Supplementary Materials

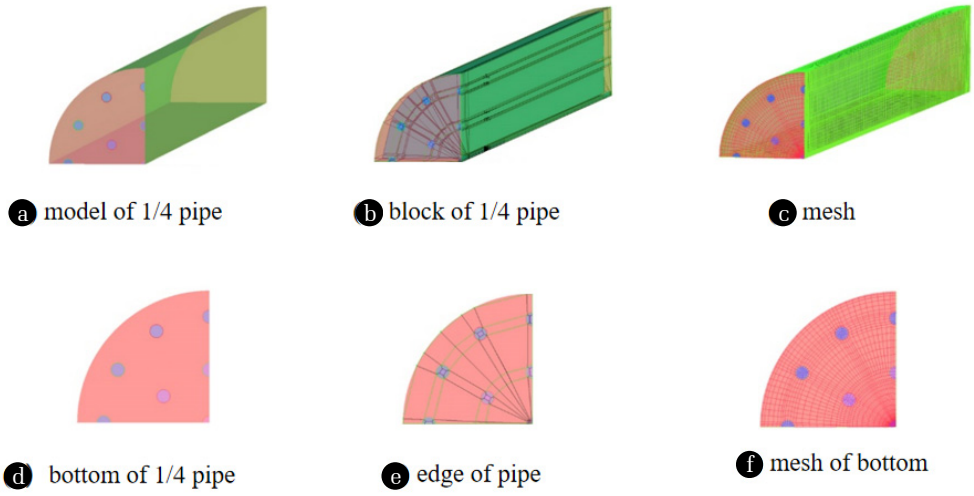

Fig. S1. Model and mesh (a) model of 1/4 pipe;(b) Block of 1/4 pipe; (c) mesh; (d) bottom of 1/4 pipe; (e) edge of pipe; (f) mesh of bottom;

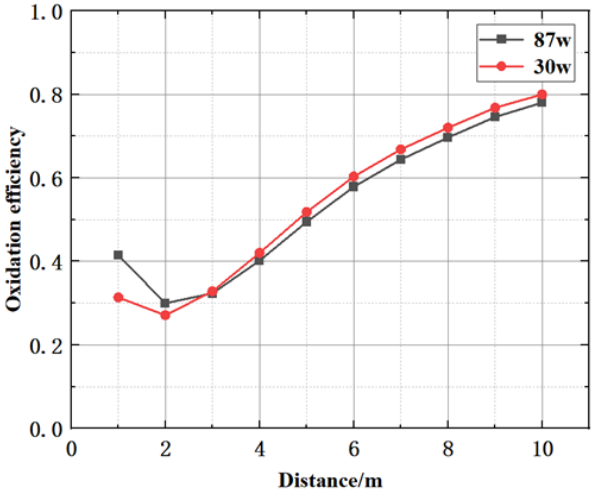

Fig. S2. Grid-independence

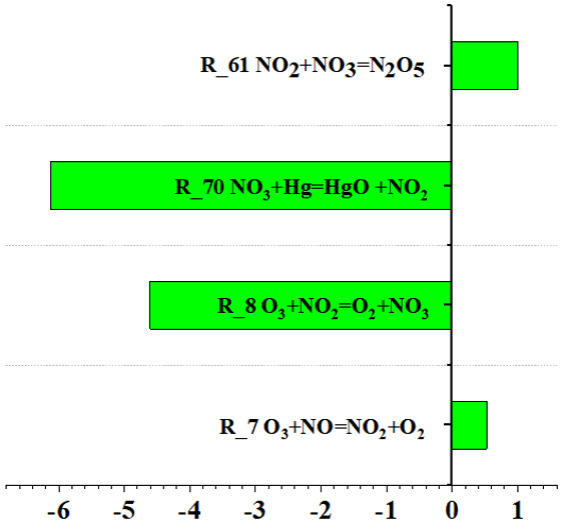

Fig. S3. Hg^0 consumption 50 % time sensitivity coefficient.

