

MINIMIZATION OF CARBON LOSS IN COAL REBURNING

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Prepared by:
Vladimir M. Zamansky and Vitali V. Lissianski

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General Electric Energy and Environmental Research Corporation
(GE EER)
18 Mason, Irvine, CA 92618

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Abstract

This project develops Fuel-Flexible Reburning (FFR), which combines conventional reburning and Advanced Reburning (AR) technologies with an innovative method of delivering coal as the reburning fuel. The overall objective of this project is to develop engineering and scientific information and know-how needed to improve the cost of reburning via increased efficiency and minimized carbon in ash and move the FFR technology to the demonstration and commercialization stage. Specifically, the project entails: (1) optimizing FFR with injection of gasified and partially gasified fuels with respect to NO_x and carbon in ash reduction; (2) characterizing flue gas emissions; (3) developing a process model to predict FFR performance; (4) completing an engineering and economic analysis of FFR as compared to conventional reburning and other commercial NO_x control technologies, and (5) developing a full-scale FFR design methodology.

The project started in August 2000 and will be conducted over a two-year period. The work includes a combination of analytical and experimental studies to identify optimum process configurations and develop a design methodology for full-scale applications. The first year of the program included pilot-scale tests to evaluate performances of two bituminous coals in basic reburning and modeling studies designed to identify parameters that affect the FFR performance and to evaluate efficiency of coal pyrolysis products as a reburning fuel.

Tests were performed in a 300 kW Boiler Simulator Facility to characterize bituminous coals as reburning fuels. Tests showed that NO_x reduction in basic coal reburning depends on process conditions, initial NO_x and coal type. Up to 60% NO_x reduction was achieved at optimized conditions.

Modeling activities during first year concentrated on the development of coal reburning model and on the prediction of NO_x reduction in reburning by coal gasification products. Modeling predicted that composition of coal gasification products depends on gasification temperature. At lower temperature yield of hydrocarbons is high which results in higher efficiency of NO_x control. As temperature decreases, yield of hydrocarbons increases and CO and H_2 yields decrease.

Table of Contents

<u>Section</u>	<u>Page</u>
Abstract	ii
Table of Contents	iii
List of Figures	iv
List of Tables	iv
List of Acronyms and Abbreviations	v
Executive Summary	vi
1.0 INTRODUCTION.....	1
2.0 APPROACH TO THE FFR DEVELOPMENT.....	1
3.0 PILOT-SCALE TESTS.....	3
3.1 Basic Coal Reburn Tests	3
3.2 FFR Tests	6
4.0 PROCESS MODEL DEVELOPMENT.....	7
4.1 Characterization of Coal Gasification Products	7
4.1.1 Composition of Coal Gasification Products.....	7
4.1.2 Rate of Coal Gasification	10
4.1.3 Heat Value of Gasification Products.....	11
4.2 Performance of Coal Gasification Products as Reburning Fuel.....	13
4.2.1 Updating the Natural Gas RCMM	13
4.2.2 FFR Model Setup	15
4.2.3 Initial Modeling Results	17
5.0 CONCLUSIONS.....	18
6.0 FUTURE WORK	19
7.0 BIBLIOGRAPHY	20
<i>Appendix A</i> Reaction Mechanism of C-H-O-N Species in Chemkin Format	A-1
<i>Appendix B</i> Thermodynamic Database for C-H-O-N Species in Chemkin Format.....	B-1

List of Figures

<u>Figure</u>	<u>Page</u>
Figure 3-1. Basic Coal Reburn performance of coal A at initial $\text{NO}_x = 430$ ppm	5
Figure 3-2. Basic Coal Reburn performance of coals A and B at initial $\text{NO}_x = 230$ ppm ...	5
Figure 3-3. Basic Coal Reburn performance of coal blend at initial $\text{NO}_x = 230$ ppm	6
Figure 4-1. Predicted equilibrium composition of gasification products	10
Figure 4-2. Predicted temperature dependence of volatile matter release in gasification of bituminous coal	11
Figure 4-3. Predicted total coal heat values and heat values of volatiles and char	13
Figure 4-4. Comparison of updated RCMM predictions with experimental data on natural gas reburning	15
Figure 4-5. Reactor diagram of model setup	16
Figure 4-6. Predicted performance of reburning as a function of gasification temperature at 20% reburning from total heat input ...	18

List of Tables

<u>Table</u>	<u>Page</u>
Table 2-1. Milestone schedule	2
Table 3-1. Test fuel analyses	4
Table 4-1. Composition of Ukrainian bituminous coal	8
Table 4-2. Equilibrium composition of coal gasification products	9
Table 4-3. Enthalpies for combustion of gasification products	12

