



## Pelagia Research Library

Der Chemica Sinica, 2011, 2 (1): 164-170



# Acetaldehyde combustion using platinum catalyst

Sanchita Chauhan

University Institute of Chemical Engineering and Technology, Panjab University, Chandigarh,  
INDIA

---

### ABSTRACT

Catalytic Converters are extensively used for reduction of the pollutants released from various sources to the atmosphere. These converters become effective in minimising the pollutant concentration only after they achieve their operating temperature. During this cold start period hydrocarbons are released untreated to the atmosphere. This paper deals with the oxidation of hydrocarbon acetaldehyde, a VOC during the cold start period. Mathematical modeling is a good way of analysing the converter behaviour without performing very expensive and time consuming experiments. A one-dimensional computer model that takes into account the mass and the heat transfer between the gas phase and the catalyst is considered. The equations form a set of ordinary and partial differential equations, which are non-linear and coupled. These equations are solved using Runge kutta and Backward Implicit scheme.

**Keywords:** Acetaldehyde, modeling, converter, quasi steady state, catalyst loading.

---

### INTRODUCTION

VOC's are important air pollutants in urban atmosphere. They are defined as organic compounds with high vapor pressure that are easily vaporized under an ambient temperature and pressure conditions [1]. They are released mostly from vehicular exhaust and industrial processes. Ethanol-fueled passenger cars are found to produce high emissions of aldehydes in comparison to gasoline-fueled cars [2].

Use of catalytic converters has proved to be a very good way of reducing emissions from the vehicular exhaust. Modeling of converters as compared to experimental testing is not only inexpensive but also time saving [3]. The monolith behaviour during warm up period can be adequately predicted by using a one-dimensional model [4].

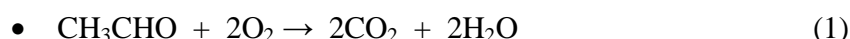
In the present paper modeling for VOC acetaldehyde is considered in a ceramic cordierite converter. A one dimensional model is used to simulate the thermal and conversion characteristics of the converter operating under warm up conditions. The change in acetaldehyde concentration due to catalytic oxidation reaction is analysed with respect to operating temperature and the effect of catalyst loading on reducing cold start period is analysed.

## MATHEMATICAL MODEL

In one-dimensional modeling only axial gradients are considered for gas concentration, gas temperature and catalyst temperature.

Assumptions made during modeling include [5]:

❖ An irreversible oxidation reaction of VOC acetaldehyde is considered to be taking place:



❖ Catalytic reactions are assumed to be first order in fuel concentration and zero order with respect to oxygen concentration under lean conditions is represented by [1]:

$$\bullet (-r)(C_s, T_s) = k_0 \exp(-E/RT_s) C_s \quad (2)$$

where pre-exponential factor  $k_0$  and activation energy  $E$  are taken as 46.18 m/s and 36374 J/gmol.

- ❖ A cylindrical channel is considered in which the catalytic reactions take place.
- ❖ Washcoat is assumed to be very thin (10 $\mu$ m in thickness) and diffusion in wash coat is neglected.
- ❖ Accumulation of mass and energy in the gas phase is negligible.
- ❖ As compared to convective transport, the axial diffusion of mass and heat transfer in gas phase is very small, therefore neglected.
- ❖ Noble metal concentration is kept constant along the length of the converter.
- ❖ Catalyst does not deactivate.
- ❖ Monolith is assumed to be adiabatic.
- ❖ Heat transfer by radiation within the channel is neglected.
- ❖ Heat exchange between the substrate and the surroundings at both the inlet and the outlet faces of the monolith is neglected.

