Mathematical modeling of automotive catalytic converter for catalytic combustion of the volatile organic compound (voc) methane

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Abstract. Monolithic catalytic converters are used to minimize the emission of air pollutants to the environment. Volatile organic compounds (VOCs) are seen to be released in considerable amounts from these catalytic converters during the warm-up period. In this paper, the conversion of a slow oxidizing volatile organic compound (VOC) methane is analysed with numerical simulation using a noble metal catalyst (Pt/$\delta$-Al$_2$O$_3$) and metal oxide catalyst CuO/$\delta$-Al$_2$O$_3$. The transient, one-dimensional monolith model is developed using gas-phase energy balance, solid-phase energy balance, and gas-phase mass balance. The unsteady state analysis consists of a system of partial differential equations (PDEs). These equations are solved using an Implicit Scheme with the help of Matlab software. The conversion of methane is analysed with reaction temperature for both Pt/$\delta$-Al$_2$O$_3$ catalyst and CuO/$\delta$-Al$_2$O$_3$ catalyst. Also, the effect of the ageing of catalysts on catalytic converter performance was analysed.

1. Introduction

Pollution is a leading environmental concern that contributes to many health problems such as vascular diseases, respiratory diseases, and lung cancer. In India, Air pollution is also a severe health issue. As stated by the WHO, 14 out of the world's 20 most polluted cities were in India in 2019 and city Ghaziabad leading cities within India [1]. Due to the urbanization, the rapid developments in the transportation and industrial sectors have contributed to the quick rise in ambient air pollution in India [2]. Emissions from vehicles are one of the essential reasons for air pollution in India. 20% of poorly maintained vehicles contribute about 60% of the vehicle’s emission in India. The main reasons for the rise in emissions from cars have been the hasty growing motor vehicle population, insufficient public transport, urban development, congestion, and poor fuel quality [3].

Greenhouse Gas Emissions (GHGs) are also severely related to air pollution and climate changes all over the world. Green House Gases (GHGs) emissions are also a significant concern in India. India comes among the top ten contributors to the GHGs [4]. Methane is a greenhouse gas that affects the environment by contributing to global warming [5]. "VOC (CH$_4$) is a significantly more potent greenhouse gas than carbon dioxide (CO$_2$)". Global warming potential (GWP) for CH$_4$ over a 100-year time horizon is 28 times more than CO$_2$, and over a 20-year time, the horizon is 84 times more than CO$_2$ [6].

The Catalytic combustion of the VOCs shows substantial potential to destroy harmful pollutants at lower concentrations, following the progressively strict environmental guidelines. A catalytic converter is a device which removes the harmful pollutants by converting them into less toxic
pollutants [7]. The catalytic converters used for the catalytic oxidation of \( \text{CH}_4 \) offer many benefits such as small pressure drop and more surface area for reactions [8,9]. Metal oxides and Noble metals are the most widely used catalysts for catalytic combustion [10,11]. Noble metal catalysts (Pt and Pd) are the most active and suitable catalysts for such applications. For methane oxidation CuO/Al\(_2\)O\(_3\) has better activity as a comparison to other metal oxides but less than Noble metal catalyst [12].

Modeling is preferred over experiments to improve the monoliths design because the experimental optimizations are expensive and very time-consuming. Numerical simulations also help to lessen the number of tests and interpret the aspects of some parameters else neglected [13,14]. In this paper, the methane conversion is analysed with reaction temperature for both Pt/\(\delta\)-Al\(_2\)O\(_3\) catalyst and CuO/\(\delta\)-Al\(_2\)O\(_3\) catalyst. Also, the effect of changing the catalyst loading on catalytic converter performance was analysed during the warm-up period.

