Biomass Reburning: Modeling/Engineering Studies

**Quarterly Report
January 1 - March 31, 1998**

**By
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ABSTRACT

This project is designed to develop engineering and modeling tools for a family of NO_x control technologies utilizing biomass as a reburning fuel. The second reporting period (January 1 - March 31) included kinetic modeling of the reburning process while firing natural gas and biomass.

Modeling was done with a kinetic mechanism that combined reactions relevant to reburning from GRI-Mech 2.11 with SNCR reactions. Experimental data obtained in a 1 MMBtu/h Boiler Simulator Facility (BSF) for reburning with natural gas and biomass were modeled using the ODF kinetic code. System was treated as a series of four one-dimensional reactors.

Modeling of natural gas reburning qualitatively agrees with experimental data for a wide range of initial conditions. Modeling of furniture waste reburning does not qualitatively match experimental data due to a number of model simplifications.

Future work will concentrate on improving the basic reburning model to give quantitative agreement with experiments and on search for better representation of biomass composition in kinetic modeling.

Experimental data on biomass reburning are included in Appendix 3. These data were obtained during the reporting period in the scope of a coordinated program funded by the U.S. Department of Agriculture.

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1.0 Introduction

The objective of kinetic modeling is to create a model for predicting the NO_x control performance via reburning and advanced reburning. The model will include homogeneous reactions in the reburning and overfire air zones and, if required, heterogeneous processes on the surface of biomass particles with formation of char and tar compounds.

This report describes an initial attempt of chemical kinetic modeling of biomass reburning. The model includes only gas phase reactions. Modeling was done with a kinetic mechanism that combined reactions relevant to reburning from GRI-Mech 2.11 (*Bowman et al., 1997*) with SNCR reactions from *Miller and Glarborg, 1996*. The total mechanism included 418 reactions of 64 chemical species (Appendix 1). Thermodynamic data used in calculations are shown in Appendix 2. Since the kinetic mechanism extends to only C_1 and C_2 hydrocarbons, the biomass fuel was represented by a mixture of decomposition products, thus assuming rapid breakdown of the reburning fuel. The fuel oxygen was assumed to form CO in the substoichiometric environment. The remaining hydrocarbon component had a C:H ratio 2:3 and was represented by a mixture of C_2H_4 and C_2H_2 .

2.0 Model Description and Results for Natural Gas Reburning

Since the experimental performance of biomass as a reburning fuel is compared with that of natural gas, the kinetic model was first applied to natural gas reburning.

Experimental data used for comparison with modeling predictions (*Zamansky et al., 1997*) were obtained in the Boiler Simulator Facility (BSF) described earlier (*Ho et al., 1993*). The BSF has a full load firing capacity of 300 kW. It is designed to provide subscale simulation of the flue gas temperatures and compositions found in a conventional utility boiler.

The EER chemical kinetic code ODF, for “One Dimensional Flame” (*Kau and Tyson, 1987*) was employed. ODF treats a system as a series of one-dimensional reactors. Each reactor may be perfectly mixed (well-stirred) or unmixed (plug flow). Each ODF reactor may be assigned a variety of thermodynamic characteristics, including adiabatic, isothermal, or specified profiles of temperature or heat flux, and/or pressure. Process streams may be added over any interval of the plug flow reactor, with arbitrary mixing profiles along the reactor length. The flexibility in model setup allows for many different chemical processes to be simulated in a wide variety of environments.

The basic reburning process was treated as series of four reactors. Each reactor described one of the physical and chemical processes occurring in a boiler: addition of reburning fuel, NO_x reduction as a result of the reaction with the reburning fuel, addition of overfire air (OFA), and oxidation of partially oxidized products.

The mixture entering the first reactor corresponded to products of methane combustion in air with the following mixture composition ($\text{SR}_1 = 1.1$):

$$8.72\% \text{ CH}_4 - 19.18\% \text{ O}_2 - \text{balance N}_2$$

Assuming that the combustion process in the primary zone is complete, mixture with $\text{SR}_1 = 1.1$ generates about 8% CO_2 and 15% H_2O . At the same time, 1.74% O_2 is left which is available for oxidation of the reburning fuel. The initial amount of NO was varied in calculations from 100 to 600 ppm. Therefore, the premixed reactants entering the first reactor can be described as:

$$1.74\% \text{ O}_2 - 100\text{-}600 \text{ ppm NO} - 8\%\text{CO}_2 - 15\% \text{ H}_2\text{O} - \text{balance N}_2$$

The reburning fuel (natural gas) was added to the main stream of reactants in the first reactor. Composition of natural gas was assumed to be 90.7% CH_4 + 7.5% C_2H_6 + 1.5%

$\text{N}_2 + 0.25\% \text{CO}_2 + 0.05\% \text{O}_2$. The amount of the reburning fuel varied to provide a stoichiometric ratio SR_2 at the beginning of the first reactor from 0.84 to 0.99.

Physically, the process in the first reactor can be described as mixing of the reburning fuel with the main stream of gases. Proper modeling of mixing requires a combination of kinetic and gasdynamic equations, a feasible but not simple undertaking for a detailed chemical mechanism. As a first approximation, the gasdynamic mixing process was simulated by assuming that mixing just retards the rate at which the additive is delivered to the system, so that the initial concentration of the additive in each experiment increased within mixing time from zero to its final value (distributed reagent injection). Calculations were done for mixing times changing from 0 ms (instantaneous mixing) to 150 ms. Estimation of mixing time made using a droplet evaporation model for typical BSF conditions gave a value of 100 ms. Mixing was modeled in a one dimensional approximation, meaning that one or more reagents were added to the main stream over period of time, and at each moment mixing was assumed to be instantaneous. Temperatures of the main gas stream and injected substances were assumed to be the same.

Three different mixing models were utilized. In the first one natural gas was added at a constant rate to the stream of NO , O_2 , H_2O , CO_2 and N_2 over the period of mixing time. The second model was similar to the first one, except that the rate of natural gas addition linearly increased in time from 0 to its final value. The third model assumed that a mixture of NO , O_2 , CO_2 , H_2O and N_2 was slowly added to the stream of natural gas (so-called inverse mixing). This arrangement is opposite to real physical processes occurring in the BSF where reburning fuel is injected into the main stream, but from the kinetic point of view it provided description of the mixing process close to the real one: a high concentration of natural gas and low concentration of NO in the area of mixing.

The second reactor described the process of NO removal in the reburning zone after the reburning fuel and flue gas are mixed. The third reactor described the process of OFA mixing with flue gas. The mixing process was always described as OFA being added to the main stream of gas with a constant rate. The amount of OFA added varied such that the total mixture composition (including previously added fuel) at the beginning of the third reactor corresponded to $\text{SR}_3 = 1.15$. The fourth reactor described oxidation of products of incomplete combustion.

Temperature measurements in the BSF showed that the temperature along the reactor decrease with approximately linear rate. All calculations reported here were done with a constant rate of 300 K/s. Calculations with -250 K/s rate showed similar results.

Calculations showed that the mixing process in the reburning zone significantly affects modeling predictions, while mixing in the OFA zone has only minor effect on NO removal. Figure 1 shows the influence of mixing time in both zones on NO removal. Introduction of mixing in calculations significantly improves process performance. The significant effect of mixing in the reburning zone can be explained taking into account the fact that the value of mixing time is longer than the characteristic time of the chemical reaction. Since the temperature in the OFA zone is lower and the corresponding time of the chemical reaction is longer, mixing in the OFA zone has only a minor effect on NO removal.

Figure 1. Predicted effect of mixing time in reburning and OFA zones on NO removal. Reburning fuel is injected at 1700 K, OFA at 1422 K. $SR_2 = 0.99$, $[NO]_0 = 600$ ppm.

Figure 2 shows how the physical mode of mixing in the reburning zone affects NO removal. Inverse addition of the reburning fuel results in the best performance of the process. However, the difference in NO removal for different mixing modes is relatively small. For the purpose of simplicity all results reported here refer to the addition of natural gas to the flue gas with constant rate (first mixing model).

Figure 3 shows comparison of experimental results on basic reburning with modeling predictions. The model gives a close description of the experiments on basic reburning. For SR_2 slightly less than unity the model gives slightly steeper than experimental dependence of NO removal efficiency on the amount of the reburning fuel added. For rich mixture compositions ($SR_2 < 0.86$) the model underpredicts NO removal efficiency. These deviations can be explained by simplification of the mixing process in the current model.

Figure 4 shows influence of OFA injection temperature on NO removal. Injection of OFA at lower temperatures is more favorable. However, at lower temperatures efficiency of CO conversion to CO_2 is reduced. An optimum temperature that provides efficient $CO \rightarrow CO_2$ conversion and at the same time results in effective NO_x reduction has to be found for process optimization.

Figure 5 shows dependence of NO removal efficiency on the initial amount of NO. Modeling underpredicts NO removal efficiency for $SR_2 = 0.89$ (please see also Fig. 3). However, it gives similar to the experiment dependence of process efficiency on the initial amount of NO.

