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Analysis through an analytical solution for the SCR reaction network using HPM

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ABSTRACT: *In this study, we investigated the analytical and a numerical solution was performed to study of the SCR reaction network. The SCR reaction network and their kinetic expressions are based on the system of nonlinear reaction diffusion equations. The dimensional, nonlinear, system of ordinary differential equations with an initial condition is solved analytically and numerically using Homotopy perturbation method and Matalb program. Analytical results are compared with the numerical results, a satisfactory agreement is noted. These analytical results are useful to understand the behavior of the system.*
KEYWORDS: *Kinetic model, Mathematical modeling, Non-linear differential equation, Homotopy perturbation method.*

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I. INTRODUCTION

Recently many researchers compared SCR activities and hydrothermal stabilities of Cu/CHA with other Cu^{2+} ion-exchanged zeolites, especially Cu/ZSM-5 and Cu/beta [1-4]. In 2005, the SCR technology was brought to the market for heavy duty vehicles already, based on the use of similar formulation on honeycomb monolith catalysts [5]. However, the low stability of vanadia at high temperature and more and stricter NO_x emission regulations for both heavy and low duty vehicles, whichr equires higher activity at low temperature, have motivated the introduction of zeolitebased catalysts promoted by transition metals, as iron [6–8] and copper [9–11]. Unai De-La-Torre et.al.,[12] have been proposed a steady-state global kinetic model for the NO_x NH_3-SCR reaction system in excess of oxygen.

In this present work, the analytical solution for concentration of NH_3, NO, NO_2 *and* N_2O involved in the reaction systems for global kinetic model considering steady state regime has been proposed. The nonlinear equations in global kinetic model depicted by the mathematical model have been solved by Homotopy perturbation method [13 - 24]. These analytical results are useful to understand and optimize the behavior of $C_{NH_3}, C_{NO}, C_{NO_2}$ *and* C_{N_2O} in global kinetic model. The information gathered from the theoretical modeling is fruitful in experimental design, optimization and prediction of the SCR reaction network.

II. FORMULATION OF THE PROBLEM AND ANALYSIS

In the SCR reaction network, there are seven reactions estimate in the global kinetic model and parameter estimation as follows [12]:

$NH_3 + 3/4\ O_2 \rightarrow 1/2\ N_2 + 3/2\ H_2O$
$NO + 1/2\ O_2 \rightleftarrows NO_2$
$NH_3 + NO + 1/4\ O_2 \rightarrow N_2 + 3/2\ H_2O$
$2\ NH_3 + NO + NO_2 \rightarrow 2N_2 + 3\ H_2O$ (1)
$4\ NH_3 + 3\ NO_2 \rightarrow 7/2\ N_2 + 6H_2O$
$3\ NH_3 + 4NO_2 \rightarrow 7/2\ N_2O + 9/2\ H_2O$
$2N_2O \rightarrow 2N_2 + O_2$

For the above reaction schemes, the kinetic equations for NH_3, NO, NO_2 and N_2O are as follows[12]:

$$r_1 = \frac{k_1 C_{NH_3} C_{O_2}}{1 + K_{NH_3} C_{NH_3}}; r_2 = k_2 \left(C_{NO} C_{O_2}^{0.5} - C_{NO_2} / K_{NO}^{eq.}\right); r_3 = \frac{k_3 C_{NH_3} C_{NO} C_{NO_2}}{1 + K_{NH_3} C_{NH_3}}; r_4 = \frac{k_4 C_{NH_3} C_{NO} C_{NO_2}}{1 + K_{NH_3} C_{NH_3}};$$

$$r_5 = \frac{k_5 C_{NH_3} C_{NO_2}}{1 + K_{NH_3} C_{NH_3}}; r_6 = \frac{k_6 C_{NH_3} C_{O_2}}{1 + K_{NH_3} C_{NH_3}}; r_7 = k_7 C_{N_2O} C_{NO_2}. \quad (2)$$

where $C_{NH_3}, C_{NO}, C_{NO_2}$ *and* C_{N_2O} represent the concentration of NH_3, NO, NO_2 *and* N_2O respectively.

