MODIFIED VARIATIONAL ITERATION METHOD FOR SOLVING NONLINEAR PARTIAL DIFFERENTIAL EQUATION DESCRIBING OIL SHALE PYROLYSIS

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Abstract

The paper presents a modification of variational iteration method by Taylor's series for finding the solution of the nonlinear partial differential equation describing the modeling of oil shale pyrolysis. The modification takes care of the nonlinear exponential part of the partial differential equation which could be complicated to solve. The results obtained using modified variational iteration method shows that the concentration of oil increases as the temperature increases.

Introduction

Several problems arising in science and engineering modeled by differential equationleads to nonlinear partial differential equations (PDEs). In various fields of physics and engineering several methods have been used to solve PDEs and these are mostly applicable to linear or polynomials nonlinearity type equations (Sweilam & Khader, 2007). In this work we consider the variational iteration method with exponential nonlinearities. Variational iteration method is a useful instrument for solving nonlinear PDEs (Elham & Hossein, 2011) and has been applied to PDEs with polynomial nonlinearities (Yulitaet al., 2009). A modification is made by replacing the exponential part with an appropriate polynomial. In order to show the efficiency, the mathematical modeling of oil shale pyrolysis is considered (Inokuti & Sekine, 1998).

Oil shale is any sedimentary rock containing various amounts of solid organic material that yields petroleum products, along with a variety of solid by-products (Pankay, 2012). Pyrolysis is the process in which the oil shale is heated in the absence of oxygen until its kerogen decomposes into condensable and non-condensable combustible oil shade gas (Dexun, et al., 2017).

The aim of this work is to analyse the effects ofdimensional activation energy, heating rate parameter, and the Arrhenius pre-exponential factor on the oil shale pyrolysis process.

Model Formulation

FollowingWang, **et al.**, (2016) the equation describing oil shale pyrolysis is given by

$$\frac{dc}{dT} = \left(\frac{Ac_0}{H}\right)\exp\left(\frac{-E}{RT} - \frac{A}{H}\int_0^T \exp\left(\frac{-E}{RT}\right)dT\right) \quad (1)$$

where T is thetemperature, H is the heating rate, E is theactivation energy, A is the Arrhenius pre-exponential factor, and R is gas constant.
We simplify (1) using the approximation:

$$\int_0^T \exp\left(\frac{-E}{RT}\right)dT = \left(\frac{RT^2}{E}\right)\exp\left(\frac{-E}{RT}\right) \quad (2)$$

Substituting (2)into (1), we have

$$\frac{dc}{dT}=\left(\frac{Ac_0}{H}\right)\exp\left(\frac{-E}{RT}-\left(\frac{ART^2}{HE}\right)\exp\left(\frac{-E}{RT}\right)\right) \quad (3)$$

The initial condition is taken as

$$c(T_0)=c_0 \quad (4)$$

Method of Solution

Non-dimensionalization

Here, we non -dimensionalized, (3)and(4) using the following set of dimensionless variables: $\phi=\frac{c}{c_0}$, $\theta=\frac{E}{RT^2}(T-T_0)$ (5)

and wehave

$$\left.\begin{aligned}\frac{c_0}{\varepsilon T_0}\frac{\partial\phi}{\partial\theta}&=\left(\frac{Ac_0}{H}\right)\exp\left(-\frac{1}{\varepsilon}+\frac{\theta}{1+\varepsilon\theta}-\beta\left(1+2\varepsilon\theta+\varepsilon^2\theta^2\right)e^{\frac{0}{1+\varepsilon\theta}}\right)\\ \Rightarrow\frac{\partial\phi}{\partial\theta}&=\left(\frac{A\varepsilon T_0}{H}\right)\exp\left(-\frac{1}{\varepsilon}+\frac{\theta}{1+\varepsilon\theta}-\beta\left(1+2\varepsilon\theta+\varepsilon^2\theta^2\right)e^{\frac{0}{1+\varepsilon\theta}}\right)\\ \frac{\partial\phi}{\partial\theta}&=\alpha\exp\left(-\frac{1}{\varepsilon}+\frac{\theta}{1+\varepsilon\theta}-\beta\left(1+2\varepsilon\theta+\varepsilon^2\theta^2\right)e^{\frac{0}{1+\varepsilon\theta}}\right)\end{aligned}\right\} \quad (6)$$

