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MATHEMATICAL MODELING OF NONLINEAR BOUNDARY VALUE PROBLEM IN Mn-Cu CATALYTIC COMBUSTION OF VOLATILE ORGANIC COMPOUNDS USING ASYMPTOTIC METHODS

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Abstract

The Article describes the kinetic approach to ethanol and ethyl acetate combustion using a Mn-Cu catalyst. Catalytic combustion is an established process for removing volatile organic compounds. Acetaldehyde is an intermediate product of ethanol oxidation. The kinetic mechanism of this model is expressed in terms of a nonlinear equation in planar coordinates. Approximate analytical solutions for the concentrations of ethanol, ethyl acetate, and acetaldehyde are derived using asymptotic methods. Analytical results are verified to be accurate through a direct comparison with numerical simulation. This paper aims to provide a kinetic evaluation of the combustion of ethanol over a Mn-Cu catalyst. The study was conducted to estimate the appropriate kinetic parameters and formulate reasonable reaction rate expressions.

Keywords: Catalytic Combustion, Mathematical modeling, Nonlinear differential equations.

I. Introduction

Various chemical and printing processes release CO and volatile organic compounds (VOCs), such as ethyl acetate and ethanol. Future regulations on VOC emissions will become stricter due to increasing concerns about photochemical smog, tropospheric ozone, air toxics, and unpleasant odours. CO is one of the primary ingredients in the waste gas from aldehyde production, and ethanol and ethyl acetate are the predominant VOCs in several industry segments. Catalytic incineration offers a competitive means of lowering CO and VOC emissions. Nowadays, supported precious metal catalysts are most frequently employed in catalytic incineration [II].

Thermal combustion is the most comprehensive technique for reducing volatile organic compounds (VOCs). Still, it is not practical due to the requirement of high temperatures above 1273 K. When VOC concentrations are low, catalytic combustion is the most promising method for their removal. Because catalytic combustion produces nitrogen oxides at considerably lower temperatures, it benefits the environment. The printing process and the use of several chemicals release volatile organic compounds (VOCs), including ethanol and ethyl acetate. Ethyl acetate and ethanol are the most common volatile organic compounds (VOCs) in various areas of the printing industry. Furthermore, the complete oxidation of ethanol has mainly been investigated in regulating emissions from ethanol-fuelled vehicles [VIII].

Volatile organic compounds (VOCs), released from various industrial operations, constitute a significant category of air pollutants. Two of these VOCs—ethanol and/or ethyl acetate—are particularly frequently used as solvents in the printing industry. The most commonly used method to eliminate these kinds of VOCs is catalytic combustion [XII]. This field's research efforts focus on developing new catalytic materials that exhibit high activity at moderate temperatures and have low manufacturing costs. Morales et al. have developed an effective Mn and Cu catalyst in which a trace of copper prevents manganese oxide from developing a crystalline structure[X]. Nevertheless, few studies have focused on determining the kinetic parameters that are necessary for the design and optimisation of catalytic reactors. This contribution aims to present kinetic research on ethanol combustion on a Mn /Cu catalyst [VII]

Additionally, acetaldehyde was detected in substantial quantities. It reacts more slowly than ethanol. Acetaldehyde is the species that is most difficult to eliminate. The distinct ethanol concentration is the cause of the variation in the acetaldehyde mole fraction. Numerous experiments using various catalyst types have documented the formation of acetaldehyde [V]. Although carbon monoxide has been detected previously [XIII], neither acetic acid nor carbon monoxide was found in this study. The primary reaction route on the catalyst under examination involves ethanol, which first yields acetaldehyde, which is then oxidised to produce CO2 and H2O products.

Delimaris et al. investigated the oxidation of ethanol, toluene, and ethyl acetate, as well as the dynamic behaviour of the urea combustion method [VI]. J. Mariani developed a nonlinear differential equation as a mathematical model that connects the molar concentrations within the catalyst particle [III]. Campesi et al. used a Mn Cu catalyst to study the combustion of an ethanol and ethyl acetate combination [IV]. A mathematical explanation of concentration using spherical geometry was developed by Meena et al. [IX]. There is no straightforward or closed-form analytical solution available for the concentrations. According to current studies, analytical procedures for the concentrations in planar have not yet been devised.

We present our results using HPM and AGM to solve the nonlinear differential equation of catalytic combustion of volatile organic compounds analytically under steady-state conditions. The validity of the proposed methods will be investigated through direct comparison with numerical results obtained using MATLAB.

II. Mathematical Model

The process of oxidizing ethanol to carbon dioxide is depicted in the following reaction scheme:

$$C_2H_6O + 1/2\ O_2 \rightarrow C_2H_4O + H_2O \tag{1.a}$$

$$C_2H_4O + 5/2\ O_2 \rightarrow 2CO_2 + 2H_2O \tag{1.b}$$

Equation (a) is a partial oxidation process where ethanol is transformed into acetaldehyde with the release of water, and equation (b) is a complete oxidation of acetaldehyde, which means that all of the carbon in acetaldehyde is converted to carbon dioxide and all of the hydrogens are converted to water. This is a typical combustion reaction where the substance is fully oxidized, and no other by-products remain.

