Theoretical Analysis of Selective Catalytic Reduction Catalysts

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ABSTRACT: A theoretical analysis of the selective catalytic reduction (SCR) process is presented to assist in the selection of a catalyst for efficient control of NO_x from flue gases. It is a two-dimensional (2D) numerical model accounting for the simultaneous effects of external diffusion and catalytic chemical kinetics. Experimental data of SCR performance employing different types of catalysts are taken from the literature and analyzed for their NH_3 adsorption constant and effective-rate constant. The catalysts' characteristics are then used to predict their SCR performance. Good agreement is obtained between model results and experimental observations on the NO removals. The activites of the catalysts are compared and strategies affecting SCR performance are discussed. It is shown that the effective reaction rate of a catalyst is the key parameter influencing its activity. The catalyst preparation procedure as well as the V_2O_5 content are important for determining its NO removal rate.

INTRODUCTION

The selective catalytic reduction (SCR) process is a widely used flue gas treatment technology. Many SCR devices have been installed and operated in the United States, Japan, Germany, Taiwan, and other countries. Its nitrogen oxides (NO_x) removal efficiency is the highest among commercialized flue gas treatment technologies. The control efficiency of an SCR device can be well above 85% with proper design and operation. The NO_x in flue gas is removed by the injection of ammonia (NH_3). The NH_3 and NO_x gaseous molecules react in a heterogeneous catalytic reactor, and nontoxic N_2 and H_2O gases are formed during the catalytic reaction. For commercial applications, catalysts are used as monolithic materials with honeycomb structures or in parallel-plate geometry (Boer et al. 1990). The catalysts used are Ti-W-V based oxides or zeolite-based systems. Marangozis (1992) evaluated the intrinsic rate of 27 catalysts and indicated that the best catalysts appear to be those containing V_2O_5 spported by TiO_2 or Al_2O_3. The performance of V_2O_5-TiO_2 based catalysts does not necessarily correlate to their V_2O_5 content. On the other hand, Svachula et al. (1993) evaluated the performance of commercialized catalysts. They found that the activity of catalysts increases when the V_2O_5 content is increased.

Cho (1994) discussed operating parameters that affect the performance of an SCR system. NO_x removal depends on the amount of injected NH_3, the type of catalysts, the residence time of the gas in the reactor, and the specific surface area of the catalysts. Cho (1994) indicated that increasing the ammonia injection quantity leads to better SCR performance. This phenomeonon has been seen in the literature for NH_3/NO inlet molar ratio (α) of less than 1. But experimental studies also revealed that for $\alpha \geq 1$, the NH_3 concentration has almost no effect on the NO removal (Lefers et al. 1991; Beeckman and Hegedus 1991; Svachula et al. 1993).

There are several theoretical models discussed on the SCR performance. Buzanowski and Yang (1990) presented theoretical and experimental results for the SCR system. The results showed that external diffusion limitation was minimal in their
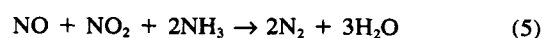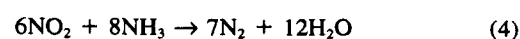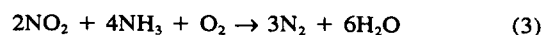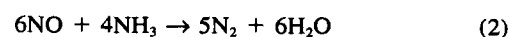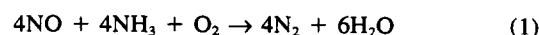
study. However, the channel pitch they employed is too narrow to be applied to a commercial SCR device. Therefore, the question remains as to whether external diffusion limitation is negligible in a real SCR system. Beeckman and Hegedus (1991) employed a one-dimensional (1D) lumped parameter model for the SCR design. They used a mass transer coefficient to represent the flow characteristics and the chemical kinetics in the SCR system. Their model accounted for external diffusion in the gas phase and intraphase diffusional phenomena. However, the adequacy of the 1D model was not addressed in their study. Later on Tronconi and Forzatti (1992) discussed the adequacy of lumped parameter models. They indicated that maximum error was found at Damkohler numbers of around 1. The Damkohler number in a real SCR system is usually on the order of unity.

Commercialized SCR catalysts are usually demonstrated at different operation conditions. This leads to a problem in the comparison and selection of catalysts with high SCR performance. The purpose of this study is to present a theoretical analysis to assist in the selection of SCR catalysts. A two-dimensional (2D) diffusion equation is employed, which accounts for simultaneous effects of external diffusion and chemical kinetic limitations in the SCR process. The 2D model has the advantage of minimizing uncertain design parameters (for example, the mass transer coefficient and the effective diffusion coefficient) for the SCR system as compared to the 1D lumped parameter model. A comparison of different catalysts is also made in terms of the NO conversion rate.

