

# One-dimensional Modeling for Removal of Volatile Organic Compounds (VOCs) in a Catalytic Converter

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**Abstract.** Emission of air pollutants like volatile organic compounds (VOCs) from the vehicular exhaust is a foremost concern of environmentalists. The steady increase of these pollutants has caused a radical increase in the level of air pollution in the atmosphere. Modeling for the reduction of VOCs were carried out using Pt/ $\delta$ -Al<sub>2</sub>O<sub>3</sub> catalyst for controlling its emissions to the environment. A one-dimensional unsteady-state model for predicting the oxidation of VOC emissions in the catalytic converter was developed during the warm-up period using material balance and energy balance equations. These equations consist of a set of partial differential equations which are combined and solved using numerical methods of partial differential equations.

**Keywords:** one-dimensional, volatile organic compounds (VOCs), modeling, numerical methods

## 1. Introduction

Air pollution is said to exist if the levels of harmful gases, solid, or liquids present in the atmosphere are high enough to affect humans, other organisms, building, monuments etc. <sup>[1]</sup> The mean percentage contribution from the vehicle exhausts was found to be 33% of total non-methane hydrocarbons (NMHCs) in Mumbai. <sup>[2]</sup> Air pollutants, like sulphur oxides (SO<sub>x</sub>), nitrogen oxide (NO<sub>x</sub>), carbon monoxide (CO), ozone (O<sub>3</sub>), volatile organic compounds (VOCs), heavy metals and particulate matter etc. affect the climate in different ways, depending on their specific properties such as their chemical constituents, reaction properties, release amount, stay time in the atmosphere, capability to be transported over long or short distances and their subsequent impacts on living organism. <sup>[3]</sup>

VOC ethane is the most abundant non-methane hydrocarbon. Ethane is also of interest in atmospheric interaction as a major source of PAN in the remote troposphere. <sup>[4]</sup> Catalysts used in catalytic oxidation reactions are usually noble metals or transition metal oxides that are supported on a different substrate. <sup>[5]</sup> Platinum-based catalysts are very energetic for oxidative removal of small amounts of VOCs like ethane from gaseous or liquid streams. <sup>[6]</sup>

In this paper, one-dimensional modeling and simulation were carried out to guess the converter behaviour during the warm-up period to bring a reduction in the ethane emissions release to the atmosphere. Also, the effect of changes in entering gas temperature on the reduction of these VOC's emissions is analyzed.

## 2. Rate kinetics

The reaction of VOC oxidation to form a less harmful gas carbon dioxide and water is being considered.



here  $i=2$  and  $j=6$  for ethane.

The presence of catalyst helps in lowering the activation energy of the reaction and makes it proceed at a lower temperature. Rate expression for the catalytic reaction is given as:

$$(-r)_{voc} = k P_{C_2H_6}^a P_{O_2}^b \quad (2)$$

Values used are:  $K = 6.457 \times 10^{13} \text{ mol/cm}^2 \cdot \text{h} \cdot \text{KPa}^{-5}$ ;  $(-\Delta H) = -372.78 \text{ cal/gmole}$ ;  
 $\alpha = 1.1$ ,  $\beta = -0.6$

### 3. Mathematical modeling

#### 3.1 One-dimensional Model

A One-dimensional model is interpreted in axial gradients for reacting gas concentration, gas temperature and solid catalyst temperature. The catalytic converter is working under warm-up conditions and the processes which included in the model are gas-solid heat and mass transfer, axial heat conductive transfer in the solid and the chemical reaction in presence of a solid catalyst. [8]

#### 3.2 Assumptions

Some major assumptions made during modeling include: [8-9]

1. axial diffusion of mass and heat transfer in the gas phase is negligible.
2. The concentration of noble metal catalyst was kept constant and the solid catalyst does not deactivate.
3. Monolith is cylindrical with circular cross-section channels
4. Gas phase concentration, gas temperature, gas velocity and the solid temperature are uniform across the monolith cross-section at any axial position.
5. The heat released due to the catalytic reactions inside the wash coat was totally transported to the gas phase by convective heat transfer.
6. Heat transfer due to the radiation inside the channels and heat exchange between the substrate and the surroundings at both inlet and an outlet face of the monolith is ignored.
7. Non-uniform flow distribution inside the catalytic converter is neglected because the entire monolith is represented as one single channel.

#### 3.3 Modeling Equations for Gas and Solid phase

Change in gas concentrations and gas temperature with time derivative is considered while solving mass and energy balance equations.