The non-linear differential equation that reaction rate for each component in the medium is evaluated as:

$$\frac{dC_{NH_3}}{d[W/Q]} = -\left(r_1 + r_3 + 2r_4 + 4r_5 + 3r_6\right) \tag{3}$$

$$\frac{dC_{NO}}{d[W/Q]} = -\left(r_2 + r_3 + r_4\right) \tag{4}$$

$$\frac{dC_{NO_2}}{d[W/Q]} = r_2 - r_4 + 3\,r_5 - 4r_6 \tag{5}$$

$$\frac{dC_{N_2O}}{d[W/Q]} = \frac{7}{2}r_6 - 2r_7 \tag{6}$$

The corresponding an initial condition for the Eqns. (3)–(6) is follows [12]:

at [W/Q] = 0; $C_{NH_3} = a_1, C_{NO} = a_2, C_{NO_2} = a_3$ *and* $C_{N_2O} = a_4$ (7)

Analytical expressions of the concentration using the Homotopy Perturbation method

In this section, the Homotopy perturbation method (refer Supplementary method of the manuscript) is used to solve nonlinear differential equation. We have solved the non-linear differential equations (3) – (6) with an initial condition, using this method. The analytical expression of the concentrations of species NH_3, NO, NO_2 and N_2O respectively can be obtained as follows:

$$\begin{aligned} C_{NH_3} &= a_1 e^{-k_1 c_{o_2}[W/X]} - \frac{K_{NH_3} k_1 c_{o_2} a_1^2}{k_1 c_{o_2}}\left(e^{-2k_1 c_{o_2}[W/X]} - e^{-k_1 c_{o_2}[W/X]}\right) + \frac{k_3 c_{o_2} a_1 a_2}{k_2 c^{0.5}_{o_2}}\left(e^{-\left(k_1 c_{o_2} + k_2 c^{0.5}_{o_2}\right)[W/X]} - e^{-k_1 c_{o_2}[W/X]}\right) \\ &+ \frac{2k_4 a_1 a_2 a_3}{k_2 c^{0.5}_{o_2} + \frac{k_2}{K^{eq.}_{NO}}}\left(e^{-\left(k_1 c_{o_2} + k_2 c^{0.5}_{o_2} + K^{eq.}_{NO}\right)[W/X]} - e^{-k_1 c_{o_2}[W/X]}\right) + \frac{(4k_5 + 3k_6) a_1 a_3}{\frac{k_2}{K^{eq.}_{NO}}}\left(e^{-\left(k_1 c_{o_2} + K^{eq.}_{NO}\right)[W/X]} - e^{-k_1 c_{o_2}[W/X]}\right) \end{aligned} \tag{8}$$

$$\begin{aligned} C_{NO} &= a_2\, e^{-k_2 c^{0.5}_{o_2}[W/X]} - \frac{\frac{k_2}{K^{eq.}_{NO}} a_1}{k_1 c_{o_2} - \frac{k_2}{K^{eq.}_{NO}}}\left(e^{-\frac{k_2}{K^{eq.}_{NO}}[W/X]} - e^{-k_2 c^{0.5}_{o_2}[W/X]}\right) + \frac{k_3 a_1 a_2}{k_1}\left(e^{-\left(k_1 c_{o_2} + k_2 c^{0.5}_{o_2}\right)[W/X]} - e^{-k_2 c^{0.5}_{o_2}[W/X]}\right) \\ &- \frac{\frac{k_2}{K^{eq.}_{NO}} K_{NH_3} a_1 a_3}{k_1 c_{o_2} - k_2 c^{0.5}_{o_2} + \frac{k_2}{K^{eq.}_{NO}}}\left(e^{-\left(k_1 c_{o_2} + \frac{k_2}{K^{eq.}_{NO}}\right)[W/X]} - e^{-k_2 c^{0.5}_{o_2}[W/X]}\right) + \frac{k_4 a_1 a_2 a_3}{k_1 c_{o_2} + \frac{k_2}{K^{eq.}_{NO}}}\left(e^{-\left(k_1 c_{o_2} + k_2 c^{0.5}_{o_2} + \frac{k_2}{K^{eq.}_{NO}}\right)[W/X]} - e^{-\frac{k_2}{K^{eq.}_{NO}}[W/X]}\right) \end{aligned} \tag{9}$$

