \quad (9)$$

($n+1$) Equations can be made from Equation 4 to Equations 8 and 9, so that ($n+1$) unknown coefficients of Eq.(3), for example $a_0, a_1, a_2 \dots a_n$ will be computed. The answer of the nonlinear differential Equation 1 will be gained by determining coefficients of Equation 3.

$$(V \rho C_p + V_m \rho_m C_{pm}) \frac{dT}{dt} = q \rho C_p (T_f - T) + V K_0 e^{-E/RT} \cdot \frac{C_A}{(I + K_0 e^{-E/RT})^2} (-\Delta H) + A_c U (T - T_c) \quad (14)$$

where $\Delta H, U, A_h, T_w, V, V_m, \rho, \rho_m, q, C_{Af}, T_f$ and A_c are the heat of chemical reaction, the total coefficient of heat transmission, the heat exchange rate, the external wall temperature of the reactor, the volume of the reaction mixture, the volume of the metal parts of the reactor (stirrer and cooling coil), the density of the reaction and metal parts, volumetric flow rate of feed, the feed concentration of reactant A, feed temperature and area of transfer between the reactor and the cooling coil, respectively.

The dimensionless form of Equations 13 and 14 can be written as follow:

$$f(t): \frac{dX_A(\tau)}{d\tau} = [X_{Af} - X_A(\tau)] - \frac{\alpha_0 e^{-\frac{\gamma}{Y(\tau)}} X_A(\tau)}{\{I + K_0 e^{-\frac{\gamma}{Y(\tau)}} X_A(\tau)\}^2} \quad (15)$$

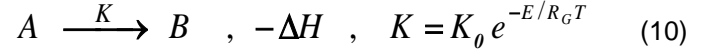
$$g(t): (I + L_m) \frac{dY(\tau)}{d\tau} = [Y_{Af} - Y(\tau)] - \frac{\alpha_0 e^{-\frac{\gamma}{Y(\tau)}} X_A(\tau)}{\{I + K_0 e^{-\frac{\gamma}{Y(\tau)}} X_A(\tau)\}^2} - K_c (Y(\tau) - Y_c) \quad (16)$$

The dimensional parameters are defined as follows:

THEORETICAL FORMULATION

Mixed flow to chemical reaction

The mixed chemical reactor is considered for chemical reaction is shown in Figure 1. The chemical reaction is considered as follows:



Supposing the kinetics of the reaction are non-monotonic for component (A) which is considered as:

$$r_A = \frac{K C_A}{(1 + K C_A)^2} \quad (11)$$

$$or \quad r_A = K_0 e^{-E/R_G T} \frac{C_A}{(1 + K_0 e^{-E/R_G T} C_A)^2} \quad (12)$$

Using the energy and mass balance equations for the reactor leads to the following equations:

$$V \frac{dC_A}{dt} = q(C_{Af} - C_A) - V K_0 e^{-E/RT} \cdot \frac{C_A}{(I + K_0 e^{-E/RT})^2} \quad (13)$$

$$\tau = \frac{t q}{V}, \quad \alpha_0 = \frac{V K_0}{q}, \quad L_m = \frac{V_m \rho_m C_{pm}}{V \rho C_p}, \quad \gamma = \frac{E}{R_G T_{ref}}, \quad X_A = \frac{C_A}{C_{ref}}, \quad Y = \frac{T}{T_{ref}} \quad (17)$$

$$\beta = \frac{(-\Delta H) C_{ref}}{\rho C_p T_{ref}}, \quad X_{Af} = \frac{C_{Af}}{C_{ref}}, \quad Y = \frac{T}{T_{ref}}, \quad K_c = \frac{A_c U}{q \rho C_p}$$

It is worthy to note that the subscript *ref* in Equation 17 denotes the reference parameter.

