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Computational Modeling and Experimental Studies on
NO_x Reduction Under Pulverized Coal Combustion Conditions

Technical Progress Report
First Quarter

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1. Introduction

This is the first quarterly report of the three-year program entitled "Computational Modeling and Experimental Studies on NO_x Reduction Under Pulverized Coal Combustion Conditions" which began on February 1, 1995. This program involves computer simulation studies to aid in planning and conducting a series of experiments that will extend our knowledge of reburning process. The objective of this work is to find nitric oxide reduction effectiveness for various reburning fuels and identify both homogeneous and heterogeneous reaction mechanisms characterizing NO reduction.

To begin with, computer simulation studies have been undertaken. The updated version of CHEMKIN II (1994) package has been acquired from Sandia National Laboratories and put to use for the preliminary runs involving reburning of nitric oxide with methane. This report presents results from these computations.

Three specific activities will be performed during the next quarter - i) computer simulation of NO reburning with a combination of methane/acetylene ii) updating the reaction mechanism based on the further examination of literature and iii) planning the experiments for nitric oxide reduction with a combination of methane/acetylene.

2. Reaction Mechanism

A detailed reaction mechanism involving hydrocarbon and nitrogen containing species is prepared to study reburning. This is very similar to that of Kilpinen et al (1992). While efforts are being made to update this mechanism based on the most recent literature, the preliminary runs on reburning with methane show promising results. Listed in Table 1 is the reaction mechanism used for the computations in this report.

The reaction mechanism will be updated constantly. Existing rate constants data will be checked against several recent publications which include (a) a paper by Byne and Dean (1993) who used a large hydrocarbon mechanism that consisted of 497 reactions and 135 species, (b) summary table of evaluated kinetic data for combustion modeling by Baulch et al (1994), (c) specific reaction rate constants for $\text{CH}_4 - \text{O}_2$ system used by Lee and Chung (1994), (d) ammonia oxidation reaction mechanism employed by Vandooren et al (1994) (e) detailed kinetic modeling of chemistry and temperature effects on ammonia oxidation by Lindstedt et al (1994) and (f) several mechanism and modeling studies conducted by Glarborg et al (1994).

3. Computational Method/Tool

The updated version of CHEMKIN II has been acquired from Sandia National Laboratories and loaded on the CRAY-Y MP Supercomputer located in the University of Mississippi. This employs VODE, an updated version of LSODE to solve the initial value problem for stiff or nonstiff systems of first order ordinary differential equations.

We have employed an adiabatic system with constant pressure to define the reactor for NO reburning with methane. The input concentrations for various reburning stoichiometric ratios (0.7 to 1.05) were calculated and supplied to the program. The CHEMKIN package handles the chemical reaction mechanism (which is given in the previous section) and then allows VODE to calculate the temperature and species concentrations at various residence times.

We have used SENKIN program also to solve this initial value problem which gave identical results. The program SENKIN uses the DASAC software to solve the nonlinear

ODE that describe the temperature and species concentrations.

So far we are involved with time evolution of a homogeneous reacting gas mixture in a closed system. As the project progresses, we will be also working with SURFACE CHEMKIN to do surface kinetics and address heterogenous reactions.

4. Results on NO Reburning with Methane

A typical input concentration for $SR2=0.7$ are 15.9% CO_2 , 1.83% O_2 , 1000 ppm NO, 5.38% CH_4 , and 76.79% inert gas. Similarly $SR2=0.9$ would represent the composition of flue gas as 16.45% CO_2 , 1.87% O_2 , 1000 ppm NO, 2.14% methane and 79.42% N_2/He . With varying $SR2$ conditions the program is run for three residence times (0.1 s, 0.2 s and 0.3 s) at the reactor temperature of 1373 K (1100 C). Also, the program is run for three temperatures, (1000 C, 1100 C and 1200 C) keeping the residence time as 0.2 s. The concentrations of NO_2 and N_2O were found to be negligible for all the cases. The three nitrogen containing species that are significant are NO, HCN and NH_3 and the concentrations of each versus $SR2$ are shown in the following figures.