$$\begin{aligned} C_{NO_2} &= a_3 e^{-\frac{k_2}{K^{eq.}_{NO}}[W/X]} + \frac{k_2 c^{0.5}_{o_2} a_1}{k_1 c_{o_2} - \frac{k_2}{K^{eq.}_{NO}}}\left(e^{-k_1 c_{o_2}[W/X]} - e^{-\frac{k_2}{K^{eq.}_{NO}}[W/X]}\right) - \frac{k_2 c^{0.5}_{o_2} K_{NH_3} a_1^2}{2k_1 c_{o_2} - \frac{k_2}{K^{eq.}_{NO}}}\left(e^{-2k_2 c^{0.5}_{o_2}[W/X]} - e^{-\frac{k_2}{K^{eq.}_{NO}}[W/X]}\right) \\ &+ \frac{k_4 a_1 a_2 a_3}{k_1 c_{o_2} + k_2 c^{0.5}_{o_2}}\left(e^{-\left(k_1 c_{o_2} + k_2 c^{0.5}_{o_2} + \frac{k_2}{K^{eq.}_{NO}}\right)[W/X]} - e^{-\frac{k_2}{K^{eq.}_{NO}}[W/X]}\right) + \frac{3k_5 a_1 a_3}{k_1 c_{o_2}}\left(e^{-\left(k_1 c_{o_2} + \frac{k_2}{K^{eq.}_{NO}}\right)[W/X]} - e^{-\frac{k_2}{K^{eq.}_{NO}}[W/X]}\right) \end{aligned} \tag{10}$$

$$C_{N_2O} = a_4 - \frac{7k_6 a_1 a_3 + 4k_7 K_{NH_3} a_1 a_3 a_4}{2k_1 c_{o_2} + 2\frac{k_2}{K^{eq.}_{NO}}}\left(e^{-\left(k_1 c_{o_2} + \frac{k_2}{K^{eq.}_{NO}}\right)[W/X]} - 1\right) + \frac{2k_7 a_3 a_4}{\frac{k_2}{K^{eq.}_{NO}}}\left(e^{-\frac{k_2}{K^{eq.}_{NO}}[W/X]} - 1\right) \tag{11}$$

Eqns. (8) – (11) satisfy the initial condition (7). These equations represent the reliable and closed-form of analytical expression of concentrations for all possible values of the parameters.

III. NUMERICAL SIMULATION

The non-linear differential Eqns. (3) – (6) for the given initial conditions Eqns. (7) are being solved numerically. The function pdex, in MATLAB software which is a function of solving the initial value problems for non-linear ordinary differential equations is used to solve these equations. The numerical solutions are compared with analytical results using Homotopy perturbation method as shown in Figs. (1) – (4) and it gives a satisfactory result. The MATLAB program is also given in Appendix B.

IV. RESULT AND DISCUSSION

The non-linear differential Eqns. (3) - (6) depending on the concentration of NH_3, NO, NO_2 and N_2O in the global kinetic model subject to the initial condition Eqn. (7) have been solved analytically using Homotopy perturbation method. Since the derived solution is very comprehensive, it is very hard to analyze by seeing the expression, so the predictions have been depicted as graphs in Fig.1- Fig.4. In order explore the results; the analytical solutions were carried out for different values of the parameters involved in the system. To see the accuracy and efficiency of the analytical solution derived is compared with the numerical solution (function pdepe, Finite element method in MATLAB), which shows the good accuracy of derived expression i.e. analytical solution matched well with numerical solution which is projected in Fig.1-Fig.4.

Figure 1 represents that the Concentration of species NH_3 versus space time [W/Q] in global kinetic model. From Fig.1 (a), concentration of species NH_3 decreases from one sharply and becomes steady state when [W/Q] ≅ 1. The concentration of species NH_3 decreases when the Kinetic rate constant k_1 increases. Fig. 1(b), it is inferred that the concentration of species NH_3 increases when the Kinetic rate constants k_5 increases for the some fixed values. In Fig. 1(c), it is labeled that the concentration of NH_3 decreases when the equilibrium constant K_{NH_3} decreases for the fixed value of other parameter.

Figure 2 exhibits the concentration of species NO in the global kinetic model versus space time [W/Q] for different values of k_2 and K_{NH_3}. From Figures 2(a), it is inferred that the concentration of species NO increases when the Kinetic rate constant k_2 increases for the fixed values of other parameter. In Figures 2(b), we show that the concentration of species NO in the global kinetic model for various values of the equilibrium constant K_{NH_3} and for some fixed values of other parameter. From this figure, we conclude that the concentration of species NO increases when the equilibrium constant K_{NH_3} decreases.

