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ANALYTICAL SOLUTION FOR THE SYSTEM OF LANE–EMDEN TYPE EQUATION WITH BOUNDARY CONDITION INSIDE THE CATALYST PARTICLE BY VARIATIONAL ITERATION METHOD

K. M. DHARMALINGAM AND K. VALLI[1]

ABSTRACT. In this paper, we describe the problem of ethanol, acetaldehyde, and ethyl acetate inside the catalyst particle. This model represents a non-linear term related to reactor particle. A Better approximation analytic solution for non-linear differential equations of the molar concentration profiles are derived using Variational Iteration Method. Furthermore, the derived solutions are validated and compared with numerical simulation (by MATLAB software–Runge–Kutta 4th order method). These solutions are good enough to predict the behaviour of the system. The influence of dimensionless reaction parameters are discussed and presented graphically. The obtained solutions are more reliable and easy to predict the dynamic behaviour of the system by varying the parameters.

1. INTRODUCTION

The control of Volatile Organic Compounds (VOCs) releasing from the many chemicals, petrochemical, and allied industries is very challenging in air pollution in the century years [1–8]. In the 1950's, Norb Ruff has developed the Catalytic combustion to control the emission of organic components in industrials

[1]*corresponding author*

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which are based on the catalyst particle and diminishes the operating temperature in the combustion process. Furthermore, Campesi et al. [9] discussed the kinetic combustion of ethanol and ethyl acetate mixtures over a MnCu catalyst and developed the mathematical model from the kinetic combustion.

This model contains the nonlinear differential system related to the kinetic combustion of ethanol and ethyl acetate mixtures. In this paper, we will analyze the kinetic combustion reactions in the catalyst combustion [10]. The concentration of ethanol and ethyl acetate mixtures in the inside catalyst combustion are represented by Lane–Emden equation with the boundary condition. Furthermore, we will derive the analytic expression for the Lane–Emden equation by the Variational iteration method [11–20]. These analytical results are very much useful in chemical engineering for the reason of diffusion reactor model analysis [21].

2. NOTATIONS

We introducing the following dimensionless variables:

$$E=\frac{C_{Et}}{C^b_{Et}}; Ac=\frac{C_{Ac}}{C^b_{Ac}}; EC=\frac{C_{EA}}{C^b_{EA}}; \beta_1=k_{C,Et}C^b_{Et}; \beta_2=k_{C,Ac}C^b_{Ac}; \beta_3=k_{C,EC}C^b_{EC};$$

$$\phi_1^2=\frac{k_{ref_1}C^b_{Et}R^2}{D_{ef,Et}C^b_{Et}}; \phi_2^2=\frac{k_{ref_2}C^b_{Ac}R^2}{D_{ef,Ac}C^b_{Ac}}; \phi_3^2=\frac{k_{ref_1}C^b_{Et}R^2}{D_{ef,Ac}C^b_{Ac}}; \phi_4^2=\frac{k_{ref_1}C^b_{EC}R^2}{D_{ef,Ac}C^b_{EC}};$$

$$\gamma_1=\frac{E_1}{R_G}\left(\frac{1}{T}-\frac{1}{T_{ref}}\right); \gamma_2=\frac{E_2}{R_G}\left(\frac{1}{T}-\frac{1}{T_{ref}}\right); \gamma_3=\frac{E_3}{R_G}\left(\frac{1}{T}-\frac{1}{T_{ref}}\right); x=\frac{z}{R}$$

The system nonlinearities are

$$F_1\left(E(x),Ac(x),EC(x)\right)=\phi_1^2e^{-\gamma_1}f_1\left(E(x),Ac(x),EC(x)\right)$$

$$F_2\left(E(x),Ac(x),EC(x)\right)=\phi_2^2e^{-\gamma_2}f_2\left(E(x),Ac(x),EC(x)\right) - \phi_3^2e^{-\gamma_1}f_3\left(E(x),Ac(x),EC(x)\right)$$

$$F_3\left(E(x),Ac(x),EC(x)\right)=\phi_4^2e^{-\gamma_3}f_3\left(E(x),Ac(x),EC(x)\right)$$

where

$$f_1\left(E(x),Ac(x),EC(x)\right)=\frac{E(x)}{1+\beta_1E(x)+\beta_2Ac(x)+\beta_3EC(x)}$$

$$f_2\left(E(x),Ac(x),EC(x)\right)=\frac{Ac(x)}{1+\beta_1E(x)+\beta_2Ac(x)+\beta_3EC(x)}$$

$$f_3\left(E(x), Ac(x), EC(x)\right) = \frac{EC(x)}{1+\beta_1 E(x)+\beta_2 Ac(x)+\beta_3 EC(x)}$$