Figure 2. Influence of mixing mode in the reburning zone on NO removal. Mixing time is 100 ms. $SR_2 = 0.99$, $[NO]_0 = 600$ ppm.

Figure 3. Comparison of experimental results on basic reburning with modeling predictions. Reburning fuel is added at 1700 K, OFA at 1422 K. $[NO]_0 = 600$ ppm.

Figure 4. Comparison of experimental results on basic reburning with modeling predictions. Reburning fuel is added at 1700 K, $[\text{NO}]_0 = 600$ ppm.

Figure 5. Effect of the initial NO concentration on basic reburning. $\text{SR}_2 = 0.89$, $T_1 = 1700$ K, $T_2 = 1550$ K.

Conclusions derived from modeling of natural gas reburning are the following:

- The model qualitatively agrees with experimental data for a wide range of initial conditions and thus correctly represents main features of the reburning process.
- The model can be used for qualitative comparison with experimental data on biomass reburning.

3.0 Kinetic Modeling of Biomass Reburning

The kinetic mechanism developed for natural gas reburning was used for modeling of biomass reburning. Experimental data used for comparison with modeling were obtained within the framework of Phase II SBIR project “Advanced Biomass Reburning for High Efficiency NO_x Control” sponsored by the U.S. Department of Agriculture. All calculations were made for furniture manufacturing waste with composition shown in Table 3.1 Appendix 3.

The biomass fuel was represented by a mixture of decomposition products. The fuel oxygen was assumed to form CO, the remaining hydrocarbon component had a C:H ratio of approximately 2:3 and so was represented by a mixture of C₂H₄ and C₂H₂. The composition of decomposition products corresponding to the ultimate analysis shown in Table 3.1 was 69%CO + 24%C₂H₄ + 7%C₂H₂.

The procedure for modeling of biomass reburning was the same as for natural gas. The system was treated by the ODF kinetic code as series of four reactors with mixing of reburning fuel and OFA assuming distributed addition reagents over 100 ms mixing time in mixing zones (reactors one and three).

Figure 6 shows comparison of modeling predictions with experimental results on furniture waste reburning. The modeling data do not quantitatively match the experimental data. There are several reasons for this. The model contains simplifications, the most notable of which is the treatment of biomass as a mixture of CO, C₂H₄ and C₂H₂. Even though such treatment correctly represents C, H and O balance found in biomass produced from furniture waste, it ignores contribution of oxygen present in biomass into the reburning process (oxygen present in the form of CO does not participate in C₂H₄ and C₂H₂ oxidation since at high temperatures CO is simply oxidized to CO₂). Another disadvantage of such representation is that the carbon present in CO does not produce HCCO which is mainly responsible for NO removal in reburning zone.

4.0 Future Work

Future work will concentrate on improving the basic reburning model. Since the model generally agrees with experimental data for a wide range of initial conditions, we expect that significant improvement of modeling predictions can be achieved by variation of rate coefficient expressions of key reactions. Sensitivity analysis will be performed to identify most important reburning reactions. Model of inverse mixing represents the mixing process more realistically, it will be applied to a wide range of initial conditions.

Another direction of future work will be to search for better representation of biomass composition in kinetic modeling. Replacement of biomass by a mixture of decomposition products seems to be a promising approach. However, the composition of decomposition products should be better defined to be able to better predict the performance of biomass found in experiments. If necessary, heterogeneous processes on the surface of biomass particles with formation of char and tar compounds will be introduced into the model.

Figure 6. Performance of furniture waste reburning. Symbols are experiments, dashed line represents calculations. Reburning fuel is injected at 1700 K, OFA at 1450 K. $[\text{NO}]_0 = 400$ ppm.

5.0 References

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Appendix 1

Kinetic Mechanism (in Chemkin format, $k = AT^n \exp(-E/RT)$ / cm; mol; s; K)

REACTIONS	A	n	E
2O+M<=>O2+M	1.200E+17	-1.000	.00
H2/ 2.40/ H2O/15.40/ CH4/ 2.00/ CO/ 1.75/ CO2/ 3.60/ C2H6/ 3.00/ AR/ .83/			
O+H+M<=>OH+M	5.000E+17	-1.000	.00
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/			
O+H2<=>H+OH	5.000E+04	2.670	6290.00
O+HO2<=>OH+O2	2.000E+13	.000	.00
O+H2O2<=>OH+HO2	9.630E+06	2.000	4000.00
O+CH<=>H+CO	5.700E+13	.000	.00
O+CH2<=>H+HCO	8.000E+13	.000	.00
O+CH2 (S) <=>H2+CO	1.500E+13	.000	.00
O+CH2 (S) <=>H+HCO	1.500E+13	.000	.00
O+CH3<=>H+CH2O	8.430E+13	.000	.00
O+CH4<=>OH+CH3	1.020E+09	1.500	8600.00
O+CO+M<=>CO2+M	6.020E+14	.000	3000.00
H2/2.00/ O2/6.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/3.50/ C2H6/3.00/ AR/ .50/			
O+HCO<=>OH+CO	3.000E+13	.000	.00
O+HCO<=>H+CO2	3.000E+13	.000	.00
O+CH2O<=>OH+HCO	3.900E+13	.000	3540.00
O+CH2OH<=>OH+CH2O	1.000E+13	.000	.00
O+CH3O<=>OH+CH2O	1.000E+13	.000	.00
O+CH3OH<=>OH+CH2OH	3.880E+05	2.500	3100.00
O+CH3OH<=>OH+CH3O	1.300E+05	2.500	5000.00
O+C2H<=>CH+CO	5.000E+13	.000	.00
O+C2H2<=>H+HCCO	1.020E+07	2.000	1900.00
O+C2H2<=>OH+C2H	4.600E+19	-1.410	28950.00
O+C2H2<=>CO+CH2	1.020E+07	2.000	1900.00
O+C2H3<=>H+CH2CO	3.000E+13	.000	.00
O+C2H4<=>CH3+HCO	1.920E+07	1.830	220.00
O+C2H5<=>CH3+CH2O	1.320E+14	.000	.00
O+C2H6<=>OH+C2H5	8.980E+07	1.920	5690.00
O+HCCO<=>H+2CO	1.000E+14	.000	.00
O+CH2CO<=>OH+HCCO	1.000E+13	.000	8000.00
O+CH2CO<=>CH2+CO2	1.750E+12	.000	1350.00
O2+CO<=>O+CO2	2.500E+12	.000	47800.00
O2+CH2O<=>HO2+HCO	1.000E+14	.000	40000.00
H+O2+M<=>HO2+M	2.800E+18	-.860	.00
O2/ .00/ H2O/ .00/ CO/ .75/ CO2/1.50/ C2H6/1.50/ N2/ .00/ AR/ .00/			
H+2O2<=>HO2+O2	3.000E+20	-1.720	.00
H+O2+H2O<=>HO2+H2O	9.380E+18	-.760	.00
H+O2+N2<=>HO2+N2	3.750E+20	-1.720	.00
H+O2+AR<=>HO2+AR	7.000E+17	-.800	.00
H+O2<=>O+OH	8.300E+13	.000	14413.00
2H+M<=>H2+M	1.000E+18	-1.000	.00
H2/ .00/ H2O/ .00/ CH4/2.00/ CO2/ .00/ C2H6/3.00/ AR/ .63/			
2H+H2<=>2H2	9.000E+16	-.600	.00
2H+H2O<=>H2+H2O	6.000E+19	-1.250	.00
2H+CO2<=>H2+CO2	5.500E+20	-2.000	.00
H+OH+M<=>H2O+M	2.200E+22	-2.000	.00
H2/ .73/ H2O/3.65/ CH4/2.00/ C2H6/3.00/ AR/ .38/			
H+HO2<=>O+H2O	3.970E+12	.000	671.00
H+HO2<=>O2+H2	2.800E+13	.000	1068.00
H+HO2<=>2OH	1.340E+14	.000	635.00