Figs. 3 show the concentration of species NO_2 versus space time [W/Q]. From Figure 3(a) and 3(b), it is described that the concentration of species NO_2 slowly reaches the constant when the Kinetic rate constant of reaction k_2 and k_4 decreases for the fixed value of other parameter.

Figure 4 represents the concentration of species N_2O versus space time [W/Q] for different values of k_6 and k_7. From Fig. 4(a), it is inferred that the concentration of NH_3 decreases when the Kinetic rate constant k_6 decreases for the fixed value of other parameter.

In Fig. 4(b), it is described that the concentration of species N_2O slowly reaches the constant when the Kinetic rate constant of reaction k_7 decreases for the fixed value of other parameter.

V. CONCLUSION

In this work, steady state nonlinear differential equations in global kinetic model have been solved analytically. Homotopy perturbation method was employed to solve the system of non-linear differential equations of SCR reaction network. Better approximate analytical expressions corresponding to concentration of NH_3, NO, NO_2 and N_2O in global kinetic model are derived. Closing matching of the analytical result with numerical solution gives assurance that our analytical result are useful to simulate the dynamic performance of system using the parameters and also useful to predict and understand the behavior of the system.

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Appendix A: Analytical solutions for the concentrations in SCR reaction network

In this Appendix, the steps leading to Eqns. (3) - (6) with an initial condition Eqn. (7) are derived. In order to solve Eqn. (3) by means of the Homotopy method, we first construct a Homotopy as follows:

$$(1-p)\left[\frac{dC_{NH_3}}{d[W/Q]}\right]+p\left[\frac{dC_{NH_3}}{d[W/Q]}+\frac{\begin{matrix}k_1C_{NH_3}C_{O_2}+k_3C_{NH_3}C_{NO}C_{NO_2}+2k_4C_{NH_3}C_{NO}C_{NO_2}\\+4k_5C_{NH_3}C_{NO_2}+3k_6C_{NH_3}C_{O_2}\end{matrix}}{1+K_{NH_3}C_{NH_3}}\right]=0 \tag{A1}$$

where $p\in[0,\ 1]$ is an embedding parameter, The solution of Eqn.(A1) is constructed as a power series in $\left[\left(C_{NH_3}\right)_i\right]_0^N$ viz

$$C_{NH_3}=\left(C_{NH_3}\right)_0+p\left(C_{NH_3}\right)_1+p^2\left(C_{NH_3}\right)_2+p^3\left(C_{NH_3}\right)_0+..... \tag{A2}$$

Here $\left(C_{NH_3}\right)_0$ is the zero-order approximation when p=0. Substituting Eqn.(A2) into Eqn.(A1) and comparing the coefficient of powers of p, we obtain

$$p^0:\frac{d\left(C_{NH_3}\right)_0}{d[W/Q]}=0 \tag{A3}$$

$$p^1:\frac{d\left(C_{NH_3}\right)_1}{d[W/Q]}+\frac{\begin{matrix}k_1\left(C_{NH_3}\right)_0C_{O_2}+k_3\left(C_{NH_3}\right)_0\left(C_{NO}\right)_0\left(C_{NO_2}\right)_0+2k_4\left(C_{NH_3}\right)_0\left(C_{NO}\right)_0\left(C_{NO_2}\right)_0\\+4k_5\left(C_{NH_3}\right)_0\left(C_{NO_2}\right)_0+3k_6\left(C_{NH_3}\right)_0C_{O_2}\end{matrix}}{1+K_{NH_3}\left(C_{NH_3}\right)_0}=0 \tag{A4}$$

The initial approximations are as follows:

at [W/Q] = 0; $\left(C_{NH_3}\right)_0=a_1$ and $\left(C_{NH_3}\right)_i=0$ for all i=1,2,3,…..