THEORY

Physical and Chemical Mechanisms of SCR Process

In the SCR process the NO_x species are reduced by injection of NH_3, ultimately to N_2 gas, over a heterogeneous catalyst in the presence of O_2. Possible reactions in the SCR process are (Cho 1994)

$$4NO + 4NH_3 + O_2 \rightarrow 4N_2 + 6H_2O \tag{1}$$

$$6NO + 4NH_3 \rightarrow 5N_2 + 6H_2O \tag{2}$$

$$2NO_2 + 4NH_3 + O_2 \rightarrow 3N_2 + 6H_2O \tag{3}$$

$$6NO_2 + 8NH_3 \rightarrow 7N_2 + 12H_2O \tag{4}$$

$$NO + NO_2 + 2NH_3 \rightarrow 2N_2 + 3H_2O \tag{5}$$

All possible reactions yield nontoxic N_2 and H_2O gaseous molecules. The results of SCR performance tests in actual applications indicated that the reaction represented by (1) is the dominant reaction. Therefore, only reaction (1) is considered in this study during model development.

The SCR reaction is a heterogeneous catalytic reaction that can be represented by six diffusion and reaction steps: (1) the NO and NH_3 reagents diffuse to the catalytic wall; (2) the reagents diffuse into the intraparticle surface of the catalyst via pore diffusion; (3) the reagents are adsorbed onto the catalytic surface; (4) the chemical reaction occurs on the catalytic surface; (5) the reaction product is desorbed from the intraparticle surface; and (6) the reaction product diffuses from the catalytic surface to the main flue gas stream.

It is seen that steps 1, 2, and 6 are physical diffusion processes, while steps 3, 4, and 5 are related to surface chemical reaction processes. The NO_x removing rate by the SCR process may be controlled by one or more of the previously mentioned steps. In this study, the six steps of diffusion and chemical reactions are reduced to three steps by using an overall effective rate for steps 2-5. The external diffusion effect in the bulk gas and the effective chemical reaction at the catalytic wall are distinguished by this approach.

Model Assumptions

The following assumptions are made in developing a mathematic model to predict the system performance of an SCR process:

- A monolithic shape catalyst with a honeycomb support is used in the model study.
- Constant fluid properties, i.e., the fluid density and diffusion coefficients of the reagents are constants at a given temperature and pressure.
- Conditions are isothermal in the system.
- There is negligible axial diffusion as compared to the convection term in the axial main flow direction.
- There is steady-state operation of the SCR system.
- Irreversible first-order kinetics are applied with respect to NO concentration at the catalytic wall.

Adsorption and Chemical Behaviors on Catalytic Surfaces

A Rideal model is the usual assumption for a heterogeneous catalytic reaction in the SCR system (Tronconi and Forzatti 1992; Beeckman and Hegedus 1991). That is, NH_3 molecules are selectively adsorbed onto the catalytic surface, then NO molecules react with the NH_3 molecules. This is a valid assumption for flue gas concentrations of H_2O and O_2 of greater than 5 and 2%, respectively (Svachula et al. 1993). The reaction rate of NO, R_{NO}, is expressed as

$$R_{NO} = K_C C_{NO} \theta_{NH_3} \qquad (6)$$

and

$$\theta_{NH_3} = \frac{K_{NH_3} C_{NH_3}}{1 + K_{NH_3} C_{NH_3}} = \frac{K^*_{NH_3} \alpha}{1 + K^*_{NH_3} \alpha} \qquad (7)$$

where C_{NO} and C_{NH_3} = NO and NH_3 gas concentations, respectively; θ_{NH_3} = fractional surface coverage of ammonia adsorbed on the active sites of the catalyst; K_{NH_3} = adsorption constant of NH_3 gas; K_{NH_3} = dimensionless adsorption constant, which is defined as $K^*_{NH_3} = K_{NH_3} C^0_{NO}$; and K_C = effective rate constant. The value of K_C represents the overall rate from steps 2 to 5 as discussed in the previous section. Therefore, it is a combined effect of intrinsic chemical kinetic and intraparticle (pore) diffusion in the monolithic catalyst.

Model Development

A schematic diagram of the SCR model is shown in Fig. 1. The geometry of the catalytic support is made of square ducts.
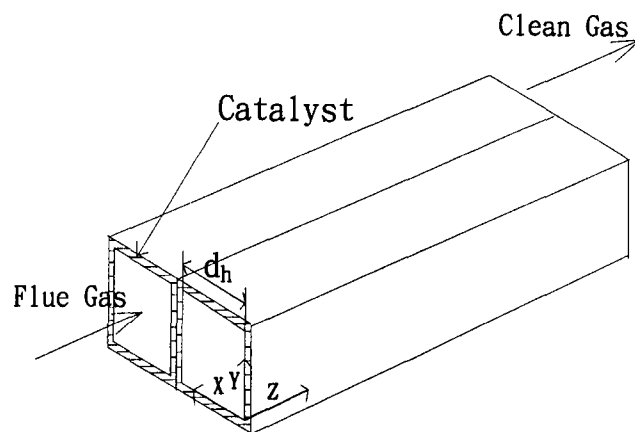
FIG. 1.   Schematic Diagram of SCR Design Model