The initial conditions in plug chemical reactor are described as follows:

$$X_A(t) = X_{A0}, \quad Y(t) = Y_0 \quad at \quad t = 0 \quad (18)$$

And the following physical values are considered for the presented problem:

$$\begin{aligned} X_{A0} = 0.2, \quad Y_0 = 1.5, \quad \gamma = 0.5, \quad K_c = 0.5, \quad L_m = 1.4, \quad \alpha_0 = 0.2 \\ X_{Af} = 0.7, \quad Y_c = 1.2, \quad Y_f = 2, \quad K_0 = 0.1 \end{aligned} \quad (19)$$

Solving the nonlinear differential equation by AGM

In the AGM calculation procedure, there is no need to use

the Taylor series expansion for the exponential term $\exp(\gamma/Y(\tau)) = e^{-\frac{\gamma}{Y(\tau)}}$; whereas in the other methods such as Homotopy Perturbation Method (HPM), (Adomian's Decomposition Method (ADM), VIM and DTM (Differential Transform Method), we should convert such terms into polynomials using Taylor series expansions. As a result, the obtained solution by AGM is more accurate and precise in comparison with the afore-mentioned methods. On the basis of the given explanations in the previous section, the answer of Equation 16 in this method is considered by the AGM as polynomials series with constant coefficients as follows:

$$X_A(t) = \sum_{k=0}^6 a_k t^k = a_0 + a_1 t + a_2 t^2 + a_3 t^3 + a_4 t^4 + a_5 t^5 + a_6 t^6 + \dots$$

$$Y(t) = \sum_{k=0}^6 b_k t^k = b_0 + b_1 t + b_2 t^2 + b_3 t^3 + b_4 t^4 + b_5 t^5 + b_6 t^6 + \dots$$

(20)

The constant coefficients of Equation 20 which are $\{a_0, a_1, \dots, a_6$ and $b_0, b_1, \dots, b_6\}$ can easily be computed by applying boundary conditions according to the physical aspects of the problem.

Applying initial or boundary conditions in AGM

Based on the given explanations in the previous section, the constant coefficients $\{a_0, a_1, \dots, a_6$ and $b_0, b_1, \dots, b_6\}$ of Equation 20 are achieved with respect to the given initial conditions and these initial conditions are applied the following two ways.

a) The initial conditions are applied on Equation 20 in the form of:

$$X_A(t=0) = 0.2 \quad \rightarrow \quad a_0 = 0.2 \quad (21)$$

$$Y(t=0) = 1.5 \quad \rightarrow \quad b_0 = 1.5 \quad (22)$$

b) The application of initial or boundary conditions on the main differential equations which in this case are Equations 15 and 16 and also on their derivatives is done in the following general form:

$$f(X_{A(IC)}) \rightarrow f(X_{A(IC)})=0, \quad f'(X_{A(IC)})=0, \quad f''(X_{A(IC)})=0, \dots$$

$$g(Y_{(IC)}) \rightarrow f(Y_{(IC)})=0, \quad f'(Y_{(IC)})=0, \quad f''(Y_{(IC)})=0, \dots$$

(23)

where (IC) is the abbreviation of initial conditions.

Therefore, after substituting Equation 20 which has

been considered as the answer of the main differential equation into $f(t)$ and $g(t)$, the initial conditions are applied on the obtained equation and also on its derivatives as follows:

$$f(X_{A(t=0)}): a_1 \{10 + a_0 e^{-\frac{0.5}{b_0}}\}^2 = 70 - 100a_0 - e^{-\frac{1}{2b_0}} (6a_0 + 20a_0^2) + e^{-\frac{1}{b_0^2}} (0.7a_0^2 - a_0^3)$$

(24)

$$g(Y_{A(t=0)}): 2.4b_1 \{10 + a_0 e^{-\frac{0.5}{b_0}}\}^2 = 260 - 150b_0 a_0^2 + e^{-\frac{1}{2b_0}} (72a_0 - 30a_0 b_0)$$

$$+ e^{-\frac{1}{b_0^2}} (2.6a_0^2 - 1.5b_0)$$

(25)