H+H2O2<=>HO2+H2	1.210E+07	2.000	5200.00
H+H2O2<=>OH+H2O	1.000E+13	.000	3600.00
H+CH<=>C+H2	1.100E+14	.000	.00
H+CH2 (+M)<=>CH3 (+M)	2.500E+16	-.800	.00
LOW / 3.200E+27 -3.140 1230.00/			
TROE/ .6800 78.00 1995.00 5590.00 /			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/			
H+CH2 (S)<=>CH+H2	3.000E+13	.000	.00
H+CH3 (+M)<=>CH4 (+M)	1.270E+16	-.630	383.00
LOW / 2.477E+33 -4.760 2440.00/			
TROE/ .7830 74.00 2941.00 6964.00 /			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/			
H+CH4<=>CH3+H2	6.600E+08	1.620	10840.00
H+HCO (+M)<=>CH2O (+M)	1.090E+12	.480	-260.00
LOW / 1.350E+24 -2.570 1425.00/			
TROE/ .7824 271.00 2755.00 6570.00 /			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/			
H+HCO<=>H2+CO	7.340E+13	.000	.00
H+CH2O (+M)<=>CH2OH (+M)	5.400E+11	.454	3600.00
LOW / 1.270E+32 -4.820 6530.00/			
TROE/ .7187 103.00 1291.00 4160.00 /			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/			
H+CH2O (+M)<=>CH3O (+M)	5.400E+11	.454	2600.00
LOW / 2.200E+30 -4.800 5560.00/			
TROE/ .7580 94.00 1555.00 4200.00 /			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/			
H+CH2O<=>HCO+H2	2.300E+10	1.050	3275.00
H+CH2OH (+M)<=>CH3OH (+M)	1.800E+13	.000	.00
LOW / 3.000E+31 -4.800 3300.00/			
TROE/ .7679 338.00 1812.00 5081.00 /			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/			
H+CH2OH<=>H2+CH2O	2.000E+13	.000	.00
H+CH2OH<=>OH+CH3	1.200E+13	.000	.00
H+CH2OH<=>CH2 (S) +H2O	6.000E+12	.000	.00
H+CH3O (+M)<=>CH3OH (+M)	5.000E+13	.000	.00
LOW / 8.600E+28 -4.000 3025.00/			
TROE/ .8902 144.00 2838.00 45569.00 /			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/			
H+CH3O<=>H+CH2OH	3.400E+06	1.600	.00
H+CH3O<=>H2+CH2O	2.000E+13	.000	.00
H+CH3O<=>OH+CH3	3.200E+13	.000	.00
H+CH3O<=>CH2 (S) +H2O	1.600E+13	.000	.00
H+CH3OH<=>CH2OH+H2	1.700E+07	2.100	4870.00
H+CH3OH<=>CH3O+H2	4.200E+06	2.100	4870.00
H+C2H (+M)<=>C2H2 (+M)	1.000E+17	-1.000	.00
LOW / 3.750E+33 -4.800 1900.00/			
TROE/ .6464 132.00 1315.00 5566.00 /			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/			
H+C2H2 (+M)<=>C2H3 (+M)	5.600E+12	.000	2400.00
LOW / 3.800E+40 -7.270 7220.00/			
TROE/ .7507 98.50 1302.00 4167.00 /			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/			
H+C2H3 (+M)<=>C2H4 (+M)	6.080E+12	.270	280.00
LOW / 1.400E+30 -3.860 3320.00/			
TROE/ .7820 207.50 2663.00 6095.00 /			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/			
H+C2H3<=>H2+C2H2	3.000E+13	.000	.00
H+C2H4 (+M)<=>C2H5 (+M)	1.080E+12	.454	1820.00

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LOW / 1.200E+42 -7.620 6970.00/
TROE/ .9753 210.00 984.00 4374.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
H+C2H4<=>C2H3+H2 1.325E+06 2.530 12240.00
H+C2H5 (+M) <=>C2H6 (+M) 5.210E+17 -.990 1580.00
LOW / 1.990E+41 -7.080 6685.00/
TROE/ .8422 125.00 2219.00 6882.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
H+C2H5<=>H2+C2H4 2.000E+12 .000 .00
H+C2H6<=>C2H5+H2 1.150E+08 1.900 7530.00
H+HCCO<=>CH2 (S) +CO 1.000E+14 .000 .00
H+CH2CO<=>HCCO+H2 5.000E+13 .000 8000.00
H+CH2CO<=>CH3+CO 1.130E+13 .000 3428.00
H+HCCOH<=>H+CH2CO 1.000E+13 .000 .00
H2+CO (+M) <=>CH2O (+M) 4.300E+07 1.500 79600.00
LOW / 5.070E+27 -3.420 84350.00/
TROE/ .9320 197.00 1540.00 10300.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
OH+H2<=>H+H2O 2.160E+08 1.510 3430.00
2OH (+M) <=>H2O2 (+M) 7.400E+13 -.370 .00
LOW / 2.300E+18 -.900 -1700.00/
TROE/ .7346 94.00 1756.00 5182.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
2OH<=>O+H2O 3.570E+04 2.400 -2110.00
OH+HO2<=>O2+H2O 2.900E+13 .000 -500.00
OH+H2O2<=>HO2+H2O 1.750E+12 .000 320.00
DUPLICATE
OH+H2O2<=>HO2+H2O 5.800E+14 .000 9560.00
DUPLICATE
OH+C<=>H+CO 5.000E+13 .000 .00
OH+CH<=>H+HCO 3.000E+13 .000 .00
OH+CH2<=>H+CH2O 2.000E+13 .000 .00
OH+CH2<=>CH+H2O 1.130E+07 2.000 3000.00
OH+CH2 (S) <=>H+CH2O 3.000E+13 .000 .00
OH+CH3 (+M) <=>CH3OH (+M) 6.300E+13 .000 .00
LOW / 2.700E+38 -6.300 3100.00/
TROE/ .2105 83.50 5398.00 8370.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
OH+CH3<=>CH2+H2O 5.600E+07 1.600 5420.00
OH+CH3<=>CH2 (S) +H2O 2.501E+13 .000 .00
OH+CH4<=>CH3+H2O 1.000E+08 1.600 3120.00
OH+CO<=>H+CO2 4.760E+07 1.228 70.00
OH+HCO<=>H2O+CO 5.000E+13 .000 .00
OH+CH2O<=>HCO+H2O 3.430E+09 1.180 -447.00
OH+CH2OH<=>H2O+CH2O 5.000E+12 .000 .00
OH+CH3O<=>H2O+CH2O 5.000E+12 .000 .00
OH+CH3OH<=>CH2OH+H2O 1.440E+06 2.000 -840.00
OH+CH3OH<=>CH3O+H2O 6.300E+06 2.000 1500.00
OH+C2H<=>H+HCCO 2.000E+13 .000 .00
OH+C2H2<=>H+CH2CO 2.180E-04 4.500 -1000.00
OH+C2H2<=>H+HCCOH 5.040E+05 2.300 13500.00
OH+C2H2<=>C2H+H2O 3.370E+07 2.000 14000.00
OH+C2H2<=>CH3+CO 4.830E-04 4.000 -2000.00
OH+C2H3<=>H2O+C2H2 5.000E+12 .000 .00
OH+C2H4<=>C2H3+H2O 3.600E+06 2.000 2500.00
OH+C2H6<=>C2H5+H2O 3.540E+06 2.120 870.00
OH+CH2CO<=>HCCO+H2O 7.500E+12 .000 2000.00
2HO2<=>O2+H2O2 1.300E+11 .000 -1630.00

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DUPLICATE				
2HO2<=>O2+H2O2	4.200E+14	.000	12000.00	
DUPLICATE				
HO2+CH2<=>OH+CH2O	2.000E+13	.000	.00	
HO2+CH3<=>O2+CH4	1.000E+12	.000	.00	
HO2+CH3<=>OH+CH3O	2.000E+13	.000	.00	
HO2+CO<=>OH+CO2	1.500E+14	.000	23600.00	
HO2+CH2O<=>HCO+H2O2	1.000E+12	.000	8000.00	
C+O2<=>O+CO	5.800E+13	.000	576.00	
C+CH2<=>H+C2H	5.000E+13	.000	.00	
C+CH3<=>H+C2H2	5.000E+13	.000	.00	
CH+O2<=>O+HCO	3.300E+13	.000	.00	
CH+H2<=>H+CH2	1.107E+08	1.790	1670.00	
CH+H2O<=>H+CH2O	1.713E+13	.000	-755.00	
CH+CH2<=>H+C2H2	4.000E+13	.000	.00	
CH+CH3<=>H+C2H3	3.000E+13	.000	.00	
CH+CH4<=>H+C2H4	6.000E+13	.000	.00	
CH+CO (+M) <=>HCCO (+M)	5.000E+13	.000	.00	
LOW / 2.690E+28 -3.740 1936.00/				
TROE/ .5757 237.00 1652.00 5069.00 /				
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/				
CH+CO2<=>HCO+CO	3.400E+12	.000	690.00	
CH+CH2O<=>H+CH2CO	9.460E+13	.000	-515.00	
CH+HCCO<=>CO+C2H2	5.000E+13	.000	.00	
CH2+O2<=>OH+HCO	1.320E+13	.000	1500.00	
CH2+H2<=>H+CH3	5.000E+05	2.000	7230.00	
2CH2<=>H2+C2H2	3.200E+13	.000	.00	
CH2+CH3<=>H+C2H4	4.000E+13	.000	.00	
CH2+CH4<=>2CH3	2.460E+06	2.000	8270.00	
CH2+CO (+M) <=>CH2CO (+M)	8.100E+11	.500	4510.00	
LOW / 2.690E+33 -5.110 7095.00/				
TROE/ .5907 275.00 1226.00 5185.00 /				
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/				
CH2+HCCO<=>C2H3+CO	3.000E+13	.000	.00	
CH2 (S) +N2<=>CH2+N2	1.500E+13	.000	600.00	
CH2 (S) +AR<=>CH2+AR	9.000E+12	.000	600.00	
CH2 (S) +O2<=>H+OH+CO	2.800E+13	.000	.00	
CH2 (S) +O2<=>CO+H2O	1.200E+13	.000	.00	
CH2 (S) +H2<=>CH3+H	7.000E+13	.000	.00	
CH2 (S) +H2O (+M) <=>CH3OH (+M)	2.000E+13	.000	.00	
LOW / 2.700E+38 -6.300 3100.00/				
TROE/ .1507 134.00 2383.00 7265.00 /				
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/				
CH2 (S) +H2O<=>CH2+H2O	3.000E+13	.000	.00	
CH2 (S) +CH3<=>H+C2H4	1.200E+13	.000	-570.00	
CH2 (S) +CH4<=>2CH3	1.600E+13	.000	-570.00	
CH2 (S) +CO<=>CH2+CO	9.000E+12	.000	.00	
CH2 (S) +CO2<=>CH2+CO2	7.000E+12	.000	.00	
CH2 (S) +CO2<=>CO+CH2O	1.400E+13	.000	.00	
CH2 (S) +C2H6<=>CH3+C2H5	4.000E+13	.000	-550.00	
CH3+O2<=>O+CH3O	2.675E+13	.000	28800.00	
CH3+O2<=>OH+CH2O	3.600E+10	.000	8940.00	
CH3+H2O2<=>HO2+CH4	2.450E+04	2.470	5180.00	
2CH3 (+M) <=>C2H6 (+M)	2.120E+16	-.970	620.00	
LOW / 1.770E+50 -9.670 6220.00/				
TROE/ .5325 151.00 1038.00 4970.00 /				
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/				
2CH3<=>H+C2H5	4.990E+12	.100	10600.00	

