

# NH<sub>3</sub> SNCR을 이용한 NO<sub>x</sub> 제거 : 실험 및 모사

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## NH<sub>3</sub>-based SNCR of NO<sub>x</sub> : Experimental and Simulation

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본 연구에서는 SNCR 공정에서 온도, NSR, 산소 농도가 질소산화물 제거 효율에 미치는 영향을 실험과 CHEMKIN-II 프로그램을 사용하여 수치적으로 조사하였다. 산소가 없는 조건에서 NO 제거 효율은 반응기 온도에 따라 증가하였다. 반면 산소농도가 4%일 때, NO 제거 효율은 900~950 °C에서 최대를 나타내었다. 산소의 존재는 저온에서 NO 제거를 증가시키는 것으로 나타났다. 산소농도와 무관하게 NO 제거 효율은 NSR에 따라 증가하였다. CHEMKIN-II에 의해 예측된 NO 제거 효율의 온도와 NSR-의존성은 실험결과와 유사하였다.

In this study, effects of temperature, NSR, and oxygen concentration on the NO<sub>x</sub> removal efficiency of an SNCR process were investigated experimentally as well as numerically using CHEMKIN-II program. The NO removal efficiency increased with the reactor temperature under oxygen-free condition, whereas when the oxygen concentration was 4%, the NO removal efficiency showed a maximum value at 900~950 °C. The pressure of oxygen was shown to enhance the NO removal at low temperature. Regardless of the oxygen concentration, the NO removal efficiency increased with NSR. The temperature- and NSR-dependencies of the NO removal efficiency predicted by CHEMKIN-II simulations were similar to that of the experimental results.

**Keywords:** NO<sub>x</sub>, selective non-catalytic reduction (SNCR), CHEKIN-II simulation

### 1. Introduction

Nitrogen oxide (NO<sub>x</sub>) is a group of gaseous air pollutants causing respiratory diseases. Together with sulfur dioxide, it is an important contributor of acid rain. Via photochemical reactions, it induces photochemical smog by promoting formation of tropospheric ozone as well as, under the presence of hydrocarbons, of PANs (peroxyacetyl nitrates) and aldehydes[1].

The selective non-catalytic reduction (SNCR) is one of the representative processes developed to remove NO<sub>x</sub>. In SNCR processes, NO<sub>x</sub> is reduced into N<sub>2</sub> via reaction with reducing agents such as NH<sub>3</sub> and urea under high temperature ranging 850~1175 °C[2]. Removal of NO can take place only within a certain temperature range called 'temperature window'[3,4], in which NH<sub>2</sub> and other radicals that play important roles in the reaction mechanism of NO<sub>x</sub> reduction can be produced. If temperature is too high, NH<sub>3</sub> is oxidized back into NO<sub>x</sub>

deteriorating the NO<sub>x</sub> removal efficiency[5].

The NO removal efficiency of the SNCR process increases with the normalized stoichiometric ratio (NSR) of reducing agent. Emission of unreacted reducing agents into the atmosphere, however, may cause secondary air pollution[6]. For example, when ammonia is used as the reducing agent, the emission standard for ammonia has to be met because ammonia itself is an air pollutant. If the region has been designated as an odor management area, the odor emission standard has to be met as well because ammonia is an odor compound. Oxygen is another important factor in SNCR processes that provides radicals required for oxidation reactions[7].

In this study, the effects of temperature, NSR, and oxygen concentration on the NO<sub>x</sub> removal efficiency of an SNCR process were investigated. For theoretical analysis, the CHEMKIN-II modeling package was used to simulate the NH<sub>3</sub>-SNCR process and the results were compared with experimental results.

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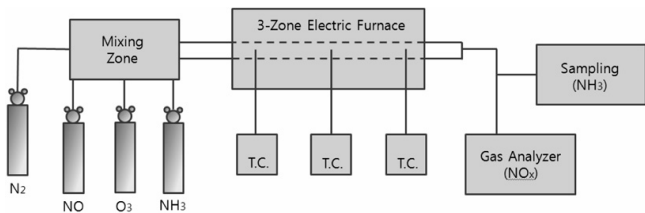


Figure 1. Schematic of the experimental setup.

## 2. Experimental

Figure 1 shows the schematic of the SNCR system used in this study.  $N_2$ , NO,  $O_2$ , and  $NH_3$  were introduced into the system as reactants. The flow rate of each reactant was controlled by a flow meter. All the reactants were mixed together in the mixing zone before entering the reactor. The tubular reactor was made of stainless steel against reactions under high temperature, with its inlet diameter and length of 8 mm and 550 mm, respectively. Because the SNCR process is sensitive to temperature, three temperature controllers were installed on the reactor to maintain temperature constant in the reactor. The residence time of the reactor was controlled to be 0.3 s.