Using the model assumptions, a three-dimensional (3D) (in space) steady-state mass transfer model can be made as

$$U \left(\frac{\partial C_i}{\partial Z} \right) = D_i \left(\frac{\partial^2 C_i}{\partial X^2} + \frac{\partial^2 C_i}{\partial Y^2} \right) \qquad (8)$$

where U = flow velocity in the ducts; D_i = diffusion coefficient of the reagents (i = NO or NH_3); Z = main flow direction; and X and Y = directions perpendicular to the main gas stream. The left-hand side term is the convection term, while two terms on the right-hand side denote the external diffusional deposition of NO and NH_3 molecules onto the catalytic wall. Eq. (8) can be normalized using the nondimensional parameters: $C^*_i = C_i/C^0_i$, $X^* = 2X/d_h$, $Y^* = 2Y/d_h$, $U^* = U/U_m$, $Z^* = ZD_{NO}/(U_m d_h^2)$, where C^0_i = reagent inlet concentration; d_h = channel pitch; and U_m = average flow velocity. As a result, the nondimensional equations for the evolution of NO and NH_3 concentrations in the SCR system are

$$U^* \frac{\partial C^*_{NO}}{\partial Z^*} = \frac{\partial^2 C^*_{NO}}{\partial X^{*2}} + \frac{\partial^2 C^*_{NO}}{\partial Y^{*2}} \qquad (9)$$

$$U^* \frac{\partial C^*_{NH_3}}{\partial Z^*} = \frac{D_{NH_3}}{D_{NO}} \left(\frac{\partial^2 C^*_{NH_3}}{\partial X^{*2}} + \frac{\partial^2 C^*_{NH_3}}{\partial Y^{*2}} \right) \qquad (10)$$

Since the entrance length is much shorter than the length of a catalyst layer (Lefers et al. 1991), the velocity profile is usually assumed to be fully developed in the SCR system. The fully developed velocity profile in a square duct is obtained from Shah and London (1978)

$$U^* = 2.0962(1 - X^{2.2})(1 - Y^{2.2}) \qquad (11)$$

The initial condition is set at the inlet of the SCR system such that

$$\text{at } Z^* = 0, \qquad C^*_i = 1 \qquad (12)$$

where the boundary conditions are that the reagent concentrations are symmetric at the centerline of the square duct; and the depositon flux is controlled by the effective rate of catalytic reaction between NO and NH_3 on the catalytic surface

$$\text{at } X^* = 1, \qquad \frac{\partial C^*_i}{\partial X^*} = 0 \qquad (13)$$

$$\text{at } Y^* = 1, \qquad \frac{\partial C^*_i}{\partial Y^*} = 0 \qquad (14)$$

$$\text{at } X^* = 0 \text{ or } 2, \qquad -\frac{\partial C^*_i}{\partial X^*} = Da_i R^* \qquad (15)$$

$$\text{at } Y^* = 0 \text{ or } 2, \qquad -\frac{\partial C^*_i}{\partial Y^*} = Da_i R^* \qquad (16)$$

where Da_i $(=K_C d_h/2D_i)$ = Damkohler number for species i; and R^*_{NO} $(=R_{NO}/K_C C^0_{NO})$ = dimensionless reaction rate for NO. Using the forward-time and centered-space (FTCS) finite-difference method, (9) and (10) become 2D in space in terms of the numerical method. Provided that the characteristics of the SCR catalyst are known, (9) and (10) can be solved simultaneously and the NO and NH_3 concentration profiles in any location of the SCR system can be obtained readily.