The oxidation of ethyl acetate results in the production of CO_2 , represented by the following reaction(c) scheme

$$C_4H_8O_2 + 5O_2 \rightarrow 4CO_2 + 4H_2O \tag{1.c}$$

The following are the ethanol, acetaldehyde, and ethyl acetate's reaction rate r_1, r_2, r_3 are

$$r_1 = \frac{K_{ref\,1}\exp[-(E_1/R_g)(1/T-1/T_{ref})]C_{ethanol}}{1+K_{c,ethanol}C_{ethanol}+K_{c,ethanol}C_{acetaldehyde}+K_{c,ethanol}C_{ethyl\,acetate}} \tag{2.1}$$

$$r_2 = \frac{K_{ref\,2}\exp[-(E_2/R_g)(1/T-1/T_{ref})]C_{acetaldehyde}}{1+K_{c,ethanol}C_{ethanol}+K_{c,ethanol}C_{acetaldehyde}+K_{c,ethanol}C_{ethyl\,acetate}} \tag{2.2}$$

$$r_3 = \frac{K_{ref\,3}\exp[-(E_3/R_g)(1/T-1/T_{ref})]C_{ethyl\,acetate}}{1+K_{c,ethanol}C_{ethanol}+K_{c,ethanol}C_{acetaldehyde}+K_{c,ethanol}C_{ethyl\,acetate}} \tag{2.3}$$

$C_{ethanol}$,$C_{acetaldehyde}$, $C_{ethyl\,acetate}$ indicates the concentrations of molar content within the catalyst. E_1,E_2, E_3 represent activation energy. $K_{c,ethanol}$ $K_{c,acetaldehyde}$, $K_{c,ethyi\,acetate}$ are the ethanol, acetaldehyde, and ethyl acetate's absorption equilibrium constants, respectively. $K_{ref\,1}$, $K_{ref\,2}$,$K_{ref\,3}$ refers to the reparametrized pre-exponential factor, R_g refers to the gas constant, T_{ref} represents the reference temperature, and T refers to the temperature.

The governing nonlinear equation for reaction-diffusion inside the catalyst particle in polar coordinates is as follows.

$$\frac{d^2C_{ethanol}}{dy^2} = \frac{r_1}{D_{ef,ethanol}} \tag{2.4}$$

$$\frac{d^2C_{acetaldehyde}}{dy^2} = \frac{r_2 - r_1}{D_{ef,acetaldehyde}} \tag{2.5}$$

$$\frac{d^2C_{ethl\,acetate}}{dy^2} = \frac{r_3}{D_{ef,ethl\,acetate}} \tag{2.6}$$

$D_{ef,ethanol}$, $D_{ef,acetaldehyde}$, $D_{ef,ethl\,acetate}$ are the concentrations effective diffusivities.

The boundary conditions for the non-dimensional equations (2.4-2.6) are

At $y = R$; $C_{ethanol} = {C^b}_{ethanol}$,$C_{acetaldehyde} = {C^b}_{acetaldehyde}$,

$$C_{ethyl\ acetate} = {C^b}_{ethyl\ acetate} \tag{2.7}$$

$$\text{At } y = 0;\ \frac{dC_{ethanol}}{dy} = 0,\ \frac{dC_{acetaldehyde}}{dy} = 0,\ \frac{dC_{ethayl\ acetate}}{dy} = 0 \tag{2.8}$$

Where $C_{ethanol}$, $C_{acetaldehyde}$, $C_{ethyl\ acetate}$ are the bulk solution and R is the catalyst particle radius.

By establishing the following parameters, we transform the nonlinear differential equations (2.4 - 2.8) into dimensionless form:

$$\varphi_1 = \frac{R^2 K_{ref\ 1}}{D_{ef,ethanol}},\ \varphi_2 = \frac{R^2 K_{ref\ 2}}{D_{ef,acetaldehyde}},\ \varphi_3 = \frac{R^2 K_{ref\ 3}}{D_{ef,ethyl\ acetate}},$$

$$\alpha_1 = K_{c,ethanol}{C^b}_{ethanol},\ \alpha_2 = K_{c,acetaldehyde}{C^b}_{acetaldehyde},$$

$$\alpha_3 = K_{c,ethyl\ acetate}{C^b}_{ethyl\ acetate},$$

$$x = \frac{y}{R},\ u = \frac{C_{ethanol}}{{C^b}_{ethanol}},\ v = \frac{C_{eacetaldehyde}}{{C^b}_{acetaldehyde}},\ \text{w}= \frac{C_{ethyi\ acetate}}{{C^b}_{ethyl\ acetate}} \tag{2.9}$$

where u, v, w are the dimensionless concentrations, respectively. x is the dimensional radial distance. φ_1,φ_2, φ_3, γ_1, γ_2 , γ_3, α_1,α_2, α_3 are the dimensionless parameters