List of Acronyms and Abbreviations

AR	-	Advanced Reburning.
BSF	-	Boiler Simulator Facility.
CET93	-	Chemical Equilibrium and Transport.
DOE	-	Department of Energy.
FFR	-	Fuel-Flexible Reburning.
GE EER	-	General Electric Energy and Environmental Research Corp.
LNB	-	Low NO _x Burner.
NASA	-	National Aeronautic and Space Administration.
NETL	-	National Energy Technology Laboratory.
ODF	-	One Dimensional Flame.
OFA	-	Overfire Air.
PFR	-	Plug Flow Reactor.
RCMM	-	Reburning Chemistry-Mixing Model.
SCR	-	Selective Catalytic Reduction.
WSR	-	Well-Stirred Reactor.
SR	-	Stoichiometric Ratio.
UBC	-	Unburned Carbon.

Executive Summary

This project develops Fuel-Flexible Reburning (FFR), which combines conventional reburning and Advanced Reburning (AR) technologies with an innovative method of delivering coal as the reburning fuel. The FFR can be retrofit to existing boilers and can be configured in several ways depending on the boiler, coal characteristics, and NO_x control requirements. Flyash generated by the technology will be a saleable byproduct for use in the cement and construction industries. FFR can also reduce NO_x by 60%-70%, achieving an emissions level of 0.15 lb/10⁶ Btu in many coal-fired boilers equipped with Low NO_x Burners. Total process cost is expected to be one third to one half of that for Selective Catalytic Reduction (SCR). Integration of FFR with AR will result in over 85% NO_x control while producing a saleable ash byproduct.

The overall objective of this project is to develop engineering and scientific information and know-how needed to improve the cost of reburning via increased efficiency and minimized carbon in ash and move the FFR technology to the demonstration and commercialization stage. Specifically, the project entails: (1) optimizing FFR with injection of gasified and partially gasified fuels with respect to NO_x and carbon in ash reduction; (2) characterizing flue gas emissions; (3) developing a process model to predict FFR performance; (4) completing an engineering and economic analysis of FFR as compared to conventional reburning and other commercial NO_x control technologies, and (5) developing a full-scale FFR design methodology.

The project started in August 2000 and will be conducted over a two-year period. The work includes a combination of analytical and experimental studies to identify optimum process configurations and develop a design methodology for full-scale applications. The first year of the program included pilot-scale tests to evaluate performances of two bituminous coals and modeling studies designed to identify parameters that affect the FFR performance and to evaluate efficiency of coal pyrolysis products as a reburning fuel.

The experimental part of the program was performed in conjunction with commercial coal reburning (Coal Reburn) project that GE EER is performing for a commercial client. In this project GE EER investigates the potential to apply Coal Reburn technology to achieve substantial reductions in power plant NO_x emissions. The client expressed interest in FFR demonstration at a 200 MW plant if the study shows economic advantages of Coal Reburn over

other approaches to control NO_x emissions. The FFR pilot-scale tests utilized the same coals that are being tested for the commercial client.

Tests were performed in a 300 kW Boiler Simulator Facility with two coals referred here as coal A and coal B. Coal A had lower volatile matter content and higher sulfur content than coal B. Tests showed that better performance in Coal Reburn was obtained with the coal B. More volatile fuels tend to release the bound-nitrogen species and fuel fragments faster. This allows the reburning chemistry more time to occur, and enables nitrogen-bound species to be processed in an environment where they can be reduced to molecular nitrogen. Other factor that can affect reburning performance is the nitrogen content of the coal that is higher for coal A. Higher nitrogen concentrations result in poorer reburning performance.

The objective of the combined chemistry-mixing modeling was to develop a FFR model for predicting the NO_x control performance and carbon in ash. This model will be used to predict composition of coal gasification products and to optimize FFR for achieving most effective NO_x reduction at lowest carbon in ash.

Modeling activities during first year concentrated on the development of Coal Reburn model and on the prediction of NO_x reduction in reburning by coal gasification products. The model was first applied to bituminous coals. Modeling predicted that composition of coal gasification products depended on gasification temperature. At lower temperatures yield of hydrocarbons was high which resulted in higher efficiency of gasification products as a reburning fuel. As temperature increased, yield of hydrocarbons decreased and CO and H₂ yields increased.

Modeling predicted that gasification of bituminous coals at reaction time of 1 s and temperatures higher than 600 K produces enough volume of gasification products to be used as a reburning fuel at heat inputs up to 20% from total heat input.