RESULTS AND ANALYSIS

Sensitivity Analysis

Since the FTCS method is an explicit finite-difference method, it may suffer from a stability problem if the numerical step sizes are not chosen properly. The stability analysis requires that $\Delta Z^*/(\Delta X^* \Delta Y^* U^*) < 0.5$ to ensure the convergence of the solution, and it was satisfied in the model results. In addition, sensitivity analysis was conducted to obtain the step sizes for consistent results. The results are shown in Figs. 2(a) and 2(b). For fixing values of ΔX^* and δY^* at 0.1, the step size requirement of $(\Delta Z^*/U^*)$ is to be less than or equal to 1/400 for a consistent output. For fixing the value of $(\Delta Z^*/U^*)$ at 1/1,500, the output, using step size of $\Delta X^* = \Delta Y^* = 0.1$, has a maximum deviation of 0.55% as compared to that using $\Delta X^* = \Delta Y^* = 0.05$. In the following model analysis, the numerical step sizes of ΔX^* and ΔY^* are set equal at 0.1, while the step size of $(\Delta Z^*/U^*)$ is set at 1/1,500.
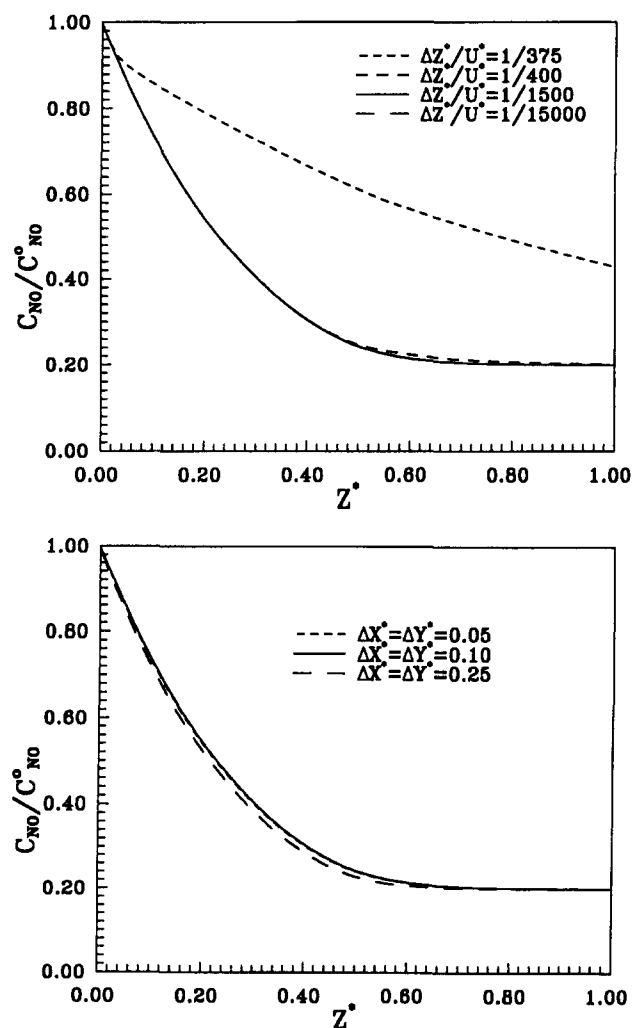
The effect of flow pattern on the model solution is also

FIG. 2. Sensitivity Analysis of Effect of: (a) $\Delta Z^*/U^*$ Step Size on Model Outputs; (b) ΔX^* (=ΔY^*) Step Size on Model Outputs
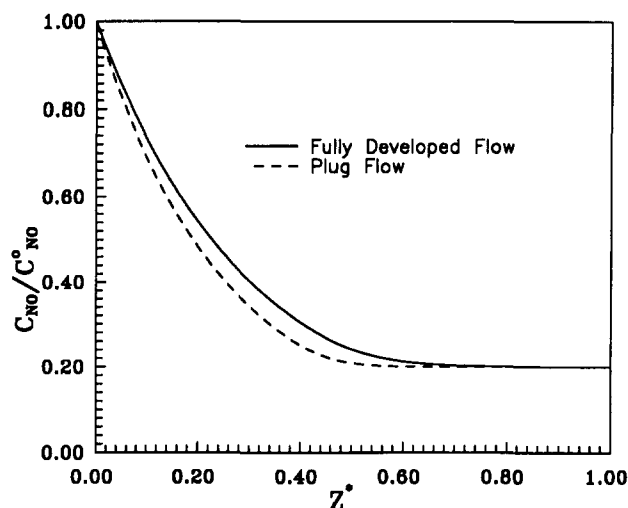

FIG. 3. Comparison Results of NO Conversion Using Fully Developed Flow Pattern and Plug Flow Pattern

evaluated. Fig. 3 shows a comparison of NO removal efficiency using fully developed laminar flow profile and plug flow profile. One can see that these two curves are in reasonable agreement. The maximum deviation, using these two flow profiles, is around 5% in terms of the NO conversion rate. In most practical applications of the SCR system, the flow pattern appears to be fully developed laminar flow. However, depending on the degree of accuracy desired in the SCR design, it may also be applicable using the plug flow profile for the sake of simplicity.

Estimation of Kinetic and Adsorption Constants

The experimental data of Buzanowski and Yang (1990), Beeckman and Hegedus (1991), and Lefers et al. (1991), as well as data taken from a local SCR study (Weng 1996) were chosen for comparison in the model study. The operation conditions of each experimental study are listed in Table 1. For a total of five V_2O_5-TiO_2 based catalysts evaluated in this study, only three (catalysts A1, A2, and B) reported their V_2O_5 contents. The manufacturing procedures of catalysts A1 and A2 are the same.