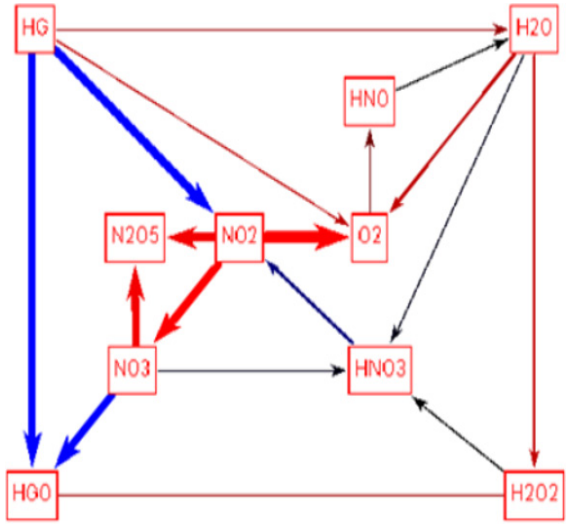

Fig. S4. Main oxidation reaction path of Hg^0. The thicker arrow denotes a faster reaction.

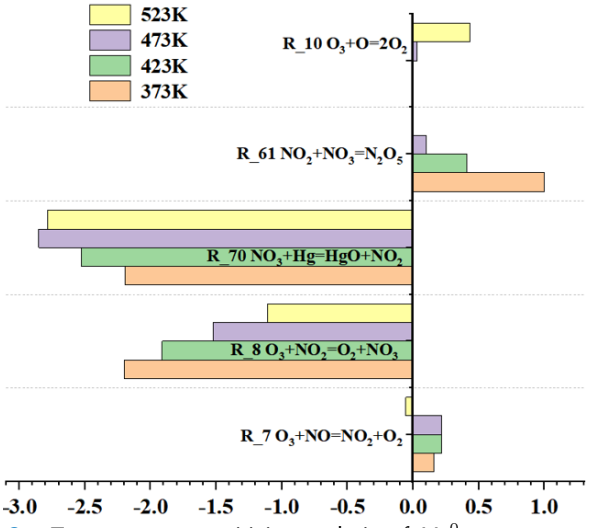

Fig. S5. Temperature sensitivity analysis of Hg^0

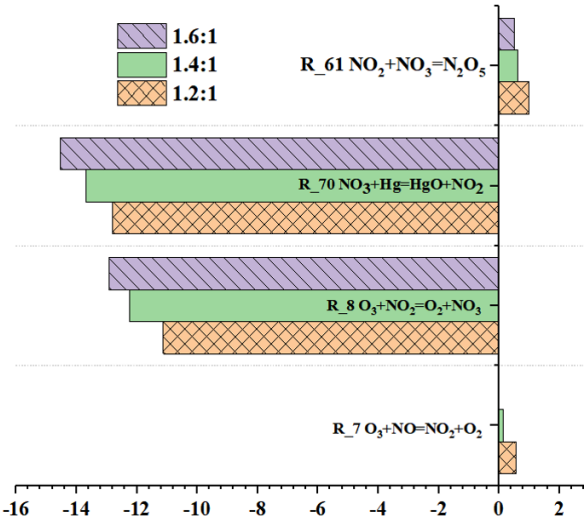

Fig. S6. Sensitivity analysis of O_3/NO at different molar ratios

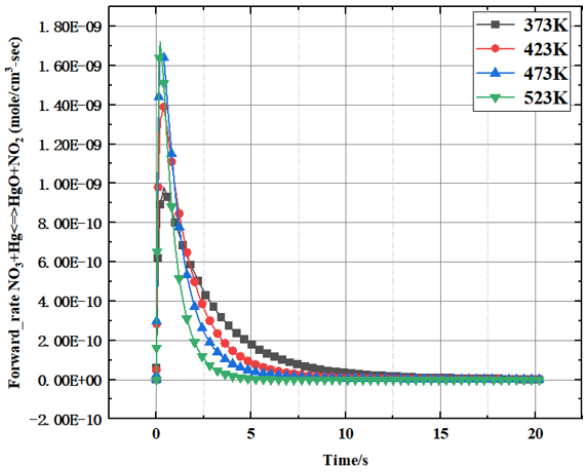

Fig. S7. Variation of key reaction rate with time

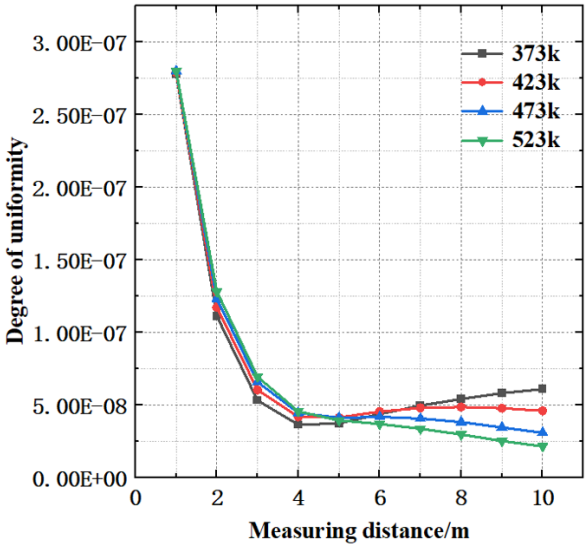

Fig. S8. Oxidation Uniformity

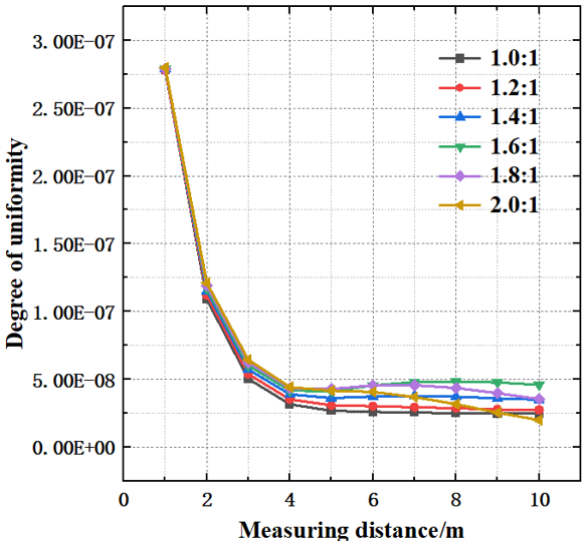

Fig. S9. Uniformity of Oxidation at Different Mole Ratios

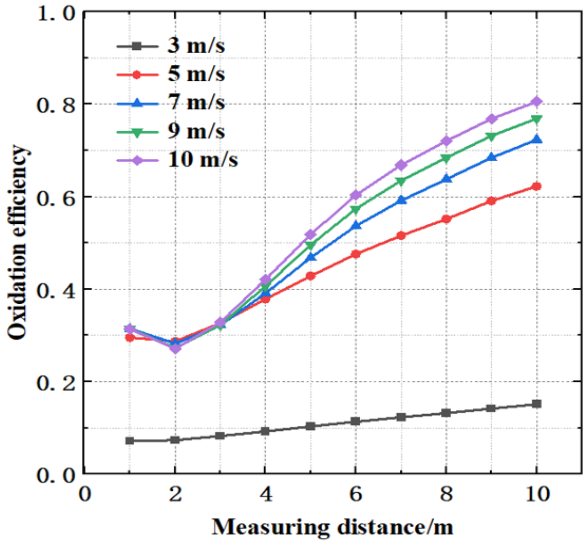

Fig. S10. Different Jet Velocity

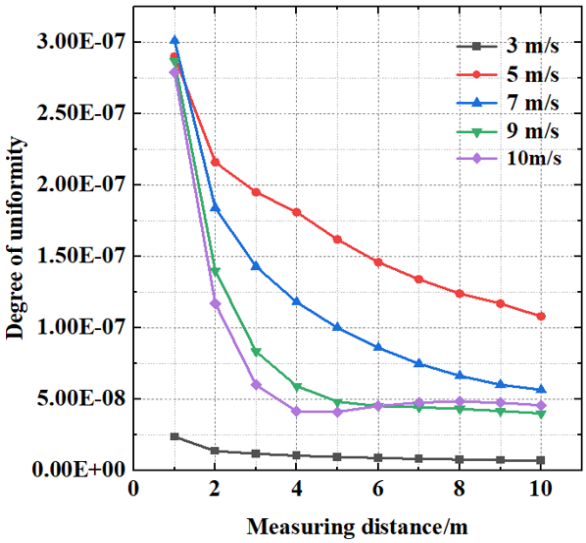

Fig. S11. Uniformity of Oxidation at Different Velocity