where

$$\alpha=\frac{A\varepsilon T_0}{H},\ \beta=\frac{ART_0^2}{HE}e^{-\frac{E}{RT_0}}$$

Therefore, the dimensionalized equation and boundary conditions are

$$\left.\begin{aligned}\frac{\partial\emptyset}{\partial\theta}&=\alpha exp\left(-\frac{1}{\varepsilon}+\frac{\theta}{1+\varepsilon\theta}-\beta(1+2\varepsilon\theta+\varepsilon^2\theta^2)e^{\frac{\theta}{1+\varepsilon\theta}}\right)\\ \emptyset(0)&=1\end{aligned}\right\} \quad (7)$$

3.2 Variational iteration method

We consider the following general nonlinear system:

$$L\phi(\theta)+N\phi(\theta)=g(\theta) \quad (8)$$

where L is the linear operator and N is the nonlinear operator, and $g(\theta)$ is the inhomogeneous term. A correction functional for (8) can be written as

$$\phi_{n+1}(\theta)=\phi_n(\theta)+\int_0^{\theta}\lambda(s)\left(L\phi_n(s)+N\tilde{\phi}_n(s)-g(s)\right)ds \quad (9)$$

The successive approximation ϕ_n, $n\geq 0$ can be established by determining λ, a general Lagrange multiplier, which will be identified optimally via the variational theory (Inokuti and Sekine, 1998). The function $\tilde{\phi}_n$ is a restricted variation, this means that $\delta\tilde{\phi}_n=0$. The Lagrange multiplier is determined using integration by parts and the successive approximations $\phi_{n+1}(\theta)$ of the solution $\phi(\theta)$ will be readily obtained upon using the Lagrange multiplier obtained and any selective function $\phi_0(\theta)$.

A modification of variational iteration method

Here, we introduce a new method for solving the nonlinear PDE (7) by introducing Taylor polynomial which takes care of the nonlinear exponential part. The modification is based on the following theorem;

Theorem 3.1 Taylor's theorem: If a function has an $(n+1)$th derivative on an interval $[a,b]$, then its value at $(b, f(b))$, can be written as a Taylor polynomial of the form $f(a)+(b-a)f'(a)+...+\frac{1}{n!}(b-a)^n f^n(a)$ plus an error term, where $f^n(a)$ is the nth derivative of $f(x)$. Let $f(x)$ be infinitely differentiable, the Taylor series will represent the function at the points for which the error goes to zero as n increases.

To modify the variational iteration method, we use Taylor's polynomials

$$\frac{\theta}{1+\varepsilon\theta}=1+\theta+0(\theta^2) \tag{10}$$

arriveat the following correction functional

$$\phi_{n+1}(\theta)=\phi_n(\theta)-\int_0^\theta\left(\frac{\partial\phi}{\partial s}-\alpha\exp\left(-\frac{1}{\varepsilon}+1+s-\beta\left(1+2\varepsilon s+\varepsilon^2 s^2\right)(1+s)\right)\right)ds \tag{11}$$

Making the correction functional stationary leads to

$$\delta\phi_{n+1}(\theta)=\delta\phi_n(\theta)-\delta\int_0^\theta\left(\frac{\partial}{\partial s}\phi_n(s)-\alpha\exp\left(-\frac{1}{\varepsilon}+1+s-\beta\left(1+2\varepsilon s+\varepsilon^2 s^2\right)(1+s)\right)\right)ds \tag{12}$$

which yields the following stationary conditions:

$$\left.\begin{array}{l} 1+\lambda(\theta)\big|_{\theta=s}=0 \\ \lambda'(\theta)=0 \end{array}\right\} \tag{13}$$