CH3+HCO<=>CH4+CO	2.648E+13	.000	.00
CH3+CH2O<=>HCO+CH4	3.320E+03	2.810	5860.00
CH3+CH3OH<=>CH2OH+CH4	3.000E+07	1.500	9940.00
CH3+CH3OH<=>CH3O+CH4	1.000E+07	1.500	9940.00
CH3+C2H4<=>C2H3+CH4	2.270E+05	2.000	9200.00
CH3+C2H6<=>C2H5+CH4	6.140E+06	1.740	10450.00
HCO+M<=>H+CO+M	1.870E+17	-1.000	17000.00
H2/2.00/ H2O/ 11.20/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/			
HCO+O2<=>HO2+CO	7.600E+12	.000	400.00
CH2OH+O2<=>HO2+CH2O	1.800E+13	.000	900.00
CH3O+O2<=>HO2+CH2O	4.280E-13	7.600	-3530.00
C2H+O2<=>HCO+CO	5.000E+13	.000	1500.00
C2H+H2<=>H+C2H2	4.070E+05	2.400	200.00
C2H3+O2<=>HCO+CH2O	3.980E+12	.000	-240.00
C2H4 (+M) <=> H2+C2H2 (+M)	8.000E+12	.440	88770.00
LOW / 7.000E+50 -9.310 99860.00/			
TROE/ .7345 180.00 1035.00 5417.00 /			
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/			
C2H5+O2<=>HO2+C2H4	8.400E+11	.000	3875.00
HCCO+O2<=>OH+2CO	1.600E+12	.000	854.00
2HCCO<=>2CO+C2H2	1.000E+13	.000	.00
! *** NH3 Reactions ***			
!			
NH3+M = NH2+H+M	2.2E16	0	93470 ! a
NH3+H = NH2+H2	6.4E05	2.39	10171 ! a
NH3+O = NH2+OH	9.4E06	1.94	6460 ! a
NH3+OH = NH2+H2O	2.0E06	2.04	566 ! a
NH3+HO2 = NH2+H2O2	3.0E11	0	22000 ! a
!			
! *** NH2 Reactions ***			
!			
NH2+H = NH+H2	4.0E13	0	3650 ! a
NH2+O = HNO+H	6.6E14	-0.5	0 ! a
NH2+O = NH+OH	6.8E12	0	0 ! a
NH2+OH = NH+H2O	4.0E06	2.0	1000 ! a
NH2+HO2 = H2NO+OH	5.0E13	0	0 ! a
NH2+HO2 = NH3+O2	1.0E13	0	0 ! a
H2NO+O = NH2+O2	2.0E14	0	0 ! c
NH2+NH2= N2H2+H2	8.5E11	0	0 ! a
NH2+NH2= NH3+NH	5.0E13	0	10000 ! a
NH2+NH2 (+M)=N2H4 (+M)	1.5E13	0	0 ! a
LOW/1.0E18 0 0/			
N2/2.5/ H2O/5/ NH3/10/			
NH2+NH = N2H2+H	5.0E13	0	0 ! a
NH2+N = N2+2H	7.0E13	0	0 ! a
NH2+NO = NNH+OH	8.9E12	-0.35	0 ! c
NH2+NO = N2+H2O	1.3E16	-1.25	0 ! a
DUP			
NH2+NO = N2+H2O	-8.9E12	-0.35	0 ! c
DUP			
NH2+NO2 = N2O+H2O	3.2E18	-2.2	0 ! a
NH2+NO2 = H2NO+NO	3.5E12	0	0 ! b
!			
! *** NH and N Reactions ***			
!			
NH+H = N+H2	3.0E13	0	0 ! a
NH+O = NO+H	9.2E13	0	0 ! a
NH+OH = HNO+H	2.0E13	0	0 ! a

NH+OH = N+H2O	5.0E11	0.5	2000	!	a
NH+O2 = HNO+O	4.6E05	2.0	6500	!	a
NH+O2 = NO+OH	1.3E06	1.5	100	!	a
NH+N = N2+H	3.0E13	0	0	!	a
NH+NH = N2+2H	2.5E13	0	0	!	a
NH+NO = N2O+H	2.9E14	-0.4	0	!	a
DUP					
NH+NO = N2O+H	-2.2E13	-0.23	0	!	
DUP					
NH+NO = N2+OH	2.2E13	-0.23	0	!	a
NH+NO2 = N2O+OH	1.0E13	0	0	!	a
N+OH = NO+H	3.8E13	0	0	!	a
N+O2 = NO+O	6.4E09	1.0	6280	!	a
N+NO = N2+O	3.3E12	0.3	0	!	a
!					
! *** NO Reactions ***					
!					
NO+O+M = NO2+M	7.5E19	-1.41	0	!	b
N2/1.7/ O2/1.5/ H2O/10/					
NO+OH+M = HONO+M	5.0E23	-2.51	-68	!	b
N2/1.0/ H2O/5.0/					
NO+HO2 = NO2+OH	2.1E12	0	-480	!	a
!					
! *** Consumption of NO2 ***					
!					
NO2+H = NO+OH	8.4E13	0	0	!	b
NO2+O = NO+O2	3.9E12	0	-238	!	b
NO2+O(+M) = NO3(+M)	1.3E13	0.00	0	!	b
LOW/1.0E28 -4.08 2470/					
N2/1.5/ O2/1.5/ H2O/18.6/					
NO2+NO2 = NO+NO+O2	1.6E12	0	26123	!	b
NO2+NO2 = NO3+NO	9.6E09	0.73	20900	!	b
!					
! *** Reactions of HNO, HONO, H2NO, NO3 ***					
!					
HNO+M = H+NO+M	1.5E16	0	48680	!	a
H2O/10/ O2/2/ N2/2/ H2/2/					
HNO+H = NO+H2	4.4E11	0.72	650	!	a
HNO+O = NO+OH	1.0E13	0	0	!	a
HNO+OH = NO+H2O	3.6E13	0	0	!	a
HNO+O2 = NO+HO2	1.0E13	0	25000	!	a
HNO+NH2= NO+NH3	2.0E13	0	1000	!	a
HNO+NO = N2O+OH	2.0E12	0	26000	!	a
HNO+NO2 = HONO+NO	6.0E11	0.00	2000	!	b
HNO+HNO = N2O+H2O	4.0E12	0	5000	!	a
HONO+H = NO2+H2	1.2E13	0.0	7350	!	b
HONO+O = NO2+OH	1.2E13	0.0	6000	!	b
HONO+OH = NO2+H2O	4.0E12	0	0	!	b
HONO+NH = NH2+NO2	1.0E13	0	0	!	b
HONO+NH2 = NH3+NO2	5.0E12	0	0	!	b
HONO+HONO=NO+NO2+H2O	2.3E12	0	8400	!	b
H2NO+M = HNO+H+M	2.5E16	0	50000	!	c
H2NO+H = HNO+H2	3.0E07	2.0	2000	!	a
H2NO+H = NH2+OH	5.0E13	0	0	!	a
H2NO+O = HNO+OH	3.0E07	2.0	2000	!	a
H2NO+OH = HNO+H2O	2.0E07	2.0	1000	!	a
H2NO+NO = HNO+HNO	2.0E07	2.0	13000	!	a
H2NO+NH2 = HNO+NH3	3.0E12	0	1000	!	a