In this study, 500 ppm of NO reacted with  $NH_3$  at different temperatures. The set-point reactor temperature was varied between 500 and 1100 °C with the interval of 50 °C. The NO removal efficiency at each set-point temperature was calculated by

$$\text{No removal efficiency (\%)} = \left( \frac{NO_{in} - NO_{out}}{NO_{in}} \right) \times 100$$

At each temperature, two different  $O_2$  concentrations, 0 and 4%, and three different NSR of  $NH_3$ , 1.0, 1.5, and 2.0, were used.

## 3. Simulation

In this study, the  $NO_x$  removal efficiency obtained under each experimental condition was compared with simulation results produced by a reaction analysis software. The reaction analysis was carried out using input information including temperature, pressure, reaction time, thermodynamic properties of the reactants (entropy, enthalpy and heat capacity), reaction mechanism composed of unit reactions, and Arrhenius equations. The CHEMKIN-II package was used as the reaction analysis software in this study. The Arrhenius equation is written as

$$k = A \times T^n \times e^{-\frac{E_a}{RT}}$$

where A is the Arrhenius coefficient, T the absolute temperature, R the gas constant,  $E_a$  the activation energy, and n a constant. The SNCR reaction mechanism and relevant constants used in this study are summarized in Table 1. The thermodynamic properties of the involved species were obtained from New Jersey Institute of Technology (NJIT) database (Table 2).

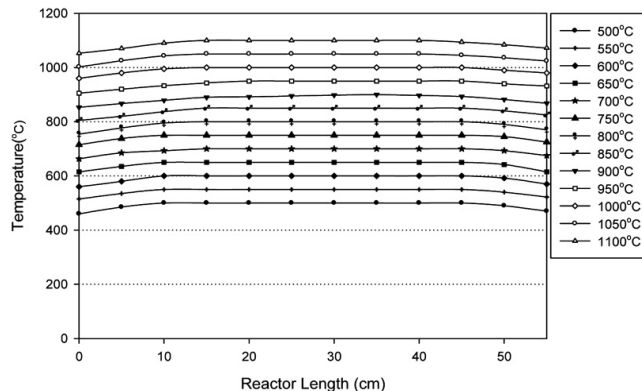


Figure 2. Temperature profile within the reactor.

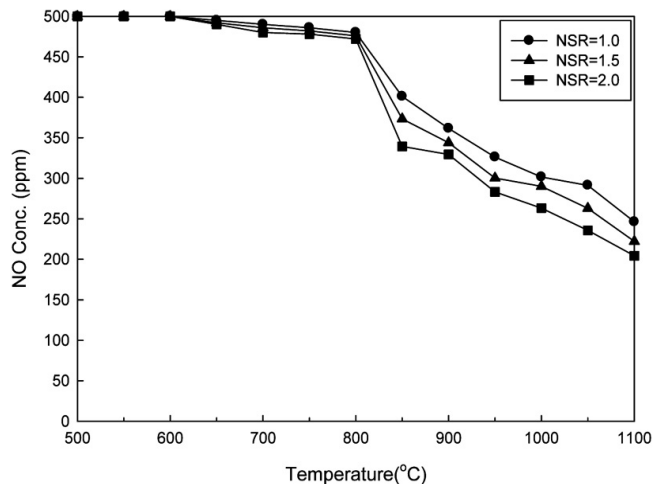


Figure 3. Outlet NO concentration as a function of temperature under the oxygen-free condition.

## 4. Results and Discussion

### 4.1. Temperature Distribution in the Reactor

One of the most important variables in the SNCR process is the temperature distribution in the reactor. The temperature was measured at every 5 cm in the reactor under different set-point temperatures between 500 and 1100 °C with an interval of 50 °C. The result is shown in Figure 2. It is shown in this figure that temperature was maintained at set-point temperature with the error within  $\pm 4\%$  throughout more than 80% of the reactor length.

### 4.2. Experimental Results

Figure 3 shows the outlet NO concentration obtained with three different NSR values of 1.0, 1.5, and 2.0 as a function of set-point reactor temperature under the oxygen-free condition. NO removal efficiency was almost zero at a temperature of 800 °C and lower. The  $NO_x$  removal became significant at 850 °C and increased with temperature thereafter. A higher NSR resulted in a higher NO removal efficiency: the removal efficiency at 1100 °C was 50.7, 55.6, and 59.1% with NSR of 1, 1.5, and 2, respectively.