2. Model rate kinetics

The following reaction represents the complete methane oxidation:

\[
\text{CH}_4 + 2\text{O}_2 \rightarrow \text{CO}_2 + 2\text{H}_2\text{O}
\]

The Rate expression for complete catalytic oxidation of methane for Pt/\(\delta\)-Al\(_2\)O\(_3\) catalyst and CuO/\(\delta\)-Al\(_2\)O\(_3\) is given by:

For Pt/\(\delta\)-Al\(_2\)O\(_3\) catalyst [15]

\[
(-r_{\text{methane}})_{\text{cat}} = k_{\text{cat}} P_{\text{CH}_4}^{0.05} P_{\text{O}_2}^{0.17} \quad \text{Here} \quad k_{\text{cat}} = k_{\text{0,cat}} e^{-E_{\text{cat}}/RT}
\]

Parameter values:
- \(\Delta H = -802.3 \text{ KJ/mole}\)
- Pre-exponential factor: \(k_{\text{0,cat}} = 1.7020 \times 10^2 \text{ mol/ Pa}^{0.5} \text{ s. cm}^2\)
- Activation energy: \(E_{\text{cat}} = 88.5 \text{ KJ/gmole}\)

For CuO/\(\delta\)-Al\(_2\)O\(_3\) catalyst [16]

\[
(-r_{\text{methane}})_{\text{cat}} = k_{\text{cat}} P_{\text{CH}_4}^{0.9} \quad \text{Here} \quad k_{\text{cat}} = k_{\text{0,cat}} e^{-E_{\text{cat}}/RT}
\]

Parameter values:
- \(\Delta H = -802.3 \text{ KJ/mole}\)
- Pre-exponential factor: \(k_{\text{0,cat}} = 6.4314 \times 10^2 \text{ mol/ atm}^{0.9} \text{ s. cm}^2\)
- Activation energy: \(E_{\text{cat}} = 96.232 \text{ KJ/gmole}\)

3. Modeling Assumption [17,18]

Some major Assumptions for modeling include:

- In the gas-phase, heat transfer through radiation is neglected.
- In the gas-phase, axial diffusion is very small, so neglected.
- Uniform gas properties are assumed.
- The concentration of catalyst is kept constant.
- Wash coat is assumed to be very thin, so diffusion is neglected inside the washcoat.
- The heat released by the reactions is entirely transferred to the gas-phase inside the wash-coat through convection.
- Flow through a single channel is assumed.
- Heat exchange among the substrate and the surroundings at both outlet and inlet faces of monolith is neglected.

4. Modeling

A 1-dimensional model for a cylindrical monolith channel for gas temperature, and solid temperature and gas concentration, is formed using assumption and only axial gradients are considered as shown in Table 1.
Table 1. Mass and Energy balance equations for catalytic reactions for Pt/δ-Al₂O₃ catalyst and CuO/δ-Al₂O₃ catalyst

Mass and energy balance equations for the catalytic reactions

Mass balance gas-phase equation
\[ \frac{\partial C_g}{\partial x} + Sk_g (C_g - C_r) = -v \rho_g C_p \frac{\partial T}{\partial x} \]

Mass balance solid-phase equation
\[ a(-r_{methane})_{cat} = Sk_g (C_g - C_r) \]

Gas-phase energy balance equation
\[ -v \rho_g C_p \frac{\partial T}{\partial x} - Sh(T_g - T_x) = \rho_g C_p \frac{\partial T}{\partial t} \]

Solid-phase energy balance equation
\[ C_p \rho_s \frac{\partial T}{\partial t} = Sh(T_g - T_x) + a(-\Delta H)(-r_{methane})_{cat} + \frac{\partial^2 T}{\partial x^2} \]

Initial conditions
\[ T_g(0,t) = T_{g0}, C_A(0,t) = C_{g0}, T_j(x,0) = T_{j0} \]

Boundary condition
\[ x = 0, \frac{\partial T}{\partial x} = 0, x = L, \frac{\partial C}{\partial x} = 0, \frac{\partial T}{\partial x} = 0, \frac{\partial T}{\partial x} = 0 \]

Table 2. Dimensionless equations for catalytic reactions for Pt/δ-Al₂O₃ catalyst and CuO/δ-Al₂O₃ catalyst

