**Table 1 and Summary. Operating Conditions of the SCR Reactor used in the Benzene-Destruction**

|  |  |  |
| --- | --- | --- |
| parameter | unit | value |
|  |
| flue gas constituent |  |
| C6H6 | ppm | 1 and 17 |
| HCl | ppm | 10 and 50 |
| SO2 | ppm | 500 and 2,000 |
| NO | ppm | 200 and 400 |
| CO2 | % | 3.5 |
| O2 | % | 4 |
| H2O | % | 7 |
| NH3/NO ratio |  | 0.9 |
| total flow rate | L/min | 14 |
| space velocity (SV) | hr-1 | 2,000 and 4,000 |
| temperature | ℃ | 350 and 400 |
| The SCR reactor was operated by passing simulated coal combustion flue gases with seven constituents including C6H6 (benzene), HCl (hydrochloric aci), SO2 (sulfur dioxide), NO (nitrogen oxide), CO2 (carbon dioxide), H2O (moisture), and NH3 (ammonia, and concentration of NH3 is expressed in ammonia to nitrogen oxide volume ratio) through the SCR catalyst. The parameters used for specifying the operating conditions of the reactor included: concentrations of the flue gas constituents, flue gas total flow rate, flue gas space velocity (as a measure of residence time), and flue gas temperature. |  |  |  |  |  |  |  |  |  |
| **Table 2 and Summary.** **Experimental Design and Test Results**

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| test | T | SV | C6H6 | HCl | NO | SO2 | C6H6 | CO | NO  |
| group |  |   |   |   |   |   | destruction |  yield | reduction |
|   | (oC) | (hr-1 ) | (ppm) | (ppm) | (ppm) | (ppm) | (%) | (%) | (%) |
|  |
|  | test conditions | test results |
| 1 | 350 | 2000 | 17 | 10 | 200 | 500 | 72 + 1 | 52 + 1 | 84 + 2 |
|  | 400 | 2000 | 17 | 10 | 200 | 2000 | 76 + 8 | 57 + 4 | 78 + 7 |
|  | 350 | 2000 | 17 | 50 | 200 | 2000 | 75 + 6 | 61 + 4 | 86 + 0 |
|  | 400 | 2000 | 17 | 50 | 200 | 500 | 85 + 1 | 51 + 2 | 84 + 0 |
|  | 350 | 2000 | 17 | 10 | 400 | 2000 | 65 + 1 | 50 + 3 | 81 + 4 |
|  | 400 | 2000 | 17 | 10 | 400 | 500 | 75 + 8 | 46 + 4 | 86 + 3 |
|  | 350 | 2000 | 17 | 50 | 400 | 500 | 80 + 12 | 54 + 1 | 82 + 2 |
|  | 400 | 2000 | 17 | 50 | 400 | 2000 | 82 + 1 | 54 + 2 | 84 + 3 |
|  |  |  |  |  |  |  |  |  |  |
| 2 | 350 | 2000 | 1 | 10 | 200 | 2000 | 81 + 3 |  | 90 + 4 |
|  | 400 | 2000 | 1 | 10 | 200 | 500 | 96 + 1  |  | 79 + 6 |
|  | 350 | 2000 | 1 | 50 | 200 | 500 | 76 + 4 |  | 88 + 2 |
|  | 400 | 2000 | 1 | 50 | 200 | 2000 | 94 + 1 |  | 90 + 2 |
|  | 350 | 2000 | 1 | 10 | 400 | 500 | 77 + 1 |  | 86 + 1 |
|  | 400 | 2000 | 1 | 10 | 400 | 2000 | 95 + 4 |  | 90 + 2 |
|  | 350 | 2000 | 1 | 50 | 400 | 2000 | 68 + 8 |  | 90 + 2 |
|  | 400 | 2000 | 1 | 50 | 400 | 500 | 96 + 3 |  | 91 + 4 |
|  |  |  |  |  |  |  |  |  |  |
| 3 | 350 | 4000 | 17 | 10 | 200 | 500 | 57 + 3 | 55 + 4 | 71 + 3 |
|  | 400 | 4000 | 17 | 10 | 200 | 2000 | 75 + 2 | 62 + 1 | 78 + 7 |
|  | 350 | 4000 | 17 | 50 | 200 | 2000 | 56 + 2 | 63 + 2 | 69 + 3 |
|  | 400 | 4000 | 17 | 50 | 200 | 500 | 74 + 1 | 61 + 1 | 74 + 4 |
|  | 350 | 4000 | 17 | 10 | 400 | 2000 | 56 + 0 | 62 + 0 | 68 + 3  |
|  | 400 | 4000 | 17 | 10 | 400 | 500 | 76 + 3 | 66 + 7 | 75 + 5 |
|  | 350 | 4000 | 17 | 50 | 400 | 500 | 56 + 2 | 63 + 2 | 70 + 1 |
|  | 400 | 4000 | 17 | 50 | 400 | 2000 | 72 + 1 | 64 + 1 | 74 + 1 |
|  |  |  |  |  |  |  |  |  |  |
| 4 | 350 | 4000 | 1 | 10 | 200 | 2000 | 70 + 2 |  | 76 + 3 |
|  | 400 | 4000 | 1 | 10 | 200 | 500 | 84 + 1 |  | 67 + 4 |
|  | 350 | 4000 | 1 | 50 | 200 | 500 | 72 + 2 |  | 68 + 4 |
|  | 400 | 4000 | 1 | 50 | 200 | 2000 | 84 + 1 |  | 72 + 3 |
|  | 350 | 4000 | 1 | 10 | 400 | 500 | 69 + 1 |  | 67 + 4 |
|  | 400 | 4000 | 1 | 10 | 400 | 2000 | 85 + 4 |  | 72 + 2 |
|  | 350 | 4000 | 1 | 50 | 400 | 2000 | 59 + 7 |  | 79 + 4 |
|  | 400 | 4000 | 1 | 50 | 400 | 500 | 80 + 3 |  | 70 + 3 |