For the first derivative,

$$f'(X_{A(t=0)}): 2a_2 b_0^2 \{1 + 0.3a_0 e^{-\frac{0.5}{b_0}} + 0.03a_0^2 e^{-\frac{1}{b_0^2}} + 0.001a_0^3 e^{-\frac{1.5}{b_0^3}}\} = -a_1 b_0^2 +$$

$$+ e^{-\frac{0.5}{b_0}} (0.3a_0 a_1 b_0^2 + 0.1b_1 a_0 + 0.2a_1 b_0^2) +$$

$$a_0 e^{-\frac{1}{b_0^2}} (0.03a_0 a_1 b_0^2 - 0.01a_0 b_0 - 0.02a_1 b_0^2) + 0.001a_1 b_0^2 a_0^3 e^{-\frac{1.5}{b_0^3}}$$

(26)

and

$$g'(Y_{(t=0)}): 4.8b_2 b_0^2 \{1 + 0.3a_0 e^{-\frac{0.5}{b_0}} + 0.03a_0^2 e^{-\frac{1}{b_0^2}} + 0.001a_0^3 e^{-\frac{1.5}{b_0^3}}\} = -1.5b_1 b_0^2 +$$

$$+ e^{-\frac{0.5}{b_0}} (0.45a_0 b_1 b_0^2 - 0.1b_1 a_0 - 0.2a_1 b_0^2) +$$

$$e^{-\frac{1}{b_0^2}} (0.045b_1 a_0^2 b_0^2 + 0.02a_0 a_1 b_0^2 + 0.01b_1 a_0^2) + 0.0015b_1 b_0^2 a_0^3 e^{-\frac{1.5}{b_0^3}}$$

(27)

And for the higher derivative, we have:

$$f^{(n)}(X_{A(t=0)}), \quad g^{(n)}(Y_{(t=0)}), \quad n = 2, 3, \dots, 6 \quad (28)$$

By solving a set of algebraic equations which is consisted of fourteen equations with fourteen unknowns, the constant coefficients $\{a_0, a_1, \dots, a_6$ and $b_0, b_1, \dots, b_6\}$ of Equation 20 can easily be yielded as follows:

$$a_0 = 0.2, a_1 = 0.427, a_2 = -0.2685, a_3 = 0.10244, a_4 = -0.02983,$$

$$a_5 = 0.007218, a_6 = -0.0015711, b_0 = 1.5, b_1 = 0.15744, b_2 = -0.03569$$

$$b_3 = 0.002043, b_4 = 0.001437, b_5 = -0.0007016, b_6 = 0.00022647$$

(29)