Figures 1 through 3 show the exit concentrations of NO, HCN and NH_3 respectively for the reactor temperature of 1373 K at varying residence times, i.e., 0.1 s, 0.2 s and 0.3 s. It can be observed that the greatest reduction of NO into mainly HCN and to some extent NH_3 takes place at the reburning stiochiometric ratio of 0.9. This reduction is very significant as Figure 1 depicts, with NO concentration being 46 ppm at 0.2 s. This phenomenon is consistent with what other researchers have observed in the past. Both HCN and NH_3 show opposite trend with NO.

The NO reduction at 0.2 s residence time is considerably higher than at 0.1 s for

stoichiometric ratios ranging from 0.7 to 0.9. However, there is no difference in NO reduction above SR2 value of 0.9. It can also be noticed that NO reduction is not much higher for the residence time of 0.3 s when compared with the reduction at 0.2 s. This difference is insignificant. Hence 0.2 s is chosen to be the optimum residence time for the reaction. Also, the residence time of 0.2 s is appropriate for experimental runs to account for non-idealities and to ensure that the equilibrium reaction for NO reduction goes close to completion.

Figures 4 through 6 depict the exit concentrations of NO, HCN, and NH₃ respectively for a residence time of 0.2 s for varying reactor temperature. The three temperatures and 1273 K, 1373 K and 1473 K. The trends are similar for all reactor temperatures. The greatest reduction of NO occurs at SR2=0.95 for lower temperatures (1273 K) and at SR2=0.9 for higher temperatures (1373 K and 1473 K). The concentration of HCN increases with increase in reactor temperature for the range 0.7 to (0.85-0.9) while it does the opposite for SR2 of 0.9-0.95. Probably this would mean that there is a shift in the mechanism at SR2 value in the neighborhood of 0.85-0.95. At $SR2 \leq 0.9$ the HCN formation is more from NO (70-80%). But above SR2 of 0.9, the NO $\rightarrow$ HCN mechanism is affected and hence the NO concentration goes up and HCN concentration goes down. Both HCN and NH₃ show similar trend with SR2, that is, as long as HCN is formed more, there is a corresponding increase in NH₃. This would mean a fragmental portion of HCN is always converted to NH₃ by some reaction. Above SR2=0.9 the HCN formation decreases and so does the NH₃. Therefore we can postulate that NO reduction goes through a series reaction as follows: $NO \rightarrow HCN \rightarrow NH_3$

5. Projections

The computer simulation will be on-going during the next quarter. Reburning with a combination of methane/acetylene and later on with ammonia will be studied. The reaction mechanism will be updated based on the further examination of literature cited. An experimental plan will be submitted to the DOE so as to start the gas phase reburning studies in the laboratory. We hope that the initial reburning experiments will be underway before the end of the next quarter.

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Table 1. Reaction Mechanism Employed Currently