The general Lagrange multiplier, therefore can be identified as

$\lambda(\theta)=-1$

using $\phi_0(\theta)=1$ as the initial approximation we obtain the following results

$$\varphi_0(\theta)=1 \tag{14}$$

$$\varphi_1(\theta)=1+\frac{1}{2\varepsilon\sqrt{\beta}}\left(\alpha\sqrt{\pi}\,e^{\frac{4\beta\varepsilon^2+1}{4\beta\varepsilon^2}}\left(-erf\left(\frac{-1+2\beta\varepsilon}{2\varepsilon\sqrt{\beta}}\right)+erf\left(\frac{2\varepsilon^2\beta\theta-1+2\beta\varepsilon}{2\varepsilon\sqrt{\beta}}\right)\right)e^{-\frac{2}{\varepsilon}}\right) \tag{15}$$

The computations (14) and (15) were done using computer symbolic algebraic package MAPLE 16 to solve (12), where $\phi(\theta)$ is the temperature.

Results and Discussion

We solve the partial differential equation (7) describing oil shale pyrolysis using a modified variational iteration method. Numerical solutions of equation (15) are computed for the values of $\beta=0.1,\ 0.3,\ 0.6$, $\varepsilon=0.4\ 0.6,\ 0.8$, $\alpha=0.1,\ 0.4,\ 0.8$, and $\theta=0..1$. The following figures explain the variation of the concentration of the oil shale pyrolysis with dimensional activation energy (ε), heating rate parameter (β), and Arrhenius pre-exponential factor, (α).