After substituting the obtained values from Equation 29

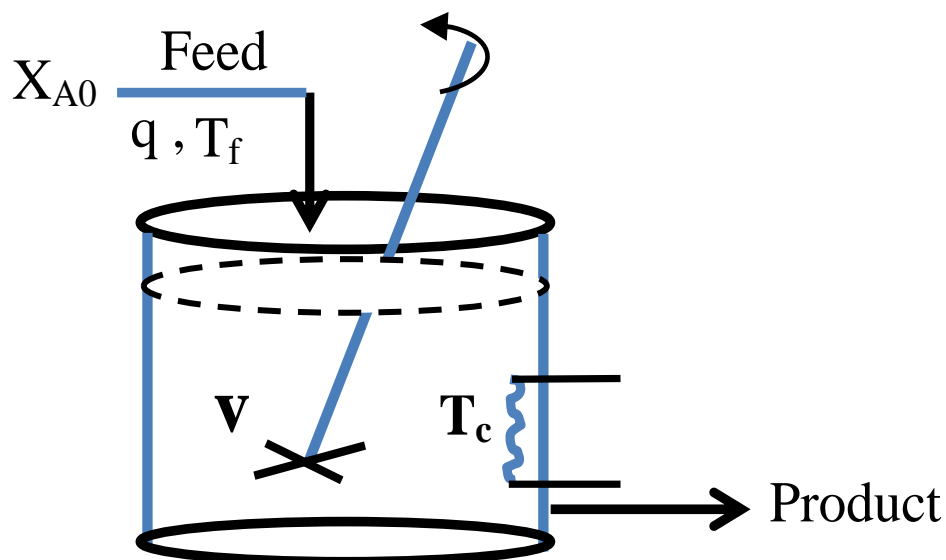


Figure 1. Schematic of the problem (mixed chemical reactor ,CSTR).

into Equation 20, the solution of the presented problem will be obtained as follows:

$$X_A(\tau) = 0.2 + 0.472\tau - 0.2685\tau^2 + 0.10244\tau^3 - 0.02983\tau^4 + 0.007218\tau^5 - 0.0015711\tau^6 \quad (30)$$

and

$$Y(\tau) = 1.5 + 0.15744\tau - 0.03569\tau^2 + 0.002043\tau^3 + 0.001437\tau^4 - 0.0007016\tau^5 + 0.00022646\tau^6 \quad (31)$$

Then, the charts of the obtained solution and its derivative are shown in Figures 2 to 8. It is evident that more reactor volume is needed in order to obtain more concentration of component (A) for this reaction. According to Figures 2 to 8, it is concluded that the more time is needed in reactor for the chemical reaction to obtain more concentration of component (A):

Numerical solution

In accordance with Equations 15 and 16 and the introduced domain $\tau \in \{0, 1.4\}$, the numerical solution of the mentioned problem is presented in Table 1.

Comparing the analytical and numerical solutions

The obtained analytical solution from Equations (30 and 31) and the numerical solution which its results have been

presented in Table 1 can be compared as shown in Figures 9 and 10.

Conclusion

Due to the complexity of solving nonlinear differential equations for chemical reactions under the presented conditions, AGM (Akbari-Ganji's Method) is used and successfully applied for the governing equations. In this study, a complicated set of nonlinear differential equations have been introduced and analyzed completely by (AGM) and also the obtained results have been compared with the numerical method (Runge-Kutta) to show the ability of AGM for solving such problems. It is concluded that AGM is a reliable and precise approach for solving miscellaneous differential equations. Moreover, a summary of the AGM excellence and its benefits is explained as: By solving a set of algebraic equations with constant coefficients, we are able to obtain the solution of nonlinear differential equation very easily which applying this procedure is possible even for researchers with intermediate mathematical knowledge. On the other hand, it should be mentioned that AGM is able to solve linear and nonlinear differential equations directly in most of the situations that means the final solution can be obtained without any dimensionless procedure. Therefore, AGM can be considered as a significant progress in nonlinear sciences. Since the shortage of boundary condition(s) in this method for solving differential equation(s) is completely terminated, AGM is operational for miscellaneous nonlinear differential equations especially in the field of chemical engineering and we are hopeful

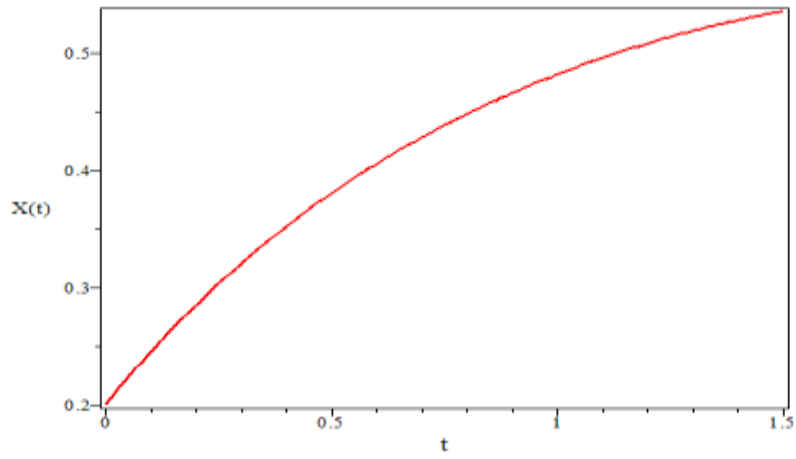


Figure 2. The chart of the obtained solution $X_A(\tau)$.