The results obtained with the oxygen concentration of 4% are shown

Table 1. Elementary Reaction Mechanism for NO<sub>x</sub> + NH<sub>3</sub> Reaction(unit : cm<sup>3</sup>-mole-sec-cal-K)

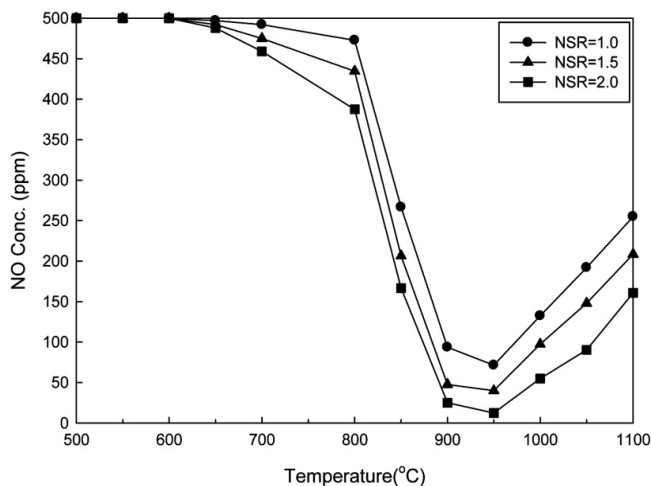
		A	n	E			A	n	E
1	NH <sub>3</sub> + M ↔ NH <sub>2</sub> + H + M	2.20E + 16	0.00	93470.0	54	HNO + NO ↔ N <sub>2</sub> O + OH	2.00E + 12	0.00	26000.0
2	NH <sub>3</sub> + H ↔ NH <sub>2</sub> + H <sub>2</sub>	6.36E + 05	2.39	10171.0	55	HNO + HNO ↔ N <sub>2</sub> O + H <sub>2</sub> O	3.95E + 12	0.00	5000.0
3	NH <sub>3</sub> + O ↔ NH <sub>2</sub> + OH	2.10E + 13	0.00	9000.0	56	H <sub>2</sub> NO + M ↔ HNO + H + M	5.00E + 16	0.00	50000.0
4	NH <sub>3</sub> + OH ↔ NH <sub>2</sub> + H <sub>2</sub> O	2.04E + 06	2.04	566.0	57	H <sub>2</sub> NO + H ↔ HNO + H <sub>2</sub>	3.00E + 07	2.00	2000.0
5	NH <sub>3</sub> + HO <sub>2</sub> ↔ NH <sub>2</sub> + H <sub>2</sub> O <sub>2</sub>	3.00E + 11	0.00	22000.0	58	H <sub>2</sub> NO + H ↔ NH <sub>2</sub> + OH	5.00E + 13	0.00	0.0
6	NH <sub>2</sub> + NO ↔ N <sub>2</sub> + H <sub>2</sub> O	3.78E + 15	-1.25	0.0	59	H <sub>2</sub> NO + O ↔ NH <sub>2</sub> + O <sub>2</sub>	7.50E + 13	0.00	0.0
7	NH <sub>2</sub> + NO ↔ NNH + OH	8.82E + 15	-1.25	0.0	60	H <sub>2</sub> NO + O ↔ HNO + OH	3.00E + 07	2.00	2000.0
8	NH <sub>2</sub> + H ↔ NH + H <sub>2</sub>	6.92E + 13	0.00	3650.0	61	H <sub>2</sub> NO + OH ↔ HNO + H <sub>2</sub> O	2.00E + 07	2.00	1000.0
9	NH <sub>2</sub> + O ↔ NH + OH	6.75E + 12	0.00	0.0	62	H <sub>2</sub> NO + NO ↔ HNO + HNO	2.00E + 07	2.00	13000.0
10	NH <sub>2</sub> + O ↔ HNO + H	6.63E + 14	-0.50	0.0	63	H <sub>2</sub> NO + NH <sub>2</sub> ↔ HNO + NH <sub>3</sub>	3.00E + 12	0.00	1000.0
11	NH <sub>2</sub> + O <sub>2</sub> ↔ HNO + OH	4.50E + 12	0.00	25000.0	64	NO <sub>2</sub> + M ↔ NO + O + M	1.10E + 16	0.00	66000.0
12	NH <sub>2</sub> + OH ↔ NH + H <sub>2</sub> O	4.00E + 06	2.00	1000.0	65	NO <sub>2</sub> + H ↔ NO + OH	3.50E + 14	0.00	1500.0
13	NH <sub>2</sub> + NH ↔ N <sub>2</sub> H <sub>2</sub> + H	5.00E + 13	0.00	0.0	66	NO <sub>2</sub> + O ↔ NO + O <sub>2</sub>	1.00E + 13	0.00	600.0
14	NH <sub>2</sub> + NH <sub>2</sub> ↔ N <sub>2</sub> H <sub>2</sub> + H <sub>2</sub>	7.20E + 13	0.00	0.0	67	N <sub>2</sub> H <sub>2</sub> + M ↔ NNH + H + M	1.00E + 17	0.00	50000.0
15	NH <sub>2</sub> + NH <sub>2</sub> ↔ NH <sub>3</sub> + NH	5.00E + 13	0.00	10000.0	68	N <sub>2</sub> H <sub>2</sub> + H ↔ NNH + H <sub>2</sub>	5.00E + 13	0.00	1000.0
16	NH <sub>2</sub> + HO <sub>2</sub> ↔ NH <sub>3</sub> + O <sub>2</sub>	1.00E + 13	0.00	0.0	69	N <sub>2</sub> H <sub>2</sub> + O ↔ NH <sub>2</sub> + NO	1.00E + 13	0.00	0.0