3. Development of the boundary value problem

In [10], the reaction schemes for the oxidation of ethanol to CO_2 and ethyl acetate to CO_2 are as follows:

$$C_2H_6O + \frac{1}{2}O_2 \rightarrow C_2H_4O + H_2O \tag{3.1}$$

$$C_2H_4O + \frac{5}{2}O_2 \rightarrow 2CO_2 + 2H_2O \tag{3.2}$$

$$C_4H_8O_2 + 5O_2 \rightarrow 4CO_2 + 4H_2O \tag{3.3}$$

From the reaction scheme Equtions (3.1) to (3.3) that formulated the mathematical model in the diffusion and reaction inside the catalyst particle can be written as follows [10]:

$$D_{ef,i}\left[\frac{1}{z^2}\frac{d}{dz}\left(z^2\frac{dC_i}{dz}\right)\right] = R_i;\ i = Et, Ac, EA\,, \tag{3.4}$$

where $D_{ef,i}$ is the effective diffusivity of substance *i = Et, Ac, EA*.
The boundary condition are as follows [10]:

$$z = R\,;\ C_i = C_i^b;\ \ i = Et, Ac, EA\,, \tag{3.5}$$

$$z = 0\,;\ \frac{dC_i}{dz} = 0;\ \ i = Et, Ac, EA\,. \tag{3.6}$$

The reaction rate R_i (*i = Et, Ac, EA*) are

$$R_{Et} = \frac{k_{ref_1} e^{\left[-(E_1/R_G)\left((1/T)-(1/T_{ref})\right)\right]} C_{Et}}{1+K_{C,Et}C_{Et}+K_{C,Ac}C_{Ac}+K_{C,EA}C_{EA}}$$

$$R_{Ac} = \frac{k_{ref_2} e^{\left[-(E_2/R_G)\left((1/T)-(1/T_{ref})\right)\right]} C_{Ac} - k_{ref_1} e^{\left[-(E_1/R_G)\left((1/T)-(1/T_{ref})\right)\right]} C_{Et}}{1+K_{C,Et}C_{Et}+K_{C,Ac}C_{Ac}+K_{C,EA}C_{EA}}$$

$$R_{EA} = \frac{k_{ref_3} e^{\left[-(E_3/R_G)\left((1/T)-(1/T_{ref})\right)\right]} C_{EA}}{1+K_{C,Et}C_{Et}+K_{C,Ac}C_{Ac}+K_{C,EA}C_{EA}}\,,$$

where C_{Et}, C_{Ac} and C_{EA} represents the molar concentrations of ethanol , acetaldehyde and ethyl acetate respectively and other designations are represent in Appendix B.
The non-linear differential reaction equations (3.1) to (3.6) will be reduced to

the following system coupled dimensionless nonlinear differential equations as follows (see Appendix A for introduce new dimensionless variables):

$$\frac{d^2E}{dx^2} + \frac{2}{x}\frac{dE}{dx} = F_1\left(E(x), Ac(x), EC(x)\right) \tag{3.7}$$

$$\frac{d^2Ac}{dx^2} + \frac{2}{x}\frac{dAc}{dx} = F_2\left(E(x), Ac(x), EC(x)\right) \tag{3.8}$$

$$\frac{d^2EC}{dx^2} + \frac{2}{x}\frac{dEC}{dx} = F_3\left(E(x), Ac(x), EC(x)\right) \tag{3.9}$$

with the boundary conditions are listed as follows:

$$x = 1\,;\;\; E = Ac = EC = 1 \tag{3.10}$$

$$x = 0\,;\;\; \frac{dE}{dx} = \frac{dAc}{dx} = \frac{dEC}{dx} = 0 \tag{3.11}$$

where the functions $E(x)$, $AC(x)$ and $EC(x)$ are the dimensionless molar concentration of the ethanol, acetaldehyde and ethyl acetate respectively, x is dimensionless axial length of the reactor inside the catalyst particle, $\gamma_i's$ and $\beta_i's$ are dimensionless parameters and ϕ_i^2 are Thiele modulus (unitless). To interpret on, consider the non-linear differential equation as follows:

$$Lu + Nu = g(t)\,,$$

where term L and N are linear and nonlinear operator respectively. We have to solve the above type of nonlinear differential equation apply the VIM, we can expressed the given Equation (3.8) as correction functional form:

$$u_{n+1}(x) = u_n(x) + \int_0^x \lambda\left(Lu_n(t) + N\tilde{u}_n(t) - g(t)\right)dt\,,$$

where constant or a function λ is a general Lagrange multiplies [22–24], the subscript n indicates the n^{th} approximation and $\tilde{u}_n$ is a restricted variation which means that $\delta\tilde{u}_n = 0$. The successive approximations u_{n+1}, for $n \geq 0$, of the solution $u(t)$ will be readily obtained upon any selective function $u_0(t)$. Consequently, the exact solution, if it exists, will be given by

$$y(x) = \lim_{n\to\infty} u_n(x)\,.$$

We apply the VIM to non-linear differential Equations (3.7) to (3.9) with initial and boundary condition equations (3.10) and (3.11). First, we determine the correction functional in the form

$$E_{n+1}(x) = E_n(x) + \int_0^x \lambda \left(E_n''(t) + \frac{2}{t} E_n'(t) - F_1\left(E_n(t), Ac_n(t), EC_n(t)\right) \right) dt$$

(3.12)

$$Ac_{n+1}(x) = Ac_n(x) + \int_0^x \lambda \left(Ac_n''(t) + \frac{2}{t} Ac_n'(t) - F_2\left(E_n(t), Ac_n(t), EC_n(t)\right) \right) dt$$

$$EC_{n+1}(x) = EC_n(x) + \int_0^x \lambda \left(EC_n''(t) + \frac{2}{t} EC_n'(t) - F_3\left(E_n(t), Ac_n(t), EC_n(t)\right) \right) dt\,,$$

where $\lambda = \frac{t(t-x)}{x}$. As a result, we obtain the following iteration formula:
We will select the zeroth approximations (which satisfy the boundary conditions) as follows:

$$\begin{aligned} E_0(x) &= E(0) + xE'(0) = \delta_1 \\ Ac_0(x) &= Ac(0) + xAc'(0) = \delta_2 \\ EC_0(x) &= EC(0) + xEC'(0) = \delta_3\,. \end{aligned}$$

This solution will accelerate the convergence of the successive approximations. where the as yet undetermined constants δ_1, δ_2 and δ_3 will be approximated by using the boundary conditions *E*(1), *Ac*(1) and *EC*(1). Thus, we obtain the following approximations:

$$\begin{aligned} E_0(x) &= \delta_1 \\ Ac_0(x) &= \delta_2 \\ EC_0(x) &= \delta_3 \\ E_1(x) &= \delta_1 + \left(\frac{\phi_1^2 e^{-\gamma_1}\delta_1}{1 + \beta_1\delta_1 + \beta_2\delta_2 + \beta_3\delta_3} \right) \frac{x^2}{6} \\ Ac_1(x) &= \delta_2 + \left(\frac{\phi_2^2 e^{-\gamma_2}\delta_2 - \phi_3^2 e^{-\gamma_1}\delta_1}{1 + \beta_1\delta_1 + \beta_2\delta_2 + \beta_3\delta_3} \right) \frac{x^2}{6} \\ EC_1(x) &= \delta_3 + \left(\frac{\phi_4^2 e^{-\gamma_1}\delta_3}{1 + \beta_1\delta_1 + \beta_2\delta_2 + \beta_3\delta_3} \right) \frac{x^2}{6} \\ &\cdots\cdots\cdots \\ &\cdots\cdots\cdots \end{aligned}$$

From these Equations (3.12), we can obtain the numerical values for δ_1,δ_2 and δ_3. Note that $\delta_i' s$ are not fixed but they are mainly depends on the parameters