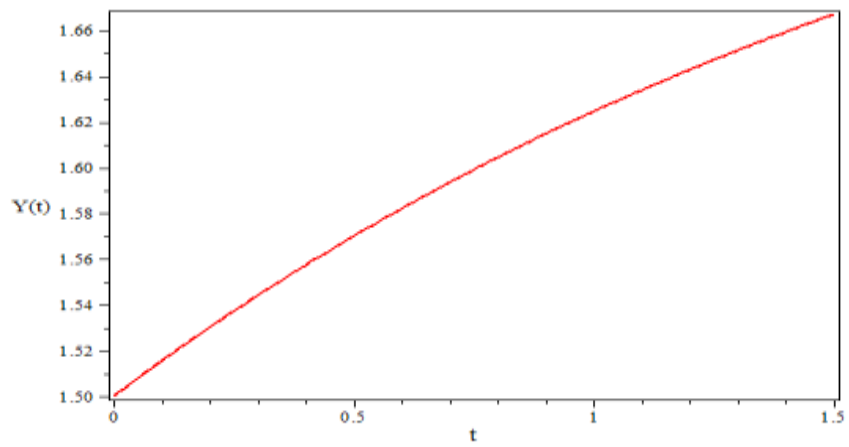


Figure 3. The chart of the temperature profile $T(^{\circ}C)$ at reactor.

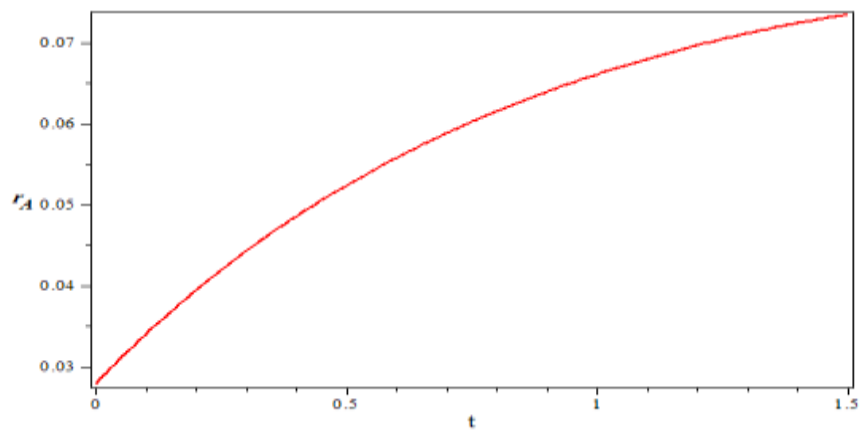


Figure 4. The chart of the A component rate $\left(\frac{mol}{litr.sec}\right)$.

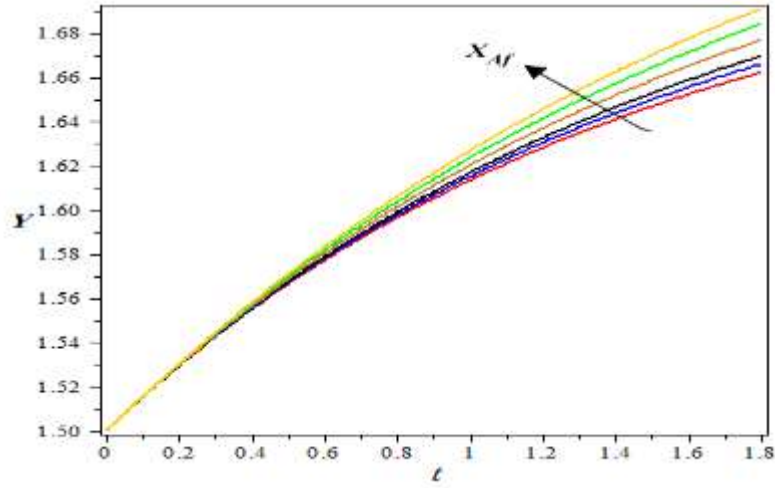


Figure 5. The chart to the component (A) percent converting.