Using equation (2.9) non-dimensional form of equations (2.4-2.8) can be written as

$$\frac{d^2u(x)}{dx^2} = \frac{\varphi_1\gamma_1 u(x)}{1+\alpha_1 u(x)+\alpha_2 v(x)+\alpha_3 w(x)} \tag{2.10}$$

$$\frac{d^2v(x)}{dx^2} = \frac{\varphi_2\gamma_2 v(x)-\varphi_1\gamma_1 u(x)}{1+\alpha_1 u(x)+\alpha_2 v(x)+\alpha_3 w(x)} \tag{2.11}$$

$$\frac{d^2w(x)}{dx^2} = \frac{\varphi_3\gamma_3 w(x)}{1+\alpha_1 u(x)+\alpha_2 v(x)+\alpha_3 w(x)} \tag{2.12}$$

The boundary condition reduces to

$$\text{When } x = 1, u = v = w = 1 \tag{2.13}$$

$$x = 0, \frac{du}{dx} = \frac{dv}{dx} = \frac{dw}{dx} = 0 \tag{2.14}$$

III. Approximate Analytical results of the concentration of ethanol, acetaldehyde, and ethyl acetate using the Akbari Ganji Method

AGM is an effective method for tackling nonlinear systems. [I, XI] AGM is a novel method for solving differential equations using algebraic expressions. Nonlinear equations typically don't have accurate solutions. An effective algebraic strategy for resolving nonlinear problems is the Akbari-Ganji method (AGM), first presented by Akbari and Ganji in 2014. It has been demonstrated that this approach can yield analytical solutions for these very accurate and approximate models. The approximate analytical solution for dimensionless concentrations is obtained using this method. To solve the differential equations, it is assumed that the proposed trial solutions for the nonlinear differential equations are given in the Equations. (2.10), (2.11), and (2.12) are as follows:

$$u(x) = A\cosh(lx) + B\sinh(lx) \tag{3.1}$$

$$v(x) = C\cosh(mx) + D\sinh(mx) \tag{3.2}$$

$$w(x) = E\cosh(nx) + E\sinh(nx) \tag{3.3}$$

Where A, B, C, D, E, F, m, n are constants. Applying the boundary constant (2.13-2.14)

We get the constant values as

$$A = \frac{1}{\cosh(l)}, B = 0, C = \frac{1}{\cosh(m)}, D = 0, E = \frac{1}{\cosh(n)}, F = 0 \tag{3.4}$$

Substituting equation (3.4) in (3.1-3.2), we get

$$u(x) = \frac{\cosh(lx)}{\cosh(l)} \tag{3.5}$$

$$v(x) = \frac{\cosh(mx)}{\cosh(m)} \tag{3.6}$$

$$w(x) = \frac{\cosh(nx)}{\cosh(n)} \tag{3.7}$$

Where l, m, n are constants

Equation (2.10) can be rearranged as follows to determine the values of l

$$l^2\left(\frac{\cosh(lx)}{\cosh(l)}\right) - \frac{\varphi_1\gamma_1\left(\frac{\cosh(lx)}{\cosh(l)}\right)}{1+\alpha_1\left(\frac{\cosh(lx)}{\cosh(l)}\right)+\alpha_2\left(\frac{\cosh(mx)}{\cosh(m)}\right)+\alpha_3\left(\frac{\cosh(nx)}{\cosh(n)}\right)} = 0 \tag{3.8}$$

At $x = 1$

$$l = \frac{\sqrt{\varphi_1\gamma_1(1+\alpha_1+\alpha_2+\alpha_3)}}{1+\alpha_1+\alpha_2+\alpha_3} \tag{3.9}$$

By solving equations (3.2) & (3.3), we get the constant values of m, n

$$m = \frac{\sqrt{-(1+\alpha_1+\alpha_2+\alpha_3)(\varphi_1\gamma_1-\varphi_2\gamma_2)}}{1+\alpha_1+\alpha_2+\alpha_3} \tag{3.10}$$

$$n = \frac{\sqrt{\varphi_3\gamma_3(1+\alpha_1+\alpha_2+\alpha_3)}}{1+\alpha_1+\alpha_2+\alpha_3} \tag{3.11}$$

Therefore, the analytical results of the concentration of ethanol, acetaldehyde, and ethyl acetate,

$$u(x) = \frac{\cosh\left(\frac{\sqrt{\varphi_1\gamma_1(1+\alpha_1+\alpha_2+\alpha_3)}}{1+\alpha_1+\alpha_2+\alpha_3}x\right)}{\cosh\left(\frac{\sqrt{\varphi_1\gamma_1(1+\alpha_1+\alpha_2+\alpha_3)}}{1+\alpha_1+\alpha_2+\alpha_3}\right)} \tag{3.12}$$

$$v(x) = \frac{\cosh\left(\frac{\sqrt{-(1+\alpha_1+\alpha_2+\alpha_3)(\varphi_1\gamma_1-\varphi_2\gamma_2)}}{1+\alpha_1+\alpha_2+\alpha_3}x\right)}{\cosh\left(\frac{\sqrt{-(1+\alpha_1+\alpha_2+\alpha_3)(\varphi_1\gamma_1-\varphi_2\gamma_2)}}{1+\alpha_1+\alpha_2+\alpha_3}\right)} \tag{3.13}$$

$$w(x) = \frac{\cosh\left(\frac{\sqrt{\varphi_3\gamma_3(1+\alpha_1+\alpha_2+\alpha_3)}}{1+\alpha_1+\alpha_2+\alpha_3}x\right)}{\cosh\left(\frac{\sqrt{\varphi_3\gamma_3(1+\alpha_1+\alpha_2+\alpha_3)}}{1+\alpha_1+\alpha_2+\alpha_3}\right)} \tag{3.14}$$

