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Effect of gas temperature on VOC emissions

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ABSTRACT

Propane is a slow oxidizing hydrocarbon, so its oxidation even in presence of catalyst platinum takes considerable time. Hence during this warm-up period it is released in considerable quantities to the atmosphere as a pollutant, before the catalyst reaches its operating temperature. Effect of varying the inlet gas temperature on the conversion of propane is analysed.

Key words: Propane, platinum, modeling, converter, warm-up.

INTRODUCTION

Vehicular pollution is one of the major sources of environmental degradation. Volatile organic compounds (VOC) include all carbon containing compounds present in the gaseous state at ambient temperatures. Propane a short chain alkane is present in both oil and natural gas. As the combustion process of propane is slower, hence it constitutes as the major VOC pollutant released from the exhaust of LPG fuelled vehicles [1].

Catalytic oxidation is recognized as one of the best methods for the abatement of VOC emissions; as it provides the potential to efficiently convert pollutants to carbon dioxide and water. In contrast to thermal incineration, the lower temperatures during catalytic oxidation result in a more economical process.

Monolithic or honeycomb catalysts, are crucial for improving our atmosphere and reducing

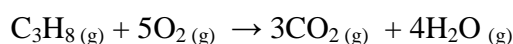
pollution. This type of the catalytic converter simultaneously meet special requirements of low pressure drop, short diffusion resistance, excellent mass transfer, high surface-to-volume ratio, easy scale-up, etc [2].

Mathematical modeling acts as an important tool in understanding the processes taking place in the converter and plays an integral part in designing and improving the already existing models. A one-dimensional model predicts the monolith performance quite accurately and requires about one-tenth computing time of the two-dimensional model. The former was found to represent the most practical model to use in modeling reactor performance while considering the initial warm-up period of an automobile from cold start [3].

In this study catalytic oxidation of propane is carried out. Platinum is considered as one of the most active material for HC oxidation. However typical catalyst requires relatively high temperatures in order to completely oxidize lower alkanes such as ethane and propane. So modeling is carried out to see the effect of inlet gas temperature on propane conversion.

REACTION KINETICS

The oxidation of propane is given by the following reaction:



The rate expression for the above catalytic reaction is given by:

$$(-r)(C_s, T_s) = k_0 \exp^{(-E_0/RT_s)} C \quad (1)$$

where, activation energy E_0 is taken as 89,849 J/gmol and the pre-exponential factor k_0 is taken as 2.40×10^7 cm/s [4].

MODELING

The model was formed taking into account the following assumptions over a single channel of the monolith:

- Catalyst does not deactivate.
- The noble metal concentration is constant.
- Diffusion in washcoat is neglected, as washcoat is very thin [5].
- Monolith is assumed to be adiabatic
- Heat exchange between the substrate and the surroundings at both inlet and outlet faces of the monolith are neglected.

Model Equations

$$\text{Mass and energy balance for gas: } v \left(\frac{\partial C_g}{\partial x} \right) + k_g S (C_g - C_s) = \left(\frac{\partial C_g}{\partial t} \right) \quad (2)$$

$$-v\rho_g C p_g \left(\frac{\partial T_g}{\partial x} \right) - hS(T_g - T_s) = \rho_g C p_g \left(\frac{\partial T_g}{\partial t} \right) \quad (3)$$

Mass and energy balance for solid: $a(-r)(C_s, T_s) = k_g S(C_g - C_s)$ (4)

$$\lambda_s \left(\frac{\partial^2 T_s}{\partial x^2} \right) + hS(T_g - T_s) + a(-\Delta H)(-r)(C_s, T_s) = \rho_s C p_s \left(\frac{\partial T_s}{\partial t} \right) \quad (5)$$

Initial and boundary conditions:

$$C_g(0, t) = C_g^0, \quad T_g(0, t) = T_g^0, \quad T_s(x, 0) = T_s^0 \quad (6)$$

$$\left(\frac{\partial C_g}{\partial x} \right)_{x=L} = 0, \quad \left(\frac{\partial T_g}{\partial x} \right)_{x=L} = 0, \quad \left(\frac{\partial T_s}{\partial x} \right)_{x=0} = 0, \quad \left(\frac{\partial T_s}{\partial x} \right)_{x=L} = 0 \quad (7)$$

All these equations (2) to (7) are first made dimensionless using the following dimensionless variables:

$$C' = \frac{C_g}{C_g^0}, \quad T'_g = \frac{T_g}{T_g^0}, \quad T'_s = \frac{T_s}{T_g^0}, \quad z = \frac{x}{L}, \quad t' = \frac{t}{t_0} \quad (8)$$