17	NH <sub>2</sub> + HO <sub>2</sub> ↔ H <sub>2</sub> NO + OH	2.50E + 13	0.00	0.0	70	N <sub>2</sub> H <sub>2</sub> + O ↔ NNH + OH	2.00E + 13	0.00	1000.0
18	NH <sub>2</sub> + N ↔ N <sub>2</sub> + 2H	7.20E + 13	0.00	0.0	71	N <sub>2</sub> H <sub>2</sub> + OH ↔ NNH + H <sub>2</sub> O	1.00E + 13	0.00	1000.0
19	NH <sub>2</sub> + NO <sub>2</sub> ↔ N <sub>2</sub> O + H <sub>2</sub> O	2.84E + 18	-2.20	0.0	72	N <sub>2</sub> H <sub>2</sub> + NO ↔ N <sub>2</sub> O + NH <sub>2</sub>	3.00E + 12	0.00	0.0
20	NH <sub>2</sub> + NH <sub>2</sub> + M ↔ N <sub>2</sub> H <sub>4</sub> + M	1.50E + 13	0.00	0.0	73	N <sub>2</sub> H <sub>2</sub> + NH ↔ NNH + NH <sub>2</sub>	1.00E + 13	0.00	1000.0
21	NNH ↔ N <sub>2</sub> + H	1.00E + 04	0.00	0.0	74	N <sub>2</sub> H <sub>2</sub> + NH <sub>2</sub> ↔ NNH + NH <sub>3</sub>	1.00E + 13	0.00	1000.0
22	NNH + O ↔ N <sub>2</sub> O + H	1.00E + 14	0.00	0.0	75	N <sub>2</sub> H <sub>3</sub> + M ↔ N <sub>2</sub> H <sub>2</sub> + H + M	3.50E + 16	0.00	46000.0
23	NNH + NH ↔ N <sub>2</sub> + NH <sub>2</sub>	5.00E + 13	0.00	0.0	76	N <sub>2</sub> H <sub>3</sub> + O ↔ N <sub>2</sub> H <sub>2</sub> + OH	5.00E + 12	0.00	5000.0
24	NNH + NH <sub>2</sub> ↔ N <sub>2</sub> + NH <sub>3</sub>	5.00E + 13	0.00	0.0	77	N <sub>2</sub> H <sub>3</sub> + O ↔ NH <sub>2</sub> + HNO	1.00E + 13	0.00	0.0
25	NNH + H ↔ N <sub>2</sub> + H <sub>2</sub>	1.00E + 14	0.00	0.0	78	N <sub>2</sub> H <sub>3</sub> + OH ↔ N <sub>2</sub> H <sub>2</sub> + H <sub>2</sub> O	1.00E + 13	0.00	1000.0
26	NNH + OH ↔ N <sub>2</sub> + H <sub>2</sub> O	5.00E + 13	0.00	0.0	79	N <sub>2</sub> H <sub>3</sub> + H ↔ NH <sub>2</sub> + NH <sub>2</sub>	1.60E + 12	0.00	0.0
27	NNH + NO ↔ N <sub>2</sub> + HNO	5.00E + 13	0.00	0.0	80	N <sub>2</sub> H <sub>3</sub> + NH ↔ NH <sub>2</sub> + N <sub>2</sub> H <sub>2</sub>	2.00E + 13	0.00	0.0
28	N <sub>2</sub> O + M ↔ N <sub>2</sub> + O + M	6.00E + 14	0.00	56100.0	81	N <sub>2</sub> H <sub>4</sub> + H ↔ N <sub>2</sub> H <sub>3</sub> + H <sub>2</sub>	1.30E + 13	0.00	2500.0
29	N <sub>2</sub> O + O ↔ NO + NO	2.90E + 13	0.00	23150.0	82	N <sub>2</sub> H <sub>4</sub> + O ↔ N <sub>2</sub> H <sub>2</sub> + H <sub>2</sub> O	8.50E + 13	0.00	1200.0
30	N <sub>2</sub> O + O ↔ N <sub>2</sub> + O <sub>2</sub>	1.40E + 12	0.00	10800.0	83	N <sub>2</sub> H <sub>4</sub> + OH ↔ N <sub>2</sub> H <sub>3</sub> + NH <sub>3</sub>	5.00E + 12	0.00	1200.0
31	N <sub>2</sub> O + OH ↔ N <sub>2</sub> + HNO <sub>2</sub>	2.00E + 12	0.00	10000.0	84	N <sub>2</sub> H <sub>4</sub> + NH <sub>2</sub> ↔ N <sub>2</sub> H <sub>3</sub> + NH <sub>3</sub>	3.90E + 12	0.00	1500.0
32	N <sub>2</sub> O + H ↔ N <sub>2</sub> + OH	7.60E + 13	0.00	15200.0	85	H + H + M ↔ H <sub>2</sub> + M	1.00E + 18	-1.00	0.0