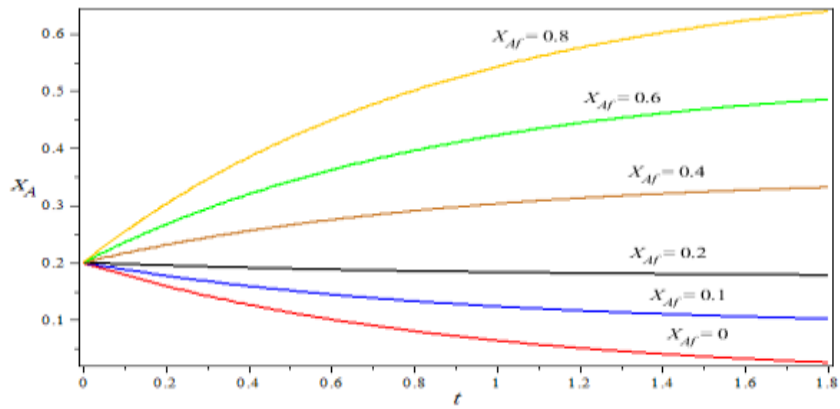


Figure 6. The chart to the component (A) percent converting for different value X_{Af} .

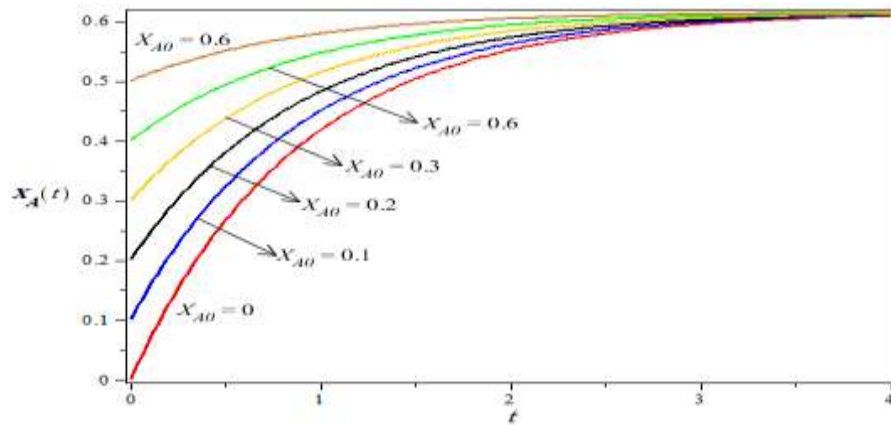


Figure 7. The chart to the component (A) for different values of X_{A0} .