Mass balance equation for gas phase:

$$\{\text{mass transport of gas}\} + \{\text{reaction term}\} = \{\text{accumulation term}\}$$

$$v \left( \frac{\partial C_g}{\partial x} \right) + k_g S (C_g - C_s) = \left( \frac{\partial C_s}{\partial t} \right) \quad (3)$$

where  $C_g$ , represents gas phase concentration (g mole/cm<sup>3</sup>),  $C_s$  represents concentration at the solid surface (g mole/cm<sup>3</sup>),  $v$  is average velocity (cm/s),  $x$  is axial length (cm),  $k_g$  is mass transfer coefficient (cm/s),  $S$  is the geometric surface area per unit volume (cm<sup>2</sup>/cm<sup>3</sup>) and  $t$  is time (sec).

Mass balance equation for solid phase:

$$a(-r) = k_g S (C_g - C_s) \quad (4)$$

where  $a$  is catalytic surface area per unit reactor volume (cm<sup>2</sup>/cm<sup>3</sup>).

Energy balance equation for gas phase:

$$\{\text{heat transport of reacting gas}\} - \{\text{Heat transport to the solid wall from the gas}\} = \{\text{accumulation of heat in the gas phase}\}$$

$$-v \rho_g C_{p_g} \left( \frac{\partial T_g}{\partial x} \right) - h S (T_g - T_s) = \rho_g C_{p_g} \left( \frac{\partial T_g}{\partial t} \right) \quad (5)$$

where  $T_s$  is solid temperature (°C),  $T_g$  is gas temperature (°C),  $C_{p_g}$  is the specific heat of gas

(J/g °C),  $\rho_g$  represents gas density (g/cm<sup>3</sup>) and h is heat transfer coefficient (J/cm<sup>2</sup>s °C).

Energy balance equation for solid phase:

{Net conductive transfer wall} + {Heat transport to the solid wall from the gas} + {amount of Heat out due to the chemical reaction} = {Net build-up of heat in the solid wall}

$$\rho_s C p_s \left( \frac{\partial T_s}{\partial t} \right) = a(-\Delta H)(-r)_{VOC} + hS(T_g - T_s) + \lambda_s \left( \frac{\partial^2 T_s}{\partial x^2} \right) \quad (6)$$

where  $\rho_s$  is solid density (g/cm<sup>3</sup>),  $C p_s$  is the specific heat of solid (J/g °C),  $\Delta H$  is the heat of reaction (J/gmole) and  $\lambda_s$  is thermal conductivity (J/cm s °C).

Initial and Boundary Conditions:

Entering ethane concentration

$$C_g(0, t) = C_g^0 \quad (7)$$

$$\text{Entering gas temperature } T_g(0, t) = T_g^0 \quad (8)$$

$$\text{Solid catalyst temperature } T_s(x, 0) = T_s^0 \quad (9)$$

At the converter entrance:

$$x = 0, \frac{\partial T_s}{\partial x} = 0 \quad (10)$$

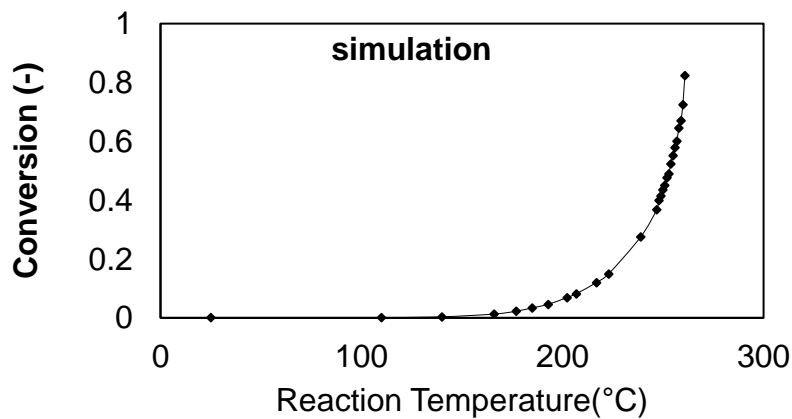
At the converter exit:

$$x = L, \frac{\partial T_s}{\partial x} = 0; \frac{\partial C_g}{\partial x} = 0; \frac{\partial T_g}{\partial x} = 0 \quad (11)$$