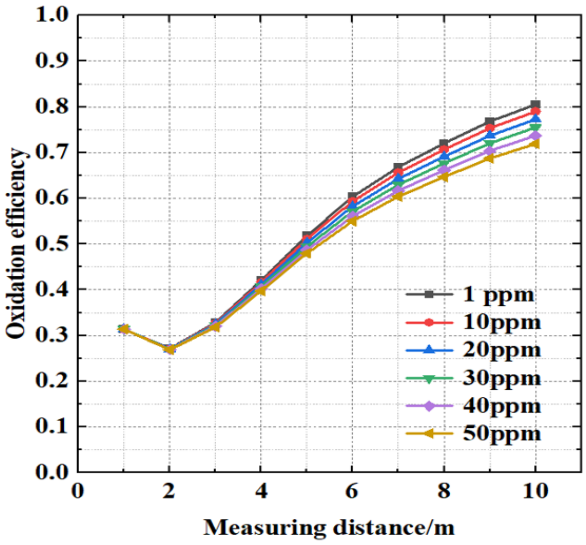

Fig. S12. Different Hg^0 Concentrations

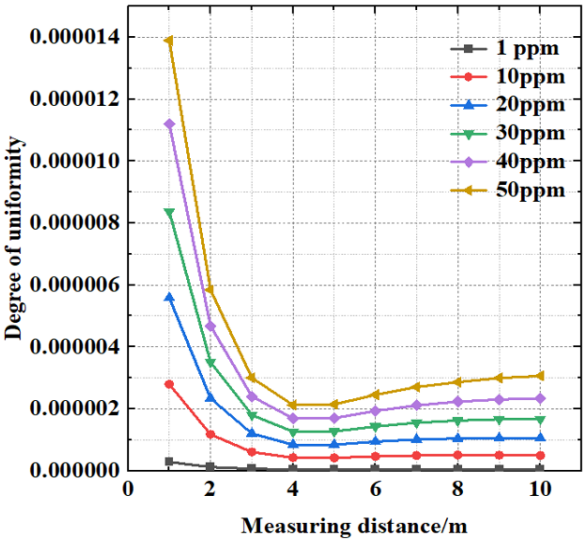

Fig. S13. Degradation Uniformity

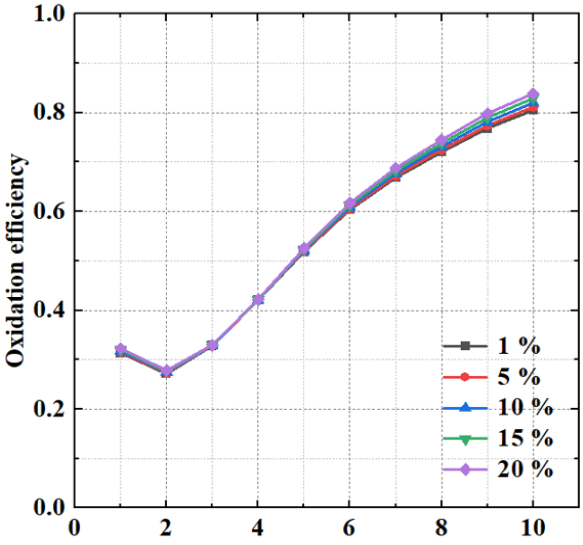

Fig. S14. Different moisture Concentration

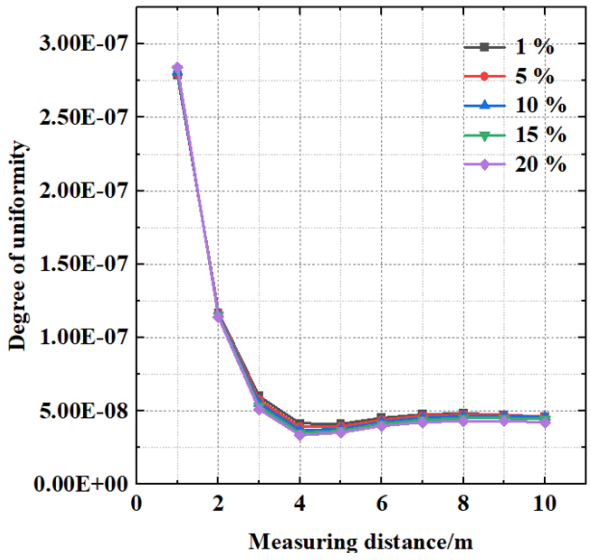

Fig. S15. Degradation uniformity

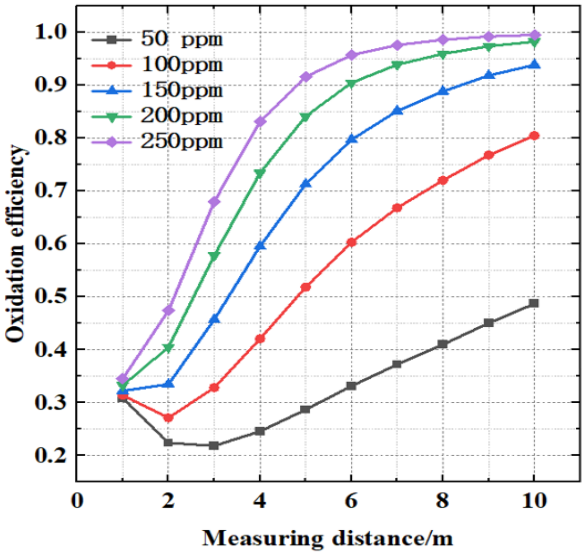

Fig. S16. Different NO concentrations

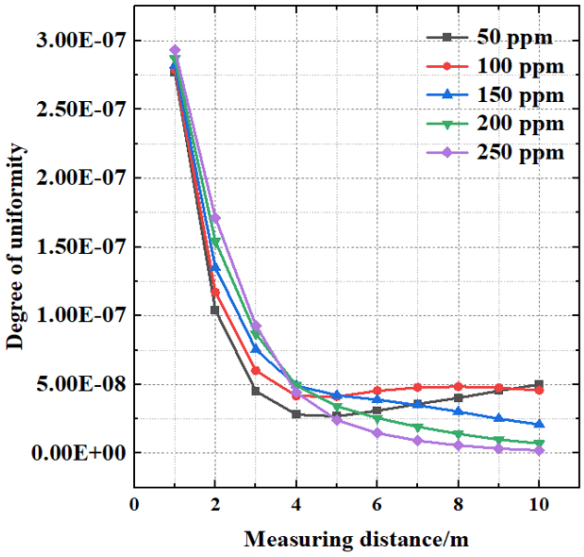

Fig. S17. Degradation uniformity

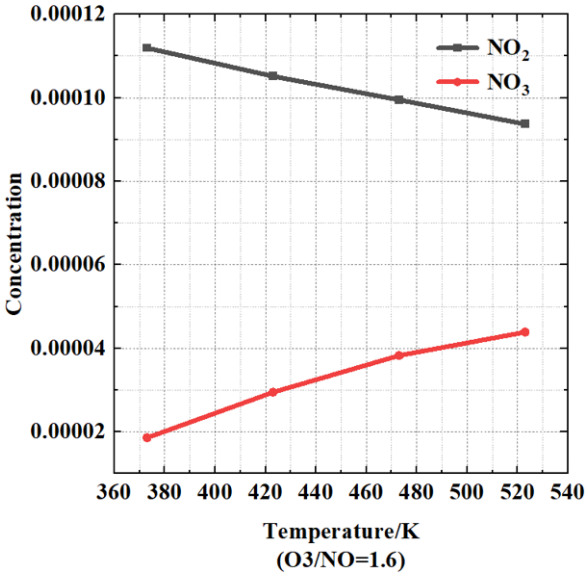

Fig. S18. The concentration of NO_3 and NO_2 at different temperatures

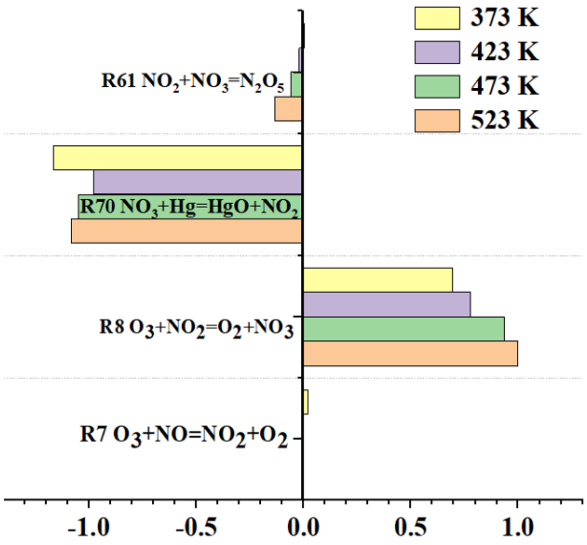

Fig. S19. NO_3 sensitivity analysis

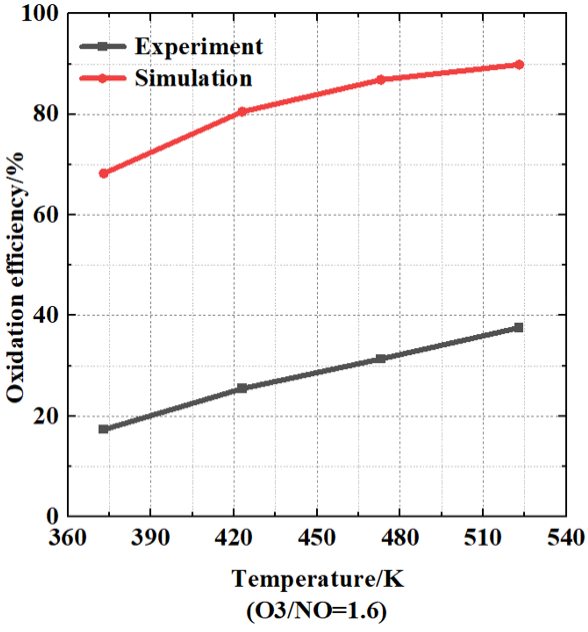

Fig. S20. Comparison of different temperatures

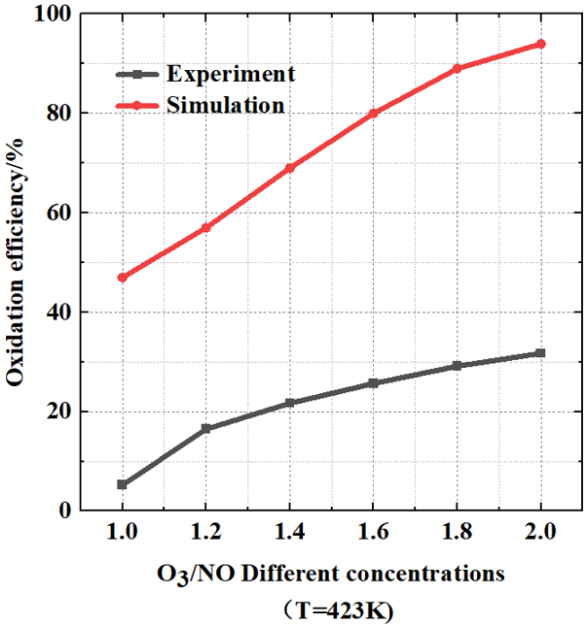

