

# 3D Numerical Simulation of Gas Flow and Selective Catalytic Reduction (SCR) of NO in the Honeycomb Reactor

Jongchol Om

Department of mechanics  
University of science  
Poyngyang, DPR of Korea  
[M15669046883@163.com](mailto:M15669046883@163.com)

Peidong Ji

State Key Laboratory of Clean Energy Utilization  
Zhejiang niversity  
Hangzhou , PR China  
[jipd@zju.edu.cn](mailto:jipd@zju.edu.cn)

Weihong Wu

State Key Laboratory of Clean Energy Utilization  
Zhejiang niversity  
Hangzhou , PR China  
[whwu2000@vip.163.com](mailto:whwu2000@vip.163.com)

**Abstract-**Selective catalytic reaction(SCR) of NO<sub>x</sub> by ammonia is a very efficient method to reduce the NO<sub>x</sub> emission from coal-fired power plants and large boilers. The ammonia is injected into the exhaust gas stream and is mixed NO<sub>x</sub>. The mixture passes through the honeycomb-type catalyst bed, where NO<sub>x</sub> reacts on the catalyst surface with adsorbed ammonia in the presence of excess oxygen, decomposing into diatomic nitrogen and water molecules, thereby reducing the NO<sub>x</sub> level in the exhaust gas. The present study discusses the NO<sub>x</sub> reduction mechanism in the honeycomb channel. In this work, 3-dimensional computational fluid dynamics (CFD) simulations are carried out to investigate the effects of the various state parameters on the De-NO<sub>x</sub> reaction at the catalyst. Research results showed that the gas temperature, flow velocity and NH<sub>3</sub>/NO<sub>x</sub> concentration ratio all are important parameters of the NO<sub>x</sub> reduction with ammonia in the honeycomb catalyst.

**Keywords-**Selective catalytic reaction(SCR); simulations; CFD; honeycomb; De-NO<sub>x</sub> reaction

## I. INTRODUCTION

Nitrogen oxides(NO<sub>x</sub>, including NO, NO<sub>2</sub> and N<sub>2</sub>O) emissions from power and chemical plants are major environmental concerns that include increasing ground level ozone, formation of acid rain, forest damage, and formation of fine particles in the atmosphere. Therefore, the technologies to reduce NO<sub>x</sub> emission are of great importance. Being one of such technologies, selective catalytic reduction(SCR) of NO<sub>x</sub>, is a very promising method, due to its high efficiency, selectivity and low expense[1-2].

Because of degradation during long-time operation, catalysts must be periodically exchanged or regenerated, hence it is needed to optimize the operation conditions of De-NO<sub>x</sub> equipment and predict the lifetime of the catalyst.

SCR performance can be improved by operating the catalysts at different temperatures to optimize their

maximum activity and gas residence time also influences catalytic activity, as well as inlet ammonia concentration.

Ammonia slip is one of the common problems with SCR system, it can occur when catalyst temperatures are not in the optimal range for the reaction, or when too much ammonia is injected into the process[3-4].

The present study investigates the effects of various parameters (temperature, inlet NH<sub>3</sub>/NO concentration ratio, gas space velocity) on the performance of honeycomb structured catalysts using three-dimensional CFD modeling and simulation.

## II. MATHEMATICAL MODEL

In present study, we ignore the heat transfer in the reactor because the concentrations of reactants are extremely low and the energy accumulation is insignificant. Furthermore, we assume a uniform catalyst distribution, an equally inlet flow over the entire cross section of the honeycomb, and an ideal homogeneous premixing of the exhaust gas and reactants. Based on these assumptions, the simulation of the physicochemical processes occurring in the whole system is reduced to the analysis of a single channel. In this model, we also assume that the diffusion in the gas phase and in the catalyst material of the reactant species obeys FICK's law and the gas flow in the honeycomb channel is turbulent[5].

### A. Reaction Kinetics

The reaction mechanism for the reduction of NO using NH<sub>3</sub> over catalyst is described as following;



The following rate equation taken from the literature on intrinsic SCR kinetics is used in this study.

$$r_1 = k_1 C_{NO} \frac{a C_{NH_3}}{1 + a C_{NH_3}} \quad (3)$$

$$r_2 = k_2 C_{NH_3} \quad (4)$$

$$k_i = A_i \exp\left(-\frac{E_i}{RT}\right), i=1,2 \quad (5)$$

$$a = A_a \exp\left(-\frac{E_a}{RT}\right) \quad (6)$$

Where  $E_i$  is the activated energy (J/mol), R is the gas constant (J/mol k) and T is the temperature (k)[6].