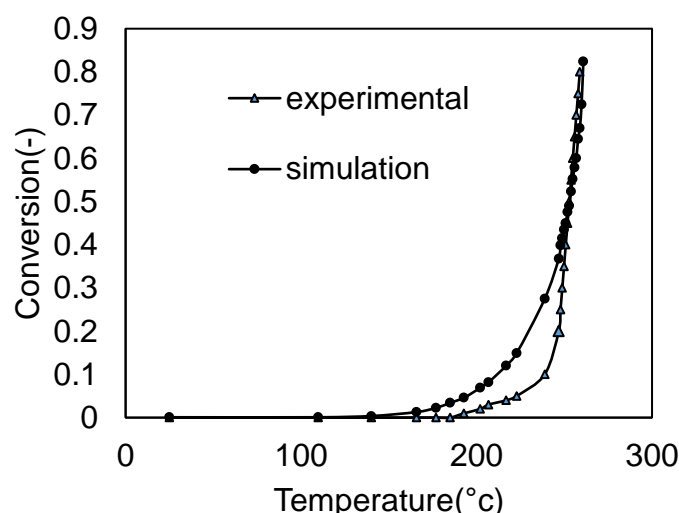
Equations (3), (4), (5) and (6) are coupled partial differential equations. All these equations are made dimensionless and solved using backward implicit scheme using Initial and Boundary Conditions.

#### 4. Results and discussion

**Fig. 1.** VOC ethane at 39 ppm<sup>[10]</sup> concentration and 250.00°C was entered in a catalytic converter initially at an ambient temperature of 25.00°C. At lower temperature, hardly any conversion takes place. As the temperature of converter reaches 184.85°C a slight conversion of about 3.40 % is observed. As the catalyst gets heated further, the exothermic catalytic reaction is initiated and rate of reaction increases due to release of heat by these reactions. About 49.00 % conversion is obtained at a temperature of 252.85°C and a temperature of 260.85°C, about 82.40% conversion is obtained.

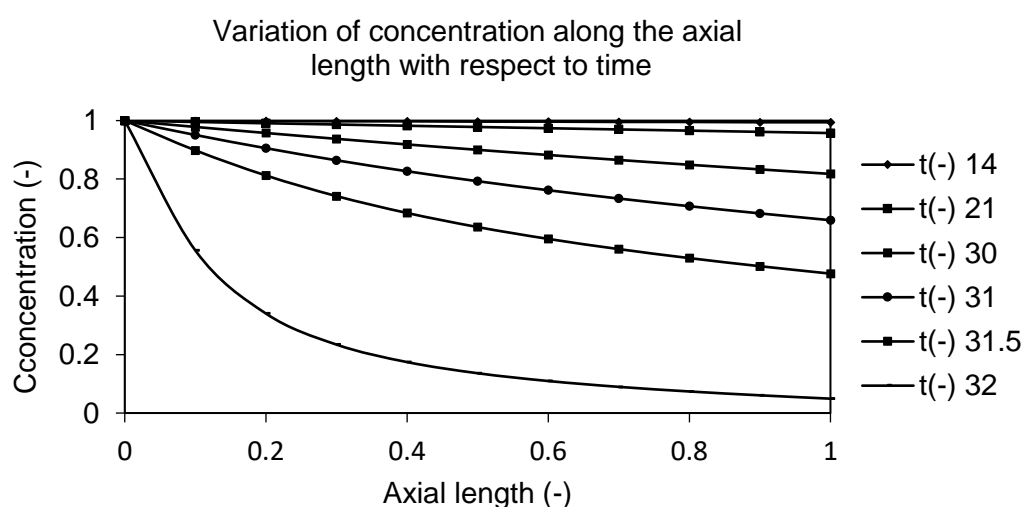


**Fig. 1.** Conversion of ethane with reaction temperature



**Fig. 2.** Comparison of modelled conversion of ethane with reaction temperature with the experimental results

**Fig. 2.**, represents the Comparison of modelled conversion of VOC ethane with reaction temperature with the experimental results using  $\text{Pt}/\delta\text{-Al}_2\text{O}_3$  as a catalyst. From the results as seen in the fig. 3. it is observed that at lower temperature  $25.00^\circ\text{C}$ , there is hardly any conversion for modelled and experimental results. The rate of reaction increases due to release of heat by these reactions as the catalyst gets heated. About 49.00 % conversion is obtained at a temperature of  $252.85^\circ\text{C}$  for modelled results and 50.00 % conversion is obtained at a temperature of  $252.85^\circ\text{C}$  for experimental results.