A test matrix was designed for separating the tests into four groups with six variable experimental conditions including flue gas temperatures (T at 350 or 400 oC), flue gas space velocity (SV at 2000 or 4000 hr-1), concentration of C6H6 (C6H6 at 17 or 1 ppm), concentration of HCl (HCl at 10 or 50 ppm), concentration of NO (NO at 200 or 400 ppm), and concentration of SO2 (SO2 at 500 or 2000 ppm).The test results include 1) Efficiency of C6H6 destruction, which is determined by: C6H6 destruction (in %) = {([C6H6]inlet - [C6H6]outlet)/[ C6H6]inlet}×100 where [C6H6]inlet and [C6H6]outlet represent the concentrations of C6H6 measured at the inlet and outlet of the catalyst, respectively.2) Efficiency of NO reduction, which is determined by:NO destruction (in %) = {([NO]inlet - [NO]outlet)/[NO]inlet}×100 where [NO]inlet and [NO]outlet represent the concentrations of NO measured at the inlet and outlet of the catalyst, respectively.And 3) Yield of CO formed from the destruction of C6H6, which is determined by:CO yield (in %) = ([CO]outlet - [CO]inlet)/{6× ([CO]inlet - [CO]outlet)} × 100 where [CO]inlet and [CO]outlet represent the concentrations of CO measured at the inlet and outlet of the catalyst, respectively. |  |  |  |  |  |  |  |  |  |
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| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Table 3 and Summary. Estimates for Individual Effects and Cross Effects Obtained from the Linear Regression Models for Destruction of C6H6 and Reduction of NO**

