https://doi.org/10.31436/iiumej.v22i1.1398

SOLUTION OF THE REVERSE FLOW REACTOR MODEL USING HOMOTOPY ANALYSIS METHOD

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(Received: 13th March 2020; Accepted: 21st July 2020; Published on-line: 4th January 2021)

ABSTRACT: Methane (CH_4) is one of the most dangerous greenhouse gases in the atmosphere. A reverse flow reactor is utilized to convert CH_4 to carbon dioxide (CO_2) as a means of reducing the effect of global warming. The dynamics of its dependent variables can be stated by a set of convective-diffusion equations. In this article, we examined analytical solutions of temperature dynamics and methane conversion for a 1-D pseudo homogeneous model without refrigeration by using the homotopy analysis method. The results show that temperature and conversion of methane will go to constant when time goes to infinity.

ABSTRAK: Metana (CH_4) merupakan salah satu gas rumah hijau paling berbahaya di atmosfera. Reaktor aliran balik telah dipakai bagi menukar CH_4 kepada CO_2 bagi mengurangkan kesan pemanasan global. Dinamik pemboleh ubah bersandar ini dapat diterangkan melalui satu set persamaan konvektif-difusi. Artikel ini akan mengkaji penyelesaian analisis dinamik suhu dan penukaran metana bagi model 1-D pseudo-homogen tanpa penyejukan dengan menggunakan kaedah analisis homotopi. Hasil kajian menunjukkan bahawa suhu dan penukaran metana akan berterusan dengan masa tak terhingga.

KEYWORDS: *analytical solution; 1-D pseudo homogeneous model; reverse flow reactor; homotopy analysis method*

1. INTRODUCTION

There are several mathematical models in differential equation form that are difficult to solve using ordinary analytic partial differential equations. Hence, various methods have been developed to solve these equations, such as the Laplace transformation method, the perturbation method, the finite difference method, etc.

One natural phenomena that gets very intensive attention is global warming caused by greenhouse gas emissions. One of the dangerous and numerous greenhouse gases in the atmosphere is methane (CH_4). Reducing the global warming effect can be achieved by converting CH_4 into carbon dioxide (CO_2) according to the oxidation (combustion) equation:

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O \qquad \Delta H_{298} = -802{,}7 \text{ kj/mol} \tag{1}$$

Every one mole of oxidized CH_4 gas will release as much heat energy of 802.7 kJ. Hence, converting CH_4 gas to CO_2 gas will reduce the heating effect by 87%. The presence of fairly small amounts of methane gas in the air (0.1–1% by volume) causes the conversion of methane gas to CO_2 gas but needs a catalyst so that the reaction can take place. On the other hand, low methane temperature (around 303 K), so far from the reaction temperature, requires preheating of the feed gas.

One technology which can be used to anticipate the negative impact and characteristic of methane is the use of a reverse flow reactor (RFR) to oxidize CH_4 into CO_2. Further explanation about RFR can be seen in [1,2]. A mathematical model illustrating the dynamics of temperature and concentration on oxidation of CH_4 through RFR has been revealed by Khinast et al. [3] and van Norden [4]. In those articles, a one-dimensional (1-D) pseudo homogeneous model was used to describe the dynamic of dependent variables in a cooled-reverse flow reactor. Previous studies [5,6] used this model to investigate operating parameter sensitivities of RFR on the behavior of dependent variables for periodic feed gas by using a numerical approach. Whereas in [7,8], this model was used to construct singular perturbation problems by considering certain assumptions for steady state conditions and solved them using asymptotic methods. While for the unsteady state case, Nuryaman [9] reported an analytical solution for conversion equation that was derived from the 1-D pseudo homogeneous model which assumed that the reaction took place spontaneously at a certain reaction rate. The homotopy perturbation method was used to get its analytical solution.

In this article, we consider the 1-D pseudo homogeneous model in [4] and we assume that the reactor is in the condition without cooling such that the equations become as follows:

$$u_t = au_{xx} - bu_x + cg(u)(1-v), \qquad x \in [0,1] \tag{2}$$

$$v_t = ev_{xx} - fv_x + l\, g(u)(1-v), \qquad t \geq 0, \tag{3}$$

$$g(u) = \frac{1{,}6656 \times 10^{-5} \exp\left(\frac{25{,}785(u-1)}{u}\right)}{1{,}6656 \times 10^{-5} + \exp\left(-\frac{25{,}785}{u}\right)} \tag{4}$$

where $u = u(x,t)$, $v = v(x,t)$ are dimensionless variables for temperature and conversion variables. Here a, b, c, e, f, and l are dimensionless parameters which values are given in Table 1, and $g(u)$ is a nonlinear function that corresponds to the rate of reaction in the RFR.