1.0 INTRODUCTION

This project develops Fuel-Flexible Reburning (FFR) technology that combines conventional reburning and Advanced Reburning (AR) technologies with an innovative method of delivering coal as the reburning fuel. In FFR solid fuel is partially gasified before injection into reburning zone of a boiler. To achieve gasification, fuel can be transported and injected by recycled flue gas stream at 600 K – 800 K. This allows the fuel to be preheated and partially pyrolyzed and gasified in the duct and then injected into the boiler as a mixture of coal, gaseous products, and char (Option No. 1). Gasification increases coal reactivity and results in lower unburned carbon (UBC) levels. As another option (Option No. 2), the gaseous and solid products can be split using cyclone separation. Indeed, coal typically consists of approximately equal fractions of volatile matter and fixed carbon. Splitting the reburning fuel stream will allow the volatile matter to be used for reburning and the fixed carbon to be injected into the high-temperature flame zone. Option No. 2 has two benefits. First, since reburning performance directly correlates with volatile matter content, this approach allows reburning to be performed with the volatile matter alone. Second, fixed carbon is primarily responsible for high UBC levels during coal reburning. Splitting off the char fraction and conveying it to the main burner zone will provide high carbon combustion efficiency. The N-agent can be injected into one or several zones of a boiler to increase the efficiency of NO_x reduction.

From an economic standpoint, advantages of the FFR technology are that it uses an inexpensive reburning fuel, it does not require micronization mills, and it generates a saleable ash byproduct. The FFR can be retrofit to existing boilers and can be configured in several ways depending on the boiler, coal characteristics, and NO_x control requirements. Flyash generated by the technology will be a saleable byproduct for use in the cement and construction industries. FFR can also reduce NO_x by 60%-70%, achieving an emissions level of 0.15 lb/10⁶ Btu in many coal-fired boilers equipped with Low NO_x Burners (LNB). Total process cost is expected to be one third to one half of that for Selective Catalytic Reduction (SCR). Integration of FFR with AR will result in over 85% NO_x control while producing a saleable ash byproduct.

The project started in August 2000 and will be conducted over a two-year period. This report summarizes work performed during first year of the project. *Section 2* describes the GE EER approach to technology development. *Section 3* presents results of pilot-scale tests to evaluate performance of two bituminous coals in Coal Reburn. *Section 4* describes modeling

activities. Summary of the first year work and plans for the second year are discussed in *Sections 5 and 6*.

2.0 APPROACH TO THE FFR DEVELOPMENT

This section describes the GE EER approach to the development of the FFR technology.

Table 2-1 presents milestone schedule for the project.

Table 2-1. Milestone schedule.

Task	Project Tasks	2000				2001				2002			
No.	<i>Calendar Quarters</i>	I	II	III	IV	I	II	III	IV	I	II	III	IV
1	Management and Reporting												
2	Reburning with Coal Gasification Products												
3	Reburning with Partial Coal Gasification Products												
4	Process Model Development												
5	Economics and Design Methodology												

The initial steps of the technical approach for this project include (1) updating chemistry-mixing reburning model developed by GE EER in previous R&D projects to include soot reactions (Task # 4) and (2) applying this model to predicting the performance of coal gasification products as a reburning fuel (Task #2). Based on previous experience with reburning modeling, such a model could predict process performance for the Option No. 2 of FFR. The chemistry-mixing model will assist in FFR optimization during the second year. Modeling will also provide a scientific understanding of the FFR process.

Pilot scale tests (Task #3) are designed to provide key engineering data required for FFR demonstration. These tests are currently in progress. Pilot-scale experiments are being conducted at the GE EER test site in Irvine, California. The 300 kW Boiler Simulator Facility (BSF) described in the First Semiannual Report¹ is used in tests. The test matrix is designed to identify optimum process configurations and to evaluate the effects of boiler parameters such as residence times, temperature effects, and coal properties. The results of this work will then be integrated into GE EER's existing reburning design methodology.

Task #5 will be conducted during the second year and will upgrade GE EER's reburning design methodology developed in previous studies with natural gas and coal reburning (Coal Reburn) to include the FFR system. In addition, a conceptual process design will be prepared for

the full-scale demonstration of FFR.

All experimental and modeling work planned for the first year was successfully completed.

The experimental part of the program is being performed in coordination with a Coal Reburn project that GE EER is performing for a commercial client. In that project GE EER investigates the potential to apply Coal Reburn technology to achieve substantial reductions in power plant NO_x emissions. The client operates a power plant with a generating capacity of 200 MW. The power plant consists of four identical front-wall fired boilers. The boilers have been equipped with Low NO_x Burners (LNB) for compliance with Title IV regulations. The primary objectives of the study are to determine the NO_x reduction performance achievable with Coal Reburn, to assess the potential impacts of Coal Reburn on boiler performance and carbon loss, and to determine the cost effectiveness of Coal Reburn in comparison to alternative NO_x control technologies. To determine how effective the plant's coals are in the reburning process, GE EER is performing pilot-scale coal characterization tests. The goal of these tests is to evaluate the NO_x reduction performance of the plant's coals as reburning fuels under conditions representative of full-scale application. The tests are being performed with the two coals fired at the plant: a high-sulfur bituminous coal from Ohio (coal A) and a low-sulfur bituminous coal from West Virginia (coal B). The selected coals are representative of the Eastern bituminous fuels fired by many utilities. The client expressed interest in the FFR demonstration at 200 MW plant if the study shows economic advantages of Coal Reburn over other approaches to control NO_x emissions.