H2NO+NO2 = HONO+HNO	6.0E11	0.00	2000	!	b
NO3+H = NO2+OH	6.0E13	0.0	0	!	b
NO3+O = NO2+O2	1.0E13	0.0	0	!	b
NO3+OH = NO2+HO2	1.4E13	0.0	0	!	b
NO3+HO2 = NO2+O2+OH	1.5E12	0.0	0	!	b
NO3+NO2 = NO+NO2+O2	5.0E10	0.00	2940	!	b
!					
! *** N2-amine Subset ***					
!					
N2H4+H = N2H3+H2	1.3E13	0	2500	!	a
N2H4+O = N2H2+H2O	8.5E13	0	1200	!	a
N2H4+OH = N2H3+H2O	4.0E13	0	0	!	b
N2H4+NH2 = N2H3+NH3	3.9E12	0	1500	!	a
N2H3+M = N2H2+H+M	3.5E16	0	46000	!	a
N2H3+H = NH2+NH2	1.6E12	0	0	!	a
N2H3+O = N2H2+OH	5.0E12	0	5000	!	a
N2H3+O = NH2+HNO	1.0E13	0	0	!	a
N2H3+OH = N2H2+H2O	1.0E13	0	1000	!	a
N2H3+OH = NH3+HNO	1.0E12	0	15000	!	a
N2H3+NH = N2H2+NH2	2.0E13	0	0	!	a
N2H2+M = NNH+H+M	5.0E16	0	50000	!	a
H2O/15.0/ H2/2.0/ N2/2.0/ O2/2.0/					
N2H2+H = NNH+H2	5.0E13	0	1000	!	a
N2H2+O = NH2+NO	1.0E13	0	1000	!	a
N2H2+O = NNH+OH	2.0E13	0	1000	!	a
N2H2+OH = NNH+H2O	1.0E13	0	1000	!	a
N2H2+NH = NNH+NH2	1.0E13	0	1000	!	a
N2H2+NH2= NNH+NH3	1.0E13	0	1000	!	a
N2H2+NO = N2O+NH2	3.0E12	0	0	!	a
NNH = N2+H	1.0E07	0	0	!	c
NNH+H = N2+H2	1.0E14	0	0	!	a
NNH+O = N2O+H	1.0E14	0	0	!	a
NNH+O = NH+NO	5.0E13	0	0	!	b
NNH+OH = N2+H2O	5.0E13	0	0	!	a
NNH+O2 = N2+HO2	2.0E14	0	0	!	c
NNH+O2 = N2+H+O2	5.0E13	0	0	!	c
NNH+NH = N2+NH2	5.0E13	0	0	!	a
NNH+NH2 = N2+NH3	5.0E13	0	0	!	a
NNH+NO = N2+HNO	5.0E13	0	0	!	a
!					
! *** N2O Subset ***					
!					
N2O+M = N2+O+M	4.0E14	0	56100	!	a
N2/1.7/ O2/1.4/ CO2/3.0/ H2O/12/				!	
N2O+H = N2+OH	3.3E10	0	4729	!	b
DUP					
N2O+H = N2+OH	4.4E14	0	19254	!	
DUP					
N2O+O = NO+NO	2.9E13	0	23150	!	a
N2O+O = N2+O2	1.4E12	0	10800	!	a
N2O+OH = N2+HO2	2.0E12	0	40000	!	b

Appendix 2

Thermodynamic Data Used for Modeling (in NASA format)

ELEMENTS

O H C N AR

SPECIES

NH3 O2 NO H2O CO2 N2
H2 H O OH HO2 H2O2
C CH CH2 CH2 (S) CH3 CH4 CO
HCO CH2O CH2OH CH3O CH3OH C2H C2H2 C2H3
C2H4 C2H5 C2H6 HCCO CH2CO HCCOH
N NH NH2 NNH N2H2 N2H3 N2H4
HNO HONO NO3 H2NO N2O NO2
AR

THERMO

300.000	1500.000	5000.000								
O	L 1/900	1	00	00	00G	200.000	3500.000	1000.000		1
	2.56942078E+00-8.59741137E-05	4.19484589E-08-1.00177799E-11	1.22833691E-15							2
	2.92175791E+04	4.78433864E+00	3.16826710E+00-3.27931884E-03	6.64306396E-06						3
	-6.12806624E-09	2.11265971E-12	2.91222592E+04	2.05193346E+00	6.72540300E+03					4
O2	TPIS89O	2	00	00	00G	200.000	3500.000	1000.000		1
	3.28253784E+00	1.48308754E-03-7.57966669E-07	2.09470555E-10-2.16717794E-14							2
	-1.08845772E+03	5.45323129E+00	3.78245636E+00-2.99673416E-03	9.84730201E-06						3
	-9.68129509E-09	3.24372837E-12-1.06394356E+03	3.65767573E+00	8.68010400E+03						4
H	L 7/88H	1	00	00	00G	200.000	3500.000	1000.000		1
	2.50000001E+00-2.30842973E-11	1.61561948E-14-4.73515235E-18	4.98197357E-22							2
	2.54736599E+04-4.46682914E-01	2.50000000E+00	7.05332819E-13-1.99591964E-15							3
	2.30081632E-18-9.27732332E-22	2.54736599E+04-4.46682853E-01	6.19742800E+03							4
H2	TPIS78H	2	00	00	00G	200.000	3500.000	1000.000		1
	3.33727920E+00-4.94024731E-05	4.99456778E-07-1.79566394E-10	2.00255376E-14							2
	-9.50158922E+02-3.20502331E+00	2.34433112E+00	7.98052075E-03-1.94781510E-05							3
	2.01572094E-08-7.37611761E-12-9.17935173E+02	6.83010238E-01	8.46810200E+03							4
OH	RUS 78O	1H	1	00	00G	200.000	3500.000	1000.000		1
	3.09288767E+00	5.48429716E-04	1.26505228E-07-8.79461556E-11	1.17412376E-14						2
	3.85865700E+03	4.47669610E+00	3.99201543E+00-2.40131752E-03	4.61793841E-06						3
	-3.88113333E-09	1.36411470E-12	3.61508056E+03-1.03925458E-01	8.81310600E+03						4
H2O	L 8/89H	2O	1	00	00G	200.000	3500.000	1000.000		1
	3.03399249E+00	2.17691804E-03-1.64072518E-07-9.70419870E-11	1.68200992E-14							2
	-3.00042971E+04	4.96677010E+00	4.19864056E+00-2.03643410E-03	6.52040211E-06						3
	-5.48797062E-09	1.77197817E-12-3.02937267E+04-8.49032208E-01	9.90409200E+03							4
HO2	L 5/89H	1O	2	00	00G	200.000	3500.000	1000.000		1
	4.01721090E+00	2.23982013E-03-6.33658150E-07	1.14246370E-10-1.07908535E-14							2
	1.11856713E+02	3.78510215E+00	4.30179801E+00-4.74912051E-03	2.11582891E-05						3
	-2.42763894E-08	9.29225124E-12	2.94808040E+02	3.71666245E+00	1.00021620E+04					4
H2O2	L 7/88H	2O	2	00	00G	200.000	3500.000	1000.000		1
	4.16500285E+00	4.90831694E-03-1.90139225E-06	3.71185986E-10-2.87908305E-14							2
	-1.78617877E+04	2.91615662E+00	4.27611269E+00-5.42822417E-04	1.67335701E-05						3
	-2.15770813E-08	8.62454363E-12-1.77025821E+04	3.43505074E+00	1.11588350E+04						4
C	L11/88C	1	00	00	00G	200.000	3500.000	1000.000		1
	2.49266888E+00	4.79889284E-05-7.24335020E-08	3.74291029E-11-4.87277893E-15							2
	8.54512953E+04	4.80150373E+00	2.55423955E+00-3.21537724E-04	7.33792245E-07						3
	-7.32234889E-10	2.66521446E-13	8.54438832E+04	4.53130848E+00	6.53589500E+03					4