Approximate analytical results for the concentration of ethanol, acetaldehyde, and ethyl acetate using the Homotopy perturbation method

Ji-Huan He proposed the homotopy perturbation method [XV, XVI, XIV] in 1998, which is a powerful and structured approach for solving nonlinear ordinary and partial differential equations. This approach combines the concepts of perturbation techniques in applied mathematics with those of homotopy in topology. HPM's primary advantage is its ability to provide accurate analytical approximations for nonlinear problems with minimal processing overhead, making it a crucial tool for scientific research and engineering applications. HPM generates a series of solutions through iterative steps in which each term improves on the previous approximations. The convergence of this series is managed by HPM, yielding an approximate analytical solution. The homotopy for equations (2.10)–(2.12) is constructed as follows.

$$(1-p)\left(\frac{d^2u}{dx^2}\right) + p\left(\frac{d^2u}{dx^2} - \frac{\varphi_1\gamma_1 u}{1+\alpha_1 u+\alpha_2 v+\alpha_3 w}\right) = 0 \tag{3.15}$$

$$(1-p)\left(\frac{d^2v}{dx^2}\right) + p\left(\frac{d^2v}{dx^2} - \frac{\varphi_2\gamma_2 v-\varphi_1\gamma_1 u}{1+\alpha_1 u+\alpha_2 v+\alpha_3 w}\right) = 0 \tag{3.16}$$

$$(1-p)\left(\frac{d^2w}{dx^2}\right) + p\left(\frac{d^2w}{dx^2} - \frac{\varphi_3\gamma_3 w}{1+\alpha_1 u+\alpha_2 v+\alpha_3 w}\right) = 0 \tag{3.17}$$

Let's now assume that equation (3.15–3.17) has a solution of

$$u = u_0 + pu_1 + p^2u_2 + \cdots \tag{3.18}$$

$$v = v_0 + pv + p^2v_2 + \cdots \tag{3.19}$$

$$w = w_0 + pw_1 + p^2w_2 + \cdots \tag{3.20}$$

Rearranging the same powers of p terms substitute (3.18-3.20) to (3.15-3.17), we get

$$p^0 : \frac{d^2u_0}{dx^2} = 0, \frac{du_0}{dx}(0) = 0, u_0(1) = 1 \tag{3.21}$$

$$p^0 : \frac{d^2v_0}{dx^2} = 0, \frac{dv_0}{dx}(0) = 0, v_0(1) = 1 \tag{3.22}$$

$$p^0 : \frac{d^2w_0}{dx^2} = 0, \frac{dw_0}{dx}(0) = 0, w_0(1) = 1 \tag{3.23}$$

$$p^1 : \frac{d^2u_1}{dx^2} - \frac{\varphi_1\gamma_1 u_0}{1+\alpha_1 u_0+\alpha_2 v_0+\alpha_3 w_0} = 0, \frac{du_1}{dx}(0) = 0, u_1(1) = 0 \tag{3.24}$$

$$p^1 : \frac{d^2v_1}{dx^2} - \frac{\varphi_2\gamma_2 v_0-\varphi_1\gamma_1 u_0}{1+\alpha_1 u_0+\alpha_2 v_0+\alpha_3 w_0} = 0, \frac{dv_1}{dx}(0) = 0, v(1) = 0 \tag{3.25}$$

$$p^1 : \frac{d^2w_1}{dx^2} - \frac{\varphi_1\gamma_1 w_0}{1+\alpha_1 u_0+\alpha_2 v_0+\alpha_3 w_0} = 0, \frac{dw_1}{dx}(0) = 0, w_1(1) = 0 \tag{3.26}$$

Solving the equation (3.21-3.26) generates the following outcomes.

$$u_0 = 1, v_0 = 1, w_0 = 1$$

$$u_1 = \frac{\varphi_1\gamma_1(x^2-1)}{2(1+\alpha_1+\alpha_2+\alpha_3)} = 0$$

$$v_1 = \frac{(\varphi_1\gamma_1-\varphi_2\gamma_2)(1-x^2)}{2(1+\alpha_1+\alpha_2+\alpha_3)} = 0$$

$$w_1 = \frac{\varphi_3\gamma_3(x^2-1)}{2(1+\alpha_1+\alpha_2+\alpha_3)} = 0$$

Therefore, the approximate analytical solution can be represented by HPM as follows:

$$u = \lim_{p\to 1} u = u_0 + u_1 = 1 + \frac{\varphi_1\gamma_1(x^2-1)}{2(1+\alpha_1+\alpha_2+\alpha_3)} \tag{3.27}$$

$$v = \lim_{p\to 1} = v_0 + v_1 = 1 + \frac{(\varphi_1\gamma_1-\varphi_2\gamma_2)(1-x^2)}{2(1+\alpha_1+\alpha_2+\alpha_3)} \tag{3.28}$$

$$w = \lim_{p\to 1} w = w_0 + w_1 = 1 + \frac{\varphi_3\gamma_3(x^2-1)}{2(1+\alpha_1+\alpha_2+\alpha_3)} \tag{3.29}$$