Significant efforts were undertaken during the first year of the program to advertise FFR and make it visible to potential users. Project plans and results were presented at the Spring Meeting of the Western States Section of the Combustion Institute in Oakland, CA in March 2001 and at the 2001 Conference on Unburned Carbon in Pittsburgh, PA sponsored by DOE NETL.

3.0 PILOT-SCALE TESTS

Tests were performed in the BSF to evaluate the performance of two bituminous coals in reburning. These basic reburning tests provided data that will be used for benchmarking the FFR technology. *Subsection 3.1* describes results of basic Coal Reburn tests while *Subsection 3.2* presents the technical approach to the FFR tests which are currently in progress.

3.1 Basic Coal Reburn Tests

Studies conducted by GE EER have shown that a number of coals can be used effectively in the reburning process. However, due to the heterogeneous nature of coal, it is difficult to predict how a specific coal will perform as a reburning fuel based upon easily characterized fuel properties. Therefore, combustion tests were performed to evaluate the reburning performance of two coals of specific interest to the commercial client. The primary objective of the basic reburning tests was to characterize the impacts of reburning process parameters on NO_x reduction under conditions typical of the full-scale boilers.

For the basic Coal Reburn experiments, the main burner was fired with natural gas. Ammonia was premixed with the combustion air to provide a controlled initial NO_x level. Two bituminous coals were tested as reburning fuels. Fuel characteristics are shown in Table 3-1. Each fuel was pulverized in a CE-Raymond deep bowl mill such that 70% passed through a 200 mesh sieve.

Table 3-1. Test fuel analyses.

		Units	Coal A	Coal B
Ultimate Analysis				
As received	C	wt %	68.92	63.11
	H	wt %	4.07	4.00
	N	wt %	1.30	1.02
	S	wt %	0.84	5.77
	Ash	wt %	14.89	17.58
	O	wt %	4.04	4.07
	H ₂ O	wt %	5.94	4.45
	HV	Btu/lb	11,912	11,269
Dry	C	wt %	73.27	66.05
	H	wt %	4.33	4.19
	N	wt %	1.38	1.07
	S	wt %	0.89	6.04
	Ash	wt %	15.83	18.40
	O	wt %	4.30	4.26
		HV	Btu/lb	12,664
Proximate Analysis				
	Volatiles	wt %	38.21	45.59
	Fixed C	wt %	61.79	54.41

The reburning fuel was injected into the furnace through an injector designed to provide rapid dispersion of the fuel into the flue gas. The transport medium for the fuel was nitrogen (to simulate recycled flue gas). The range of parameters investigated in the study represented the

range of conditions available at full-scale units. The main burner was fired at an excess air level of 10%. The reburning fuel was injected at a temperature of 1700 K at rates between 10% and 30% of the total fuel heat input. The overfire air (OFA) was injected at 1400 K, corresponding to a reburning zone residence time of 800 ms. The initial NO_x level was set at 430 ppm and 230 ppm on a dry, corrected to 3% O_2 basis.

Figure 3-1 shows reburning performance of the coal A at initial $\text{NO}_x = 430$ ppm. Figure 3-2 compares performances of coals A and B at initial $\text{NO}_x = 230$ ppm. The efficiency of NO_x reduction decreases for coal A from about 58% to 44% as initial NO_x decreases from 430 ppm to 230 ppm. The best performance was obtained with the coal B.

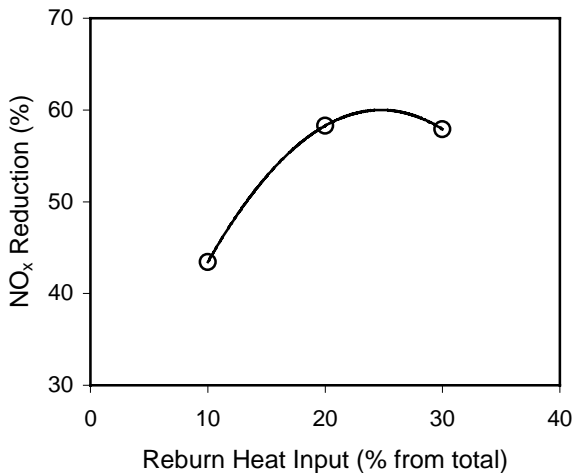


Figure 3-1. Basic Coal Reburn performance of coal A at initial $\text{NO}_x = 430$ ppm.