CH	TPIS79C	1H	1	00	00G	200.000	3500.000	1000.000	1
	2.87846473E+00	9.70913681E-04	1.44445655E-07	-1.30687849E-10	1.76079383E-14				2
	7.10124364E+04	5.48497999E+00	3.48981665E+00	3.23835541E-04	-1.68899065E-06				3
	3.16217327E-09	-1.40609067E-12	7.07972934E+04	2.08401108E+00	8.62500000E+03				4
CH2	L S/93C	1H	2	00	00G	200.000	3500.000	1000.000	1
	2.87410113E+00	3.65639292E-03	-1.40894597E-06	2.60179549E-10	-1.87727567E-14				2
	4.62636040E+04	6.17119324E+00	3.76267867E+00	9.68872143E-04	2.79489841E-06				3
	-3.85091153E-09	1.68741719E-12	4.60040401E+04	1.56253185E+00	1.00274170E+04				4
CH2(S)	L S/93C	1H	2	00	00G	200.000	3500.000	1000.000	1
	2.29203842E+00	4.65588637E-03	-2.01191947E-06	4.17906000E-10	-3.39716365E-14				2
	5.09259997E+04	8.62650169E+00	4.19860411E+00	-2.36661419E-03	8.23296220E-06				3
	-6.68815981E-09	1.94314737E-12	5.04968163E+04	-7.69118967E-01	9.93967200E+03				4
CH3	L11/89C	1H	3	00	00G	200.000	3500.000	1000.000	1
	2.28571772E+00	7.23990037E-03	-2.98714348E-06	5.95684644E-10	-4.67154394E-14				2
	1.67755843E+04	8.48007179E+00	3.67359040E+00	2.01095175E-03	5.73021856E-06				3
	-6.87117425E-09	2.54385734E-12	1.64449988E+04	1.60456433E+00	1.03663400E+04				4
CH4	L 8/88C	1H	4	00	00G	200.000	3500.000	1000.000	1
	7.48514950E-02	1.33909467E-02	-5.73285809E-06	1.22292535E-09	-1.01815230E-13				2
	-9.46834459E+03	1.84373180E+01	5.14987613E+00	-1.36709788E-02	4.91800599E-05				3
	-4.84743026E-08	1.66693956E-11	-1.02466476E+04	-4.64130376E+00	1.00161980E+04				4
CO	TPIS79C	1O	1	00	00G	200.000	3500.000	1000.000	1
	2.71518561E+00	2.06252743E-03	-9.98825771E-07	2.30053008E-10	-2.03647716E-14				2
	-1.41518724E+04	7.81868772E+00	3.57953347E+00	-6.10353680E-04	1.01681433E-06				3
	9.07005884E-10	-9.04424499E-13	-1.43440860E+04	3.50840928E+00	8.67100000E+03				4
CO2	L 7/88C	1O	2	00	00G	200.000	3500.000	1000.000	1
	3.85746029E+00	4.41437026E-03	-2.21481404E-06	5.23490188E-10	-4.72084164E-14				2
	-4.87591660E+04	2.27163806E+00	2.35677352E+00	8.98459677E-03	-7.12356269E-06				3
	2.45919022E-09	-1.43699548E-13	-4.83719697E+04	9.90105222E+00	9.36546900E+03				4
HCO	L12/89H	1C	1O	1	00G	200.000	3500.000	1000.000	1
	2.77217438E+00	4.95695526E-03	-2.48445613E-06	5.89161778E-10	-5.33508711E-14				2
	4.01191815E+03	9.79834492E+00	4.22118584E+00	-3.24392532E-03	1.37799446E-05				3
	-1.33144093E-08	4.33768865E-12	3.83956496E+03	3.39437243E+00	9.98945000E+03				4
CH2O	L 8/88H	2C	1O	1	00G	200.000	3500.000	1000.000	1
	1.76069008E+00	9.20000082E-03	-4.42258813E-06	1.00641212E-09	-8.83855640E-14				2
	-1.39958323E+04	1.36563230E+01	4.79372315E+00	-9.90833369E-03	3.73220008E-05				3
	-3.79285261E-08	1.31772652E-11	-1.43089567E+04	6.02812900E-01	1.00197170E+04				4
CH2OH	GUNL93C	1H	3O	1	00G	200.000	3500.000	1000.000	1
	3.69266569E+00	8.64576797E-03	-3.75101120E-06	7.87234636E-10	-6.48554201E-14				2
	-3.24250627E+03	5.81043215E+00	3.86388918E+00	5.59672304E-03	5.93271791E-06				3
	-1.04532012E-08	4.36967278E-12	-3.19391367E+03	5.47302243E+00	1.18339080E+04				4
CH3O	121686C	1H	3O	1	00G	300.00	3000.00	1000.000	1
	0.03770799E+02	0.07871497E-01	-0.02656384E-04	0.03944431E-08	-0.02112616E-12				2
	0.12783252E+03	0.02929575E+02	0.02106204E+02	0.07216595E-01	0.05338472E-04				3
	-0.07377636E-07	0.02075610E-10	0.09786011E+04	0.13152177E+02					4
CH3OH	L 8/88C	1H	4O	1	00G	200.000	3500.000	1000.000	1
	1.78970791E+00	1.40938292E-02	-6.36500835E-06	1.38171085E-09	-1.17060220E-13				2
	-2.53748747E+04	1.45023623E+01	5.71539582E+00	-1.52309129E-02	6.52441155E-05				3
	-7.10806889E-08	2.61352698E-11	-2.56427656E+04	-1.50409823E+00	1.14352770E+04				4
C2H	L 1/91C	2H	1	00	00G	200.000	3500.000	1000.000	1
	3.16780652E+00	4.75221902E-03	-1.83787077E-06	3.04190252E-10	-1.77232770E-14				2
	6.71210650E+04	6.63589475E+00	2.88965733E+00	1.34099611E-02	-2.84769501E-05				3
	2.94791045E-08	-1.09331511E-11	6.68393932E+04	6.22296438E+00	1.04544720E+04				4
C2H2	L 1/91C	2H	2	00	00G	200.000	3500.000	1000.000	1
	4.14756964E+00	5.96166664E-03	-2.37294852E-06	4.67412171E-10	-3.61235213E-14				2
	2.59359992E+04	-1.23028121E+00	8.08681094E-01	2.33615629E-02	-3.55171815E-05				3
	2.80152437E-08	-8.50072974E-12	2.64289807E+04	1.39397051E+01	1.00058390E+04				4

C2H3	L 2/92C	2H	3	00	00G	200.000	3500.000	1000.000	1	
	3.01672400E+00	1.03302292E-02	-4.68082349E-06	1.01763288E-09	-8.62607041E-14				2	
	3.46128739E+04	7.78732378E+00	3.21246645E+00	1.51479162E-03	2.59209412E-05				3	
	-3.57657847E-08	1.47150873E-11	3.48598468E+04	8.51054025E+00	1.05750490E+04				4	
C2H4	L 1/91C	2H	4	00	00G	200.000	3500.000	1000.000	1	
	2.03611116E+00	1.46454151E-02	-6.71077915E-06	1.47222923E-09	-1.25706061E-13				2	
	4.93988614E+03	1.03053693E+01	3.95920148E+00	-7.57052247E-03	5.70990292E-05				3	
	-6.91588753E-08	2.69884373E-11	5.08977593E+03	4.09733096E+00	1.05186890E+04				4	
C2H5	L12/92C	2H	5	00	00G	200.000	3500.000	1000.000	1	
	1.95465642E+00	1.73972722E-02	-7.98206668E-06	1.75217689E-09	-1.49641576E-13				2	
	1.28575200E+04	1.34624343E+01	4.30646568E+00	-4.18658892E-03	4.97142807E-05				3	
	-5.99126606E-08	2.30509004E-11	1.28416265E+04	4.70720924E+00	1.21852440E+04				4	
C2H6	L 8/88C	2H	6	00	00G	200.000	3500.000	1000.000	1	
	1.07188150E+00	2.16852677E-02	-1.00256067E-05	2.21412001E-09	-1.90002890E-13				2	
	-1.14263932E+04	1.51156107E+01	4.29142492E+00	-5.50154270E-03	5.99438288E-05				3	
	-7.08466285E-08	2.68685771E-11	-1.15222055E+04	2.66682316E+00	1.18915940E+04				4	
CH2CO	L 5/90C	2H	20	1	00G	200.000	3500.000	1000.000	1	
	4.51129732E+00	9.00359745E-03	-4.16939635E-06	9.23345882E-10	-7.94838201E-14				2	
	-7.55105311E+03	6.32247205E-01	2.13583630E+00	1.81188721E-02	-1.73947474E-05				3	
	9.34397568E-09	-2.01457615E-12	-7.04291804E+03	1.22156480E+01	1.17977430E+04				4	
HCCO	SRIC91H	1C	20	1	00G	300.00	4000.00	1000.000	1	
	0.56282058E+01	0.40853401E-02	-0.15934547E-05	0.28626052E-09	-0.19407832E-13				2	
	0.19327215E+05	-0.39302595E+01	0.22517214E+01	0.17655021E-01	-0.23729101E-04				3	
	0.17275759E-07	-0.50664811E-11	0.20059449E+05	0.12490417E+02					4	
HCCOH	SRI91C	20	1H	2	00G	300.000	5000.000	1000.000	1	
	0.59238291E+01	0.67923600E-02	-0.25658564E-05	0.44987841E-09	-0.29940101E-13				2	
	0.72646260E+04	-0.76017742E+01	0.12423733E+01	0.31072201E-01	-0.50866864E-04				3	
	0.43137131E-07	-0.14014594E-10	0.80316143E+04	0.13874319E+02					4	
N	J 3/61N	1	0	0	0G	300.000	5000.000	1000.000	01	
	2.50104420E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00				2	
	5.61038356E+04	4.17481974E+00	2.50104420E+00	0.00000000E+00	0.00000000E+00				3	
	0.00000000E+00	0.00000000E+00	5.61038356E+04	4.17481974E+00					4	
NH	melius/91 N	1H	1	0	0G	300.000	5000.000	1368.000	01	
	2.71207542E+00	1.33555860E-03	-3.70230207E-07	4.57845270E-11	-2.13216798E-15				2	
	4.24170243E+04	6.21142965E+00	3.49617412E+00	-2.58512197E-04	8.00229766E-07				3	
	-3.18729027E-10	3.76580317E-14	4.21181588E+04	1.91107205E+00					4	
NO	J 6/63N	10	1	0	0G	300.000	5000.000	1397.000	01	
	3.30616438E+00	1.05880379E-03	-3.35101565E-07	4.84712126E-11	-2.66276333E-15				2	
	9.80488610E+03	6.14537840E+00	3.18302768E+00	1.26159588E-03	-4.40480253E-07				3	
	6.32411494E-11	-1.29137488E-15	9.85926748E+03	6.84194428E+00					4	
N2	J 9/65N	2	0	0	0G	300.000	5000.000	1651.000	01	
	2.99595342E+00	1.23650804E-03	-3.70307892E-07	5.05346628E-11	-2.62980307E-15				2	
	-9.13275945E+02	5.68044094E+00	3.26021755E+00	5.91317615E-04	2.24046981E-07				3	
	-1.95572855E-10	3.61873253E-14	-9.99926028E+02	4.27471775E+00					4	
NH2	L 9/81N	1H	2	0	0G	300.000	5000.000	1379.000	01	
	2.81084081E+00	3.24676780E-03	-1.05043681E-06	1.56667098E-10	-8.82503591E-15				2	
	2.19519093E+04	6.57719920E+00	4.10811911E+00	-1.25157496E-03	4.38306028E-06				3	
	-2.62867774E-09	5.10376771E-13	2.16908327E+04	2.01299833E-01					4	
HNO	WA/93	H	1N	10	1	0G	300.000	5000.000	1671.000	01
	3.78577430E+00	2.86062728E-03	-1.02423922E-06	1.64463139E-10	-9.77943616E-15				2	
	1.14004149E+04	3.87180712E+00	3.33656431E+00	2.67682939E-03	5.61801303E-07				3	
	-1.11362279E-09	2.84076438E-13	1.16664200E+04	6.71330606E+00					4	
NO2	J 9/64N	10	2	0	0G	300.000	5000.000	1502.000	01	
	5.25702679E+00	1.59120496E-03	-5.75149303E-07	9.26518589E-11	-5.51558940E-15				2	
	1.98171367E+03	-2.31252539E+00	2.83832558E+00	6.42094110E-03	-3.71675448E-06				3	
	7.13464440E-10	2.36187798E-14	2.88065438E+03	1.09303839E+01					4	