Fig. S21. Comparison of different molar ratios of O_3/NO

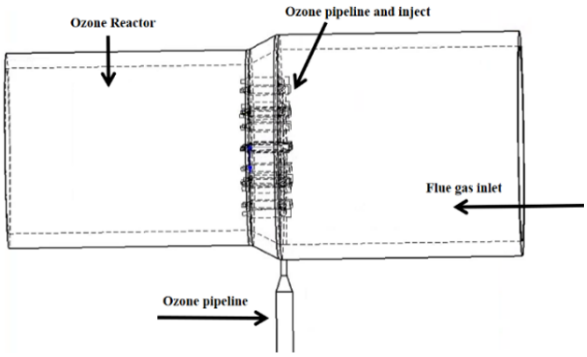

Fig. S22. Reaction pipeline

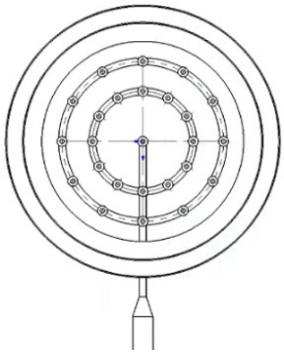

Fig. S23. Nozzle arrangement

Table S1. Detail reaction mechanism of Hg0 oxidization in flue gas by O3

No	Reaction	*A*	*b*	*E*	No	Reaction	*A*	*b*	*E*
1	$O_3+H=O_2+OH$	1.64×10^{13}	0.75	750	36	$H+HNO_2=NO_2+H_2$	1.37×10^{12}	1.55	6592
2	$O_3+H=O+HO_2$	4.52×10^{11}	0	0	37	$H+HNO_2=NO+H_2O$	3.85×10^{11}	1.89	3840
3	$O_3+OH=O_2+HO_2$	1.15×10^{12}	0	1990	38	$O_3+HNO_2=O_2+HNO_3$	3.01×10^{5}	0	0
4	$O_3+H_2O=O_2+H_2O_2$	6.62×10^{1}	0	0	39	$HNO_3+O=NO_3+OH$	1.81×10^{7}	0	0
5	$O_3+HO_2=2O_2+OH$	1.19×10^{8}	4.57	1380	40	$HNO_3+H=NO_3+H2$	3.4×10^{12}	1.53	16332