REACTIONS CONSIDERED	(k = A T**b exp(-E/RT))		
	A	b	E
1. C2H6+M=2CH3+M	5.80E+13	0	75000
2. CH4+M=CH3+H+M	4.17E+17	0	92300
H2O Enhanced by 5			
3. CH4+O2=CH3+HO2	4.00E+13	0	56910
4. CH4+H=CH3+H2	2.02E+04	3	8750
5. CH4+OH=CH3+H2O	1.90E+05	2.4	2110
6. CH4+O=CH3+OH	1.02E+09	1.5	8604
7. CH4+HO2=CH3+H2O2	1.80E+11	0	18700
8. CH4+CH2=CH3+CH3	4.30E+13	0	10030
9. CH3+CH2O=CH4+HCO	5.50E+03	2.8	5860
10. CH3+HCO=CH4+CO	1.20E+14	0	0
11. CH3+M=CH2+H+M	1.90E+16	0	91600
12. CH3+HO2=CH3O+OH	2.00E+13	0	0
13. CH3+O2=CH3O+O	2.05E+19	-1.6	29229
14. CH3+O=CH2O+H	8.40E+13	0	0
15. CH3+OH=CH2+H2O	7.50E+06	2	5000
16. CH3+H=CH2+H2	9.00E+13	0	15100
17. CH3O+M=CH2O+H+M	1.00E+14	0	25000
18. CH2OH+M=CH2O+H+M	1.00E+14	0	25000
19. CH3O+H=CH2O+H2	2.00E+13	0	0
20. CH2OH+H=CH2O+H2	3.00E+13	0	0
21. CH3O+OH=CH2O+H2O	1.00E+13	0	0
22. CH2OH+OH=CH2O+H2O	1.00E+13	0	0
23. CH3O+O=CH2O+OH	1.00E+13	0	0
24. CH2OH+O=CH2O+OH	1.00E+13	0	0
25. CH3O+O2=CH2O+HO2	6.30E+10	0	2600
26. CH2OH+O2=CH2O+HO2	1.48E+13	0	1500
27. CH2+HCO=CH3+CO	2.00E+13	0	0
28. CH2+H=CH+H2	1.00E+17	-1.2	0
29. CH2+OH=CH+H2O	1.13E+07	2	3000
30. CH2+OH=CH2O+H	3.00E+13	0	0
31. CH+O2=HCO+O	3.30E+13	0	0
32. CH+O=CO+H	1.00E+13	0.3	0
33. CH+OH=HCO+H	5.00E+13	0	0
34. CH+CO2=HCO+CO	3.40E+12	0	690
35. CH+H=C+H2	1.50E+14	0	0

36. CH+H2O=CH2O+H	5.70E+12	0	-755
37. CH+CH2O=CH2CO+H	9.46E+13	0	-515
38. CH+C2H2=C3H2+H	8.40E+13	0	0
39. CH+CH2=C2H2+H	4.00E+13	0	0
40. CH+CH3=C2H3+H	3.00E+13	0	0
41. CH+CH4=C2H4+H	6.00E+13	0	0
42. C+O2=CO+O	2.00E+13	0	0
43. C+OH=CO+H	5.00E+13	0	0
44. C+CH3=C2H2+H	5.00E+13	0	0
45. C+CH2=C2H+H	5.00E+13	0	0
46. CH2+CO2=CH2O+CO	1.10E+11	0	1000
47. CH2+O=CO+2H	1.70E+13	0.2	0
48. CH2+O=CO+H2	9.00E+12	0.2	0
49. CH2+O2=CO2+2H	1.60E+12	0	1000
50. CH2+O2=CH2O+O	5.00E+13	0	9000
51. CH2+O2=CO2+H2	6.90E+11	0	500
52. CH2+O2=CO+H2O	1.90E+10	0	-1000
53. CH2+O2=CO+OH+H	8.60E+10	0	-500
54. CH2+O2=HCO+OH	4.30E+10	0	-500
55. CH2O+M=CO+H2+M	8.30E+15	0	69550
56. CH2O+O=CO2+2H	3.50E+05	2.4	1360
57. CH2O+OH=HCO+H2O	3.43E+09	1.2	-447
58. CH2O+H=HCO+H2	2.19E+08	1.8	3000
59. CH2O+M=HCO+H+M	1.00E+16	0	80270
60. CH2O+O=HCO+OH	1.70E+16	2.3	3080
61. HCO+OH=H2O+CO	1.00E+14	0	0
62. HCO+H=CO+H2	1.19E+13	0.3	0
63. HCO+O=CO+OH	3.00E+13	0	0
64. HCO+O=CO2+H	3.00E+13	0	0
65. HCO+O2=HO2+CO	3.30E+13	-0.4	0
66. CO+O+M=CO2+M	6.17E+14	0	3000
67. CO+OH=CO2+H	1.51E+07	1.3	-758
68. CO+O2=CO2+O	2.50E+12	0	47700
69. HO2+CO=CO2+OH	5.80E+13	0	22934
70. C2H6+CH3=C2H5+CH4	5.50E-01	4	8300
71. C2H6+H=C2H5+H2	5.40E+02	3.5	5210
72. C2H6+O=C2H5+OH	1.20E+12	0.6	7310
73. C2H6+OH=C2H5+H2O	8.70E+09	1	1810
74. C2H4+OH=CH2O+CH3	5.60E+12	0	1500
75. C2H4+CH3=C2H3+CH4	6.60E+00	3.7	9500
76. C2H4+H=C2H3+H2	1.30E+06	2.5	12240
77. C2H4+OH=C2H3+H2O	9.00E+13	0	6860