ϕ_1, ϕ_2, ϕ_3, ϕ_4, γ_1, γ_2, γ_3, β_1, β_2 and β_3.
Therefore, we can represent the approximate solution functions as follows:

$$E(x) = \sum_{n=0}^{m} E_n(x) \tag{3.13}$$

$$Ac(x) = \sum_{n=0}^{m} Ac_n(x) \tag{3.14}$$

$$EC(x) = \sum_{n=0}^{m} EC_n(x) \tag{3.15}$$

MATLAB software can be used to find the numerical simulation for the non-

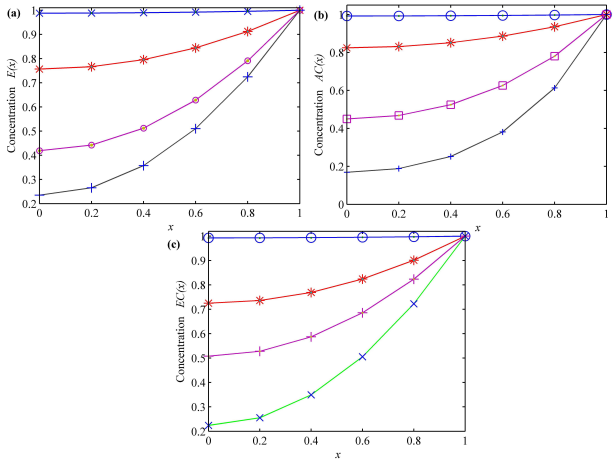

FIGURE 1. Comparison between numerically(different symbol curve) computed concentration profile with the analytical expression(soild line curve) Equations (3.13) to (3.15). The reaction/diffusion parameter is varied at (a)β_1=β_2=β_3=ϕ_2=ϕ_3= ϕ_4=γ_1 = 1, γ_2=5, γ_3=3 and ϕ_1= 1, 5, 10, 15. (b)β_1=β_3=10,β_2=1, ϕ_1=ϕ_3= ϕ_4=γ_1=γ_2=γ_3=0.001 and ϕ_2= 1, 6, 8, 10. (c)β_1=β_3=10,β_2=1, ϕ_1=ϕ_2= ϕ_3=γ_1=γ_2=γ_3=0.001 and ϕ_4= 1, 5, 10, 15.

linear differential equations with the boundary conditions (Equations (3.7) to (3.11)). For these purpose, the obtain solutions (Equations (3.13) to (3.15)) will

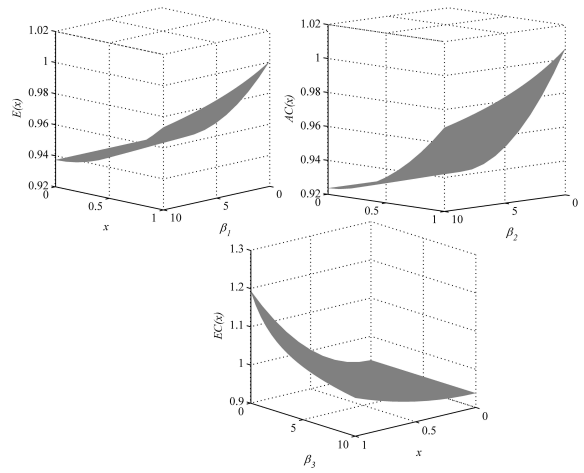

FIGURE 2. The concentration of ethanol $E(x)$, acetaldehyde $Ac(x)$ and ethyl acetate $EC(x)$ was computed against dimensionless radial distance x and using Equations (3.13) to (3.15), for various values of (a)$\beta_1=\beta_2=\beta_3=\gamma_1=\gamma_2=\gamma_3=3$, $\phi_2=15$ and $\phi_3=\phi_4=10$. (b)$\beta_1=\beta_2=\beta_3=\gamma_2=\gamma_3=3$, $\gamma_1=\phi_1=\phi_3=\phi_4=10$. (c)$\beta_1=\beta_2=\beta_3=\gamma_2=\gamma_3=3$, $\gamma_1=\phi_1=\phi_3=10$ and $\phi_2=15$.

be convergent solution or not.The convergence will be analysing in graphical representation and error calculation format.We analyse the reaction parameters in the catalyst particle for the physical point of view and these are represented graphically in figures 1- 3. Also, We have obtained numerical simulation for the Equations (3.7) to (3.11) with the help of MATLAB software. From these numerical solution is compared with our analytical results for the reason of the obtained result approximate or not.