### B. Transport Phenomena

The governing equations for the exhaust gas flow are continuity equation, momentum equation (N-S equation), and mass conservation equation of species I, which are written as

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0 \quad (7)$$

$$\rho \frac{\partial \vec{u}}{\partial t} + \rho (\vec{u} \cdot \nabla) \vec{u} = -\text{grad}(p) + (\mu + \mu_t) \Delta \vec{u} \quad (8)$$

$$\frac{\partial C_i}{\partial t} + \nabla \cdot (-D_i \nabla C_i + \vec{u} C_i) = R_i$$

$$i=\text{NO or } NH_3, R_1 = r_1, \quad R_2 = r_1 + r_2. \quad (9)$$

where  $D_i$  and  $C_i$  denote the diffusion coefficient ( $m^2/s$ ) and the specie core, respectively.

We assumed that reaction rate  $R_i$  is negligible in the gas phase and it is considerable only in the catalyst material, because the reaction rate between NO and  $NH_3$  without the catalyst is very slow.

The exhaust gas flow is usually turbulent. In this study, the turbulent flow is described as RNG  $k-\epsilon$  model.

$$\frac{\partial}{\partial t}(\rho k) + \nabla \cdot (\rho u k) = \nabla \cdot \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \nabla k \right] + P_k - \rho \epsilon \quad (10)$$

$$\frac{\partial}{\partial t}(\rho \epsilon) + \nabla \cdot (\rho u \epsilon) = \nabla \cdot \left[ \left( \mu + \frac{\mu_t}{\sigma_\epsilon} \right) \nabla \epsilon \right] +$$

$$C_1 \frac{\epsilon}{k} P_k - C_2 \rho \frac{\epsilon^2}{k} \quad (11)$$

$$\mu_t = \rho C_\mu \frac{k^2}{\epsilon} \quad (12)$$

The constants appearing in Eqs, (10)-(12) are  $C_\mu=0.09$ ,  $\sigma_k=1.0$ ,  $\sigma_\epsilon=1.30$ ,  $C_1=1.44$ , and  $C_2=1.92$ . [7]

### III. CFD SIMULATIONS AND PARAMETER VALUES

Three-dimensional simulation are carried out with the commercial CFD simulation package Ansys 14.5 Fluent.

Fig.1 shows a schematic diagram of the honeycomb element SCR reactor and the computational domain.

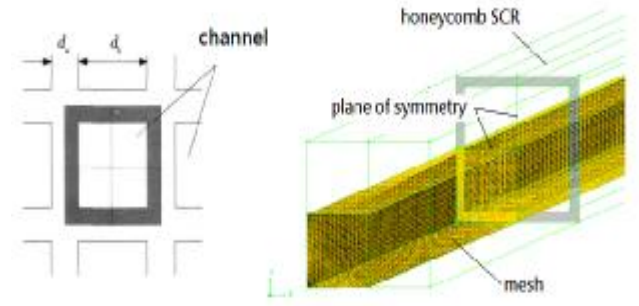


Figure 1. Honeycomb SCR channel and computational mesh.

The simulation parameters such as the inflow properties and the physical properties of the SCR reactor are listed in table 1 and 2.

Table 1. Physical property of the SCR [8-9]

Kinetic parameter	Physical meaning	value	unit
$E_1$	Activate energy	41900	j/mol
$E_2$	Activate energy	85400	j/mol
$k_1$	Rate constant	$1.19 \times 10^4$	j/mol
$k_2$	Rate constant	$6.73 \times 10^7$	$s^{-1}$
$k_r$	reaction constant	2.57	$s^{-1}$
$A_a$	constant	$\times 10^{-17}$	$m^2/mol$
$E_a$	Activate energy	$-2.37 \times 10^5$	j/mol
$S_g$	BET surface	73.75	$m^2/g$
$V_g$	Totalpore volume	0.1658	$cm^3/g$

The discretization of the governing equations and the boundary conditions was established on the basis of the geometrical symmetry. The elements of mesh all are hexahedron and the mesh number is  $80 \times 80 \times 600$ , about 3.80million.

For considering the interface between the catalyst and the gas phase, we can be written as follow:

$$D_e \frac{\partial C_i}{\partial n} = D_g \frac{\partial C_i}{\partial n} \quad (13)$$

Where n: normal vector,  $D_e$ : diffusion coefficient in the catalyst,  $D_g$ : diffusion coefficient in gas phase.