For a quasi steady state model the time derivative terms in gas phase mass and energy balances are neglected.

$$\text{i.e., } \frac{\partial C_g}{\partial t} = 0 \quad (3)$$

$$\text{and } \frac{\partial T_g}{\partial t} = 0 \quad (4)$$

**Mass and energy balance equations for gas phase:**

$$v\left(\frac{\partial C_g}{\partial x}\right) + k_g S(C_g - C_s) = 0 \quad (5)$$

$$-v\rho_g C p_g \left(\frac{\partial T_g}{\partial x}\right) - hS(T_g - T_s) = 0 \quad (6)$$

**Mass and energy balance equations for solid phase:**

$$a(-r)(C_s, T_s) = k_g S(C_g - C_s) \quad (7)$$

$$\rho_s C p_s \left(\frac{\partial T_s}{\partial t}\right) = a(-\Delta H)(-r)(C_s, T_s) + hS(T_g - T_s) + \lambda_s \left(\frac{\partial^2 T_s}{\partial x^2}\right) \quad (8)$$

**Initial and boundary conditions:**

Entering acetaldehyde concentration at all times

$$C_g(0, t) = C_g^0 \quad (9)$$

Entering gas temperature at all times

$$T_g(0, t) = T_g^0 \quad (10)$$

Solid catalyst temperature at the start

$$T_s(x, 0) = T_s^0 \quad (11)$$

Lagging solid catalyst at entry and exit

$$x = 0, \frac{\partial T_s}{\partial x} = 0 \quad (12)$$

$$x = L, \frac{\partial T_s}{\partial x} = 0 \quad (13)$$

The governing Eqs. (5) to (13) are made dimensionless by using the following dimensionless variables:

$$C' = \frac{C_g}{C_g^0}, \quad T_g' = \frac{T_g}{T_g^0}, \quad T_s' = \frac{T_s}{T_s^0}, \quad z = \frac{x}{L}, \quad t' = \frac{t}{t^0} \quad (14)$$

**Dimensionless mass and energy balance equations for gas and solid phase:**

$$\left(\frac{\partial C'}{\partial z}\right) = -\gamma_1 C' e^{(-E/RT_s)} \quad (15)$$

$$\left(\frac{\partial T'_g}{\partial z}\right) = -\alpha_{22}(T'_s - T'_g) \quad (16)$$

$$\left(\frac{\partial T'^2_s}{\partial z^2}\right) = -\alpha_3 C' e^{(-E/RT_s)} + \alpha_{33}(T'_s - T'_g) + \delta_3 \left(\frac{\partial T'_s}{\partial t'}\right) \quad (17)$$

where,  $\gamma_1$ ,  $\alpha_{22}$ ,  $\alpha_3$ ,  $\alpha_{33}$  and  $\delta_3$  are dimensionless numbers as shown in Table 1.

**Dimensionless initial and boundary conditions:**

$$C'(0, t') = 1.0 \quad (18)$$

$$T'_g(0, t') = \frac{T_g}{T_g^0} \quad (19)$$

$$T'_s(z, 0) = \frac{T_s}{T_s^0} \quad (20)$$

$$\text{at } z = 0, \frac{\partial T'_s}{\partial z} = 0 \quad (21)$$

$$\text{at } z = 1.0, \frac{\partial T'_s}{\partial z} = 0 \quad (22)$$

**NUMERICAL SCHEME**

The dimensionless Eqs. (15) and (16) are ODEs and Eq. (17) is a PDE. As these equations are coupled; hence they are solved at the same time. The ODEs do not have a time derivative term but as these equations are coupled with the PDE, the time derivative present in the later gets introduced in the iterated results for the ODEs. The ODEs (15) and (16) are solved using Runge-Kutta method of fourth order and the PDE (17) by using backward implicit scheme [6].