Dimensionless Equations

Combining equations (2) and (4) for dimensionless mass balance equation:

$$\left(\frac{\partial C'}{\partial z} \right) = -\delta_1 \left(\frac{\partial C'}{\partial t'} \right) - \psi_1 C' e^{(-E_0/RT_s)} \quad (9)$$

where ψ_1 and δ_1 are dimensionless numbers and their values are given by:

$$\psi_1 = \frac{Lak_0}{v} \quad (10)$$

$$\delta_1 = \frac{L}{vt_0} \quad (11)$$

Dimensionless energy balance equation for gas phase:

$$\left(\frac{\partial T'_g}{\partial z} \right) = -\delta_2 \left(\frac{\partial T'_g}{\partial t'} \right) - \delta_{22}(T'_g - T'_s) \quad (12)$$

where δ_{22} and δ_2 are dimensionless numbers and their values are given by:

$$\delta_{22} = \frac{SLh}{v(\rho_g C p_g)} \quad (13)$$

$$\delta_2 = \frac{L}{vt_0} \quad (14)$$

Dimensionless energy balance equation for solid phase:

$$\left(\frac{\partial T'^2_s}{\partial z^2} \right) = -\psi_2 C' e^{(-E_0/RT_s)} + \alpha_1 (T'_s - T'_g) + \delta_3 \left(\frac{\partial T'_s}{\partial t'} \right) \quad (15)$$

where ψ_2 , α_{33} and δ_3 are dimensionless numbers and their values are given by:

$$\psi_2 = (C_g^0) \frac{aL^2(-\Delta H)k_0}{\lambda_s T_g^0} \quad (16)$$

$$\alpha_1 = \frac{ShL^2}{\lambda_s} \quad (17)$$

$$\delta_3 = \frac{(\rho_s C_{p_s})L^2}{\lambda_s t_0} \quad (18)$$

Dimensionless initial conditions and boundary conditions:

$$C'(0, t') = 1.0 \quad (19)$$

$$T_g'(0, t') = \frac{T_g}{T_g^0} \quad (20)$$

$$T_s'(z, 0) = \frac{T_s}{T_s^0} \quad (21)$$

$$\text{at } z = 0, \quad \frac{\partial T_s'}{\partial z} = 0 \quad (22)$$

$$\text{at } z = 1.0, \quad \frac{\partial T_s'}{\partial z} = 0 \quad (23)$$

$$\text{at } z = 1.0, \quad \frac{\partial C'}{\partial z} = 0 \quad (24)$$

$$\text{at } z = 1.0, \quad \frac{\partial T_g'}{\partial z} = 0 \quad (25)$$

METHODOLOGY OF SOLUTION

The coupled partial differential equations (9), (12) and (15) along with the initial and boundary conditions in equations (19) to (25) are used for calculating the gas concentration, the gas temperature and the solid catalyst temperature using the Backward implicit scheme. The method used is central difference in space and backward difference in time. These partial differential equations are discretized along with the initial and boundary conditions resulting in the following equations:

Mass balance for propane in gas phase:

$$\left[\frac{(C'_{j,j+1} - C'_{j,j-1})}{2k} \right] + \delta_1 \left[\frac{(C'_{j,j} - C'_{j-1,j})}{h} \right] = -\psi_1 C'_{j-1,j} e^{-\left[\frac{E_0}{R(T_{s,j-1,j} + 273)} \right]} \quad (26)$$

At I=1 inlet dimensionless concentration of propane is taken as 1.0000 and at the converter exit I = M, equation (24) becomes:

$$\left[\frac{(C'_{j,j} - C'_{j,j-1})}{k} = 0 \right] \quad (27)$$

Energy balance for the gas phase:

$$\left[\frac{(T'_{g,J,I+1} - T'_{g,J,I-1})}{2k} \right] + \delta_2 \left[\frac{(T'_{g,J,I} - T'_{g,J-1,I})}{h} \right] = -\delta_{22} (T'_{g,J,I} - T'_{s,J,I}) \quad (28)$$

At $I = 1$, gas temperature is 450°C at the entrance and at $I = M$ equation (25) can be written as:

$$\left[\frac{(T'_{g,J,I} - T'_{g,J,I-1})}{k} \right] = 0 \quad (29)$$

Energy balance for the solid phase:

$$\begin{aligned} & \left[\frac{T'_{s,J,I+1} - 2T'_{s,J,I} + T'_{s,J,I-1}}{k^2} \right] + \alpha_1 [T'_{g,J,I} - T'_{s,J,I}] + \psi_2 C'_{sJ-1,I} e^{\left(\frac{E_0}{R(T'_{s,J-1,I} + 273)} \right)} \\ & - \delta_3 \left[\frac{T'_{s,J,I} - T'_{s,J-1,I}}{h} \right] = 0 \end{aligned} \quad (30)$$