TABLE 2. Numerical Simulation condition

Parameters	value
Length of SCR layer	600mm
Cell size	$6 \times 6$ mm
Thickness	1mm
Gas velocity	0.1 – 10 m/s
temperature	300 – 400 °C
NO	1000 ppm
$NH_3$	900 – 1100 ppm
Tortuosity	4
Porosity	0.4

Since the diffusion coefficient and the gas viscosity are dependent of temperature, in this study the following corrections are used in this work[10-11].

$$D_e = \frac{\epsilon}{\tau} \times 9.70 \times 10^3 \times \bar{T} \times \sqrt{\frac{T}{M_i}} \quad (14)$$

$$D_g = 2.695 \times 10^{-5} \frac{\sqrt{T^3 ((M_1 + M_2) / (2 \times 10^3 M_1 M_2))}}{p \sigma_1 \sigma_2 \Omega_D} \quad (15)$$

$$\ln \mu = A_0 + B_0 \ln T + \frac{B_1}{T} + \frac{B_2}{T^2} \quad (16)$$

$$A_0=1.209188, B_0=0.6916243, B_1 \times 10^{-3}=0.0576372, \\ B_2 \times 10^{-5} = -0.1429573.$$

Where  $\epsilon$  and  $\tau$  are the tortuosity and the porosity,  $M_i$  and  $M_g$  present the molar mass (kg/mol) of gas species, respectively. And  $\sigma_i$  and  $\sigma_g$  are the diameters(m) of the gas species. Besides,  $P$  is the pressure (Pa) and  $\Omega_D$  is collision integrals[8].

#### IV. RESULT AND DISCUSSION

Fig .2shows the flow velocity profile in a honeycomb channel. The development of the velocity distribution can be portrayed by a sequence of velocity profiles along the channel.

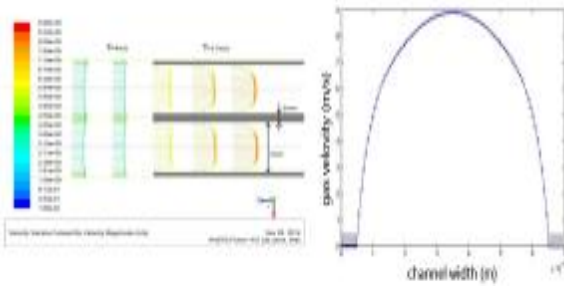


Figure2.gas velocity profile in the honeycomb chanel.

It is clearly seen that the gas inflow at the inlet cross section has homogeneous velocity 4m/s, but the maximum speed of the developed flow in a channel is 8.9m/s.It is clear that the gas flow non-uniformly enters the channel and it is gradually developed up to the point ,60mm from the inlet, since the velocity profile has two peaks at upstream and it has one peak at downstream in this figure.

Fig .3 shows the decrease of the NO concentration profiles at various axial positions along the channels with two catalyst layerswhen the inlet gas temperature is 380°C,the flow velocity is 4m/s ,and inlet NO and  $\text{NH}_3$ concentration both are 1000ppm respectively.

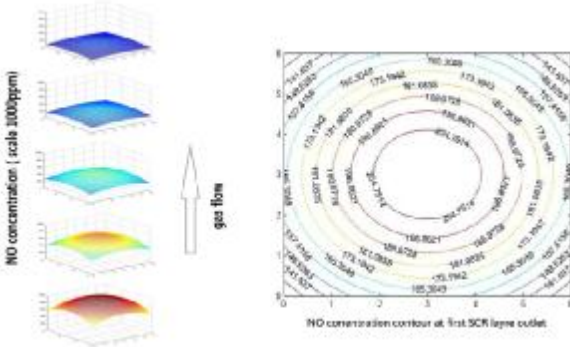


Figure 3.Developing NO concentration profile in a channel and No concentration contour at the outlet section.

After the exhaust gas passes through the first catalyst layer, then continually passes through the second one. The results show that the NO conversion of the first layer and the second layer is 82.7% and 97% , respectively.

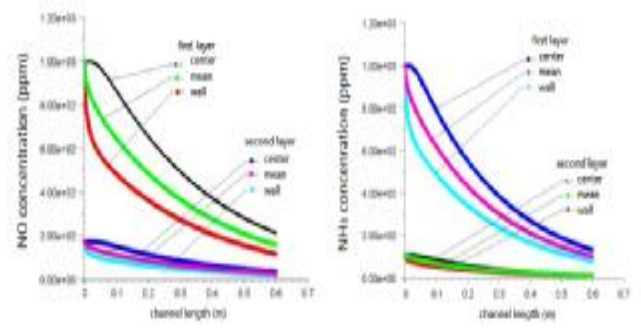


Figure 4.concentrations of NO and  $\text{NH}_3$  along the length of the channel

Furthermore, the NO reduction reaction is suppressed in the corner region due to the flow stagnation.