6	$O_3+N=O_2+NO$	6.00×10^{7}	0	0	41	$HNO_3+H=NO_2+H_2O$	8.39×10^{9}	3.29	6255
7	$O_3+NO=NO_2+O2$	1.8×10^{12}	0	2722	42	$HNO_3+NO=NO_2+HNO_2$	4.48×10^{3}	0	0
8	$O_3+NO_2=O_2+NO_3$	7.22×10^{10}	0	4870	43	$HNO_3+OH=NO_3+H_2O$	4.82×10^{8}	0	0
9	$O_3=O_2+O$	2.0×10^{15}	0	23250	44	$HNO_3+OH=NO_2+H_2O_2$	4.82×10^{8}	0	0
10	$O_3+O=2O_2$	4.82×10^{12}	0	4093.	45	$HNO_3=NO_2+OH$	6.90×10^{17}	0	45730
11	$H+O_2+M=HO_2+M$	3.61×10^{17}	-0.72	0	46	$HNO+O=NO+OH$	2.29×10^{13}	0	0
12	$H+H+M=H_2+M$	1.0×10^{18}	-1.0	0	47	$HNO+HNO=N_2O+H_2O$	2.55×10^{7}	3.98	1188
13	$H+H+H_2=H_2+H_2$	9.2×10^{16}	-0.6	0	48	$HNO+H=NO+H_2$	2.7×10^{13}	0.72	651
14	$H+H+H_2O=H_2+H_2O$	6.0×10^{19}	-1.25	0	49	$HNO+NO_2=NO+HNO_2$	6.03×10^{11}	0	1980
15	$H+OH+M=H_2O+M$	1.6×10^{22}	-2.0	0	50	$HNO+OH=NO+H_2O$	4.82×10^{13}	0	990