78. $\text{CH}_2 + \text{CH}_3 = \text{C}_2\text{H}_4 + \text{H}$	4.20E+13	0	0
79. $\text{C}_2\text{H}_5 + \text{M} = \text{C}_2\text{H}_4 + \text{H} + \text{M}$	1.00E+17	0	31000
80. $\text{C}_2\text{H}_5 + \text{H} = 2\text{CH}_3$	2.30E+12	0.5	0
81. $\text{C}_2\text{H}_5 + \text{O}_2 = \text{C}_2\text{H}_4 + \text{HO}_2$	8.43E+11	0	3875
82. $\text{C}_2\text{H}_2 + \text{O} = \text{CH}_2 + \text{CO}$	1.70E+08	1.6	2210
83. $\text{C}_2\text{H}_2 + \text{O} = \text{HCCO} + \text{H}$	2.50E+08	1.6	2210
84. $\text{H}_2 + \text{C}_2\text{H} = \text{C}_2\text{H}_2 + \text{H}$	4.09E+05	2.4	864
85. $\text{C}_2\text{H}_3 + \text{M} = \text{C}_2\text{H}_2 + \text{H} + \text{M}$	8.00E+14	0	31550
86. $\text{C}_2\text{H}_3 + \text{H} = \text{C}_2\text{H}_2 + \text{H}_2$	4.00E+13	0	0
87. $\text{C}_2\text{H}_3 + \text{O} = \text{CH}_2\text{CO} + \text{H}$	3.30E+13	0	0
88. $\text{C}_2\text{H}_3 + \text{O}_2 = \text{C}_2\text{H}_2 + \text{HO}_2$	4.00E+12	0	-250
89. $\text{C}_2\text{H}_3 + \text{OH} = \text{C}_2\text{H}_2 + \text{H}_2\text{O}$	5.00E+12	0	0
90. $\text{OH} + \text{C}_2\text{H}_2 = \text{C}_2\text{H} + \text{H}_2\text{O}$	3.37E+07	2	14000
91. $\text{OH} + \text{C}_2\text{H}_2 = \text{CH}_2\text{CO} + \text{H}$	2.18E-04	4.5	-1000
92. $\text{CH}_2\text{CO} + \text{H} = \text{CH}_3 + \text{CO}$	1.13E+13	0	3428
93. $\text{CH}_2\text{CO} + \text{H} = \text{HCCO} + \text{H}_2$	5.00E+13	0	8000
94. $\text{CH}_2\text{CO} + \text{O} = \text{HCCO} + \text{OH}$	1.00E+13	0	8000
95. $\text{CH}_2\text{CO} + \text{O} = \text{CH}_2\text{O} + \text{CO}$	1.50E+12	0	1350
96. $\text{CH}_2\text{CO} + \text{OH} = \text{HCCO} + \text{H}_2\text{O}$	7.50E+12	0	3000
97. $\text{CH}_2\text{CO} + \text{M} = \text{CH}_2 + \text{CO} + \text{M}$	1.50E+15	0	57600
98. $\text{C}_2\text{H} + \text{O}_2 = \text{CO} + \text{HCO}$	5.00E+13	0	1500
99. $\text{C}_2\text{H} + \text{C}_2\text{H}_2 = \text{C}_4\text{H}_2 + \text{H}$	4.00E+13	0	0
100. $\text{O} + \text{HCCO} = \text{H} + 2\text{CO}$	1.00E+14	0	0
101. $\text{HCCO} + \text{O}_2 = 2\text{CO} + \text{OH}$	1.60E+12	0	854
102. $\text{CH} + \text{HCCO} = \text{C}_2\text{H}_2 + \text{CO}$	5.00E+13	0	0
103. $2\text{HCCO} = \text{C}_2\text{H}_2 + 2\text{CO}$	1.00E+13	0	0
104. $\text{C}_2\text{H} + \text{O} = \text{CH} + \text{CO}$	5.00E+13	0	0
105. $\text{C}_2\text{H} + \text{OH} = \text{HCCO} + \text{H}$	2.00E+13	0	0
106. $2\text{CH}_2 = \text{C}_2\text{H}_2 + 2\text{H}$	1.00E+12	0.6	0
107. $\text{CH}_2 + \text{HCCO} = \text{C}_2\text{H}_3 + \text{CO}$	3.00E+13	0	0
108. $\text{C}_4\text{H}_2 + \text{OH} = \text{C}_3\text{H}_2 + \text{HCO}$	3.00E+13	0	0
109. $\text{C}_3\text{H}_2 + \text{O}_2 = \text{HCO} + \text{HCCO}$	1.00E+13	0	0
110. $\text{C}_4\text{H}_2 + \text{O} = \text{C}_3\text{H}_2 + \text{CO}$	2.70E+13	0	1700
111. $\text{C}_2\text{H}_2 + \text{M} = \text{C}_2\text{H} + \text{H} + \text{M}$	4.20E+16	0	107000
112. $\text{C}_2\text{H}_4 + \text{M} = \text{C}_2\text{H}_2 + \text{H}_2 + \text{M}$	1.50E+15	0	55440
113. $\text{C}_2\text{H}_4 + \text{M} = \text{C}_2\text{H}_3 + \text{H} + \text{M}$	1.40E+16	0	81280
114. $\text{H}_2 + \text{O}_2 = 2\text{OH}$	1.70E+13	0	47780
115. $\text{OH} + \text{H}_2 = \text{H}_2\text{O} + \text{H}$	6.40E+06	2	2961
116. $\text{O} + \text{OH} = \text{O}_2 + \text{H}$	4.50E+14	-0.5	600
117. $\text{O} + \text{H}_2 = \text{OH} + \text{H}$	5.06E+04	2.7	6290
118. $\text{H} + \text{O}_2 + \text{M} = \text{HO}_2 + \text{M}$	7.00E+17	-0.8	0