NNH	Melius93N	2H	1	0	OG	300.000	5000.000	1571.000	01
	4.16742317E+00	2.46673021E-03	-8.65307320E-07	1.36642746E-10	-8.02228303E-15				2
	2.83839159E+04	2.06116000E+00	3.73530535E+00	1.00340348E-03	3.26619841E-06				3
	-2.89569645E-09	6.96522384E-13	2.87981268E+04	5.28804396E+00					4
N2O	J12/64N	2O	1	0	OG	300.000	5000.000	1389.000	01
	5.34204014E+00	1.90604176E-03	-6.74838906E-07	1.07237509E-10	-6.32392655E-15				2
	7.86113134E+03	-5.23705883E+00	2.69094434E+00	8.36738233E-03	-6.74046569E-06				3
	2.71424228E-09	-4.38174973E-13	8.74933506E+03	8.89673234E+00					4
NH3	J 9/65N	1H	3	0	OG	300.000	5000.000	1389.000	01
	2.97970284E+00	5.36649578E-03	-1.72269060E-06	2.55767504E-10	-1.43684720E-14				2
	-6.74869189E+03	4.46279267E+00	3.24695599E+00	3.11219422E-03	1.94311272E-06				3
	-1.94660247E-09	4.40577561E-13	-6.64082103E+03	3.66779173E+00					4
H2NO	M/JB86	N	1H	2O	1	OG	300.000	5000.000	1398.000
	4.26222939E+00	4.60071183E-03	-1.52686779E-06	2.32081624E-10	-1.32607907E-14				2
	6.26937941E+03	1.89523882E+00	2.62132814E+00	8.05594293E-03	-4.34199752E-06				3
	1.31067689E-09	-1.79413169E-13	6.89825870E+03	1.08768221E+01					4
HONO	NBS	N	1H	1O	2	OG	300.000	5000.000	1377.000
	6.11754445E+00	3.00786121E-03	-1.06923897E-06	1.70344657E-10	-1.00625644E-14				2
	-1.17949476E+04	-6.16262788E+00	2.75201621E+00	1.05958045E-02	-7.62288678E-06				3
	2.77356136E-09	-4.14321183E-13	-1.05902472E+04	1.20246757E+01					4
N2H2	J12/65N	2H	2	0	OG	300.000	5000.000	1391.000	01
	4.17789510E+00	4.56480666E-03	-1.41875536E-06	2.10366577E-10	-1.19629007E-14				2
	2.33992310E+04	4.99620907E-01	1.86991331E+00	9.88823409E-03	-6.18682259E-06				3
	2.19505186E-09	-3.35933023E-13	2.42170286E+04	1.29348918E+01					4
N2H3	J12/65N	2H	3	0	OG	300.000	5000.000	1408.000	01
	5.17455613E+00	6.20839945E-03	-2.04623019E-06	3.09591864E-10	-1.76333264E-14				2
	2.19580913E+04	-4.69414951E+00	1.55383758E+00	1.53873331E-02	-1.11813107E-05				3
	4.51731686E-09	-7.65249835E-13	2.31503729E+04	1.45063790E+01					4
N2H4	J12/65N	2H	4	0	OG	300.000	5000.000	1399.000	11
	6.51535328E+00	7.45035248E-03	-2.52984543E-06	3.90697765E-10	-2.25791189E-14				2
	8.55432595E+03	-1.19149920E+01	8.18811840E-01	2.28521917E-02	-1.91832580E-05				3
	8.76414899E-09	-1.63696490E-12	1.03626512E+04	1.80013590E+01					4
AR	L 5/66AR	1	0	0	OG	300.000	5000.000	1000.000	01
	2.50104420E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00				2
	-7.45686328E+02	4.36103010E+00	2.50104420E+00	0.00000000E+00	0.00000000E+00				3
	0.00000000E+00	0.00000000E+00	-7.45686328E+02	4.36103010E+00					4
NO3	121286N	1O	3		G	0300.00	5000.00	1000.00	1
	0.07120307E+02	0.03246228E-01	-0.14316134E-05	0.02797053E-08	-0.02013007E-12				2
	0.05864479E+05	-0.12137301E+02	0.12210763E+01	0.01878797E+00	-0.13443212E-04				3
	0.12746013E-08	0.13540601E-11	0.07473144E+05	0.01840202E+03					4

Appendix 3

Experimental Data on Biomass Reburning

Experimental data reported here are obtained within the framework of Phase II SBIR project “Advanced Biomass Reburning for High Efficiency NO_x Control” sponsored by the U.S. Department of Agriculture.

3.0 Pilot Scale Test Results

A series of pilot scale tests was conducted in the BSF to characterize biomass reburn performance as a function of key process variables. The reburn fuel of primary interest was a pelletized furniture waste. For comparison, several tests were also conducted with natural gas and walnut shells. An initial brief series of tests was performed using natural gas as the main fuel in order to provide baseline performance data. More detailed applications tests were then performed using pulverized coal as the main fuel. The following sections describe test fuel characteristics and results of the biomass reburning test series with natural gas and coal as primary fuels.

3.1 Test Fuel Characteristics

Reburn fuels tested included furniture waste pellets, walnut shells, and natural gas. Main fuels tested included bituminous Illinois coal, bituminous Ohio coal, and natural gas. Table 3.1 presents analytical data for each of the solid fuels. The furniture waste had notably high volatiles, low total ash and low fuel nitrogen, as well as somewhat high chlorine. The furniture waste ash was high in both sodium and potassium.

All solid fuels were pulverized for the tests. The coals were pulverized in a bowl mill such that 70% passed through a 200 mesh sieve. The furniture waste and walnut shells were pulverized in a hammer mill. Size distribution was varied by installing different screens in the hammer mill and by running samples through the mill multiple times. For the furniture waste four grinds were tested: 9%, 21%, 27%, and 48% through 200 mesh. The 48% < 200 mesh grind was used for most of the tests. The walnut shells were more brittle than the furniture waste pellets and provided a finer size distribution. For the walnut shells a single grind of 55% < 200 mesh was tested.