IV. Validation

The validation approach has received a lot of attention in the literature. Equations (2.10)–(2.12) and (2.13)–(2.14) represent the newly created approximate analytical formulations for the concentrations utilizing the HPM and the Akbari Ganji method, respectively. Tables 1–3 present a comparison of the numerical and analytical concentrations of ethanol, acetaldehyde, and ethyl acetate, as determined by the AGM and HPM methods, for varying values of the diffusion parameter φ_i. According to the table I-III, the typical relative errors are less than 1%. The numerical responses of Equations are compared with our results (3.12-3.14) and (3.27-3.29) to demonstrate the efficiency of our present approach. Using MATLAB, the numerical solutions are determined. These figures lead us to the conclusion that the analytical and numerical solutions are similar.

Table 1: Comparison between analytical results for different diffusion parameter φ_1 with the concentration of ethanol and for fixed parameters $\gamma_1 = 0.1, \alpha_1, \alpha_2, \alpha_3$=0.1

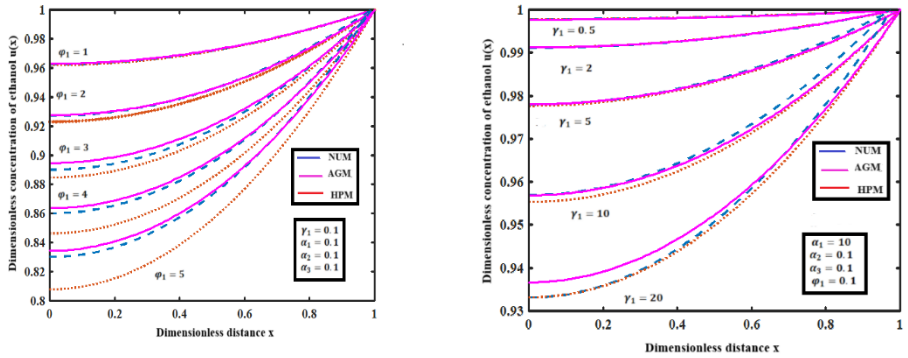
X	$\varphi_1 = 2$					$\varphi_1 = 4$					$\varphi_1 = 6$				
	NUM	AGM	HPM	ERR % AGM	ERR % HPM	NUM	AGM	HPM	ERR % AGM	ERR % HPM	NUM	AGM	HPM	ERR % AGM	ERR % HPM
0	0.9277	0.9277	0.9231	0	0.50	0.86	0.8637	0.8562	0.43	0.44	0.83	0.8343	0.8177	0.52	1.50
0.2	0.9306	0.9306	0.9262	0	0.48	0.8657	0.8691	0.8624	0.39	0.38	0.8369	0.8409	0.8155	0.48	2.62
0.4	0.9394	0.9394	0.9356	0	0.41	0.8826	0.8855	0.8813	0.33	0.15	0.8579	0.8607	0.8391	0.33	2.24
0.6	0.9541	0.9541	0.9513	0	0.29	0.9118	0.9118	0.9027	0	1.00	0.893	0.894	0.8783	0.11	1.67
0.8	0.9747	0.9747	0.9733	0	0.14	0.9526	0.9526	0.9466	0	0.63	0.9428	0.9413	0.9333	0.16	1.02
1	1	1	1	0	0	1	0.9972	1	0.28	0	1	1	1	0	0
	AVG ERR %			0	0.30	AVG ERR %			0.24	0.44	AVG ERR %			0.26	1.51

TABLE 2: Comparison between analytical results for different diffusion parameter φ_2 with the concentration of acetaldehyde and for fixed parameters $\gamma_1, \gamma_2 = 0.1, \alpha_1, \alpha_2, \alpha_3$=1

X	$\varphi_2 = 5$					$\varphi_2 = 7$					$\varphi_2 = 10$				
	NUM	AGM	HPM	ERR % AGM	ERR % HPM	NUM	AGM	HPM	ERR % AGM	ERR % HPM	NUM	AGM	HPM	ERR % AGM	ERR % HPM
0	0.952	0.952	0.95	0	0.21	0.9294	0.9294	0.925	0	0.48	0.8972	0.8972	0.8875	0	1.09
0.2	0.9539	0.9539	0.952	0	0.20	0.9323	0.9323	0.9281	0	0.45	0.9013	0.9013	0.8921	0	1.03
0.4	0.9598	0.9598	0.9538	0	0.63	0.9408	0.9408	0.9372	0	0.38	0.9137	0.9137	0.9059	0	0.86
0.6	0.9695	0.9695	0.9684	0	0.11	0.9551	0.9551	0.9525	0	0.27	0.9345	0.9345	0.9288	0	0.61
0.8	0.9833	0.9833	0.9826	0	0.07	0.9753	0.9753	0.974	0	0.13	0.9639	0.9639	0.961	0	0.30
1	1	1	1	0	0	1	1	1	0	0	1	1	1	0	0
	AVG	ERR	%	0	0.20	AVG	ERR	%	0	0.29	AVG	ERR	%	0	0.65