H2O Enhanced by 18.6

CO2	Enhanced by	4.2		
H2	Enhanced by	2.86		
CO	Enhanced by	2.11		
N2	Enhanced by	1.26		
119. H+HO2=2OH		2.50E+14	0	1900
120. O+HO2=OH+O2		4.80E+13	0	1000
121. OH+HO2=H2O+O2		5.00E+13	0	1000
122. 2OH=O+H2O		2.10E+08	1.4	-400
123. 2H+M=H2+M		1.00E+18	-1	0
H2	Enhanced by	0		
H2O	Enhanced by	0		
CO2	Enhanced by	0		
124. 2H+H2=2H2		9.20E+16	-0.6	0
125. 2H+H2O=H2+H2O		6.00E+19	-1.3	0
126. 2H+CO2=H2+CO2		5.49E+20	-2	0
127. H+OH+M=H2O+M		7.50E+23	-2.6	0
H2O	Enhanced by	5		
128. 2O+M=O2+M		1.89E+13	0	-1788
129. H+HO2=H2+O2		2.50E+13	0	700
130. 2HO2=H2O2+O2		2.00E+12	0	0
131. H2O2+M=2OH+M		1.20E+17	0	45500
132. H2O2+H=HO2+H2		1.70E+12	0	3750
133. H2O2+O=HO2+OH		9.60E+06	2	3974
134. H2O2+OH=H2O+HO2		1.00E+13	0	1800
135. CH+N2=HCN+N		3.00E+11	0	13600
136. CN+N=C+N2		1.90E+15	-0.6	0
137. CH2+N2=HCN+NH		1.00E+13	0	74000
138. H2CN+M=HCN+H+M		3.00E+14	0	22000
139. C+NO=CN+O		3.70E+13	0	0
140. CH+NO=HCN+O		1.10E+14	0	0
141. CH2+NO=HCNO+H		1.39E+12	0	-1100
142. CH3+NO=HCN+H2O		5.30E+11	0	15000
143. CH3+NO=H2CN+OH		5.30E+11	0	15000
144. HCCO+NO=HCNO+CO		2.00E+13	0	0
145. HCNO+H=HCN+OH		1.00E+14	0	12000
146. HNCO+O=NCO+OH		3.20E+12	0	10300
147. HNCO+OH=NCO+H2O		2.60E+12	0	5540
148. CH2+N=HCN+H		5.00E+13	0	0
149. CH+N=CN+H		1.30E+13	0	0
150. CO2+N=NO+CO		1.90E+11	0	3400
151. HCCO+N=HCN+CO		5.00E+13	0	0
152. CH3+N=H2CN+H		3.00E+13	0	0