**Fig. 3.** Concentration variation along the axial length with respect to time for  $\text{Pt}/\delta\text{-Al}_2\text{O}_3$  catalyst

**Fig. 3.**, represents the concentration variation of the entering gas ethane along the axial length of the catalytic converter with respect to dimensionless time. The inlet dimensionless value of ethane concentration is considered as 1.0000. There is hardly any change in the concentration of VOC ethane initially up to dimensionless time 14.00. The dimensionless concentrations are 0.9991, 0.9980, 0.9964, 0.9953, and 0.9943 at axial distances 0.10, 0.30, 0.60, 0.80 and 1.00, respectively at dimensionless time 14.00. At axial distance 0.70 the dimensionless concentrations are 0.9959, 0.9167, 0.8175 and 0.5606 at dimensionless time 14.00, 24.00, 30.50 and 31.50 respectively.

The catalytic conversion increases due to the exothermic nature of catalytic reaction as the catalyst temperature increases with increase in dimensionless time. As the reacting gas ethane passages along the converter length it interacts with more surface area of a catalyst which offers more area for catalytic reaction and due to this, there is a decrease in its concentration along the length of the catalytic converter.

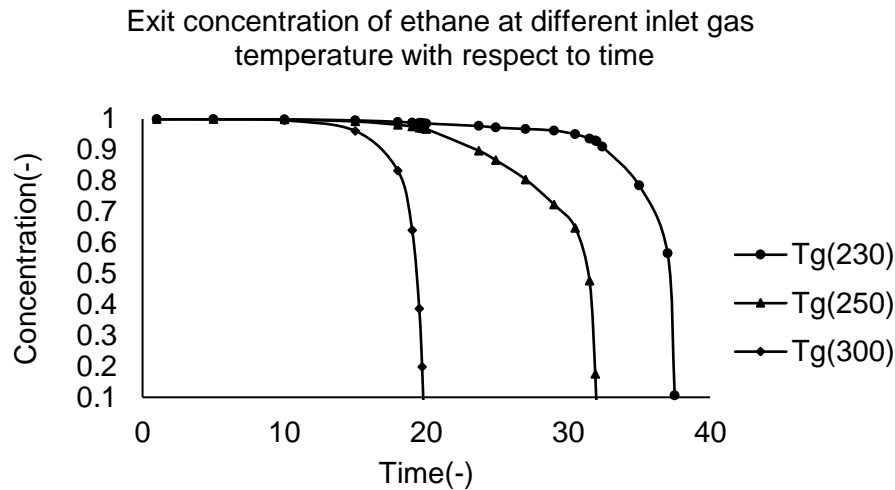


Fig. 4. Exit concentration of ethane at different inlet gas temperature with respect to time

**Fig. 4.**, represents the variation in ethane exit concentration at different inlet gas temperature along dimensionless time. Results are analyzed for inlet gas temperature for 230.00°C, 250.00°C, and 300.00°C. At the very start, there is no much variation in catalytic conversion due to change in inlet gas temperature. the exit dimensionless ethane concentrations are 0.9990, 0.9985 and 0.9956 for inlet gas temperature 230.00°C, 250.00°C and 300.00°C respectively at dimensionless time 10.00.

Though, the effect of an increase in inlet gas temperature on the catalytic conversion of reacting gas becomes more noticeable with the rise in time. The exit dimensionless ethane concentration is 0.9863, 0.9697 and 0.0642 for inlet gas temperature at 230.00°C, 250.00°C, and 300.00°C respectively at dimensionless time 19.80. Catalytic conversion is found to be quicker at higher inlet gas temperatures because additional heat is supplied to the solid catalyst surface, therefore, bring it faster to its operational temperature. The catalytic reactions triggered quickly which causes the desired conversion in a shorter duration of time

#### 4. Conclusions

A one-dimensional model for predicting the oxidation of ethane emissions in the converter was developed during the warm-up period using Pt/ $\delta$ -Al<sub>2</sub>O<sub>3</sub> catalyst. Variation in gas concentration along the length with respect to time was analyzed during the warm-up period. The VOC concentration decreased as a rise in the catalyst temperature due to the exothermic reaction and contact with more catalyst surface area, which offers more surface area for catalytic reaction. The effect of inlet gas temperature on the warm-up period was also examined. It was perceived that higher conversion of VOC ethane produces when the inlet gas temperature is increased. So, increase in the inlet gas temperature reduces the time required to achieve the desired conversion of VOC ethane.

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