Equations in dimensionless form for catalytic reactions

Dimensionless mass balance equation for gas-phase
\[ \frac{\partial C}{\partial z} = -A_1 \frac{\partial C_g}{\partial t} - (A_2 (M_j)_{cat} e^{E_{cat} / RT}) \]

Energy balance dimensionless equation for gas-phase
\[ \frac{\partial T}{\partial z} = -B_1 \frac{\partial T}{\partial t} - B_2 (T_g - T_x) \]

Solid-phase dimensionless energy balance equation
\[ \frac{\partial^2 T}{\partial z^2} = C_3 \frac{\partial T}{\partial t} + C_2 (T_g - T_x) - C_2 (M_j)_{cat} e^{E_{cat} / RT} \]

Boundary and initial conditions in dimensionless form
\[ T_g(0,t) = \frac{T_{g0}}{T_g}, C_g(0,t) = 1.0, T_j(0,t) = \frac{T_{j0}}{T_g}, \]
\[ z = 0, \frac{\partial T}{\partial x} = 0, z = L, \frac{\partial T}{\partial x} = 0, \frac{\partial C}{\partial x} = 0, \frac{\partial T}{\partial x} = 0 \]

Dimensionless numbers used in dimensionless equations for Pt/δ-Al₂O₃ catalyst

\[ A_1 = \frac{L}{v \rho \theta}, A_2 = \frac{L}{v \rho \theta} \frac{\partial (M_j)_{cat} e^{E_{cat} / RT}}{\partial t}, B_1 = \frac{L}{v \rho \theta}, B_2 = \frac{ShL}{v \rho \theta} \frac{\partial (M_j)_{cat} e^{E_{cat} / RT}}{\partial t}, \]
\[ C_1 = \frac{ShL}{\lambda_j} \frac{\partial (M_j)_{cat} e^{E_{cat} / RT}}{\partial t}, C_2 = \frac{\partial (M_j)_{cat} e^{E_{cat} / RT}}{\partial t} \frac{\partial (M_j)_{cat} e^{E_{cat} / RT}}{\partial t}, C_3 = \frac{\partial (M_j)_{cat} e^{E_{cat} / RT}}{\partial t} \frac{\partial (M_j)_{cat} e^{E_{cat} / RT}}{\partial t} \]

Dimensionless numbers used in dimensionless equations for CuO/δ-Al₂O₃ catalyst
\[
A_1 = \frac{L}{Vt_0}, A_2 = \frac{aLK_{\text{cat}}C_0^{0.1}R^{0.9}T_0^{0.9}}{V}, B_1 = \frac{L}{Vt_0}, B_2 = \frac{ShL}{vC_p\rho_g}, \\
D_1 = \frac{ShL^2}{\lambda_g}, D_2 = \frac{aK_{\text{cat}}C_0^{0.1}R^{0.9}T_0^{0.9}(-\Delta H)}{\lambda_gT_0}, D_3 = \frac{L^2C_p\rho_s}{\lambda_sI_0}
\]

Here \((M_1')\) for \(\text{Pt/}\delta-\text{Al}_2\text{O}_3\) catalyst = 0.0140 + 1.0653\(C_j^g\) - 0.1015\(C_j^g\) + 0.0306\(C_j^g\) - 0.0055\(C_j^a\)

\((M_1')\) for \(\text{CuO/}\delta-\text{Al}_2\text{O}_3\) catalyst = 0.0298 + 1.0742\(C_j^g\) - 0.1465\(C_j^g\) + 0.0512\(C_j^a\) - 0.0087\(C_j^a\)