Table 1: The dimensionless parameter values of RFR [4]

No	Parameter	Values
1	a	6.9393×10^{-4}
2	b	0.1749
3	c	1.5577×10^{-6}
4	e	2.4038×10^{-3}
5	f	174.06
6	l	0.01

Based on equations (2)-(3) and under the certain assumptions, in this article, we investigate an analytical solution by applying the homotopy analysis method (HAM). In recent years, HAM can be applied for solving various linear and nonlinear systems, and homogeneous and nonhomogeneous equations [10]. The HAM is used to solve problems using the determination of series convergence with respect to an embedded parameter [11]. In fact, the homotopy method is easier to use in solving difficult problems. Therefore, the HAM method will be applied herein solving the RFR model.

2. METHODOLOGY

The Homotopy Analysis Method (HAM) was designed firstly in 1992 by Liao [12] and was then modified in 1997 [13]. This is a semi-analytics technique for solving ordinary nonlinear problems or partial differential equations. Homotopy can be defined as a link between two different objects in mathematics that have the same characteristics in several aspects [13].

The HAM is based on concepts in topology and differential geometry to produce a series convergence of a nonlinear system. The concept of homotopy is then traced back to Jules Henri Poincare, a French mathematician. Homotopy explains a kind of deformation variation in mathematics. For example, a circle can be deformed continuously into an ellipse, and the shape of a coffee cup can be deformed continuously into a donut shape.

Suppose there are zero*th*-order differential equations:

$$N_k[z_k(\omega,\tau)] = 0, \quad k = 1, 2, \dots, m \tag{5}$$

where N_k are nonlinear operators that represent the whole equations, ω and τ denote the independent variables, and $z_k(\omega,\tau)$ are unknown functions. Liao constructed the deformation equations as

$$(1-q)L\big[\phi_k(\omega,\tau;q) - z_{k,0}(\omega,\tau)\big] = q\hbar_k N_k[\phi_k(\omega,\tau;q)] \tag{6}$$

where q is an embedding parameter, $q \in [0,1]$, $\hbar_k$are nonzero auxiliary functions, L is an auxiliary linear operator, $z_{k,0}(\omega,\tau)$ are initial guesses of $z_k(\omega,\tau)$, and $\phi_k(\omega,\tau;q)$ are unknown functions. One has great freedom to choose auxiliary objects such as $\hbar_k$ and L. Obviously, when $q = 0$ and $q = 1$, ϕ_k hold:

$$\phi_k(\omega,\tau;0) = z_{k,0}(\omega,\tau) \text{and } \phi_k(\omega,\tau;1) = z_k(\omega,\tau) \tag{7}$$

Thus, if q increases from 0 to 1, then the solutions $\phi_k(\omega,\tau;q)$ move from $z_{k,0}(\omega,\tau)$ to $z_k(\omega,\tau)$. $\phi_k(\omega,\tau;q)$ are then expanded in Taylor series with respect to q, and then becomes

$$\phi_k(\omega,\tau;q) = z_{k,0}(\omega,\tau) + \sum_{n=1}^{+\infty} z_{k,n}(\omega,\tau)q^n \tag{8}$$

where

$$z_{k,n} = \frac{1}{n!}\frac{\partial^n \phi_k(\omega,\tau;q)}{\partial q^n}\Big|_{q=0}. \tag{9}$$

When $\hbar_k$, L, $z_{k,0}(\omega,\tau)$, and $\phi_k(\omega,\tau;q)$are properly chosen, then Equation (8) converges at $q = 1$ and

$$\phi_k(\omega,\tau;1) = z_{k,0}(\omega,\tau) + \sum_{n=1}^{+\infty} z_{k,n}(\omega,\tau) \tag{10}$$

which has to be one of the solutions. As $\hbar_k = -1$, Equation (6) becomes

$$(1-q)L\big[\phi_k(\omega,\tau;q) - z_{k,0}(\omega,\tau)\big] + qN_k[\phi_k(\omega,\tau;q)] = 0 \tag{11}$$

The governing equations can be deduced from the zero*th*-order deformation Equation (6). Define the vectors

$$\overrightarrow{z_{k,m}} = \{z_{k,0}(\omega,\tau), z_{k,1}(\omega,\tau), \dots, z_{k,m}(\omega,\tau)\} \tag{12}$$