33	NH + O <sub>2</sub> ↔ HNO + O	1.00E + 13	0.00	12000.0	86	H + H + H <sub>2</sub> ↔ H <sub>2</sub> + H <sub>2</sub>	9.20E + 16	-0.60	0.0
34	NH + O <sub>2</sub> ↔ NO + OH	7.60E + 10	0.00	1530.0	87	H + H + H <sub>2</sub> O ↔ H <sub>2</sub> + H <sub>2</sub> O	6.00E + 19	-1.25	0.0
35	NH + OH ↔ HNO + H	2.00E + 13	0.00	0.0	88	H + O + M ↔ OH + M	6.20E + 16	-0.60	0.0
36	NH + OH ↔ N + H <sub>2</sub> O	5.00E + 11	0.50	2000.0	89	H + OH + M ↔ H <sub>2</sub> O + M	1.60E + 22	-2.00	0.0
37	NH + H ↔ N + H <sub>2</sub>	3.00E + 13	0.00	0.0	90	H + O <sub>2</sub> + M ↔ OH + O + M	4.69E + 17	-0.72	0.0
38	NH + O ↔ NO + H	9.20E + 13	0.00	0.0	91	H <sub>2</sub> + O <sub>2</sub> ↔ OH + OH	1.70E + 13	0.00	47780.0
39	NH + N ↔ N <sub>2</sub> ↔ H	3.00E + 13	0.00	0.0	92	O + O + M ↔ O <sub>2</sub> + M	1.89E + 13	0.00	-1788.0
40	NH + NH ↔ N <sub>2</sub> + 2H	2.54E + 13	0.00	0.0	93	O + OH ↔ H + O <sub>2</sub>	4.00E + 14	-0.50	0.0
41	NH + NO ↔ N <sub>2</sub> + OH	2.40E + 15	-0.80	0.0	94	O + H <sub>2</sub> ↔ H + OH	5.06E + 04	2.67	6300.0
42	NH + NO ↔ N <sub>2</sub> O + H	2.90E + 14	-0.40	0.0	95	OH + H <sub>2</sub> ↔ H <sub>2</sub> O + H	1.17E + 09	1.30	3626.0
43	NH + NO <sub>2</sub> ↔ N <sub>2</sub> O + OH	1.00E + 13	0.00	0.0	96	OH + OH ↔ H <sub>2</sub> O + O	6.00E + 08	1.30	0.0
44	N + OH ↔ NO + H	3.80E + 13	0.00	0.0	97	HO <sub>2</sub> + H ↔ H <sub>2</sub> + O <sub>2</sub>	1.25E + 13	0.00	0.0
45	N + O <sub>2</sub> ↔ NO + O	6.40E + 09	1.00	6280.0	98	HO <sub>2</sub> + H ↔ OH + OH	1.40E + 14	0.00	1073.0
46	N + NO ↔ N <sub>2</sub> + O	3.27E + 12	0.30	0.0	99	HO <sub>2</sub> + O ↔ OH + O <sub>2</sub>	1.40E + 14	0.00	1073.0
47	HNO + M ↔ H + NO + M	1.50E + 16	0.00	48680.0	100	HO <sub>2</sub> + OH ↔ H <sub>2</sub> O + O <sub>2</sub>	5.00E + 13	0.00	1000.0
48	HNO + O ↔ NO + OH	1.00E + 13	0.00	0.0	101	HO <sub>2</sub> + NO ↔ NO <sub>2</sub> + OH	2.11E + 12	0.00	-479.0
49	HNO + H ↔ NO + H <sub>2</sub>	5.00E + 12	0.00	0.0	102	HNO <sub>2</sub> + HNO <sub>2</sub> ↔ H <sub>2</sub> O <sub>2</sub> + O <sub>2</sub>	2.00E + 12	0.00	0.0
50	HNO + O <sub>2</sub> ↔ NO + HNO <sub>2</sub>	1.00E + 13	0.00	25000.0	103	H <sub>2</sub> O <sub>2</sub> + M ↔ OH + OH + M	1.30E + 17	0.00	45500.0
51	HNO + OH ↔ NO + H <sub>2</sub> O	3.60E + 13	0.00	0.0	104	H <sub>2</sub> O <sub>2</sub> + H ↔ HO <sub>2</sub> + H <sub>2</sub>	1.60E + 12	0.00	3800.0
52	HNO + HO <sub>2</sub> ↔ NO + H <sub>2</sub> O <sub>2</sub>	3.15E + 11	0.50	1976.0	105	H <sub>2</sub> O <sub>2</sub> + OH ↔ H <sub>2</sub> O + HO <sub>2</sub>	1.00E + 13	0.00	18000.0
53	HNO + NH <sub>2</sub> ↔ NO + NH <sub>3</sub>	2.00E + 13	0.00	1000.0					