**Table 3.** The discretized dimensionless equations for catalytic reactions for \(\text{Pt/}\delta-\text{Al}_2\text{O}_3\) catalyst

| Discretized dimensionless equations for \(\text{Pt/}\delta-\text{Al}_2\text{O}_3\) catalyst |
| --- |
| **Discretized mass balance equation for solid-phase** |
| \(A_1[\frac{dC_i}{dt}] = \left[\frac{C_{i+1} - C_{i-1}}{2k}\right] - A_2[-0.02432 + 1.07449C_i^j] - 0.02178C_j^g - 0.04266C_j^g + 0.01796C_j^a [e^{\frac{E_{\text{act}}}{RT_i}}] \) |
| At \(i=1\), dimensionless concentration of methane = 1.0000 |
| At \(i=n\), \(\frac{C_i^j - C_{i-1}^j}{k} = 0\) |
| **Discretized gas-phase energy balance equation** |
| \(B_1[\frac{dT_i^g}{dt}] = \left[\frac{T_{i+1}^g - T_{i-1}^g}{2k}\right] - B_2[-T_i^s + T_i^g] \) |
| At \(i=1\), incoming gas temperature = 655K, At exit \(i=n\), \(\frac{T_i^g - T_{i+1}^g}{k} = 0\) |
| **Discretized energy balance equation for solid-phase** |
| \(C_i[\frac{dT_i^s}{dt}] = \left[\frac{T_{i+1}^s + T_{i-1}^s - 2T_i^s}{k^2}\right] + C_1[T_{i+1}^s - T_{i-1}^s] + C_2[-0.02432 + 1.07449C_i^j - 0.02178C_j^g - 0.04266C_j^g + 0.01796C_j^a [e^{\frac{E_{\text{act}}}{RT_i}}] \) |
| At \(i = 1\), initial solid temperature = 298K, \(\frac{T_{i+1}^s - T_{i-1}^s}{k} = 0\) |
| At \(i=n\), \(\frac{-T_i^s + T_{i-1}^s}{k} = 0\) |
Table 4. Dimensionless equations for catalytic reactions in discretized terms for CuO/δ-Al₂O₃ catalyst

Discretized dimensionless equations for CuO/δ-Al₂O₃ catalyst

Discretized mass balance equation for solid-phase

\[
A_i \frac{dC_i}{dt} = \left( \frac{C_{i+1} - C_{i-1}}{2k} \right) - A_i \left[ 0.0298 + 1.0742C_i - 0.1465C_i^2 + 0.0512C_i^3 - 0.0087C_i^4 \right] \left[ e^{\frac{E_{act}}{RT}} \right]
\]

At \( i = 1 \), dimensionless concentration of methane = 1.0000
At converter exit \( i = n \), \( \frac{C_i - C_{i-1}}{k} = 0 \)

Discretized gas-phase energy balance equation

\[
B_i \frac{dT_i}{dt} = \left( \frac{T_{i+1} - T_{i-1}}{2k} \right) - B_i \left[ T_i - T_{i+1} + T_{i-1} \right]
\]

At \( i = 1 \), incoming gas temperature = 820K, At exit \( i = n \), \( \frac{T_i - T_{i+1}}{k} = 0 \)

Discretized energy balance equation for solid-phase

\[
C_j \frac{dT_j}{dt} = \left( \frac{T_{j+1} + T_{j-1} - 2T_j}{k^2} \right) + C_j \left[ T_i - T_j \right] + C_j \left[ 0.0298 + 1.0742C_j - 0.1465C_j^2 + 0.0512C_j^3 - 0.0087C_j^4 \right] \left[ e^{\frac{E_{act}}{RT}} \right]
\]

At \( j = 1 \), initial solid temperature = 298K, \( \frac{T_{j+1} - T_j}{k} = 0 \)
At \( j = n \), \( \frac{-T_{j+1} + T_j}{k} = 0 \)