16	$H+O+M=OH+M$	6.2×10^{16}	-0.6	0	51	$H+HO_2=OH+OH$	8.22×10^{12}	0.75	0
17	$O+O+M=O_2+M$	1.89×10^{13}	0	-1788.	52	$NO_2+HO_2=HNO_2+O_2$	2.2×10^{-1}	0	0
18	$H_2O_2+M=OH+OH+M$	1.3×10^{17}	0	45500.	53	$NO+HO_2=HNO+O_2$	5.84×10^{5}	0	5600
19	$H_2+O_2=2OH$	1.7×10^{13}	0	47780.	54	$NO+HO_2=NO_2+OH$	6.32×10^{11}	0.58	1430
20	$OH+H_2=H_2O+H$	1.17×10^{9}	0	3626.	55	$NO+HO_2=HNO_3$	3.47×10^{12}	0	-5720
21	$O+OH=O_2+H$	3.61×10^{14}	-0.5	0	56	$H_2O+HO_2=H_2O_2+OH$	2.80×10^{13}	0	32790
22	$O+H_2=OH+H$	5.06×10^{4}	2.67	6290.	57	$H_2O_2+HO_2=O_2+H_2O+OH$	6.03×10^{10}	0	0
23	$O+HO_2=O_2+OH$	1.4×10^{13}	0	1073.	58	$OH+HO_2=O_2+H_2O$	4.28×10^{13}	-0.21	110
24	$2OH=O+H_2O$	6.0×10^{8}	1.3	0	59	$HO_2+HO_2=H_2O_2+O_2$	1.87×10^{12}	0	1540
25	$H+HO_2=H_2+O_2$	1.25×10^{13}	0	0	60	$HO_2=H+O_2$	1.45×10^{16}	-1.18	48490