in Figure 4. Similar to the oxygen-free case, the NO<sub>x</sub> removal efficiency was considerable at temperature of 850 °C and higher. Showing the maximum NO removal efficiency at 950 °C, however, further increase of reactor temperature resulted in reduction of removal effi-

ciency contrary to the oxygen-free case. The NO removal efficiency increased with NSR value in this case, too: the removal efficiency at 950 °C was 85.7, 92.0, and 97.5% with NSR of 1.0, 1.5, and 2.0, respectively.

**Table 2. Thermochemical Data for NO<sub>x</sub> + NH<sub>3</sub> Reaction**

Species	$\Delta H_f$ (298.15 K) (kcal/mol · K)	S (298.15 K) (cal/mol · K)	Cp						
			300	400	500	600	800	1000	1500
NH <sub>3</sub>	-10.98	46.05	8.53	9.28	10.03	10.78	12.22	13.49	15.78
NH <sub>2</sub>	45.50	46.53	8.13	8.38	8.63	8.90	9.56	10.21	11.53
NO	21.59	50.36	7.01	7.19	7.36	7.53	7.84	8.08	8.51
N <sub>2</sub>	0.00	45.79	6.86	7.00	7.14	7.27	7.53	7.80	8.27
NNH	58.61	53.66	8.32	8.82	9.36	9.88	10.86	11.53	12.43
N <sub>2</sub> O	19.63	52.56	9.25	10.07	10.88	11.57	12.51	13.10	13.94
NO <sub>2</sub>	7.91	57.39	8.92	9.63	10.33	10.93	11.79	12.34	13.08
H <sub>2</sub> NO	15.89	56.60	8.48	9.50	10.52	11.52	13.36	14.87	17.07
HNO	23.80	52.75	8.37	8.88	9.39	9.88	10.71	11.41	12.48
N <sub>2</sub> H <sub>2</sub>	50.00	52.22	8.75	9.85	10.85	11.85	13.50	14.84	16.85
N <sub>2</sub> H <sub>3</sub>	48.09	54.64	10.47	12.12	13.76	15.20	17.33	18.93	21.58
N <sub>2</sub> H <sub>4</sub>	22.80	57.03	12.21	14.43	16.64	18.52	21.13	22.99	26.32
NH	84.24	43.30	6.98	7.00	7.01	7.05	7.25	7.46	8.06
H <sub>2</sub> O	-57.82	45.12	8.11	8.29	8.47	8.68	9.25	9.85	11.19
HO <sub>2</sub>	3.80	54.76	8.44	8.96	9.47	9.95	10.71	11.38	12.39
H <sub>2</sub> O <sub>2</sub>	-32.54	55.69	10.43	11.36	12.29	13.10	14.32	15.21	16.86
H <sub>2</sub>	0.00	31.23	6.91	6.94	6.97	7.01	7.13	7.27	7.68
O <sub>2</sub>	0.00	49.02	7.01	7.24	7.47	7.68	8.03	8.30	8.73
H	52.13	27.40	4.97	4.97	4.97	4.97	4.97	4.97	4.97
OH	9.49	43.90	6.96	7.00	7.03	7.08	7.22	7.36	7.80
N	113.03	36.63	4.97	4.97	4.97	4.97	4.97	4.97	4.97
O	59.59	38.50	5.24	5.17	5.10	5.05	5.02	5.00	4.97

**Figure 4. Outlet NO concentration as a function of temperature with the oxygen concentration of 4%.**

### 4.3. Simulation Results

Figure 5 compares the model estimated outlet NO concentrations with measurements at different temperatures with NSR of 1.0 (a), 1.5 (b), and 2.0 (c). For all cases, the inlet NO concentration was 500 ppm and N<sub>2</sub> was used as the balance gas under oxygen-free condition. The model predicted well the increasing trend of NO removal efficiency

with temperature. The temperature at which the NO removal efficiency became significant, however, was predicted to be much higher (950~1000 °C) by the model than that shown by measurements (800~850 °C). Except the case with high temperature and high NSR, the model-predicted NO removal efficiency was lower than measured ones. Experiments were carried out only up to the temperature of 1100 °C due to the limitation of heating instrument, but the model simulations were performed up to 1300 °C. As is shown in Figure 5, the NO removal efficiency was predicted to increase rapidly over 1100 °C reaching 100% at 1300 °C when NSR was 1.5 or 2.