TABLE 3: Comparison between analytical results for different diffusion parameter φ_3 with the concentration of ethyl acetate and for fixed parameters $\gamma_1 = 0.01, \alpha_1, \alpha_2, \alpha_3$=1

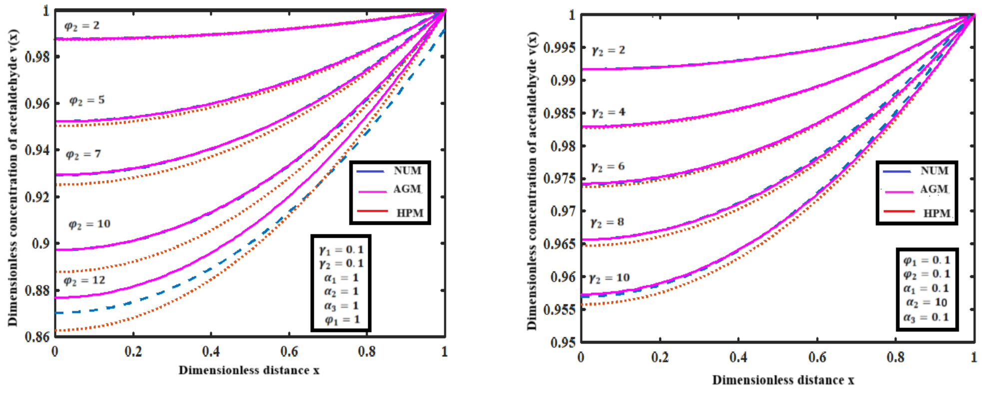
X	$\varphi_2 = 5$					$\varphi_2 = 7$					$\varphi_2 = 10$				
	NUM	AGM	HPM	ERR % AGM	ERR % HPM	NUM	AGM	HPM	ERR % AGM	ERR % HPM	NUM	AGM	HPM	ERR % AGM	ERR % HPM
0	0.952	0.952	0.95	0	0.21	0.9294	0.9294	0.925	0	0.48	0.8972	0.8972	0.8875	0	1.09
0.2	0.9539	0.9539	0.952	0	0.20	0.9323	0.9323	0.9281	0	0.45	0.9013	0.9013	0.8921	0	1.03
0.4	0.9598	0.9598	0.9538	0	0.63	0.9408	0.9408	0.9372	0	0.38	0.9137	0.9137	0.9059	0	0.86
0.6	0.9695	0.9695	0.9684	0	0.11	0.9551	0.9551	0.9525	0	0.27	0.9345	0.9345	0.9288	0	0.61
0.8	0.9833	0.9833	0.9826	0	0.07	0.9753	0.9753	0.974	0	0.13	0.9639	0.9639	0.961	0	0.30
1	1	1	1	0	0	1	1	1	0	0	1	1	1	0	0
	AVG	ERR	%	0	0.20	AVG	ERR	%	0	0.29	AVG	ERR	%	0	0.65



(a) (b)

Fig. 1. Ethanol concentration $u(x)$ plotted against dimensionless distance$x$.

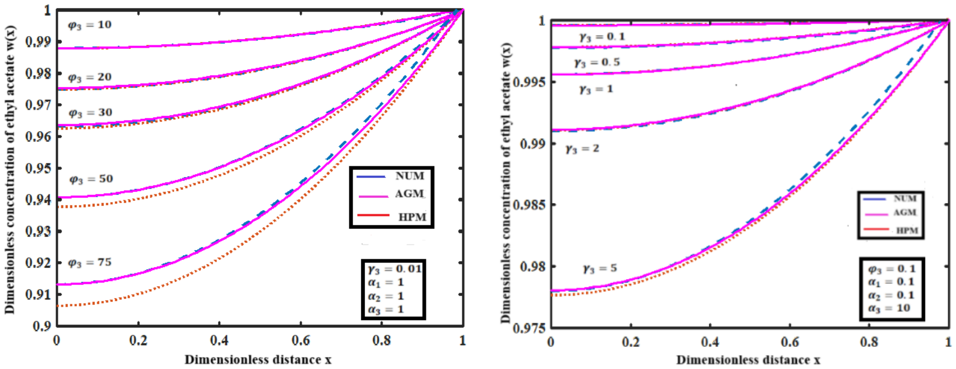
Figure 1 illustrates the dimensionless concentration of ethanol versus the dimensional radial distance x. Figure 1 confirms that for fixed values of γ_1 and $\alpha_1, \alpha_2, \alpha_3$and the non-dimensional concentration $u(x)$, it drops as the dimensionless diffusion parameter $\varphi_1$rises. This means that the dimensionless parameter φ_1 is inversely related to the dimensionless concentration of ethanol $u(x)$. The concentration of ethanol becomes steady when$\varphi_1 \leq 1$. Fig. (b) shows that the non-dimensional ethanol concentration decreases as the diffusion parameter γ_1 increases.



(a) (b)

Fig. 2. Concentration profile of acetaldehyde $v(x)$ plotted against dimensionless distance$x$.