Table 5. Parameters used in the model [17,18]

| Parameters | Value |
|------------|-------|
| L          | 10 cm |
| λ          | 0.01675 J/ K. cm.s |
| a          | 268 (cm²/cm³) |
| h          | 0.0169 J/s. K cm² |
| v          | 1800 (cm/s) |
| S          | 23.02 (cm²/cm³) |
| \( \rho_g \) \( \text{C}_p \) \( g \) | \( 1.225 \times 10^{-3} \) (J/ K cm³) |
| \( \rho_s \) \( \text{C}_p \) \( s \) | 1.678 (J/ K cm³) |
| \( t_0 \) | 0.1 |
5. Methodology for solving dimensionless coupled equations
Dimensionless equations in Table 2 are coupled with partial differential equations (PDEs), which are solved by implicit schemes by finite difference approximation with the Matlab software using data cited in the literature in Table 5. In Table 3 and Table 4, spatial derivatives in equations are substituted with central finite-difference approximations and boundary conditions with backward finite difference approximations for axial length. Discretization leads to the formation of systems of ordinary differentials equations (ODEs) in time and which are solved by numerical integration by calling ode23tb solver, which is an implementation of the TR-BDF2 method [19,20,21].

6. Result and Discussions

In Figure 1, the concentration of the entering methane gas is taken as 75 ppm [22] at 655 K. Figure 1 shows the comparison of the experimental result of methane conversion with the modeled results in converter at a temperature of 298K. Hardly any conversion has been seen below 555K temperature for experimental and modeled results. Conversion values are 0.10% for experimental and 2.92% for modeled results at temperature 560 K. As soon as the catalytic reaction starts, the reaction rate increases by the exothermic catalytic on the release of heat. At a temperature of 643K, about 70.00% conversion is achieved for experimental results, and 70.93% conversion is achieved for the modeled results. About 80.00% methane conversion for experimental results and 75.58% VOC methane conversion is achieved for modeled results at the temperature of 645K, and both results are found in the agreement.

In Figure 2, the concentration of the entering methane gas is taken as 75 ppm [22] at 820 K. Figure 2 shows the comparison of the experimental result of methane conversion with the modeled results in converter at a temperature of 298K using CuO/δ-Al2O3 catalyst. Hardly any conversion has been seen below 560K temperature for experimental and modeled results. Conversion values are 10.00 % for experimental and 4.00 % for modeled results at temperature 675 K. As soon as the catalytic reaction starts, the reaction rate increases by the exothermic reaction on the release of heat. At a temperature of 783 K, about 70.00% conversion is achieved for experimental results, and 62.40% conversion is achieved for the modeled results. About 80.00% methane conversion for the
experimental results and 79.33% VOC methane conversion is achieved for modeled results at the temperature of 796K, and both results are found in the agreement.

![Graph](image-url)

**Figure 2.** Comparison of modeled and experimental results for methane conversion with reaction temperature using CuO/δ-Al₂O₃ catalyst

Figure 3 shows the comparison of modeled methane conversion for Pt/δ-Al₂O₃ catalyst and CuO/δ-Al₂O₃ catalyst with reaction temperature. From figure 3, it is observed that lesser temperature is required for the Pt/δ-Al₂O₃ catalyst for the removal of VOC methane in comparison of the CuO/δ-Al₂O₃ catalyst. Temperature range (298K to 647K) is required for methane conversion from 0 to 80% for Pt/δ-Al₂O₃ catalyst, and the temperature range (298 to 797 K) is required for methane conversion from 0 to 80% for CuO/δ-Al₂O₃ catalyst. About 50.00% methane conversion is obtained for Pt/δ-Al₂O₃ catalyst at the temperature of 632 K and CuO/δ-Al₂O₃ catalyst at the temperature of 772 K. About 80% VOC methane conversion is obtained for Pt/δ-Al₂O₃ catalyst at the temperature of 647 K and CuO/δ-Al₂O₃ catalyst at the temperature of 797 K. From the results it is observed that Pt/δ-Al₂O₃ catalyst has a better activity for the removal of VOC methane over CuO/δ-Al₂O₃ catalyst.