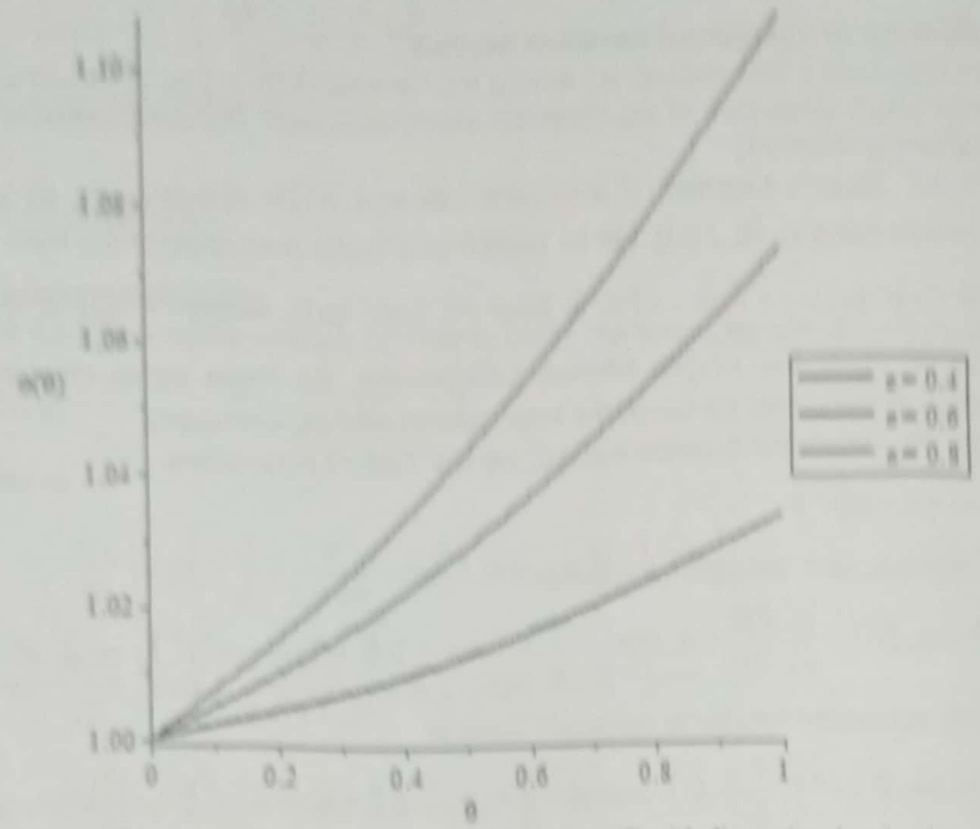

Figure 1: Variation of the concentration of oil shale, φ(θ) with dimensional activation energy, ε

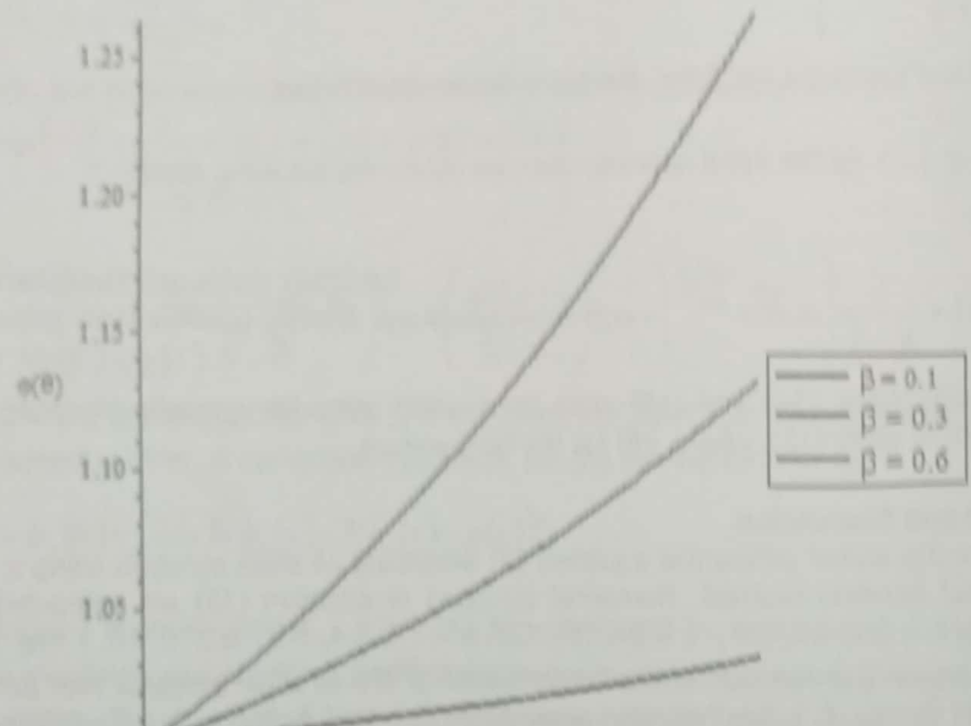

Figure 2: Variation of the concentration of oil shale, φ(θ) with heating rate parameter, β