153. C2H3+N=HCN+CH2	2.00E+13	0	0
154. HCN+OH=CN+H2O	1.45E+13	0	10929
155. OH+HCN=HOCN+H	5.85E+04	2.4	12500
156. OH+HCN=HNCO+H	1.98E-03	4	1000
157. OH+HCN=NH2+CO	7.83E-03	4	4000
158. HOCN+H=HNCO+H	1.00E+13	0	0
159. HCN+O=NCO+H	1.38E+04	2.6	4980
160. HCN+O=NH+CO	3.45E+03	2.6	4980
161. HCN+O=CN+OH	2.70E+09	1.6	29200
162. CN+H2=HCN+H	2.95E+05	2.5	2237
163. CN+O=CO+N	1.80E+13	0	0
164. CN+O2=NCO+O	5.60E+12	0	0
165. CN+OH=NCO+H	6.00E+13	0	0
166. HO2+NO=NO2+OH	2.11E+12	0	-479
167. NO2+H=NO+OH	3.50E+14	0	1500
168. NO2+O=NO+O2	1.00E+13	0	600
169. NO2+M=NO+O+M	1.10E+16	0	66000
170. NCO+H=NH+CO	5.00E+13	0	0
171. NCO+O=NO+CO	3.20E+13	0	0
172. NCO+N=N2+CO	2.00E+13	0	0
173. NCO+OH=NO+CO+H	1.00E+13	0	0
174. NCO+M=N+CO+M	3.10E+16	-0.5	47700
175. NCO+NO=N2O+CO	1.00E+13	0	-390
176. NCO+H2=HNCO+H	8.58E+12	0	9000
177. HNCO+H=NH2+CO	1.10E+14	0	12720
178. NH+O2=HNO+O	1.00E+13	0	12000
179. NH+O2=NO+OH	7.60E+10	0	1530
180. NH+O=NO+H	2.00E+13	0	0
181. NH+NO=N2O+H	2.40E+15	-0.8	0
182. N2O+OH=N2+HO2	2.00E+12	0	10000
183. N2O+H=N2+OH	1.90E+06	2.4	13500
184. N2O+M=N2+O+M	9.30E+14	0	59300
185. N2O+O=N2+O2	1.00E+14	0	28200
186. N2O+O=2NO	1.00E+14	0	28200
187. NH+OH=HNO+H	2.00E+13	0	0
188. NH+OH=N+H2O	5.00E+11	0.5	2000
189. NH+H=N+H2	1.00E+14	0	0
190. NH2+O=HNO+H	7.90E+14	-0.5	0
191. NH2+O=NH+OH	7.00E+12	0	0
192. NH2+OH=NH+H2O	4.00E+06	2	1000
193. NH2+H=NH+H2	6.92E+13	0	3650
194. NH2+NO=NNH+OH	6.40E+15	-1.3	0