(A5)

Upon solving the Eqn. (A3) and Eqn. (A4), and employing the initial conditions (Eqn. (A5)), the following equations for concentrations are deduced:

$$\left(C_{NH_3}\right)_0=a_1e^{-k_1c_{o_2}[W/X]} \tag{A6}$$

$$\begin{aligned}\left(C_{NH_3}\right)_1=&-\frac{K_{NH_3}k_1c_{o_2}a_1^2}{k_1c_{o_2}}\left(e^{-2k_1c_{o_2}[W/X]}-e^{-k_1c_{o_2}[W/X]}\right)+\frac{2k_4a_1a_2a_3}{k_2c_{o_2}^{0.5}+\frac{k_2}{K_{NO}^{eq.}}}\left(e^{-\left(k_1c_{o_2}+k_2c_{o_2}^{0.5}+K_{NO}^{eq.}\right)[W/X]}-e^{-k_1c_{o_2}[W/X]}\right)\\&+\frac{k_3c_{o_2}a_1a_2}{k_2c_{o_2}^{0.5}}\left(e^{-\left(k_1c_{o_2}+k_2c_{o_2}^{0.5}\right)[W/X]}-e^{-k_1c_{o_2}[W/X]}\right)+\frac{(4k_5+3k_6)a_1a_3}{\frac{k_2}{K_{NO}^{eq.}}}\left(e^{-\left(k_1c_{o_2}+K_{NO}^{eq.}\right)[W/X]}-e^{-k_1c_{o_2}[W/X]}\right)\end{aligned} \tag{A7}$$

Using the basic assumptions underlying the Homotopy perturbation method, we obtain

$$C_{NH_3}([W/Q]) = p \overset{\lim}{\rightarrow} 1 C_{NH_3}([W/Q]) \approx \left(C_{NH_3}([W/Q])\right)_0 + \left(C_{NH_3}([W/Q])\right)_1 \quad \text{(A8)}$$

Substituting Eqn.(A6) and Eqn.(A7) in Eqn.(A8), Eqn.(8) of the text is obtained. Similarly, we obtain Eqns.(8) – (10).

Appendix B: Scilab/Matlap program for the numerical solution of nonlinear differential equation (3) – (6).

```
function may2018
options= odeset ('RelTol',1e-6,'Stats','on');
%initial conditions
Xo = [1;0.001;0.001;0.001];
tspan = [0,1];
tic
[t,X] = ode45(@TestFunction,tspan,Xo,options);
toc
figure
hold on
plot(t, X(:,1),'-')
%plot(t, X(:,2),'-')
%plot(t, X(:,3),'-')
%plot(t, X(:,4),'-')
legend('x1','x2','x3','x4')
ylabel('x')
xlabel('t')
return
function[dx_dt]= TestFunction(t,x)
co2 = 1; co21 = 0.001; kn =1; kneq = 0.001; k1 = 15; k2 = 0.001; k3 = 0.001; k4 = 0.001; k5 = 0.001; k6 =0.001;k7=0.001;
dx_dt(1)=(k1*co2*x(1)+k3*co2*x(1)*x(2)+2*k4*x(1)*x(2)*x(3)+4*k5*x(1)*x(3)+3*k6*x(1)*x(3))/(1+kn*x(1));
dx_dt(2) = -k2*(x(2)*co21-x(3)/kneq)-(k3*co2*x(1)*x(2)+k4*x(1)*x(2)*x(3))/(1+kn*x(1));
dx_dt(3)=k2*(x(2)*co21-x(3)/kneq)-(k4*x(1)*x(2)*x(3)+3*k5*x(1)*x(3)+4*k6*x(1)*x(3))/(1+kn*x(1));
dx_dt(4) = -2*k7*x(3)*x(4)+(7/2)*(k6*x(1)*x(3))/(1+kn*x(1));
dx_dt = dx_dt';
return
```

Appendix C

Nomenclature

C_i	Concentration of i species calculated in the kinetic model where i = NH_3, NO, NO_2 and N_2O	mol/m^3
k_1, k_5, k_6 & k_7	Kinetic rate constants of reaction 1,5,6&7	$m^6\ g^{-1}\ h^{-1}\ mol^{-1}$
k_2	Kinetic rate constants of reaction 2	$m^{4.5}\ m^{-3}\ h^{-1}\ mol^{-0.5}$
k_3, k_4	Kinetic rate constants of reaction 3 and 4	$m^9\ g^{-1}\ h^{-1}\ mol^{-2}$
K_{NH_3}	Equilibrium constant of NH_3	$m^3\ mol^{-1}$
$K^{eq.}_{NO}$	Equilibrium constant of NO	$m^{1.5}\ mol^{-0.5}$
r_j	Rate of reaction j. where j = 1 to 7	$mol\ g^{-1}\ h^{-1}$
W/Q	Space time	(g cat.) h m^{-3}