Figure 6 shows the same results as those of Figure 5 but for the O<sub>2</sub> concentration of 4%. The temperature dependency of the NO removal efficiency was predicted by the model very similarly with the measurement. Both measurements and model simulations showed that the NO removal efficiency had its maximum value at a temperature of 900~950 °C. The value of the maximum removal efficiency was similar between measurements and model simulations. When the removal efficiency was low at higher or lower temperature, however, the difference between measurements and model predictions was larger. The model predicted the maximum efficiency temperature accurately except for the case of NSR = 2, where the model-predicted maximum efficiency temperature (900 °C) was lower than measured one (950 °C). At all NSR values tested, the model could not predict slow reaction

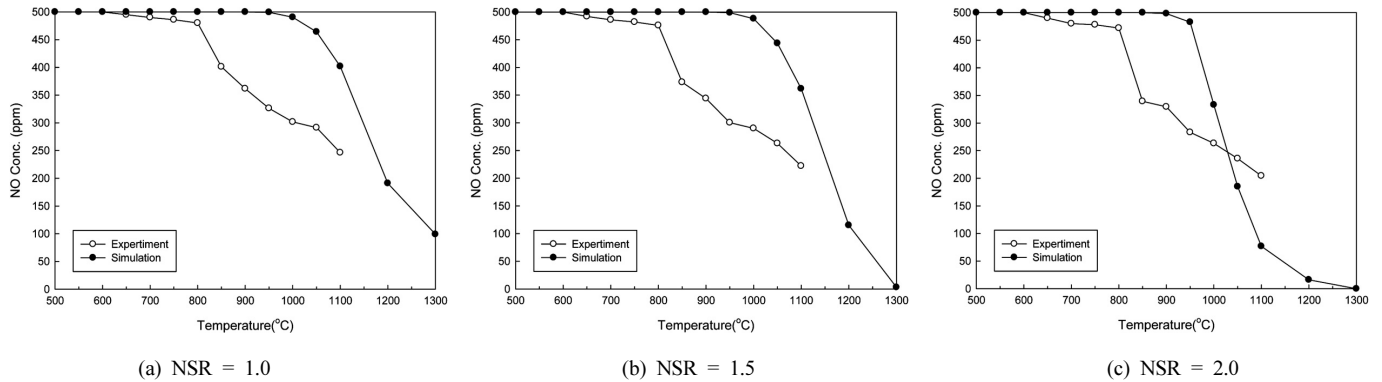


Figure 5. Comparison of measured and simulated outlet NO concentration under the oxygen-free condition.

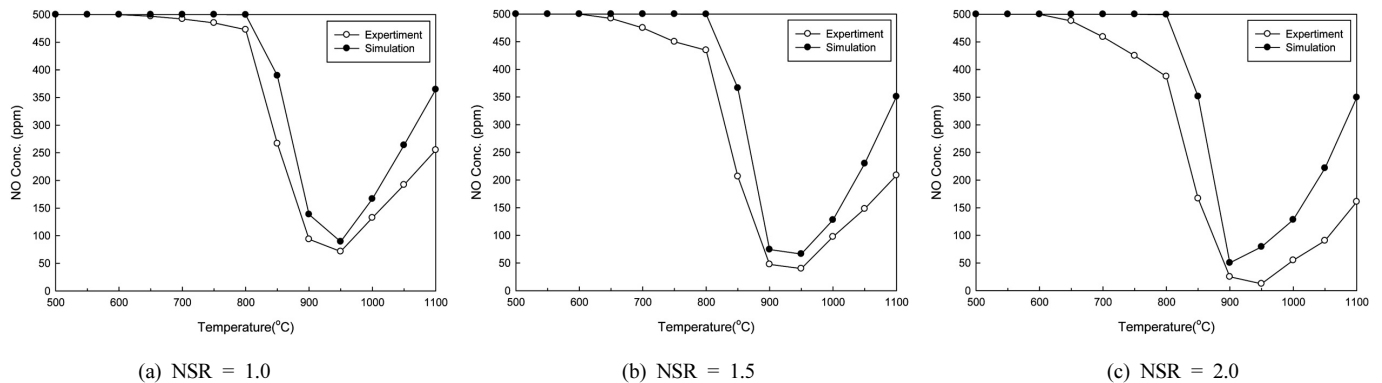


Figure 6. Comparison of measured and simulated outlet NO concentration with the oxygen concentration of 4%.