195. $\text{NH}_3 + \text{OH} = \text{NH}_2 + \text{H}_2\text{O}$	2.04E+06	2	566
196. $\text{NH}_3 + \text{H} = \text{NH}_2 + \text{H}_2$	6.36E+05	2.4	10171
197. $\text{NH}_3 + \text{M} = \text{NH}_2 + \text{H} + \text{M}$	1.40E+16	0	90600
198. $\text{NNH} = \text{N}_2 + \text{H}$	1.00E+04	0	0
199. $\text{NNH} + \text{NO} = \text{N}_2 + \text{HNO}$	5.00E+13	0	0
200. $\text{NNH} + \text{H} = \text{N}_2 + \text{H}_2$	1.00E+14	0	0
201. $\text{NNH} + \text{OH} = \text{N}_2 + \text{H}_2\text{O}$	5.00E+13	0	0
202. $\text{NNH} + \text{O} = \text{N}_2\text{O} + \text{H}$	1.00E+14	0	0
203. $\text{HNO} + \text{M} = \text{H} + \text{NO} + \text{M}$	1.50E+16	0	48680
H_2O Enhanced by	10		
O_2 Enhanced by	2		
N_2 Enhanced by	2		
H_2 Enhanced by	2		
204. $\text{HNO} + \text{OH} = \text{NO} + \text{H}_2\text{O}$	3.60E+13	0	0
205. $\text{HNO} + \text{H} = \text{H}_2 + \text{NO}$	5.00E+12	0	0
206. $\text{N} + \text{NO} = \text{N}_2 + \text{O}$	3.27E+12	0.3	0
207. $\text{N} + \text{O}_2 = \text{NO} + \text{O}$	6.40E+09	1	6280
208. $\text{N} + \text{OH} = \text{NO} + \text{H}$	3.80E+13	0	0
209. $\text{NO} + \text{NH}_2 = \text{N}_2\text{O} + \text{H}_2$	5.00E+13	0	24640
210. $\text{NO} + \text{N}_2\text{H}_2 = \text{N}_2\text{O} + \text{NH}_2$	3.00E+12	0	0
211. $\text{NO}_2 + \text{NH}_2 = \text{N}_2\text{O} + \text{H}_2\text{O}$	1.90E+20	-3	0
212. $\text{HNO} + \text{NO} = \text{N}_2\text{O} + \text{OH}$	2.00E+12	0	26000
213. $\text{HNO} + \text{HNO} = \text{N}_2\text{O} + \text{H}_2\text{O}$	4.00E+12	0	5000
214. $\text{N}_2\text{O} + \text{CO} = \text{N}_2 + \text{CO}_2$	5.00E+13	0	44000
215. $\text{HCCO} + \text{OH} = \text{HCO} + \text{CO} + \text{H}$	1.00E+13	0	0
216. $\text{HCO} + \text{M} = \text{CO} + \text{H} + \text{M}$	2.50E+14	0	16802
217. $\text{NH}_3 + \text{O} = \text{NH}_2 + \text{OH}$	2.10E+13	0	9000
218. $\text{NO} + \text{NH}_2 = \text{N}_2 + \text{H}_2\text{O}$	6.20E+15	-1.3	0

NOTE: A units mole-cm-sec-K, E units cal/mole

Figure 1. Effect of residence time on NO exit concentration in reburning by methane (Input NO Concentration: 1000 ppm; Reactor Temperature: 1373 K)

Figure 2. Effect of residence time on HCN exit concentration in reburning by methane (Input NO Concentration: 1000 ppm; Reactor Temperature: 1373 K)

Figure 3. Effect of residence time on NH₃ exit concentration in reburning by methane (Input NO Concentration: 1000 ppm; Reactor Temperature: 1373 K)

Figure 4. Effect of reactor temperature on NO exit concentration in reburning by methane (Input NO Concentration: 1000 ppm; Residence Time: 0.2 s)

Figure 5. Effect of reactor temperature on HCN exit concentration in reburning by methane (Input NO Concentration: 1000 ppm; Residence Time: 0.2 s)

Figure 6. Effect of reactor temperature on NH₃ exit concentration in reburning by methane (Input NO Concentration: 1000 ppm; Residence Time: 0.2 s)