26	$H_2O_2+H=HO_2+H_2$	1.6×10^{12}	0	3800.	61	$NO_2+NO_3=N_2O_5$	7.98×10^{17}	-3.9	0
27	$N+O_2=NO+O$	6.40×10^{9}	1.0	6280	62	$N+NO_2=O+O+N_2$	1.30×10^{-1}	0	0
28	$N+OH=NO+H$	3.80×10^{13}	0	0	63	$NO_2+H=NO+OH$	2.41×10^{14}	0	680
29	$NO+M=N+O+M$	9.64×10^{14}	0	620910	64	$NO+NO=O_2+N_2$	3.10×10^{13}	0	63190
30	$N+HO_2=NO+OH$	1.00×10^{13}	0	8390	65	$NO+N_2O=NO_2+N_2$	1.73×10^{11}	2.23	46300
31	$NO+N=N_2+O$	3.27×10^{12}	0.30	0	66	$O_3+Hg=HgO+O_2$	5.08×10^{7}	0	2796
32	$NO+O(+M)=NO_2(+M)$	1.30×10^{15}	-0.75	0	67	$OH+Hg=HgO+H$	2.14×10^{10}	0	-584
33	$NO+OH=HNO_2$	5.45×10^{17}	0	0	68	$H_2O_2+Hg=HgO+H_2O$	5.12×10^{5}	0	0
34	$O+HNO_2=NO_2+OH$	1.21×10^{13}	0	5938	69	$NO_2+Hg=HgO+NO$	1.81×10^{13}	0	171390
35	$H+HNO_2=HNO+OH$	7.57×10^{12}	0.86	4914	70	$NO_3+Hg=HgO+NO_2$	1.49×10^{14}	0	26136