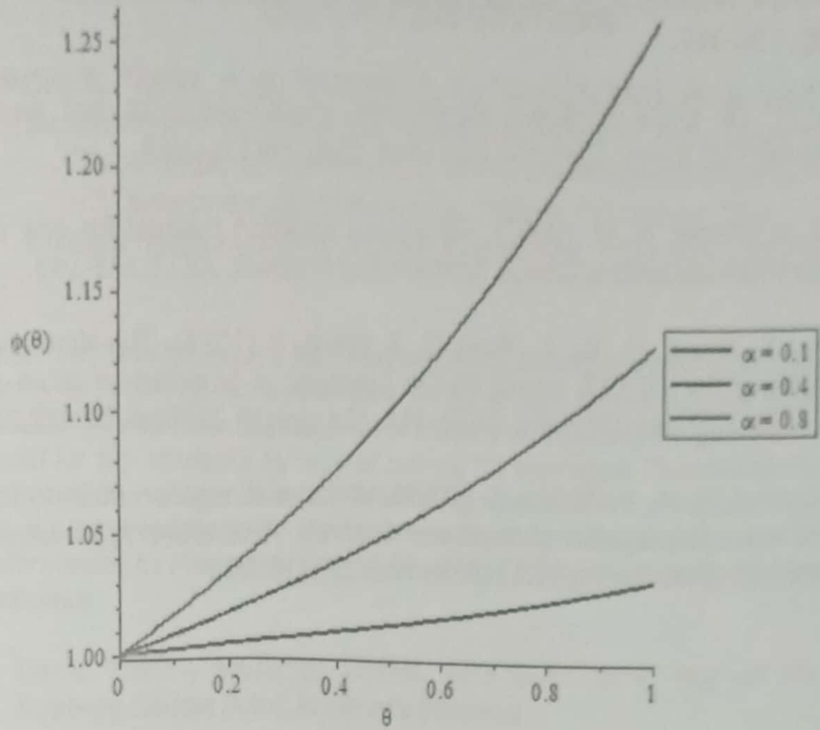

Figure 3: Variation of the cncentration of oil shale pyrolysis, φ(θ) with Arrhenius pre-exponential factor, α

Figure 1 shows the effect of dimensional activation energy, (ε) on the concentration of oil. It is observed that the concentration of oil increases as temperature, θ and increases as dimensional activation energy, ε increases.

Figure 2 shows the effect of heating rate parameter, (β) on the concentration of oil. It is observed that the concentration of oil increases as temperature, θ increases and as heating rate parameter, β increases.

Figure 3 shows the effect of Arrhenius pre-exponential factor, (α) on the concentration of oil. It is observed that the concentration of oil increases as temperature, θ increases and as Arrhenius pre-exponential factor, α increases.

Conclusion

In this paper, the mathematical model of oil shale pyrolysis is presented. We used a modified iteration method to obtain the numerical solution of the model. The governing parameters for the problem under study are the dimensional activation energy, heating rate parameter, and the Arrhenius pre-exponential factor. The oil temperature profiles are significantly influenced by this parameter. Increase in temperature leads to more production of oil shale.

References

Dexun, L., Shusheng, T., Qun, Z., Hongyan, W., Zazhong, D., Nan, W., Feng, L. (2017). Pyrolysis mechanisim and kinetic model of Mudanjiang oil shale in Singhao, China. *SAGE Journal*, *35*(4), 504-515.

Elham, S., & Hossein, J. (2011). Variational iteration method: A tool for solving partial differential eqautions. *The Journal of Mathematics and Computer Science*, 2(2), 388-393.

Inokuti, M., & Sekine, T. M. (1998). General use of the Lagrange multiplier in nonlinear mathematical physics, in: S. Nemat-Nasser (Ed.), Variational methods in mechanics of solids. pp. 156-162.

Pankay T. (2012). *Oil shale pyrolysis: Benchscale experimental studies and modeling.* Unpublished PhD thesis, The University Utah, Salt Lake City, USA.

Sweilam, N. H., & Khader, M. M. (2007). Variational iteration method for one dimensional nonlinear thermoelasticity. *Chaos, Solitons and Fractals, 32*(1), 145-149.

Wang, Q., Wang, Y., Zhang, H., Xu, X., Yang, Q., & Wang, P. (2016). The simulation study of application of the FG-DVC model to the pyrolysis of Huadian oil shale of China at different heating rates. *Oil shale, 33*(2), 111-124. doi:10.3176/oil.2016.2.02

Yulita, M. R., Noorani, S. M., & Hashim, I. (2009). Variational iteration method for fractional heat and wave like equations. *Nonlinear Analysis: Real World Applications, 10*,1854-1869. doi:http://dx.doi.org/10.1016.nonrwa.2008.02.026