There are two unknown parameters: the effective rate constant (K_C) and the NH_3 adsorption constant (K_{NH_3}). They can be determined by fitting the laboratory data with model simulations. Using the least-squares method, the values of K_C and K_{NH_3} were obtained for each operation temperature. The relative square of errors (s^2) between the model simulations and experimental data of NO conversion are less than 5×10^{-4} for all tests. The values of K_C and K_{NH_3} at different operation

TABLE 1. Experimental Conditions of SCR Performance Data Used in the Model Study

Catalyst (1)	Composition (2)	Temperature (°C) (3)	Feed ratio NH_3/NO (α) (4)	Channel pitch d_h (cm) (5)
A1[a]	1.0% V_2O_5/TiO_2	100–300	1.0	0.14
A2[a]	3.45% V_2O_5/TiO_2	100–300	1.0	0.14
B[b]	0.8% V_2O_5/TiO_2	281–380	0.6–1.2	0.60
C[c]	V_2O_5/TiO_2	300–400	0.3–1.5	0.60
D[d]	V_2O_5/TiO_2	320–380	1.0	0.29

[a]Buzanowski and Yang (1990).
[b]Beeckman and Hegedus (1991).
[c]Lefers et al. (1991).
[d]Weng (1996).

temperatures were then regressed using the adsorption equation and Arrhenius equation

$$K_{NH_3} = K_0 \exp\left(\frac{-\Delta H}{RT}\right) \qquad (17)$$

$$K_C = k_0 \exp\left(\frac{-E}{RT}\right) \qquad (18)$$

where ΔH = heat of adsorption; E = activation energy; K_0 and k_0 = preexponential factors in the adsorption equation and the Arrhenius equation, respectively; T = reaction temperature (K) and R = gas constant. The logarithmic plots of K_{NH_3} and K_C as an inverse function of temperature for catalysts B and D are shown in Figs. 4(a) and 4(b). Each symbol in Figs. 4(a) and 4(b) represents the least-squares result obtained from three to five experimental data operated under the same temperature. Lines are the linear regression results of (17) and (18). Due to the unavailability of SCR performance data, only three sets of temperature variation data are plotted. But one can see from Figs. 4(a) and 4(b) that the adsorption equation and Arrhenius equation apply reasonably well to the experimental observations. The value of K_C increases as the temperature increases, and the value of K_{NH_3} decreases as temperature increases. The regression results of the values of K_0, k_0, ΔH, and E for all catalysts employed in this study are listed in Table 2. The correlation coefficients (r^2) for the regression analysis are
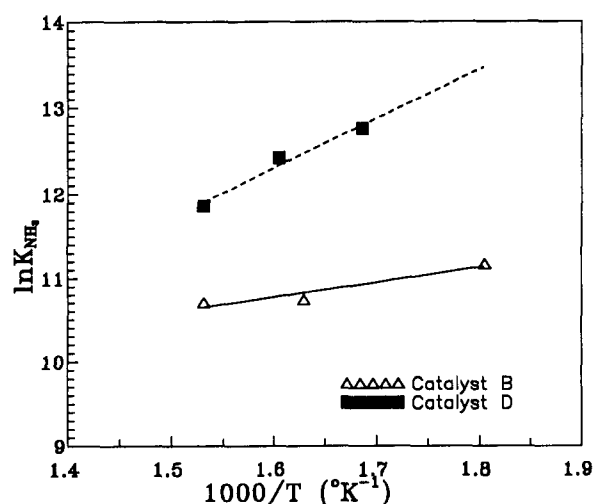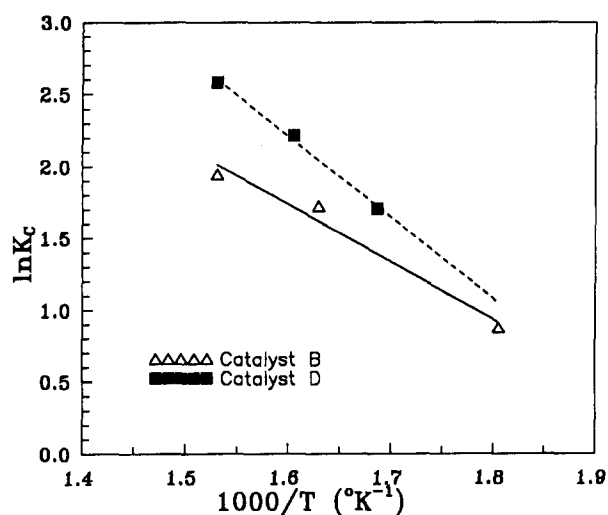
TABLE 2. Regression Results of Adsorption Equation and Arrhenius Equation