The analytical results for the fixed bed laboratory reactor model using Equations (3.7) to (3.11) are validated against the numerical results. Our analytical expression of dimensionless concentration of the ethanol $E(x)$, acetaldehyde $Ac(x)$ and ethyl acetate $EC(x)$ are compared with simulation results in Tables 1 and 2 for various values of the dimensionless parameters $\phi_i's$, $\gamma_i's$ and $\beta_i's$ respectively. From these tables, it can be noticed our analytical results match es quite well with the numerical results. The relative error between our analytical and numerical result does not exceed 1.5% for all values of parameters considered in the simulation.

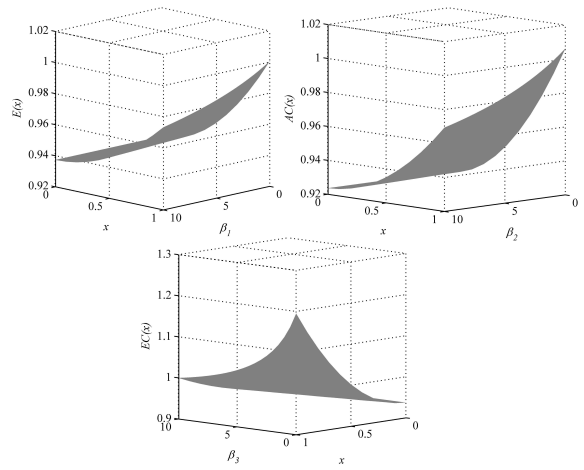

FIGURE 3. The concentration of ethanol $E(x)$, acetaldehyde $Ac(x)$ and ethyl acetate $EC(x)$ was computed against dimensionless radial distance x and using Equations(3.13) âĂŞ (3.15), for various values of (a)β_2=1, β_3=10,γ_1=γ_2=γ_3=3, ϕ_1=ϕ_3=ϕ_4=10 and ϕ_2=15. (b)β_1=0.1, β_3=10,γ_1=γ_2=γ_3=3, ϕ_1=ϕ_3=ϕ_4=10 and ϕ_2=15. (c)β_1=0.1, β_2=1,γ_1=γ_2=γ_3=3, ϕ_1=ϕ_3=ϕ_4=10 and ϕ_2=15.

Comparison between VIM and numerical results for various values of the reaction parameters is shown in Fig.1 and Table 1 and 2. The obtained results in comparison with numerical simulations represented that VIM has been enough accuracy and efficiency so it would be applicable for solving strongly nonlinear equations of coupled system. The dimensionless concentration $E(x)$, $Ac(x)$ and $EC(x)$ as attain maximum ($\approx$ 1) for the dimensionless reaction parameters $\phi_i's$, $\gamma_i's$ and $\beta_i's$ are greater than 0.001.

In Figures 2 and 3, we represent graphically the dimensionless concentrations $E(x)$, $Ac(x)$ and $EC(x)$ against dimensionless radial distance x and reaction diffusion parameters $\phi_i's$ and $\beta_i's$. From these figures, it is observed that the behaviour for reaction diffusion parameter in various values and also it is applicable in chemical engineering for the reason of diffusion reactor model analysis.

TABLE 1. Error calculation E(x) and Ac(x) respectively with the numerical and analytical results for various values of parameters $\phi_i's$, $\gamma_i's$ and $\beta_i's$.