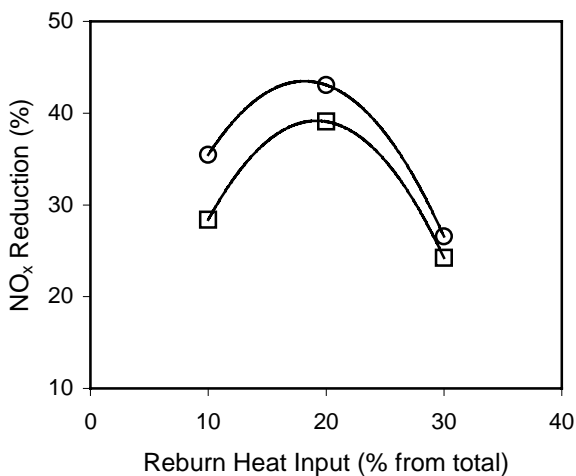


Figure 3-2. Basic Coal Reburn performance of coals A (rectangles) and B (circles) at initial $\text{NO}_x = 230$ ppm.

It is believed that these results could be explained taking into account the composition and volatility of each reburning fuel. More volatile fuels tend to release the bound-nitrogen

species and fuel fragments faster. This allows the reburning chemistry more time to occur, and enables nitrogen-bound species to be processed in an environment where they can be reduced to molecular nitrogen. Other factor that can affect reburning performance is the nitrogen content of the coal which is higher for coal A: higher nitrogen concentrations result in poorer reburning performance.

Figure 3-3 shows performance of a blend of coals A and B at initial $\text{NO}_x = 230$ ppm. The blend consisted of 70% A / 30% B. Performance of the blend was similar to that of coal B at 20% and 30% reburn heat input and similar to that of coal A at 10% reburn heat input. The coal blend provided the highest NO_x reduction among tested coals at initial $\text{NO}_x = 230$ ppm.

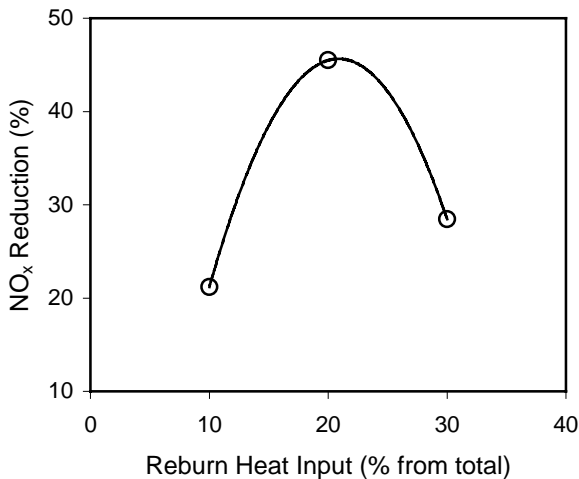


Figure 3-3. Basic Coal Reburn performance of coal blend at initial $\text{NO}_x = 230$ ppm.

3.2 FFR Tests

Specific objectives of these tests are to determine main process parameters that affect FFR efficiency and to optimize FFR for achieving maximum NO_x reduction at minimum carbon in ash. The BSF was modified to enable coal gasification before injection into the reburning zone. Nitrogen was used as a reburning fuel transport medium. Nitrogen was first preheated by passing it through a U-tube inserted into the BSF furnace at 1400 K. The nitrogen then passes through an electrical heating system which consists of a 10 cm diameter, 1.25 m long pipe in which three 2500 W heating elements have been installed in parallel. Pulverized coal is then added to the preheated nitrogen. The coal and nitrogen enter an insulated chamber that is 10 cm in diameter. Its length can be varied up to 1.4 m to vary the residence time of coal gasification.

The nitrogen/coal/gasification products stream is then conveyed through an injector into the furnace.

Tests on the effect of coal gasification on NO_x reduction and carbon in ash are currently in progress, and the results will be presented in the next report.

4.0 PROCESS MODEL DEVELOPMENT

The objective of the modeling task was to develop a FFR model for predicting the NO_x control performance and carbon in ash. This model will be used to predict composition of coal gasification products and to optimize FFR for achieving most effective NO_x reduction at lowest carbon in ash.