The nth order deformation can be found by differentiating (6) n times with respect to q and then putting $q = 0$. After that divide it by $n!$ such that

$$L\left[z_{k,n}(\omega,\tau) - \chi_n z_{k,n-1}(\omega,\tau)\right] = \hbar_k R_{k,n}(\overrightarrow{z_{\iota,n-1}}) \tag{13}$$

where

$$R_{k,n}\left(\overrightarrow{z_{k,n-1}}\right) = \frac{1}{(n-1)!}\frac{\partial^{n-1}N_k[\phi_k(\omega,\tau;q)}{\partial q^{n-1}}|_{q=0} \tag{14}$$

and

$$\chi_n = \begin{cases} 0, n \leq 1 \\ 1, n > 1 \end{cases} \tag{15}$$

Note that $z_{k,n}(\omega,\tau)$ $(n \geq 1)$ are governed by (13) with boundary conditions coming from the original problem.

3. RESULT AND DISCUSSION

Consider the 1-D pseudo homogeneous model in Equations (2)-(3). By using a rescaling process and the assumption that the reaction rate takes place at certain temperature such that the nonlinear term approach to one. We obtain a dimensionless equation set that illustrates the dynamics of temperature and conversion of methane gas to methane oxidation using RFR without cooling as follows:

$$u_t - au_{xx} + bu_x + cv - c = 0 \tag{16}$$

$$v_t - ev_{xx} + fv_x + lv - l = 0 \tag{17}$$

where $u = u(x,t), v = v(x,t)$ are dimensionless variables for temperature and conversion and a, b, c, e, f, and l are dimensionless parameters which values given in Table 1. In this case, initial conditions are

$$u(x,0) = \beta,\ \beta > 1 \tag{18}$$

where β is constant and

$$v(x,0) = 0 \tag{19}$$

The linear operator

$$L[\varphi_k(x,t;q)] = \frac{\partial\varphi_k(x,t;q)}{\partial t}, k = 1,2 \tag{20}$$

with $L[p_k] = 0$, where $p_k(k = 1,2)$ are integral constants.

The nonlinear operator

$$N_1[\varphi_1(x,t;q)] = \frac{\partial\varphi_1(x,t;q)}{\partial t} - a\frac{\partial^2\varphi_1(x,t;q)}{\partial x^2} + b\frac{\partial\varphi_1(x,t;q)}{\partial x} + c\varphi_2(x,t;q) - c \tag{21}$$

$$N_2[\varphi_2(x,t;q)] = \frac{\partial\varphi_2(x,t;q)}{\partial t} - e\frac{\partial^2\varphi_2(x,t;q)}{\partial x^2} + f\frac{\partial\varphi_2(x,t;q)}{\partial x} + l\varphi_2(x,t;q) - l \tag{22}$$

Using the above definition, we construct the zeroth-order deformation equations

$$(1-q)L\left[\varphi_k(x,t;q) - z_{k,0}(x,t)\right] = qh_k N_k[\varphi_k(x,t;q)], k = 1,2$$

https://doi.org/10.31436/iiumej.v22i1.1398

When $q = 0$ and $q = 1$, respectively, yields

$$\varphi_1(x,t;0) = z_{1,0}(x,t) = u_0(x,t)$$
$$\varphi_2(x,t;0) = z_{2,0}(x,t) = v_0(x,t)$$
$$\varphi_1(x,t;1) = u(x,t)$$
$$\varphi_2(x,t;1) = v(x,t)$$

After expanding $\varphi_k(x,t;q)$in Taylor series with respect to q, it yields

$$\varphi_k(x,t;q) = z_{k,0}(x,t) + \sum_{n=1}^{+\infty} z_{k,n}(x,t)q^n$$

where

$$z_{k,n}(x,t) = \frac{1}{n!}\frac{\partial^n \varphi_i(x,t;q)}{\partial q^n}|_{q=0}$$

The above series will converge at $q = 1$, so that

$$u(x,t) = z_{1,0}(x,t) + \sum_{n=1}^{+\infty} z_{1,n}(x,t)$$
$$v(x,t) = z_{2,0}(x,t) + \sum_{n=1}^{+\infty} z_{2,n}(x,t)$$

These are the solution of the nonlinear equation systems (16, 17). Now, we define the vector

$$\overrightarrow{z_{k,m}} = \{z_{k,0}(x,t), z_{k,1}(x,t), \dots, z_{k,m}(x,t)\}$$