Concentration $E(x)$				Concentration $Ac(x)$			
$\phi_2=\phi_3=\phi_4=\gamma_1=\gamma_2=\gamma_3=0.0001$, $\beta_1=\beta_3=10$, $\beta_2=1$ and $\phi_1=15$.				$\phi_1=\phi_3=\phi_4=\gamma_1=\gamma_2=\gamma_3=0.0001$, $\beta_1=\beta_3=10$, $\beta_2=1$ and $\phi_2=8$.			
$\delta_1=0.1174635034$,$\delta_2=0.5015671968$ $\delta_3=0.4990224959$				$\delta_1=0.4999999963$,$\delta_2=0.3401746555$ $\delta_3=0.4999999963$			
x	Num.	VIM	% Error	x	Num.	VIM	%Error
0.0	0.2349	0.2349	0.0000	0.0	0.6803	0.6803	0.0000
0.2	0.2655	0.2655	0.0000	0.2	0.6931	0.6932	0.0144
0.4	0.3573	0.3572	0.0288	0.4	0.7315	0.7317	0.0273
0.6	0.5104	0.5104	0.0000	0.6	0.7954	0.7955	0.0126
0.8	0.7246	0.7245	0.0138	0.8	0.8849	0.8849	0.0000
1.0	1.0000	1.0000	0.0000	1.0	1.0000	1.0000	0.0000
Average Error %			0.0071	Average Error %			0.0090

TABLE 2. Error calculation EC(x) with the numerical and analytical results for various values of parameters $\phi_i's$, $\gamma_i's$ and $\beta_i's$.

$\phi_1=\phi_2=\phi_3=\gamma_1=\gamma_2=\gamma_3=0.0001$, $\beta_1=\beta_3=10$, $\beta_2=1$ and $\phi_1=5$.			
$\delta_1=0.4999999963$,$\delta_2=0.3958863145$, $\delta_3=0.4999999963$			
x	Num.	VIM	% Error
0	0.7910	0.7910	0.0000
0.2	0.7990	0.7990	0.0000
0.4	0.8232	0.8230	0.0243
0.6	0.8647	0.8646	0.0156
0.8	0.9300	0.9300	0.0000
1.0	1.0000	1.0000	0.0000
Average Error %			0.0071

4. Concluding comments

In this work, the variational iteration method (VIM) is successfully applied to the concentration of the ethanol $E(x)$, ethyl acetate $EC(x)$ and acetaldehyde $Ac(x)$ with the boundary conditions. Comparisons have been done among VIM and numerical method by different reaction parameters values. Data from error figures represent that obtained solutions with VIM has minor differences with numerical simulations. Furthermore, according to achieved results, these works are useful to understand the behaviour of the system. Also, it will be obvious that VIM is convenient analytical method and due to its accuracy, efficiency and convergence it could be applicable for solving strongly nonlinear differential equations.

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APPENDIX A:NOMENCLATURE

$D_{ef,i}$	Effective diffusivities of *i*(=ethanol, ethyl acetate and acetaldehyde)(cm^2/s)
C_i	Concentration of *i*(=ethanol, ethyl acetate and acetaldehyde)$(mol\ m^{-3})$
$K_{C,i}$	Adsorption equilibrium constant of *i*(=ethanol, ethyl acetate and acetaldehyde)$(m^3 mol^{-1})$
$K_{ref,1}$	Reparameterized pre exponential factor of step 1 at a reference temperature T_{ref} (s^{-1})
$K_{ref,2}$	Reparameterized pre exponential factor of step 2 at a reference temperature T_{ref} $(mols^{-1}m^{-3})$
E_1&E_2	Activation Energy $(Jmol^{-1})$
T_{ref}	Reference temperature(*K*)
T	Temperature(*K*)
R_G	Gas Constant(*J / (mol k)*)
z	Axial length of the reactor(*cm*)
C_i^b	Molar Concentration of *i*(=ethanol, ethyl acetate and acetaldehyde)$(mol\ m^{-3})$
R	Particle radius(*cm*)
E	Dimensionless molar concentration of ethanol (unitless)
EA	Dimensionless molar concentration of ethyl acetate (unitles)
AC	Dimensionless molar concentration of acetaldehyde (unitless)
x	Dimensionless distance (unitless)
$\gamma_i's$ & $\beta_i's$	Dimensionless parameters (unitless)
ϕ_i^2's	Thiele modulus (unitless)

DEPARTMENT OF MATHEMATICS
THE MADURA COLLEGE, MADURAI, TAMIL NADU, INDIA
E-mail address: kmdharma6902 @ yahoo.in

DEPARTMENT OF MATHEMATICS
THE MADURA COLLEGE, MADURAI, TAMIL NADU, INDIA
E-mail address: vallimadhavan.tnj@gmail.com