Figure 4 shows the VOC methane exit concentration for the aged catalyst and fresh catalyst to time for both Pt/δ-Al₂O₃ and CuO/δ-Al₂O₃ catalyst. Conversion is faster due to higher catalyst loading, which increases the rate of the catalytic reaction. Data cited in the literature about catalyst loading levels suggest that for the aged catalyst, the value of standard loading is (∼268 cm² catalyst/cm³). For fresh catalyst, its value is about 8 times to the standard loading (∼2144 cm² catalyst/cm³) [23,24]. The catalyst loading declines with time due to many factors such as the age of the vehicle, poisoning and sintering at high temperatures [25,26,27]. At dimensionless time 40.00, the exit dimensionless methane concentrations are 0.2728 and 0.8546 for the fresh and the aged Pt/δ-Al₂O₃ catalyst and 0.9602 and 0.9950 for the fresh and the aged CuO/δ-Al₂O₃ catalyst, respectively. At dimensionless time 43.70, the exit dimensionless methane concentrations are 0.1054 and 0.7685 for the fresh and the aged Pt/δ-Al₂O₃ catalyst and 0.9404 and 0.9913 for the fresh and the aged CuO/δ-Al₂O₃ catalyst, respectively. It is observed that methane conversion is faster for Pt/δ-Al₂O₃ catalyst as compared to CuO/δ-Al₂O₃ catalyst for both fresh and aged catalysts. From the results, it is concluded that even-aged Pt/δ-Al₂O₃ catalyst has superior activity as a comparison to the fresh CuO/δ-Al₂O₃ catalyst.
8

Figure 3. Comparison of methane conversion with reaction temperature For Pt/δ-Al₂O₃ catalyst and CuO/δ-Al₂O₃ catalyst

7. Conclusion
In the present study, mathematical modeling and numerical simulation for VOC methane are carried out using the unsteady state model for both Pt/δ-Al₂O₃ and CuO/δ-Al₂O₃ catalyst. Initially, the catalytic oxidation of methane is not substantial through the warm-up time of the catalytic converter for both the catalysts. Due to the lower early temperature of the catalytic converter, some more time is
required for preheating, so it could reach its operational temperature after that an apparent methane conversion is observed due to the beginning of catalytic reactions. Calculations based on the mathematical model confirm that methane conversion is faster for Pt/δ-Al₂O₃ catalyst as compared to CuO/δ-Al₂O₃ catalyst. Also, it is concluded that the warm-up time is more for the in-use aged catalyst as compared to the fresh catalysts. Pt/δ-Al₂O₃ catalyst has a superior activity for the elimination of VOC methane over CuO/δ-Al₂O₃ catalyst even for the in-use aged catalyst.

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Nomenclature
\[ a \] - Catalytic surface area, (cm\(^2\)/cm\(^3\))
\[ C_g \] - Gas concentration, (gmol/cm\(^3\))
\[ \lambda \] - Thermal conductivity, (J/cm K s)
\[ t \] - Time, (s)
\[ L \] - Monolith Length, (cm)
\[ k_{cat} \] - Rate constant, (mol/cm\(^2\). s. Pa\(^{0.5}\))
\[ k_{pre exp} \] - preexponential factor for reactions, (mol/cm\(^2\). s. Pa\(^{0.5}\))
\[ k_g \] - Mass transfer coefficient, (cm/s)
\[ v \] - Gas velocity, (cm/s)
\[ E_a \] - Activation energy, (cal/gmole)
\[ C_p \] - Specific heat, (J/g K).
\[ h \] - Heat transfer coefficient, (J/K cm\(^2\) s)
\[ R \] - Gas constant, J/gmole (K)
\[ T_g \] - Gas temperature, (K)
\[ S \] - Geometric surface area, (cm\(^2\)/cm\(^3\))
\[ T_s \] - Solid temperature, (K)
\[ x \] - Axial coordinate, (cm)
\[ \Delta H \] - Heat of reaction, (cal/gmole)
\[ \rho \] - Density, (g/cm\(^3\))
\[ C_g' \] - Concentration in dimensionless term
\[ T_g' \] - Gas temperature in dimensionless term
\[ T_s' \] - Solid temperature in dimensionless term
\[ z \] - Axial coordinates in dimensionless term
\[ t' \] - Time in dimensionless term

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