Figure 2 shows the concentration of acetaldehyde $v(x)$ for different values of φ_2 and γ_2 . According to Figure 2(a), as the non-dimensional diffusion parameter $\varphi_2$increases, the acetaldehyde concentration drops. In Figure 2(b), as the dimensionless parameter γ_2 rises, the non-dimensional concentration of acetaldehyde decreases. In this case, the dimensional concentration of acetaldehyde is reciprocally proportional to the dimensional parameters φ_2 and γ_2



(a) (b)

Fig. 3. Concentration profile of ethanol $w(x)$ plotted against dimensionless distance x.

A graph illustrating the relationship between the distance x and the concentration of ethyl acetate $w(x)$, across various parameters, is shown in Figure 3. In Figure 3 (a), the ethyl acetate concentration falls as the value of the non-dimensional diffusion parameter φ_3 rises. The ethyl acetate concentration does not change significantly with dimensionless distance and stabilises at $\varphi_3 \leq 2$. Figure 3(b) displays the normalised concentration for various values of γ_3. As the diffusion parameter γ_3 increases, figure 3(b) indicates that the ethyl acetate $w(x)$ concentration decreases.

V. Residual Analysis for Stability Demonstration

To assess the stability and robustness of the analytical solutions derived using the Akbari–Ganji Method (AGM) and the Homotopy Perturbation Method (HPM), we analyse the residual functions corresponding to each species: ethanol $u(x)$, acetaldehyde $v(x)$, and ethyl acetate $w(x)$. The residuals are defined as the deviation from the original governing nonlinear differential equations (2.10–2.12) when the approximate solutions are substituted. Mathematically, for ethanol:

$$R_u(x) = \frac{d^2u}{dx^2} + A_1 u(x) + B_1 v(x) + C_1 w(x) \qquad (5.1)$$

With similar expressions for $R_v(x)$ and $R_w(x)$. These residuals were computed symbolically and evaluated numerically over the domain $x \in [0,1]$.

The maximum absolute residuals for the approximate solutions obtained via AGM and HPM were computed for all species. For ethanol concentration $u(x)$, AGM yielded a maximum residual of 0.016, while HPM resulted in 0.022. In the case of acetaldehyde $v(x)$, the residuals were 0.026 and 0.031 for AGM and HPM, respectively. For ethyl acetate $w(x)$, AGM produced a residual of 0.018, compared to 0.025 from HPM. These results indicate that both methods provide highly accurate approximations, with AGM demonstrating superior performance across all species.

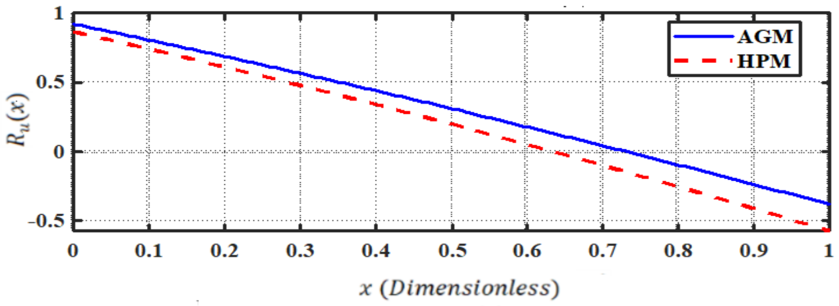


Figure 4(a) :Residual Comparison of $u(x)$

(a)

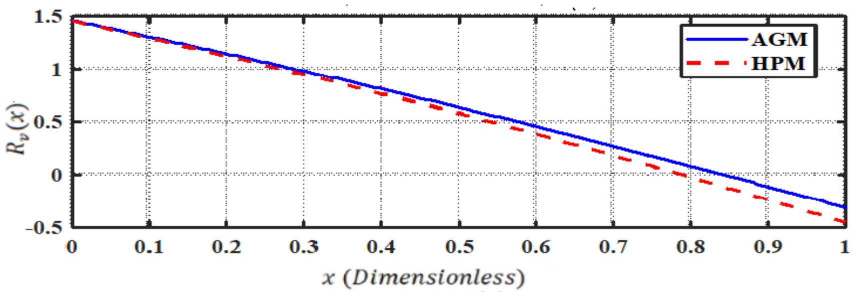


Figure 4(b) : Residual Comparison of $v(x)$

(b)

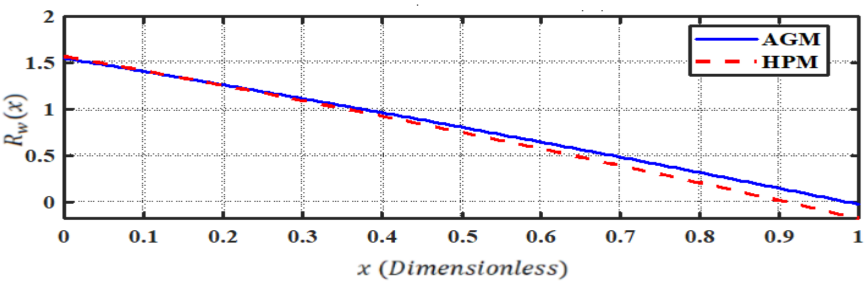


Figure 4(c) : Residual Comparison of $w(x)$

(c)

Fig. 4. (a-c). Comparison of residual errors for the Approximate Generalized Method (AGM) and Homotopy Perturbation Method (HPM) applied to the dimensionless functions $u(x)$,$v(x)$ and $w(x)$, using the parameter sets:$A_1 = 0.5, B_1 = 0.2, C_1 = 0.8, A_2 = 1.0, B_2 = 0.2, C_2 = 0.6, A_3 = 0.3, B_3 = 0.7, C_3 = 0.9$.