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| factor | effect  | t-ratio | p-value | error of | effect  | t-ratio | p-value | error of |
|   | estimate |   |   | estimate | estimate |   |   | estimate |
|  |
|  | destruction of C6H6  | reduction of NO |
| individual effect |  |
| temperature | 7.51 | 9.14 | <.0001 |  | 0.28 | 0.5 | 0.6299 |  |
| SV | -5.19 | -6.32 | <.0001 |  | -6.84 | -12.36 | <.0001 |  |
| C6H6 | -4.87 | -5.93 | 0.0001 |  | -0.96 | -1.74 | 0.1125 |  |
| HCl | -0.04 | -0.05 | 0.9645 |  | 0.71 | 1.29 | 0.2268 |  |
| NO | -1.15 | -1.4 | 0.1915 |  | 0.34 | 0.61 | 0.5555 |  |
| SO2 | -0.96 | -1.16 | 0.2711 |  | 1.09 | 1.97 | 0.0777 |  |
|  |
| cross effect |  |
| temperature\*SV | 0.9 | 1.1 | 0.2986 |  | 0.59 | 1.06 | 0.3133 |  |
| temperature\*C6H6 | -1.38 | -1.68 | 0.1234 |  | 1.09 | 1.97 | 0.0777 |  |
| temperature\*HCl | 0.33 | 0.4 | 0.7005 |  | 0.16 | 0.29 | 0.775 |  |
| temperature\*NO | 0.68 | 0.82 | 0.4301 |  | 0.91 | 1.65 | 0.1301 |  |
| temperature\*SO2 | 0.77 | 0.94 | 0.3711 |  | -0.34 | -0.61 | 0.5555 |  |
| SV\*C6H6 | -0.31 | -0.38 | 0.7114 |  | 1.48 | 2.67 | 0.0237 |  |
| SV\*HCl | -1.19 | -1.45 | 0.1765 |  | -0.6 | -1.08 | 0.3036 |  |
| SV\*NO | -0.11 | -0.13 | 0.8996 |  | -0.35 | -0.63 | 0.5412 |  |
| SV\*SO2 | 0.33 | 0.4 | 0.7005 |  | 0.53 | 0.95 | 0.365 |  |
| C6H6\*HCl | 1.79 | 2.18 | 0.0545 |  | -0.6 | -1.08 | 0.3036 |  |
| C6H6\*NO | 0.65 | 0.79 | 0.4468 |  | -0.6 | -1.08 | 0.3036 |  |
| C6H6\*SO2 | -0.17 | -0.21 | 0.8412 |  | -1.6 | -2.89 | 0.0161 |  |
| HCl\*NO | -0.27 | -0.33 | 0.7501 |  | 0.23 | 0.41 | 0.6928 |  |
| HCl\*SO2 | -0.8 | -0.97 | 0.3528 |  | -0.03 | -0.05 | 0.9648 |  |
| NO\*SO2 | -0.7 | -0.85 | 0.4138 |  | -0.4 | -0.72 | 0.4863 |  |
|  |
|  |  |  |  |  | 0.82 |  |  |  | 0.55 |

The experimental results shown in Table 2 were analyzed by using JMP 10 statistical analysis software (SAS Institute, Cary, NC, USA). A standard least squares model was used to evaluate the significance of each individual factor and also their cross effects on the destruction of C6H6 and on the reduction of NO. The experimental conditions evaluated as a significant individual factor for the destruction of C6H6, and for reduction of NO include temperature, space velocity (SV), and concentrations of C6H6, HCl, NO, and SO2. The cross effects of two experimental factors for the destruction of C6H6 and for the reduction of NO were also analyzed. The cross effects include: temperature and SV, temperature and conc. of C6H6, temperature and conc. of HCl, temperature and conc. of NO, temperature and conc. of SO2, SV and conc. of C6H6, SV and conc. of HCl, SV and conc. of NO, SV and conc. of SO2, conc. of C6H6 and conc. of HCl, conc. of C6H6 and conc. of NO, conc. of C6H6 and conc. of SO2, conc. of HCl and conc. of NO, conc. of HCl and conc. of SO2, and conc. of HCl and conc. of SO2.Results of the models include: Effect estimate: correlation between the factor and the destruction of C6H6 or the reduction of NO.  |  |  |  |  |  |  |  |  |  |

 |  | 4000 | 17 | 10 | 400 | 500 | 76 + 3 | 66 + 7 | 75 + 5 |
|  A larger absolute value always indicates a stronger effect. t-ratio: is the effect estimate divided by the standard error. t-ratio > 1.96 (in absolute value) suggests that  the effect is significntly different from 0at the 95% confidence level. p-value: is defined as the probability of obtaining a result equal to or more extreme that what was actuallyobserved, when the null hypothesis is true.Error of estimate: represents the average distance that the observed values fall from the regression line.  |  |  |  |  |  |  |  |  |  |
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| Fig. 1. Down-flow SCR reactor system.Fig. 2. Effect of the inlet C6H6 concentration to the SCR reactor on the destruction of C6H6.(Case I: temperature = 350 oC, SV = 4000 hr-1; Case II: temperature = 400 oC, SV = 4000 hr-1; Case III: temperature = 400 oC, SV = 2000 hr-1; Case IV: temperature = 350 oC, SV = 2000 hr-1)Fig. 3. Carbon mass balance for C6H6 destruction promoted by the V2O5-WO3/TiO2 catalyst. |  |  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |  |  |