Catalyst (1)	K_{NH_3}			K_C		
	K_0 (cm³/mol) (2)	ΔH (kJ/mol) (3)	r^2 (4)	k_0 (cm/s) (5)	E_a (kJ/mol) (6)	r^2 (7)
A1	19,000	0	1.000	456.59	25.14	0.993
A2	12,202.6	−2.984	0.920	1,006.55	26.63	0.998
B	1,652.6	−14.87	0.959	3,522.52	33.42	0.987
C	20.1	−38.67	0.983	117.56	16.14	0.938
D	17.3	−46.67	0.990	68,291.94	46.29	0.998

above 0.92 for all tests. Note that the correlation coefficient of K_{NH_3} for catalyst A1 is 1.0. This indicates that its values of K_{NH_3} are constant and are not affected by temperature variations. Smaller values of ΔH also reveal that values of K_{NH_3} are less affected by temperature variation. Since catalysts A1 and A2 were manufactured under the same procedure, and the value of K_{NH_3} of catalyst A1 is not affected by the temperature variation, it is not surprising that catalyst A2 has the smallest K_{NH_3} as compared to catalysts B, C, and D.

Model Prediction

After the determination of the values of K_C and K_{NH_3} for a given type of catalyst, predictions of the SCR performance are possible. Fig. 5 shows the effect of inlet NH₃/NO molar ratio on NO conversion. The symbols are experimental performance data of catalysts B and C, and the lines are the prediction results. The operation conditions for catalyst B were: C_{NO}^0 = 1,000 ppm; gas hourly space velocity (GHSV) = 12,000 h⁻¹ (STP); and T = 341°C. For catalyst C, the operation conditions were: C_{NO}^0 = 425 ppm; GHSV = 28,813 h⁻¹ (NTP); and T = 350°C. One can see for α values of less than around 0.8, the NO conversion increases rapidly as the value of α increases. But NO conversion is almost independent of the inlet concentration of NH₃ as α continues to increase. This can be explained by the fact that the NH₃ inlet concentration only affects the value of θ_{NH_3} as it appeared in (7). Increasing the value of α so that it is greater than around 1.0 may lead the value of θ_{NH_3} to approach its asymptotic value of 1.0. After that, the NH₃-NO reaction in the SCR system becomes zero order with respect to NH₃. Therefore, an increase in the NH₃/NO injection ratio that is greater than 1.0 only results in an ammonia slip problem.

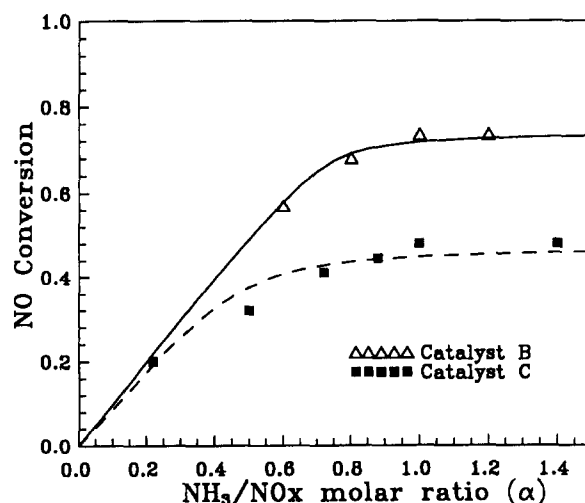Fig. 6 depicts the prediction of NO conversion as a function

FIG. 4. Variation of: (a) Effective Rate Constant (K_C) with Respect to Temperature; (b) NH₃ Adsorption Constant (K_{NH_3}) with Respect to Temperature

FIG. 5. Comparison of Model Prediction Results with Experimental Observations as a Function of NH₃/NO Inlet Ratio
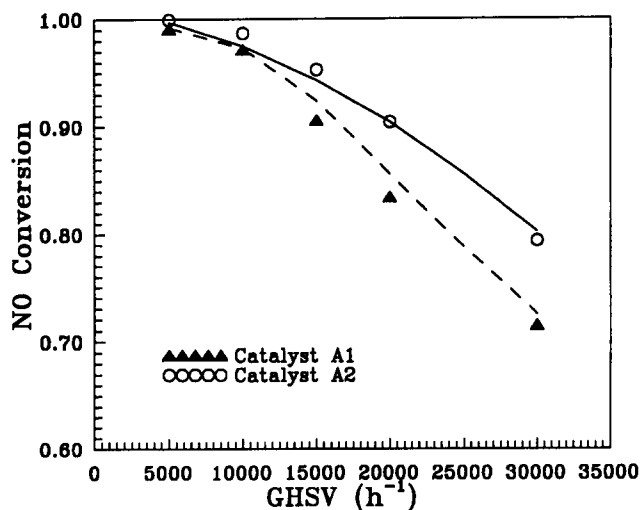
FIG. 6. Comparison of Model Prediction Results with Experimental Observations as a Function of Gas Hourly Space Velocity (GHSV)
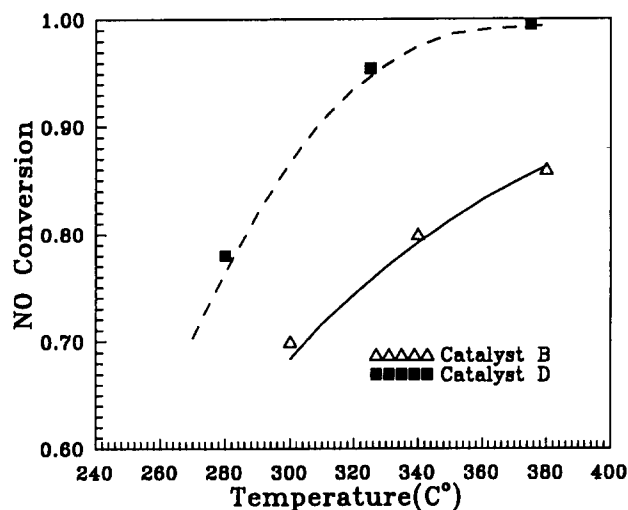