Residual curve comparison between AGM and HPM methods for the concentration profiles of ethanol, acetaldehyde, and ethyl acetate over the dimensionless domain. The residuals, defined as the deviation from the original nonlinear governing equations, are plotted to evaluate the accuracy of each method. The Akbari–Ganji Method (AGM) consistently yields lower residuals compared to the Homotopy Perturbation Method (HPM), demonstrating superior accuracy and solution stability across all species.

VI. Validation of Model Predictions with Experimental Data

A comparison was conducted between the expected conversion efficiencies of ethanol and ethyl acetate, as reported by Campesi et al. [IV], and the experimental results to further confirm the model's dependability. As illustrated in Figure 5, the present model predicts a conversion of approximately 94.7% for ethanol and 91.3% for ethyl acetate, which are in good agreement with the experimental findings of 95% and 90%, respectively. This agreement supports the model's suitability for simulating the kinetics of VOC oxidation over Mn–Cu catalysts at moderate temperatures.

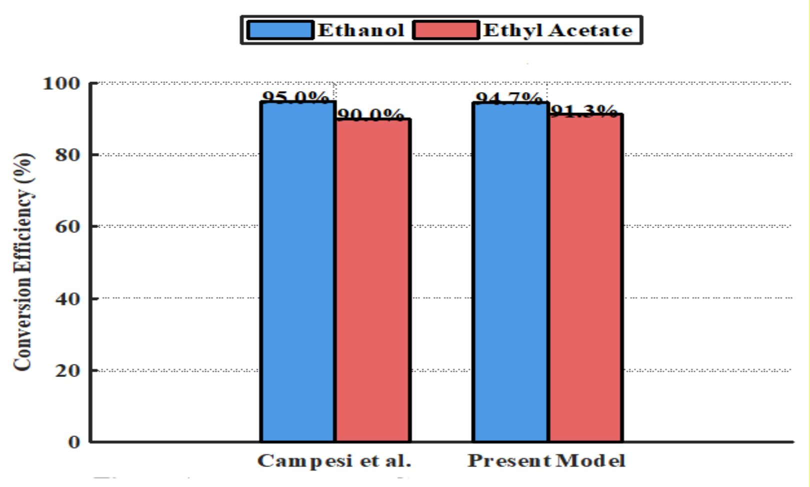


Fig. 5. Comparison of VOC Conversion Efficiency

VII. Conclusions and Future Perspectives

This study presents a theoretical analysis of VOC combustion kinetics (ethanol and ethyl acetate) over Mn–Cu catalysts using asymptotic methods. A nonlinear boundary value model describes the reaction-diffusion behaviour in planar coordinates. Analytical solutions via AGM and HPM were validated against numerical simulations, with AGM showing an error of less than 1%. The results highlight the inverse relationship between diffusion parameters and VOC concentrations, aiding in reactor design. Acetaldehyde's persistence highlights the need for catalyst optimisation to promote complete oxidation and emission control.

Future work should focus on experimental validation using data from existing studies. Incorporating transient conditions will enhance real-world relevance. Coupling particle- and reactor-scale models can improve system-level analysis. An economic assessment of catalyst design will help translate theoretical insights into practical industrial VOC control applications.

Nomenclature

Symbol		Units
$D_{ef,ethanol}$, $D_{ef,acetaldehyde}$, $D_{ef,ethl\ acetate}$	Ethanol, acetaldehyde, and ethyl acetate effective diffusivities	cm^2/s
$C_{ethanol}$, $C_{acetaldehyde}$, $C_{ethyl\ acetate}$	Ethanol, acetaldehyde, and ethyl acetate's concentration	mol/m^3
$K_{c,ethanol}$, $K_{c,acetaldehyde}$, $K_{c,ethyl\ acetate}$	Ethanol, acetaldehyde, ethyl acetate's absorption equilibrium constant	m^3/mol
$K_{ref\ 1}$	Reference temperature, re-parameterized	$T_{ref1}(S^{-1})$
$K_{ref\ 2}$	Reference temperature, re-parameterized	$T_{ref2}(S^{-1})$
$K_{ref\ 3}$	Reference temperature, re-parameterized	$T_{ref3}(S^{-1})$
$E_{1,,}, E_2, E_3$	Activation energy	J/ mol
T	Temperature	K
R_g	Gas constant	$Jk^{-1}mol^{-1}$
Y	Axial length of the reactor	(m)
R	Particle Radius	M
${C^b}_{ethanol}$, ${C^b}_{acetaldehyde}$, ${C^b}_{ethyl\ acetate}$	Molar concentration	Mol /m^3

Conflict of Interest:

There was no relevant conflict of interest regarding this paper.

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