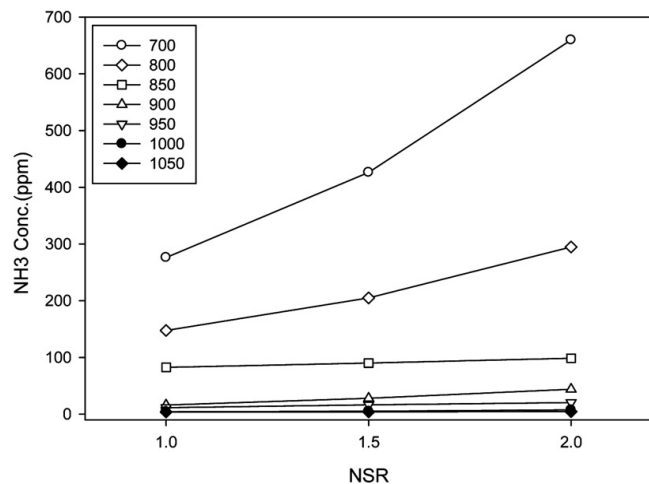


Figure 7. Outlet concentration of NH<sub>3</sub> obtained with the oxygen concentration of 4% under different temperature and NSR conditions.

that took place at low temperature range (650~800 °C) probably because the temporal or spatial fluctuation of temperature in the reactor was not taken into account in the model.

Regardless of the presence of oxygen, the NO removal efficiency increased with NSR in this study. Use of high NSR, however, may result in emission of significant amount of unreacted ammonia. Figure 7 shows the outlet concentration of NH<sub>3</sub> as a function of NSR at different temperatures. At a low temperature (900 °C or below), the concen-

tration of unreacted ammonia increased with NSR. At a higher temperature, the concentration of unreacted ammonia did not depend much on NSR. Therefore, NSR should be decided considering NO<sub>x</sub> removal efficiency, cost for use of ammonia, and air pollutant emission standard simultaneously.

## 5. Conclusions

The SNCR process was applied to NO<sub>x</sub> removal. Under oxygen-free condition, NO removal efficiency increased with reaction temperature. Simulations using the CHEMKIN-II package predicted that the NO removal efficiency would reach 100% with NSR = 1.5 or 2 at the reactor temperature of 1300 °C under oxygen-free condition, but this was not confirmed by experiments due to the limitation of the heating instrument used in this study. When the inlet oxygen concentration was set at 4%, the NO removal efficiency showed a maximum value at 900~950 °C. At a higher temperature, the NO removal efficiency was reduced due to the reaction between oxygen and ammonia producing NO. Therefore, if the SNCR is applied under the presence of oxygen, it should be operated at the maximum removal efficiency temperature. Presence of oxygen resulted in an increase of NO removal efficiency at low temperature, whereas at high temperature the oxygen-free condition was more favorable to NO removal. Considering the fuel use for maintaining the reactor temperature and aging of the instruments, operation at low temperature with appropriate concentration of oxygen is

recommended.

Regardless of the presence of oxygen, the NO removal efficiency increased with NSR. However, at 900 °C or below the concentration of unreacted ammonia also increased with NSR. At a higher temperature, the concentration of unreacted ammonia did not depend much on NSR. Therefore, NSR should be decided considering NO<sub>x</sub> removal efficiency, cost for use of ammonia, and air pollutant emission standard simultaneously.

The NO removal efficiency of the SNCR process predicted by CHEMKIN-II was close to the measured one at around the maximum removal efficiency temperature. The predictions for temperature- and NSR-dependencies of the NO removal efficiency also agreed well with the experimental results. Therefore, CHEMKIN-II may be useful for predicting the optimum reactor temperature and NSR and for estimating the NO removal efficiency before actual operation.

## References

1. J. C. Choi, C. H. Cho, K. E. Jeong, J. K. Jeon, J. H. Yim, and Y. K. Park, *J. Kor. Ind. Eng. Chem.*, **19**, 92 (2008).
2. M. T. Javed, N. Irfan, and B. M. Gibbs, *J. Env. Manage.*, **83**, 251 (2007).
3. J. A. Miller and C. T. Bowman, *Prog. Energy Combust. Sci.*, **15**, 287 (1989).
4. J. A. Silver and C. E. Kolb, *J. Phys. Chem.*, **86**, 3240 (1982).
5. R. K. Lyon and J. E. Hardy, *Ind. Eng. Chem. Fundam.*, **25**, 19 (1986).
6. P. Lodder and J. B. Lefers, *Chem. Eng. J.*, **30**, 161, (1985).
7. R. K. Lyon, *Int. J. Chem. Kinet.*, **8**, 315, (1976).