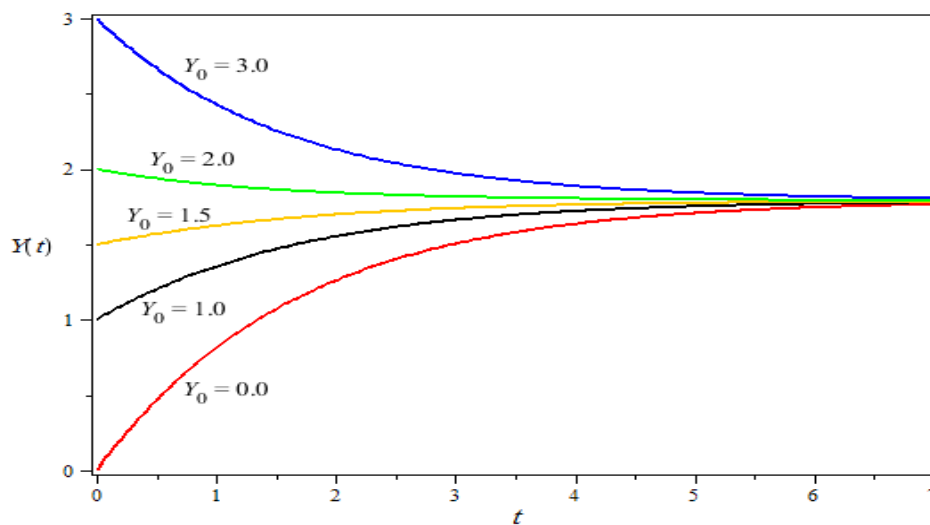


Figure 8. The chart to the component (A) for different values of Y_0 .

Table 1. The obtained results for $X_A(\tau)$, $Y(\tau)$.

τ	$X_A(\tau)$		$Y(\tau)$	
	AGM	NUM Runk45	AGM	NUM Runk45
0.00	0.20000000	0.20000000	1.50000000	1.50000000
0.28	0.31305900	0.3132269	1.54146570	1.54141198
0.56	0.39517300	0.39561012	1.5777777	1.577642105
0.84	0.45474310	0.455564743	1.60933540	1.609130103
1.12	0.49763570	0.49919756	1.63658561	1.636351816
1.40	0.52741852	0.530947229	1.65988560	1.659783591

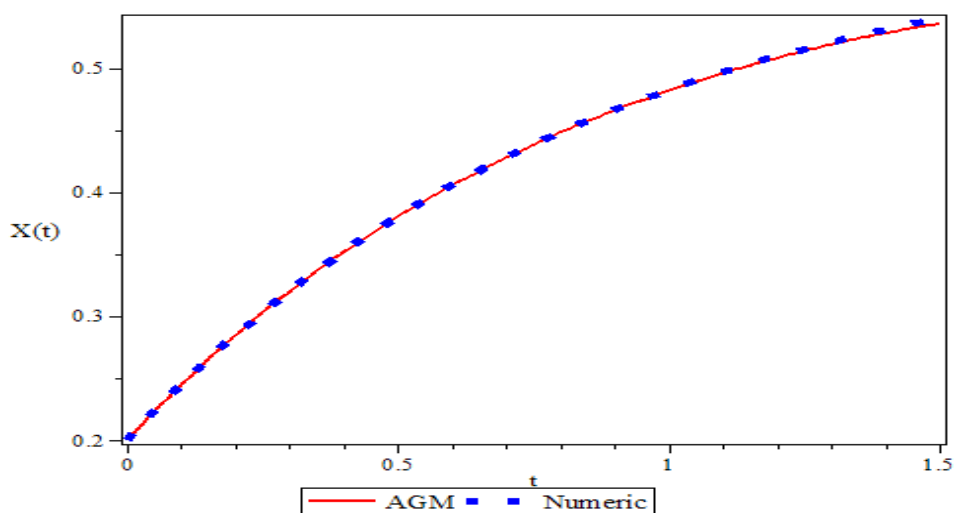


Figure 9. A comparison between AGM and numerical solution for component $X_A(\tau)$.