3.2 Results of Reburn Tests with Natural Gas Primary

The first reburning tests were conducted with natural gas as the primary fuel to provide baseline performance data. Furniture waste and natural gas were tested as reburn fuels. Test variables included reburn heat input (10% to 25%) and reburn fuel transport medium (air and nitrogen). Figure 3.1 shows reburn performance for both test fuels as a function of reburn heat input. With nitrogen transport, NO reduction provided by the furniture waste was comparable to that provided by natural gas, and in fact was better than natural gas at 10% and 15% reburning. For furniture waste reburning, maximum NO reduction was 67%, achieved at 15% reburn heat input. Furniture waste reburn performance was significantly worse with air transport than with nitrogen.

3.3 Results of Reburn Tests with Coal Primary

After the natural gas tests, a series of reburn tests was conducted with pulverized coal as the main fuel. Test variables included reburn heat input, initial NO concentration, overfire air injection temperature, and biomass particle size distribution. The majority of the tests were conducted with Illinois coal as the main fuel and furniture waste as the reburn fuel. However, for comparison several tests were also conducted with Ohio coal as the

main fuel and with natural gas and walnut shells as reburn fuels. Fly ash samples were also obtained at different reburn test conditions and analyzed for residual carbon.

3.3.1 Effect of Reburn Heat Input on Performance

Reburn heat input was varied from 10% to 25% with furniture waste and natural gas as reburn fuels and Illinois coal as the main fuel. As shown in Figure 3.2, with nitrogen transport furniture waste reburning gave a maximum of 67% NO reduction at 15% reburning. At 10% and 15% reburning, furniture waste performed better than natural gas. However, at 20% and 25% reburning the natural gas performed better. With air atomization reburn performance was consistently better with natural gas than with furniture waste.

3.3.2 Effect of Initial NO Concentration on Performance

Initial NO concentration (NO_i) was varied from 400 to 900 ppm with furniture waste and natural gas as reburn fuels and Illinois coal as the main fuel. Figure 3.3 shows NO reduction as a function of NO_i at 15% and 20% reburning. For the most part performance was fairly flat as NO_i decreased from 900 to 600 ppm, and then began to fall off as NO_i further decreased to 400 ppm. The furniture waste performed better than natural gas at 15% reburning, although natural gas was better at 20% reburning.

3.3.3 Effect of Overfire Air Injection Temperature on Performance

Reburn performance generally improves with decreasing overfire air (OFA) injection temperature, i.e. with increasing reburn zone residence time. In the current program OFA temperature was varied from 1530 to 1370 K, corresponding to a range of residence times of 0.37 to 1.20 sec. Figure 3.4 shows furniture waste reburn performance as a function of OFA temperature. NO reduction decreased with increasing OFA temperature, and this decrease was more pronounced with air as the transport medium than with nitrogen. It is also noted that these tests were performed at 20% reburning. Subsequent data analysis revealed that 15% reburning provided better NO reduction, as described above. Future OFA temperature optimization testing will be performed at 15% reburning.

3.3.4 Effect of Biomass Size Distribution on Performance

The degree to which biomass is pulverized involves trade-offs between improved reburn performance and increased fuel processing cost. To provide data to assist with making such value judgments, reburn tests were performed at different particle size distribution. Four furniture waste grinds were tested: 9%, 21%, 27%, and 48% through 200 mesh. As shown in Figure 3.5, performance improved with decreasing biomass particle size. At 15% reburning, NO reduction increased from 42% at 9% < 200 mesh to 67% at 48% < 200 mesh. The finer grinds also exhibited some advantages with respect to carbon burnout, as described in Section 3.3.7.

3.3.5 Results of Tests with Ohio Coal Primary

EER's previous reburn test work has shown that the main coal type can have an impact on reburn performance. It is believed that main fuel parameters of importance include concentrations of sulfur, chlorine, sodium, and potassium. To evaluate the effect of main coal type, a series of furniture waste reburning tests was performed with Ohio coal as the main fuel. Figure 3.6 compares results obtained with Illinois coal, Ohio coal, and natural gas as main fuels. With nitrogen atomization, NO reductions were very similar for the two main coals, with natural gas slightly better than both coals. With air atomization,

performance was slightly better with Ohio coal than with Illinois coal, and performance was better with both coals than with natural gas main fuel. Future tests will be performed to further define and expand upon these results.

3.3.6 Results of Walnut Shell Reburn Tests

A literature review of the compositions of various biomass products revealed that walnut shells have high volatiles, low nitrogen, and very high potassium content. Because these features are believed to correlate with reburn performance, it was of interest to determine how well walnut shells worked as a reburn fuel. Therefore, walnut shells were obtained from a local processing facility, pulverized, and tested in the BSF. Figure 3.7 shows walnut shell reburn performance along with that of furniture waste and gas reburning. The walnut shells provided a maximum of 65% NO reduction at 20% reburning. This maximum is about the same as that of the furniture waste, although it occurred at a higher reburn heat input. Walnut shell reburn performance was slightly better than that of natural gas at lower reburn heat inputs, and worse than gas at higher reburn heat inputs.

3.3.7 Carbon in Ash Analytical Results

Fly ash carbon content is important both from the standpoint of recovering fuel energy content and finding a market for the fly ash; fly ash can generally be sold to the construction industry if it contains less than 5% carbon. Fly ash samples were obtained and sent to a contract laboratory for carbon analysis. Test conditions included baseline coal firing, natural gas reburning, furniture waste reburning at three particle size distributions, and walnut shells reburning. For all tests Illinois coal was the main fuel. Results are summarized in Table 3.2.

Carbon in ash was slightly higher for biomass reburning than for baseline coal firing. However, carbon in ash decreased with finer reburn fuel size distributions. Carbon in ash for biomass reburning was slightly better than that for natural gas reburning, and in all cases carbon concentrations were well below 5%.

Table 3.1 - Test Fuel Analytical Properties.

Parameter	Units	Illinois Coal	Ohio Coal	Furniture Waste	Walnut Shells
<u>Proximate analysis</u>					
Ash	% dry	9.60	10.66	1.31	1.93
Volatiles	% dry	41.15	40.83	79.06	72.02
Fixed Carbon	% dry	49.25	48.51	19.63	26.05
Moisture	% as fired	6.00	8.68	6.37	12.43
<u>Ultimate analysis</u>					
Carbon	% dry	66.48	70.14	53.91	51.00
Hydrogen	% dry	4.12	4.66	6.07	5.72
Nitrogen	% dry	1.30	1.32	0.56	0.32
Sulfur	% dry	3.11	2.49	0.03	0.00
Oxygen (difference)	% dry	9.60	10.73	38.12	41.03
Ash	% dry	15.39	10.66	1.31	1.93
Chlorine	% dry	0.005	0.010	0.190	0.130
Higher Heating Value	Btu/lb dry	11,210	12,296	8,824	8,624
<u>Ash analysis</u>					
SiO ₂	% dry	60.54	55.96	13.86	34.98
Al ₂ O ₃	% dry	18.08	23.99	3.29	6.09
TiO ₂	% dry	0.87	1.31	6.72	0.21
Fe ₂ O ₃	% dry	9.45	9.92	8.25	10.71
CaO	% dry	2.56	2.43	24.10	23.25
MgO	% dry	0.69	0.73	3.00	3.16
K ₂ O	% dry	2.55	3.22	7.50	11.15
Na ₂ O	% dry	0.69	0.66	11.16	6.64
SO ₃	% dry	2.98	0.67	6.73	1.59
P ₂ O ₅	% dry	0.26	0.24	2.20	1.92
SrO	% dry	0.03	0.08	0.13	0.02
BaO	% dry	0.10	0.24	3.83	0.08
Mn ₃ O ₄	% dry	0.03	0.00	1.75	0.10
Undetermined	% dry	1.17	0.55	7.48	0.10

Table 3.2 Carbon in Ash Results

Reburn fuel	%<200 mesh	Reburn Heat Input (%)	C in Ash (%)
None (baseline)	- - -	None	0.07
Natural gas	- - -	20	0.61
Furniture waste	48%	20	0.19
Furniture waste	27%	20	0.25
Furniture waste	21%	20	0.31
Walnut shells	55%	20	0.20

Figure 3.1 Furniture waste and natural gas reburn performance with natural gas main fuel.

Figure 3.2 Furniture waste and natural gas reburn performance as a function of reburn heat input with Illinois coal main fuel.

Figure 3.3 Reburn performance as a function of initial NO_x concentration.

Figure 3.4 Biomass reburn performance as a function of overfire air injection temperature.

Figure 3.5 Furniture waste reburn performance as a function of particle size.

Figure 3.6 Furniture waste reburn performance with different main fuels.

Figure 3.7 Performance of walnut shells, furniture waste, and natural gas reburning.