FIG. 7. Comparison of Model Prediction Results with Experimental Observations as a Function of SCR Operation Temperature

of the space velocity GHSV as compared to the performance data of catalysts A1 and A2. Typical operation range of space velocity in the SCR system is $3,000-7,000$ h^{-1} (Turner 1993). The operation conditions for catalysts A1 and A2 were: C_{NO}^0 = 1,000 ppm; T = 300°C, and α = 1.0. Increasing the space velocity above this range usually yields a significant reduction in the NO conversion as seen in Fig. 6. The performance of catalyst A2 is better than catalyst A1 under the same space velocity, since catalyst A2 has a higher V$_2$O$_5$ content.

Fig. 7 shows the comparison of experimental data of catalysts B and D with model predictions on the NO conversion as a function of temperature. The operation conditions for catalyst B were: C_{NO}^0 = 1,000 ppm; GHSV = 8,600 h^{-1} (STP); and α = 1.0. For catalyst D, the operation conditions were: C_{NO}^0 = 600 ppm, GHSV = 22,500 h^{-1} (NTP); and α = 1.0. It is seen that the NO conversion of catalyst D is higher than catalyst B. It must be noted that these two experimental tests were conducted under different operation conditions. For example, the channel pitch for catalyst B was 0.6 cm, while it was 0.29 cm for catalyst D. Increasing the channel pitch tends to yield a decrease in NO conversion due to external diffusion limitation. Besides, the space velocities of these two catalysts' performance data were different. Therefore, it is not appropri-

ate to compare the performance of these two catalysts by observation of Fig. 7.

Practical Application: Evaluation of Catalyst Performance

To evaluate the performance of SCR catalysts used in this study, their NO conversion rates, as a function of temperature, are predicted under the same operation conditions. The results are shown in Fig. 8. The associated values of K_C, K_{NH_3}, and the dimensionless parameters ($K_{NH_3}^*$ and Da) are listed in Table 3. In Fig. 8, the operation conditions are at a temperature of 350°C; GHSV = 7,000 h^{-1} (NTP); C_{NO}^0 = 1,000 ppm; NH$_3$/NO inlet ratio = 1.0; and channel pitch = 0.6 cm. One can see in Fig. 8 that the performance of catalyst D appears to be the best, while catalyst A1 (whose V$_2$O$_5$ content was 1.0%) has the lowest NO removal rate. After increasing the V$_2$O$_5$ content to 3.45%, the performance of catalyst A2 is greatly increased. If one compares the SCR performance results to the data listed in Table 3, it is found that the SCR performance is affected by the effective rate constant (K_C) rather than by the NH$_3$ adsorption ability. The performance of catalyst A2 is slightly better than catalysts B and C, since it has a relatively higher value of K_C. However, it must also be noted that the V$_2$O$_5$ content in catalyst B, 0.8%, is lower than catalysts A1 and A2. But the performance of catalyst B is better than that of catalyst A1. Therefore, V$_2$O$_5$ content is not the only reason for limiting SCR performance. Since increasing the V$_2$O$_5$ content may lead to the deterioration of the SCR poisoning problem caused by catalytic reaction of NH$_3$ with SO$_2$, a catalyst with low V$_2$O$_5$
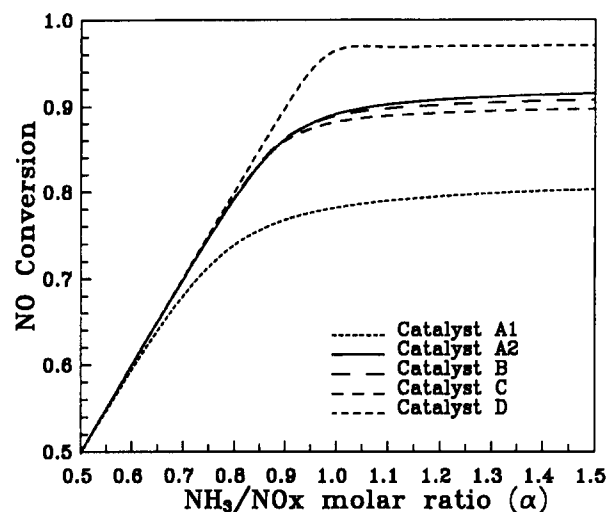