Fig .4 shows the concentration of NO and  $\text{NH}_3$  along the channel length for two catalyst layers.

Here, three curve lines represent the concentration profile in the center of channel, the profile of mean concentration at cross section and the profile of concentration at the catalyst wall surface, respectively. The concentration at the catalyst wall surface is significantly lower than other two concentrations.

Fig .5 shows the NO concentration distribution at 60mm across section from the channel inlet.

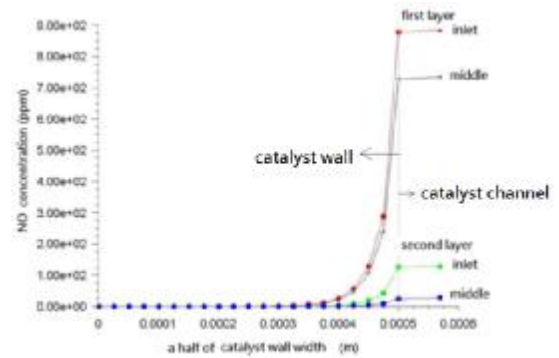


Figure 5. NO concentration profiles in the catalyst material(two SCR layers).

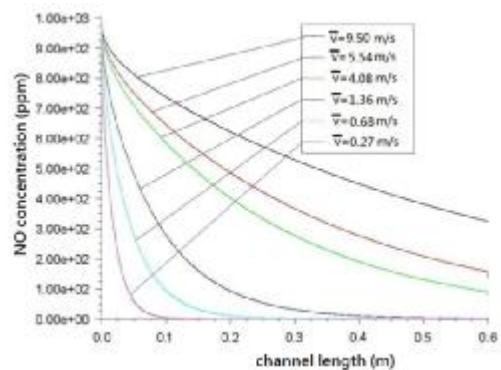


Figure 6.Effect of gas velocity on NO concentration.

It is clear that the NO reduction reaction only was occurred in the thin region of the catalyst wall. When the gas temperature is 380°C,the diffusion thickness of the reactants is about 0.25mm in the catalyst material, this value is 50% of whole catalyst volume and the others all

are the dead zones.

Fig .6 shows the NO concentration reduces along the length of the channel for different values of the inlet velocity. This simulation indicates that the increase in inlet flow velocity results in the decrease of the NO conversion because of less residence time.

The NO reduction rates under different operating temperature are illustrated in fig .7. From this figure, it can be observed that the increase of operating temperature results in the increase of the NO conversion efficiency.

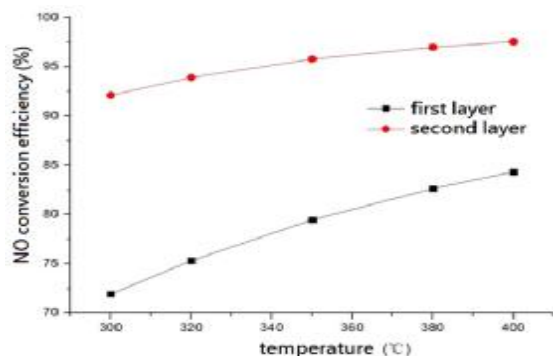


Figure 7. Effect of temperature on NO conversion efficiency.

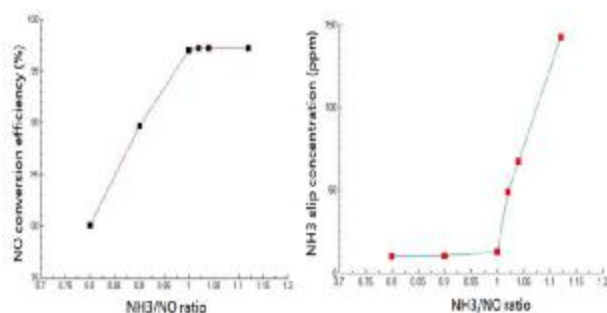


Figure 8. Effect of  $\text{NH}_3/\text{NO}$  ratio on NO conversion and  $\text{NH}_3$  slip.