Modeling activities during the first year of the project concentrated on the development of Coal Reburn model and on the prediction of NO_x reduction in FFR. The model was applied to bituminous coals. Modeling was conducted for the Ukrainian coal which was used in previous tests, as well as coals A and B. Specific objectives of modeling were to:

- (1) Predict performance of FFR in Option No. 2. Since Coal Reburn performance directly correlates with volatile matter content in coal, it is expected that Option No. 2 results in the maximum efficiency of NO_x reduction that can be achieved in FFR.
- (2) Assist in optimization of the gasification process to achieve maximum efficiency of gasification products as a reburning fuel. Parameters that have to be optimized include gasification temperature and residence time in the gasification zone. These parameters depend on the coal type, coal particle size, and targeted NO_x reduction.

The following sections describe approach used to characterize composition of coal gasification products and application of the FFR model to describe performance of reburning in Option No. 2.

4.1 Characterization of Coal Gasification Products

4.1.1 Composition of Coal Gasification Products

Composition of coal gasification products was predicted using coal proximate and ultimate analyses and CET93 equilibrium code². Characteristics of three bituminous coals used in modeling are presented in Tables 3-1 and 4-1.

NASA CET93 code was used to calculate equilibrium composition of coal gasification products. Chemical equilibrium compositions in CET93 are obtained by the method of free energy minimization. A thermodynamic state is characterized by two independent state variables, such as temperature and pressure. Thermodynamic properties of mixtures include the contribution of condensed and gaseous phases. It is assumed that gases are ideal. Thermodynamic properties of species are taken from the CET93 thermo base.

Table 4-1. Composition of Ukrainian bituminous coal.

		Units	Ukrainian coal
Ultimate Analysis			
As received	C	wt %	43.06
	H	wt %	2.79
	N	wt %	0.81
	S	wt %	1.09
	Ash	wt %	43.19
	O	wt %	4.74
	H ₂ O	wt %	4.32
	HV	Btu/lb	7,535
Dry	C	wt %	45.00
	H	wt %	2.92
	N	wt %	0.85
	S	wt %	1.14
	Ash	wt %	45.14
	O	wt %	4.95
		HV	Btu/lb
Proximate Analysis			
	Volatiles	wt%	44.15
	Fixed C	wt%	55.85

The following approach was used to calculate composition of coal gasification products:

- C, H, O, N and S content of the volatile matter was determined using coal ultimate and proximate analyses.
- These data were used to calculate equilibrium composition of gasification products using CET93.

The following assumptions were made:

- In the gasification process, the coal nitrogen is distributed mainly as nitrogen bound in char (char-N) and hydrogen cyanide³. An increasing fraction of the char-N is converted to HCN with increasing temperature⁴.

- All volatile nitrogen is released as HCN and the nitrogen release is proportional to the carbon release (in reasonable agreement with Niksa and Cho³).
- All hydrogen, oxygen and sulfur were assumed to be released as volatiles.

Table 4-2 shows predicted composition of coal gasification products. Figure 4-1 presents equilibrium compositions in a graphic form.

Table 4-2. Equilibrium composition of coal gasification products.

Coal	Species	Composition (mole fraction)				
		600 K	800 K	1000 K	1200 K	1400 K
Coal A	CH ₄	0.339	0.168	0.034	0.007	0.002
	CO	0.000	0.005	0.046	0.060	0.060
	CO ₂	0.003	0.006	0.002	0.000	0.000
	H ₂	0.042	0.249	0.435	0.477	0.483
	H ₂ O	0.094	0.064	0.015	0.001	0.000
	N ₂	0.006	0.005	0.004	0.004	0.004
	C(graphite)	0.515	0.504	0.464	0.452	0.451
Coal B	CH ₄	0.254	0.127	0.026	0.005	0.001
	CO	0.000	0.005	0.043	0.057	0.057
	CO ₂	0.003	0.006	0.002	0.000	0.000
	H ₂	0.034	0.208	0.370	0.406	0.413
	H ₂ O	0.080	0.055	0.013	0.001	0.000
	N ₂	0.006	0.005	0.004	0.004	0.004
	H ₂ S	0.061	0.051	0.042	0.041	0.039
	C(graphite)	0.561	0.543	0.499	0.486	0.485
Ukrainian coal	CH ₄	0.270	0.139	0.029	0.006	0.002
	CO	0.000	0.008	0.073	0.099	0.100
	CO ₂	0.009	0.014	0.006	0.000	0.000
	H ₂	0.036	0.223	0.409	0.454	0.460
	H ₂ O	0.136	0.091	0.022	0.002	0.000
	N ₂	0.007	0.006	0.005	0.005	0.005
	C(graphite)	0.542	0.519	0.456	0.434	0.433

Note: mole fractions of other species were less than 1×10^{-6} .