Supplementary method of the manuscript:

Basic concepts of the Homotopy perturbation method

To explain this method, let us consider the following function:

$$D_o(u) - f(r) = 0, \quad r \in \Omega \quad \text{(B1)}$$

with the boundary conditions of

$$B_o(u, \frac{\partial u}{\partial n}) = 0, \quad r \in \Gamma \quad \text{(B2)}$$

where D_o is a general differential operator, B_o is a boundary operator, $f(r)$ is a known analytical function and Γ is the boundary of the domain Ω. In general, the operator D_o can be divided into a linear part L and a non-linear part N. Eqn. (B1) can therefore be written as

$$L(u) + N(u) - f(r) = 0 \quad \text{(B3)}$$

By the Homotopy technique, we construct a Homotopy $v(r,p):\Omega\times[0,1]\to\Re$ that satisfies

$$H(v,p)=(1-p)[L(v)-L(u_0)]+p[D_o(v)-f(r)]=0. \quad \text{(B4)}$$

$$H(v,p)=L(v)-L(u_0)+pL(u_0)+p[N(v)-f(r)]=0. \quad \text{(B5)}$$

where $p\in[0,1]$ is an embedding parameter, and u_0 is an initial approximation of Eqn. (B1) that satisfies the boundary conditions. From Eqn. (B4) and Eqn. (B5), we have

$$H(v,0)=L(v)-L(u_0)=0 \quad \text{(B6)}$$

$$H(v,1)=D_o(v)-f(r)=0 \quad \text{(B7)}$$

When p=0, Eqn.(B4) and Eqn.(B5) become linear equations. When p =1, they become non-linear equations. The process of changing p from zero to unity is that of $L(v)-L(u_0)=0$ to $D_o(v)-f(r)=0$. We first use the embedding parameter p as a "small parameter" and assume that the solutions of Eqn. (B4) and Eqn. (B5) can be written as a power series in p:

$$v=v_0+pv_1+p^2v_2+... \quad \text{(B8)}$$

Setting $p=1$ results in the approximate solution of Eqn. (B1):

$$u=\lim_{p\to1}v=v_0+v_1+v_2+... \quad \text{(B9)}$$

Figures

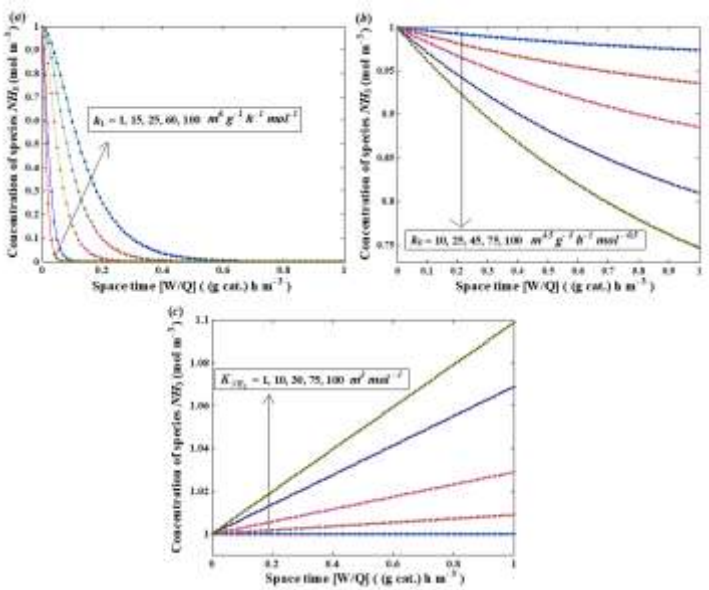

Figure.1 Plot of concentration of species NH_3 versus Space time [W/Q] with various values of the parameters and some fixed values all other parameters.

Solid lines represent numerical solutions whereas the dotted line represents analytical solutions.