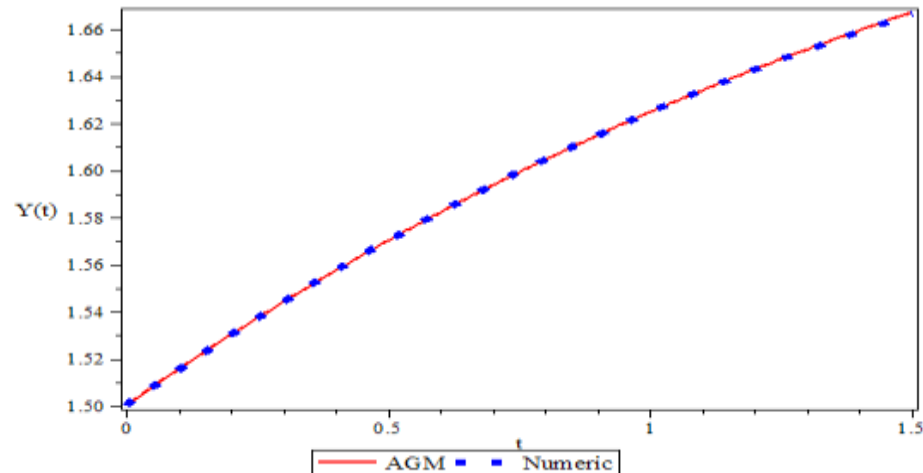


Figure 10. A comparison between AGM and numerical solution for temperature $Y(\tau)$.

that this method will be applied by enthusiastic young researchers in the near future.

CONFLICT OF INTERESTS

The authors have not declared any conflict of interests.

REFERENCES

- Abbasbandy S (2007). A numerical solution of Blasius equation by Adomian's decomposition method and comparison with homotopy perturbation method. *Chaos, Solitons and Fractals* 31:257-260.
- Adomian G (1994). *Solving Frontier Problems of Physics. The Decomposition Method*. Kluwer Academic Publishers, Boston, MA.
- Akbari MR, Ganji DD, Nimafar M, Rostami AK (2014a). Analyzing the nonlinear vibrational wave differential equation for the simplified model of Tower Cranes by Algebraic Method. *Frontiers of Mechanical Engineering* 9(1):58-70.
- Akbari MR, Ganji DD, Majidian A, Ahmadi AR (2014b). Dynamic Vibration Analysis for Non-linear Partial Differential Equation of the Beam-Columns with Shear Deformation and Rotary Inertia by AGM. *Development and Applications of Oceanic Engineering* 3:22-31.
- Akbari MR, Ganji DD, Nimafar M (2014c). Significant progress in solution of nonlinear equations at displacement of structure and heat transfer extended surface by new AGM approach. *Frontiers of Mechanical Engineering* 9(4):390-401.
- Akbari MR, Nimafar M, Ganji DD, Akbarzade MM (2014d). Scrutiny of non-linear differential equations Euler-Bernoulli beam with large rotational deviation by AGM. *Frontiers of Mechanical Engineering* 9(4):402-408.
- Chang J (2011). The exp-function method and generalized solitary solutions. *Computers and Mathematics with Applications* 61(8):2081-2084.
- Ganji DD, Hafez T, Bakhshi MJ (2007). Variational iteration method and homotopy perturbation method for nonlinear evolution equations. *Computers and Mathematics with Applications* 54(7-8):1018-1027.
- Ganji ZZ, Ganji DD, Asgari A (2009a). Finding general and explicit solutions of high nonlinear equations by the Exp-Function method. *Computers and Mathematics with Applications* 58(11-12):2124-2130.
- Ganji ZZ, Ganji DD, Bararnia H (2009b). Approximate general and explicit solutions of nonlinear BBMB equations by Exp-Function method. *Applied Mathematical Modeling* 33(4):1836-1841.
- He J (1999). Variational iteration method—a kind of non-linear analytical technique: some examples. *International Journal of Non-Linear Mechanics* 34(4):699-708.
- He J, Wu X (2006). Exp-function method for nonlinear wave equations. *Chaos, Solitons and Fractals* 30(3):700-708.
- Masdemont JJ (2010). High-order expansions of invariant manifolds of libration point orbits with applications to mission design, "An International Journal of Dynamical Systems" 20(1):59-113.
- Navarro JF (2007). On the implementation of the poincare-Lindstedt technique, *Journal of Sound and Vibration* 301:415-419.