So, the *n*th-order deformation equations is

$$L[z_{k,n}(x,t) - \chi_n z_{k,n-1}(x,t)] = \hbar_k R_{k,n}(\vec{z}_{k,n-1})$$

where

$$R_{1,n}(\vec{z}_{k,n-1}) = (z_{1,n-1})_t - a(z_{1,n-1})_{xx} + b(z_{1,n-1})_x + c(z_{2,n-1}) - c + cX_n$$
$$R_{2,n}(\vec{z}_{k,n-1}) = (z_{2,n-1})_t - e(z_{2,n-1})_{xx} + f(z_{2,n-1})_x + l(z_{2,n-1}) - l + lX_n$$

Now, the solution of the n*th*-order deformation equation for $n \geq 1$ becomes

$$z_{k,n}(x,t) = \chi_n z_{k,n-1}(x,t) + \hbar_k \int_0^t R_{k,n}(\vec{z}_{k,n-1})\, d\tau + p_k$$

where the integration constants $p_k = 0$.

We, now successively have

$$z_{1,0}(x,t) = \beta$$

$$z_{1,1}(x,t) = -cht$$

$$z_{1,2}(x,t) = -cht - ch^2 t - \frac{clh^2 t^2}{2}$$

https://doi.org/10.31436/iiumej.v22i1.1398

$$\mathrm{z}_{1,3}(\mathrm{x},\mathrm{t}) = -cht - 2ch^2t - clh^2t^2 - ch^3t - clh^3t^2 - \frac{cl^2h^3t^3}{6}$$

$$\mathrm{z}_{1,4}(\mathrm{x},\mathrm{t}) = -cht - 3ch^2t - clh^2t^2 - 3ch^3t - 3clh^3t^2 - \frac{cl^2h^3t^3}{2} - ch^4t - \frac{3clh^4t^2}{2} - \frac{cl^2h^4t^3}{2} - \frac{clh^2t^2}{2} - \frac{c[^3h^4t^4}{24}$$

$$\mathrm{z}_{1,5}(\mathrm{x},\mathrm{t}) = -cht - 4ch^2t - 2clh^2t^2 - 6ch^3t - 6clh^3t^2 - cl^2h^3t^3 - 4ch^4t - 6clh^4t^2 - 2cl^2h^4t^3 - \frac{cl^3h^4t^4}{6} - ch^5t - 2clh^5t^2 - cl^2h^5t^3 - \frac{cl^3h^5t^4}{6} - \frac{cl^4h^5t^5}{120}$$

$$\mathrm{z}_{2,0}(\mathrm{x},\mathrm{t}) = 0$$

$$\mathrm{z}_{2,1}(\mathrm{x},\mathrm{t}) = -lht$$

$$\mathrm{z}_{2,2}(\mathrm{x},\mathrm{t}) = -lht - lh^2t - \frac{l^2h^2t^2}{2}$$

$$\mathrm{z}_{2,3}(\mathrm{x},\mathrm{t}) = -lht - 2lh^2t - l^2h^2t^2 - lh^3t - l^2h^3t^2 - \frac{l^3h^3t^3}{6}$$

$$\mathrm{z}_{2,4}(\mathrm{x},\mathrm{t}) = -lht - 3lh^2t - 3lh^3t - 3l^2h^3t^2 - \frac{l^3h^3t^3}{2} - lh^4t - \frac{l^3h^4t^3}{2} - \frac{3l^2h^2t^2}{2} - \frac{3l^2h^4t^2}{2} - \frac{l^4h^4t^4}{24}$$

$$\mathrm{z}_{2,5}(\mathrm{x},\mathrm{t}) = -lht - 4lh^2t - 6lh^3t - l^3h^3t^3 - 4lh^4t - 2l^3h^4t^3 - 2l^2h^2t^2 - 6l^2h^4t^2 - \frac{l^4h^4t^4}{6} - lh^5t - l^3h^5t^3 - 6l^2h^3t^2 - \frac{l^4h^5t^4}{6} - 2l^2h^5t^2 - \frac{l^5h^5t^5}{120}$$

The solutions then have the form

$$u(x,t) = z_{1,0}(x,t) + z_{1,1}(x,t) + z_{1,2}(x,t) + z_{1,3}(x,t) + z_{1,4}(x,t) + z_{1,5}(x,t) + \cdots$$

$$v(x,t) = z_{2,0}(x,t) + z_{2,1}(x,t) + z_{2,2}(x,t) + z_{2,3}(x,t) + z_{2,4}(x,t) + z_{2,5}(x,t) + \cdots$$