(Arrhenius expression: $k=AT^{b}exp(-E/(RT))$; Preexponential factor A: $cm^3/mol/s$; Activate energy E: J/mol)

Table S2. Reduced reaction mechanism of Hg^0 oxidization in flue gas by O_3

Serial number	Reaction	A	b	E	Serial number	Reaction	A	b	E
1	$NO+M=N+O+M$	9.64E14	0	6.209E5	7	$NO_3+Hg=HgO+NO_2$	2.41E9	0	0
2	$O_3+O=2O_2$	4.82E12	0	4.09E3	8	$H_2O_2+Hg=HgO+O_2$	5.12E5	0	0
3	$2NO=O_2+N_2$	3.1E13	0	6.319E4	9	$O_3+Hg=HgO+O_2$	1.8E4	0	0
4	$O_3+NO=NO_2+O_2$	8.43E11	0	2.6E3	10	$NO_2+NO_3=N_2O_5$	7.98E17	-3.9	0
5	$O_3+NO_2=O_2+NO_3$	8.43E10	0	4.87E3	11	$O_3+H_2O=O_2+H_2O_2$	6.62E1	0	0
6	$H_2O_2+M=2OH+M$	1.3E17	0	4.55E4	12	$OH+Hg=HgO+H$	2.14E10	0	584

(Arrhenius expression: $k=AT^{b}exp(-E/(RT))$; Preexponential factor A: $cm^3/mol/s$; Activate energy E: J/mol)