Table 1: Mathematical expressions for the dimensionless numbers

Dimensionless numbers	Mathematical expression
$\gamma_1$	$\frac{Lak_0}{v}$
$\alpha_{22}$	$\frac{SLh}{v(\rho_g Cp_g)}$
$\alpha_3$	$(C_g^0) \frac{aL^2(-\Delta H)k_0}{\lambda_s T_g^0}$
$\alpha_{33}$	$\frac{ShL^2}{\lambda_s}$
$\delta_3$	$\frac{(\rho_s Cp_s)L^2}{\lambda_s t_0}$

## RESULTS AND DISCUSSION

At the start of the operation the converter is at 25<sup>0</sup>C and exhaust gas entering the converter at 400<sup>0</sup>C heats the converter. The catalytic reaction starts once the converter has attained the operating temperature. Due to the reaction a decrease in the concentration of acetaldehyde is observed. The inlet concentration of acetaldehyde (100ppm) has a dimensionless value of 1. Results as shown in Figure1 represent the onset of catalytic reaction for acetaldehyde and Figure 2 show the variation in exit concentration of acetaldehyde with time based on converter catalyst loading.

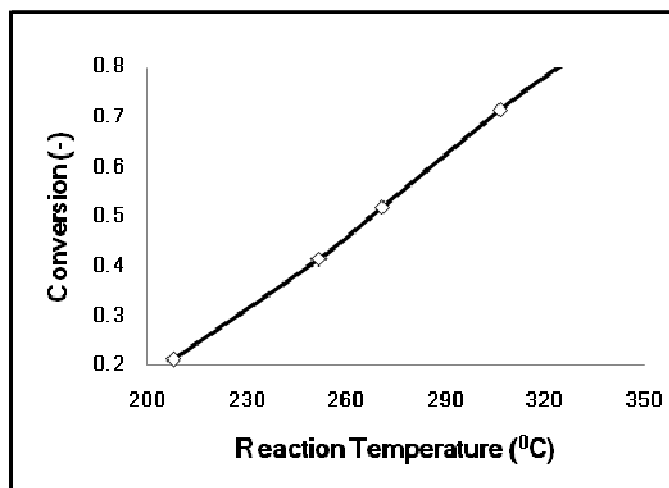


Figure 1. Effect of solid catalyst temperature on conversion of acetaldehyde

Figure 1 shows the effect of solid temperature on the conversion of acetaldehyde. Initially when the converter is at 25<sup>0</sup>C, there is negligible conversion of acetaldehyde. On heating the converter by the incoming hot gas at 400<sup>0</sup>C the converter finally reaches its operating temperature. The results show that for the solid temperature of about 200<sup>0</sup>C conversion of acetaldehyde is only

0.20. However beyond this temperature, a noticeable conversion of acetaldehyde takes place. About 50% and 80% conversion are brought about at catalyst temperatures of 270<sup>0</sup>C and 326<sup>0</sup>C respectively. The results indicate that after the operating temperature is achieved the catalytic reaction begins and the heat released by the reaction further increases the solid catalyst temperature. This brings about a faster conversion of acetaldehyde.

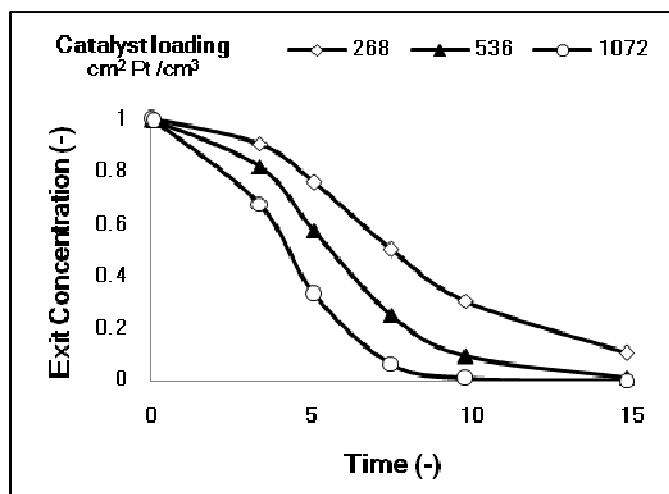


Figure 2. Variation of exit concentration of acetaldehyde with time for different catalyst loading