FIG. 8. Comparison of Performance of Five Catalysts at the Same Operation Conditions

TABLE 3. Catalysts' Characteristics as Normalized at the Same Operation Conditions

Catalyst (1)	K_C (cm/s) (2)	Da[a] (3)	K_{NH_3} (cm³/mol) (4)	$K_{NH_3}^*$[c] (5)	θ_{NH_3}[c] at α = 1.0 (6)
A1	3.56[b]	3.08[b]	19,000[b]	19.0[b]	0.950[b]
A2	5.89[b]	5.07[b]	21,710[b]	21.7[b]	0.956[b]
B	5.56	4.76	29,170	29.2	0.967
C	5.21	4.47	35,140	35.1	0.972
D	8.98	22.13	141,640	141.6	0.993

[a]Normalized at channel pitch of 0.6 cm.
[b]Extrapolation from adsorption equation and Arrhenius equation derived at temperatures of 100–300°C.
[c]At C_{NO}^0 = 1,000 ppm.

content (<2%) is usually used in an SCR application. However, if the manufacture procedure of catalysts A1 and A2 can be improved, their SCR performance may be greatly increased.

The dimensionless adsorption constant ($K^*_{NH_3}$) is a measure of the catalyst's ability to adsorb NH_3 on the V_2O_5 active sites. Values of $K^*_{NH_3}$ are given in Table 3 for NO concentrations of 1,000 ppm. The corresponding values of θ_{NH_3} at $\alpha = 1$ are also given. One can see that catalyst D has the highest value of $K^*_{NH_3}$ and its value of θ_{NH_3} at $\alpha = 1$ approaches the asymptotic value of 1.0. As a result, the performance of catalyst D is not affected by α for $\alpha > 1.0$ as seen in Fig. 8. On the other hand, catalyst A1 has the lowest value of θ_{NH_3} at $\alpha = 1$, and, therefore, increasing the value of α after $\alpha > 1.0$ slightly increases the NO conversion.

CONCLUSION

A theoretical analysis of the SCR system to improve the NO conversion was presented. A 2D numerical model was developed, which accounts for both the external diffusion limitation and the chemical kinetic limitation in the SCR process. The adsorption equation and the Arrhenius equation for determining the adsorption constant and the effective rate constant were obtained by a regression analysis for a given type of catalyst. The model results of NO conversion were then compared with experimental observations and good agreements were obtained. The analysis presented in this study can be used to select catalysts and to determine strategies that affect catalyst performance. The results revealed that the manufacturing procedure of V_2O_5-TiO_2 based catalysts is another important consideration in the determination of NO removal rates besides the V_2O_5 content.

ACKNOWLEDGMENTS

APPENDIX I. REFERENCES

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APPENDIX II. NOTATION

The following symbols are used in this paper:

C_i = gas concentration, i = NH$_3$ or NO, mol/cm^3;
C^* = dimensionless gas concentration, C_{NO}/C^0_{NO};
Da = Damkohler number, $K_C d_h/2D$;
D_i = diffusion coefficient, i = NH$_3$ or NO, cm^2/s;
d_h = channel pitch, cm;
K_C = effective chemical reaction rate, cm/s;
K_{NH_3} = adsorption constant of NH$_3$, cm^3/mol;
$K^*_{NH_3}$ = dimensionless adsorption constant, $K_{NH_3}C^0_{NO}$;
K_0 = preexponential factor of adsorption equation;
k_0 = preexponential factor of Arrhenius equation;
Q = gas flow rate, cm^3/s;
R = gas constant, 8.314 J/mol K;
R_{NO} = reaction rate of NO, mol/(cm^2/s);
R^*_{NO} = dimensionless reaction rate of NO, $R_{NO}/(C^0_{NO}K_C)$;
T = operation temperature, K;
U = flow velocity, cm/s;
U_m = average flow velocity, cm/s;
U^* = dimensionless flow velocity, U/U_m;
V = volume of SCR system, cm^3;
X = direction perpendicular to flow, cm;
X^* = dimensionless parameter of X, $2X/d_h$;
Y = direction perpendicular to flow, cm;
Y^* = dimensionless parameter of Y, $2Y/d_h$;
Z = direction of main flow, cm;
Z^* = dimensionless parameter of Z, $ZD_{NO}/U_m D^2_h$;
α = inlet molar ratio of NH$_3$/NO; and
θ_{NH_3} = fractional surface coverage of ammonia adsorbed on active sites of catalyst.

Subscripts and Superscripts

0 = initial condition; and
* = dimensionless parameter.