By putting $h = -1$, yields

$$u(x,t) = \beta + ct - \frac{clt^2}{2} + \frac{cl^2t^3}{6} - \frac{cl^3t^4}{24} + \frac{cl^4t^5}{120} - \cdots$$

$$= \beta + ct + \frac{c}{l}\left(-\frac{l^2t^2}{2} + \frac{l^3t^3}{6} - \frac{l^4t^4}{24} + \frac{l^5t^5}{120} - \cdots\right)$$

$$= \beta + ct + \frac{c}{l}(1 - lt - e^{-lt})$$

$$= \beta + ct + \frac{c}{l} - ct - \frac{ce^{-lt}}{l}$$

$$= \beta + \frac{c}{l} - \frac{ce^{-lt}}{l}$$

$$= \frac{\beta l + c - ce^{-lt}}{l}$$

$$v(x,t) = 0 + lt - \frac{l^2t^2}{2} + \frac{l^3t^3}{6} - \frac{l^4t^4}{24} + \frac{l^5t^5}{120} - \cdots$$
$$= 1 - e^{-lt}$$

Using the physical data available in Table 1, the solution graph for $u(x,t)$ and $v(x,t)$, as shown in Fig. 1 and Fig. 2.

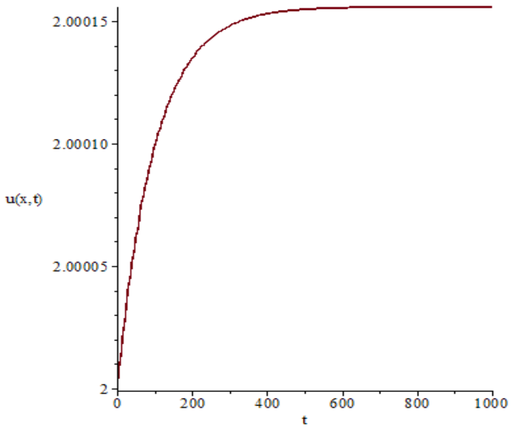

Fig. 1: The solution graph for $u(x,t)$ at certain position.

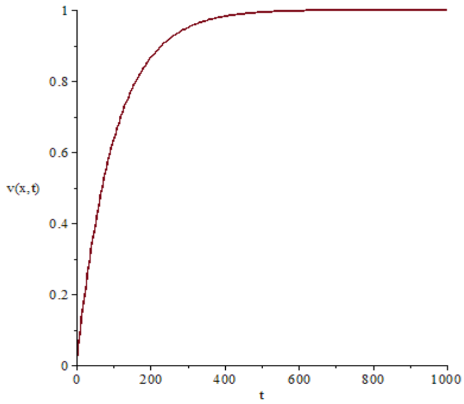

Fig. 2: The solution graph for $v(x,t)$ at certain position.

In RFR, the heat that is stored in the reactor can be used to preheat the feed. If the reaction temperature has been reached, the reactor system no longer needs a preheater for preheating the feed so that the process has high energy efficiency. This condition is illustrated by the graph $u(x,t)$.As shown in Figure 1, there is an increase in temperature within a certain time interval, after which the temperature does not increase or decrease but moves constantly. This condition has reached the steady state; thus, no preheater is needed. The $v(x,t)$graph in Figure 2 illustrates the amount of concentration that reacts. After the concentration reacts entirely within a certain time, then the graph will move constantly. When this condition is reached, it means that the feed gas has completely reacted. Thus no more heat is released so that the temperature of the reactor becomes constant.

4. CONCLUSION

In this article, we consider the 1-D pseudo homogeneous model that describes the dynamics of temperature and conversion variabls in RFR without the cooling process. Here, we consider only the feed gas flow from left to the right end of RFR. Then, we solve this model using the homotopy analysis method. Based on the description above, it can be concluded that the solution of the dimensionless equation system describing the dynamics of temperature and conversion to methane oxidation using RFR without refrigeration is obtained as $u(x,t) = \frac{\beta l + c - ce^{-lt}}{k}$ and $v(x,t) = 1 - e^{-lt}$. The solution graph of $u(x,t)$ illustrates an increase in temperature within a certain time interval, after which the temperature does not increase or decrease but it moves constantly. This condition has reached the steady state; thus, no preheater is needed. The solution graph of $v(x,t)$ describes the amount of concentration that reacts. After the concentration reacts entirely within a certain time, then the graph will move constantly. Future studies can be extended by considering the cooling process term in the 1-D pseudohomogeneous model. In the real problem, the heat energy expended during the methane oxidation should be controlled so that reactor overheating will not occur.

ACKNOWLEDGEMENT

The authors would like to thank the reviewers for invaluable suggestions and corrections. Also, the authors would like to thank Universitas Lampung for the facilities, funding through BLU Research Grants No. 2280/UN.21/PN/2019, and support during the research.

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