Figure 2. shows the effect of catalyst loading on the conversion of acetaldehyde. Three different cases are analysed with catalyst loadings 268 cm<sup>2</sup>Pt/cm<sup>3</sup>, 536 cm<sup>2</sup>Pt/cm<sup>3</sup> and 1072 cm<sup>2</sup>Pt/cm<sup>3</sup>. At dimensionless time 3.40 the exit concentrations of acetaldehyde are 0.9062, 0.8212 and 0.6744 for catalyst loadings 268 cm<sup>2</sup>Pt/cm<sup>3</sup>, 536 cm<sup>2</sup>Pt/cm<sup>3</sup> and 1072 cm<sup>2</sup>Pt/cm<sup>3</sup>. More deviation is observed in the exit concentrations as time increases. At dimensionless time 7.50 the exit concentrations of acetaldehyde are 0.5015, 0.2515 and 0.0633 for catalyst loadings 268 cm<sup>2</sup>Pt/cm<sup>3</sup>, 536 cm<sup>2</sup>Pt/cm<sup>3</sup> and 1072 cm<sup>2</sup>Pt/cm<sup>3</sup>. The results show that higher the catalyst loading faster is the conversion of acetaldehyde.

## CONCLUSION

At ambient conditions the oxidation of acetaldehyde is not appreciable during the cold start period of the converter, due to low initial temperatures of the converter. So some time is required to preheat the converter to its operating temperature after which the catalytic reactions get initiated and bring about conversion of acetaldehyde. Fresh catalyst with relatively higher catalyst loading brings about a faster conversion of acetaldehyde as compared to in use catalyst with lower values of catalyst loading.

## NOMENCLATURE

<i>a</i>	catalytic surface area per unit reactor volume (cm <sup>2</sup> /cm <sup>3</sup> )
<i>C</i>	concentration of the species (gmole/cm <sup>3</sup> )
<i>C<sub>p</sub></i>	specific heat (J/g K)
<i>E</i>	activation energy for catalytic reaction (J/gmole)

---

$h$	heat transfer coefficient (J/cm <sup>2</sup> s K)
$-\Delta H$	heat of reaction (J/gmole)
$k_g$	mass transfer coefficient (cm/s)
$k_0$	rate constant for catalytic reaction (cm/s)
$L$	length of monolith (cm)
$R$	gas constant (J/gmole K)
$S$	geometric surface area per unit reactor volume (cm <sup>2</sup> /cm <sup>3</sup> )
$T$	temperature (K)
$t$	time (s)
$v$	gas velocity (cm/s)
$x$	axial coordinates (cm)
$z$	dimensionless axial coordinates
$\lambda$	thermal conductivity (J/cm s K)
$\rho$	density (g/cm <sup>3</sup> )

**Subscript and Superscript**

$s$	solid
$g$	gas
'	dimensionless values
$0$	initial conditions

**Acknowledgement**

The support of Prof. V. K. Srivastava (Academy of Business & Engg. Sciences, Vijay Nagar, Ghaziabad) for his invaluable inputs and advice is gratefully acknowledged.

**REFERENCES**

- [1] Wang TP, Tran DV, Sakurai VM, Kameyama H, *Applied Catalysis A: General*, **2008**, 350, 150.
- [2] R.W. McCabe, P.J. Mitchell, *Ind Eng Chem Prod Res Dev*, **1983**, 22, 212.
- [3] P.M. Liang, M.D. Shane, S. Son, A.A. Adamczyk, P. Li, *SAE Paper 1999-01-3476*, **1999**, 1362.
- [4] R.H. Heck, J. Wei, J.R. Katzer, *AIChE J*, **1976**, 22, 477.
- [5] S. Chauhan, V.K. Srivastava, *Computers and Mathematics with Application*, **2008**, 55, 319.
- [6] S. Chauhan, V.K. Srivastava, *Chemical Product and Process Modeling*, **2008**, 3, Article 10, 1.