Modeling predicts that composition of gasification products depends on temperature: soot and methane are the main components at low temperatures and soot, H₂, and CO are the main components at high temperatures. This finding agrees with experimental data⁵ suggesting that yield of hydrocarbons in coal gasification is larger at low temperatures. Since it is known^{6,7} that hydrocarbons are more effective reburning fuels than H₂ and CO, these results suggest that coal

gasification at lower temperatures produces more effective reburning fuel than coal gasification at higher temperatures.

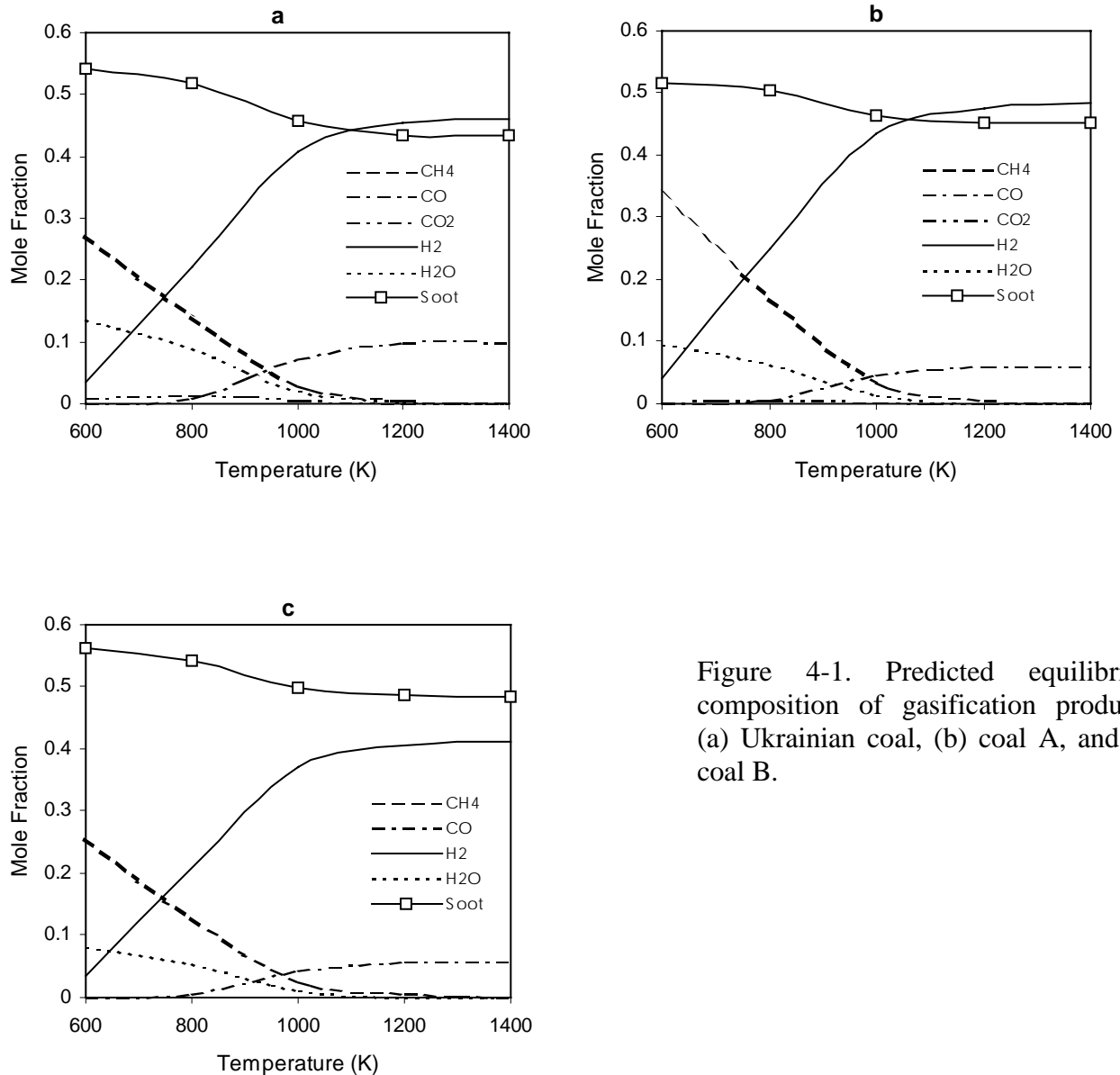


Figure 4-1. Predicted equilibrium composition of gasification products: (a) Ukrainian coal, (b) coal A, and (c) coal B.