At $J = 1$ solid temperature is 25°C all along the reactor length. At $I = 1$ and $I = M$, equations (22) and (23) can be written as:

$$\left[\frac{T'_{s,J,I+1} - T'_{s,J,I}}{k} \right] = 0 \quad (31)$$

$$\left[\frac{T'_{s,J,I} - T'_{s,J,I-1}}{k} \right] = 0 \quad (32)$$

The above equations (26) to (32) are used for calculating the gas concentration, gas temperature and the solid catalyst temperature, at any time using backward implicit scheme [6].

RESULTS AND DISCUSSION

The propane gas at 450°C enters the converter initially at 25°C . The inlet concentration of gas has a dimensionless value of 1.0000 and the results are obtained and analysed for decrease in the dimensionless concentration upto 0.1000. Fig.1 shows conversion of propane with reaction temperature. Fig. 2 and 3 show the effect of variation of gas inlet temperatures on exit concentration of propane.

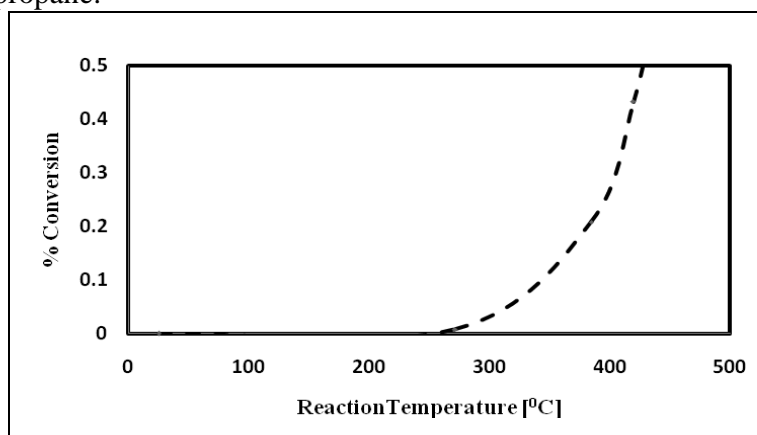


Fig. 1. Effect of Reaction Temperature on conversion of Propane

Fig.1 shows the effect of catalyst reaction temperature on conversion of propane. Up to catalyst temperature of 270°C , there is no conversion of propane and it is released untreated to the atmosphere as the catalyst is not warm enough to cause its conversion. About 50% conversion achieved around 430°C .

Fig. 2 shows the effect of inlet gas temperatures 400°C and 450°C on conversion of propane. For inlet gas temperature of 400°C , there is hardly any conversion of propane even up to dimensionless time 14.40, whereas about 90% conversion is achieved for inlet gas temperature of 450°C at dimensionless time 14.40. So a minimum inlet gas temperature is required to heat the catalyst to its operating temperature.

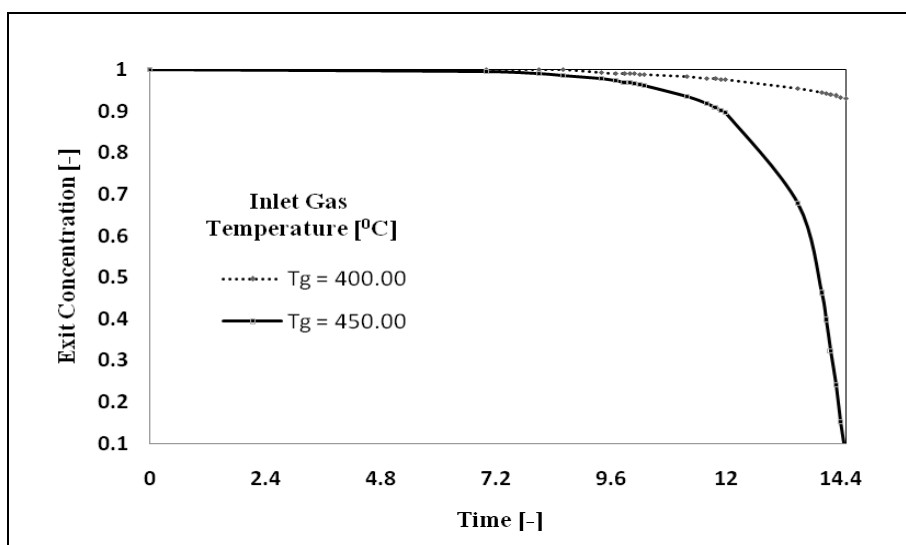


Fig. 2 Variation in Exit Concentration of propane with time for inlet gas temperatures of 400°C and 450°C