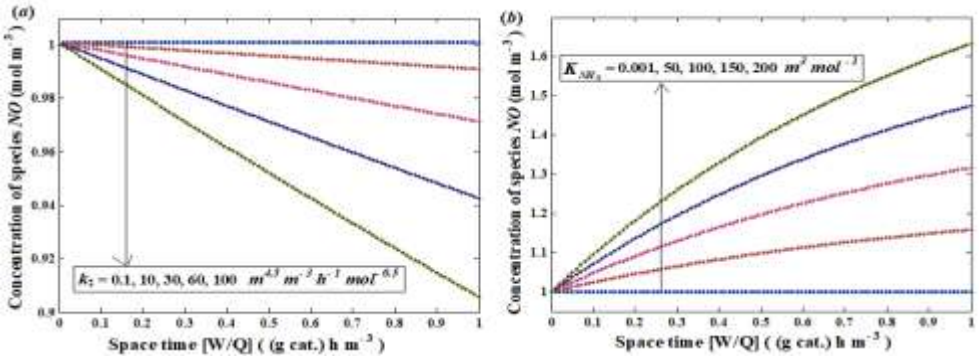

Figure.2 Plot of concentration of species NO versus Space time [W/Q] for various values of the parameters and some fixed values all other parameters.

Solid lines represent numerical solutions whereas the dotted line represents analytical solutions.

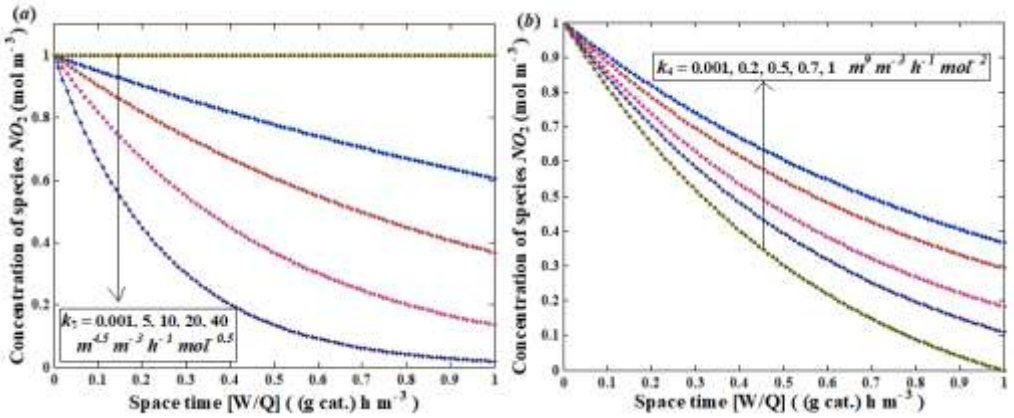

Figure.3 Plot of concentration of species NO_2 versus Space time [W/Q] for various values of the parameters and some fixed values all other parameters.

Solid lines represent numerical solutions whereas the dotted line represents analytical solutions.

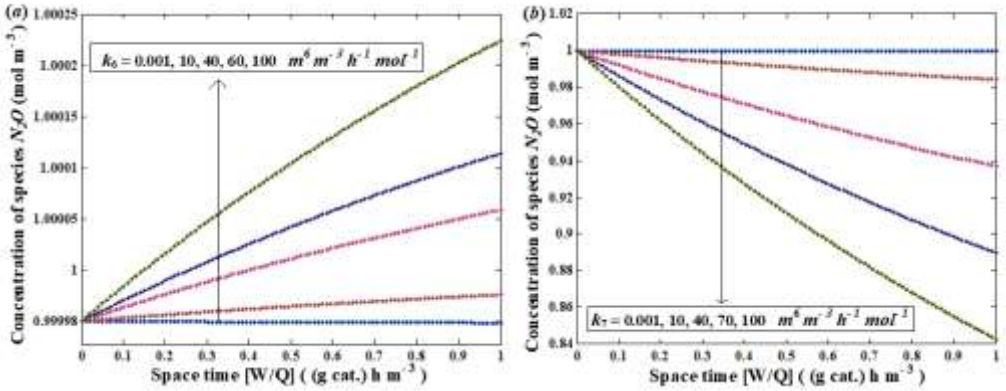

Figure.4 Plot of concentration of species N_2O versus Space time [W/Q] for various values of the parameters and some fixed values all other parameters.

Solid lines represent numerical solutions whereas the dotted line represents analytical solutions.

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