Fig .8 shows the effect of  $\text{NH}_3/\text{NO}$  ratio on the NO conversion efficiency and the ammonia slip, when the inlet gas temperature is  $380^\circ\text{C}$ , the flow velocity is  $5.5\text{m/s}$ , and inlet NO and  $\text{NH}_3$  concentration both are  $1000\text{ppm}$  respectively.

The results show that the NO conversion efficiency increases as  $\text{NH}_3/\text{NO}$  ratio is increased up to the maximum value near stoichiometric condition, and simultaneously the ammonia slip is also increased with increasing of  $\text{NH}_3/\text{NO}$  ratio.

From the simulation, when  $\text{NH}_3/\text{NO}$  ratio is 1.1,  $\text{NH}_3$  slip is  $10\text{ppm}$ , less than the accepted value and NO conversion efficiency can be reached 97.2%.

## V. CONCLUSIONS

In the present study, 3D numerical simulation was applied to investigate the effects of the various operating parameters on the selective catalytic De-NOx reaction in a honeycomb channel.

The gas flow is entirely developed up to point, 60mm from the channel inlet.

From three dimension NO and  $\text{NH}_3$  concentration profiles along the duct channel, it is clearly verified that the NO reduction reaction is suppressed in the corner

region due to the flow stagnation. This is very important for designing honeycomb SCR system.

The results show that as the gas flow velocities increase, the conversion efficiencies decrease and the ammonia slip increase. This is due to the decrease of interaction time between NO,  $\text{NH}_3$  and the catalyst.

The result shows that the SCR reaction only occurs in thin region close to the catalyst wall surface (about  $0.25\text{mm}$ ) and the rest is dead zone. Therefore, it gives the possibility of saving the catalyst resources to us.

The result shows that the NO conversion efficiency increase when the temperature of the inlet gas and  $\text{NH}_3/\text{NO}$  ratio both are increased.

The larger the  $\text{NH}_3/\text{NO}$  ratio, the more significant the  $\text{NH}_3$  slip phenomenon because of the ammonia excess, otherwise this can be avoided by using a higher operating temperature.

The results of this paper can be contributed to the improvement of SCR system in order to meet the increasingly stringent NOx emissions regulations.

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## REFERENCES

- [1] Oghare V Ogidiama, Tariq Shamim, "Performance analysis of industrial selective catalytic reduction (SCR) systems," Energy Procedia vol.61 (2014), pp.2154 – 2157
- [2] S.R. Dhanushkodi, N. Mahinpeya, b, M. Wilson, "Kinetic and 2D reactor modeling for simulation of the catalytic reduction of NOx in the monolith honeycomb reactor," process safety and environment protection vol.86 (2008), pp. 303–309
- [3] B. Roduit and A. Baiker, "3-D modeling of SCR of NOx by on vanadia honeycomb catalysts AICHE Journal Vol. 44, No. 12
- [4] Hong Mei F, Zhao Ping Z, Bao Sheng J, et al. "Numerical calculation of a honeycomb shaped catalyst denitration process," Journal of engineering for thermal energy and power, vol.22, no.4
- [5] Kenji Tanno, Ryoichi Kurose, Takenobu Michioka. "Direct numerical simulation of flow and surface reaction in de-NOx catalyst," Advanced Powder Technology vol.24 (2013), pp. 879–885
- [6] JianXun D, SongLing W, YongHua L. "Mathematical simulation study of a selective catalytic reduction based flue gas denitration process," Journal of engineering for thermal energy and power, vol.22, no.5
- [7] Tuncer Cebec. "Analysis of Turbulent Flows with Computer Programs," Oxford, UK.: 3rd ed., 2013,
- [8] JiangYo, Xiang Gao. "Study on titania-based SCR catalysts and their poisoning mechanism of potassium and lead," Ph.D. dissertation. China: Zhejiang university; 2010
- [9] G. Schaub, D. Unruh, J. Wang, T. "Kinetic analysis of selective catalytic NOx reduction (SCR) in a catalytic filter," Chemical Engineering and Processing 42 (2003), pp.365–371
- [10] Chyi-Tsong Chen, Wei-Lun Tan. "Mathematical modeling, optimal design and control of an SCR reactor for NOx removal," Journal of the Taiwan Institute of Chemical Engineers 43 (2012), pp. 409–419
- [11] Juan Yang, Hongtao Ma, et al. "SCR catalyst coated on low-cost monolith support for flue gas denitration of industrial furnaces," Chemical Engineering Journal vol.230 (2013), pp. 513–52