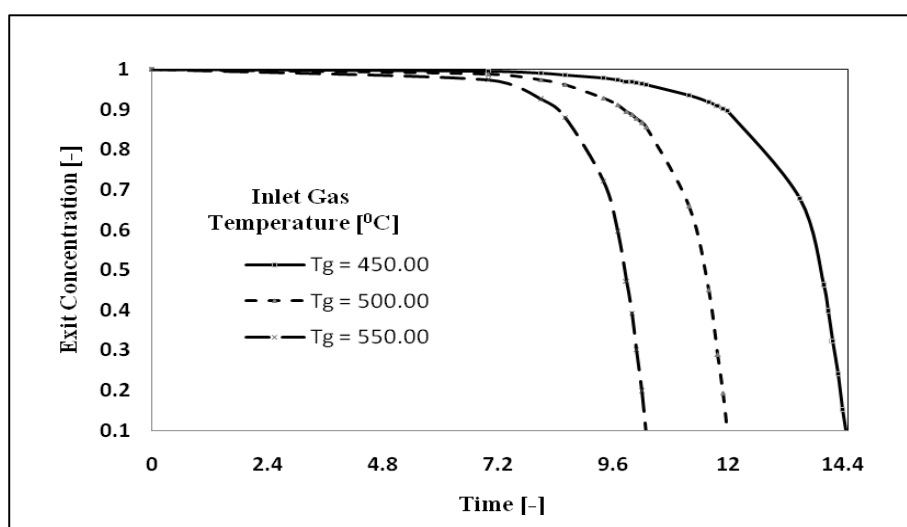


Fig. 3 Variation in Exit Concentration of propane with time for inlet gas temperatures of 450°C , 500°C and 550°C

Fig. 3 shows the effect of inlet gas temperatures 450⁰C, 500⁰C and 550⁰C on conversion of propane. For inlet gas temperature of 450⁰C at dimensionless time 14.40 about 90% conversion of propane is achieved. The same conversion can be achieved in dimensionless times 12.00 and 10.30 if the inlet gas temperatures are increased to 500⁰C and 550⁰C respectively, thereby reducing the time of release of pollutant to the atmosphere by heating the catalyst faster to its operating temperature.

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REFERENCES

- [1] B Solsona; I Vazquez; T Garcia; TE Davies; SH Taylor, *Catal. Letters*, **2007**, 116, 116-121.
- [2] V Tomasic; Z Gomzi; S Zrnecvic, *React. Kinet. Catal. Lett.*, **2002**, 77, 245-253.
- [3] RH Heck; J Wei; JR Katzer, *AIChE J.*, **1976**, 22, 477-484.
- [4] R Wanker; H Raupenstauch; G Staudinger, *Chem. Engng. Sci.*, **2000**, 55, 4709-4718.
- [5] ST Kolaczowski, *Catal. Today*, **1999**, 47, 209-218.
- [6] S Chauhan; VK Srivastava, *Int. J. of Chem. Reactor Eng.*, **2008**, 6 Article A85, 1-24.

NOMENCLATURE

a	catalytic surface area per unit reactor volume, cm ² /cm ³
C _i	concentration of the species, mol/cm ³
C _p	specific heat, J/g K
E ₀	activation energy for catalytic reaction, J/mol
h	heat transfer coefficient, J/cm ² s K
-ΔH	heat of reaction, J/mol
k _g	mass transfer coefficient, cm/s
k ₀	pre-exponential factor for catalytic reaction, cm/s
L	length of monolith, cm
R	gas constant, J/mol K
S	geometric surface area per unit reactor volume, cm ² /cm ³
T	temperature, K
t	time, s
v	gas velocity, cm/s
x	axial coordinates, cm

Greek symbols

λ	thermal conductivity, J/cm s K
ρ	density, g/cm ³

Subscripts and Superscripts

i	represents propane
s	solid
g	gas
o	initial conditions

Dimensionless numbers

C'	dimensionless concentration
T' _g	dimensionless gas temperature
T' _s	dimensionless solid temperature
z	dimensionless axial coordinates
t'	dimensionless time