4.1.2 Rate of Coal Gasification

The rate of coal gasification, however, is a function of temperature and decreases as temperature decreases. Since coal residence time in the gasification zone is limited, coal gasification at low temperatures may not be completed within allocated time and thus will not produce enough volume of gasification products to be used as a reburning fuel. Thus, the gasification process has to be optimized to (1) produce gas with highest possible hydrocarbons

content and (2) produce enough volume of gas to satisfy requirements for the reburning fuel heat input (typically 15-25% from the total heat input).

Information on the rate of coal gasification at different temperatures can be obtained from experimental data or from modeling predictions. Typically coal gasification/combustion models contain information that is unique for specific coals and can not be used for other coals. Recently Østenberg et al.⁸ developed a model for reburning with coal. The model provides a good description of reburning with gasification products and with bituminous coals. Since Ukrainian coal and coals A and B are bituminous coals, this model can be used to estimate the time required for gasification of these coals at different temperatures.

Figure 4-2 shows the predicted release of volatiles from bituminous coals as percent of the total volatile matter at 1 s residence time in the gasification zone. One second residence time was chosen because this time is expected to be typical residence time in full-scale FFR applications. Modeling predicts that gasification rate increases with temperature, and at about 900 K all volatile matter is released within 1 s. At 700 K, however, only 55% of volatile matter is released within 1 s.

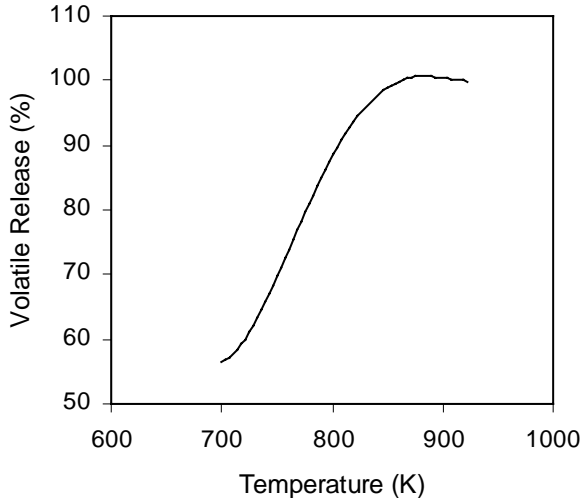


Figure 4-2. Predicted temperature dependence of volatile matter release in gasification of bituminous coal at 1 s reaction time.

4.1.3 Heat Value of Gasification Products

Since the amount of volatiles released from coal depends on temperature and residence time in the gasification zone, the heat value of gasification products also depends on these parameters. The following procedure was used to estimate the heat value of gasification products at different gasification temperatures. Table 4-3 presents reaction enthalpies (ΔH_0^{298}) of main combustible gasification products (CH_4 , CO , H_2), soot, and char. Char and soot were represented

as elemental carbon. ΔH_0^{298} values from Table 4-3 and compositions of gasification products from Table 4-2 were used to calculate the heat value of gasification products (including soot) at different temperatures. Char heat value was calculated using fixed carbon amounts from Tables 3-1 and 4-1 and ΔH_0^{298} for the reaction of elemental carbon oxidation from Table 4-3. Calculated heat values of gasification products and soot correspond to complete coal gasification. To take into account incomplete coal gasification at low temperatures, data on composition of gasification products (presented in Figure 4-2) were then used to determine heat value of gasification products at different gasification temperatures. For example, modeling predicted (Figure 4-2) that at 800 K about 90% of volatiles were gasified at residence time of 1 s. Since at this temperature about 90% of volatiles are released into the gas phase, the heat value of solid residue was taken as that of char plus 10% of the heat value of volatiles and soot (part of volatiles and soot that did not gasify within residence time of 1s).

Figure 4-3 shows predicted heat values of volatiles released from Ukrainian coal and coals A and B at different temperatures and gasification residence time of 1 s. Experimental coal heat values (Tables 3-1 and 4-1) are also shown. Total predicted heat values of volatiles (including soot) and char at all temperatures agree within 4-5% with experimental values of coal heat value (dry) (squares in Figure 4-3). This agreement suggests that assumptions made to estimate heat value of gasification and solid products at different gasification temperatures were reasonable.

Table 4-3. Enthalpies for combustion of gasification products.

Reactions of Gasification Products	ΔH_0^{298} , Btu/lb
$\text{CO} + 0.5\text{O}_2 = \text{CO}_2$	0.05
$\text{H}_2 + 0.5\text{O}_2 = \text{H}_2\text{O}$	0.255
$\text{CH}_4 + 2\text{O}_2 = \text{CO}_2 + 2\text{H}_2\text{O}$	0.106
$\text{C} + \text{O}_2 = \text{CO}_2$ (soot)	0.069
$\text{C} + \text{O}_2 = \text{CO}_2$ (char)	0.069

Data presented in Figure 4-3 suggests that at temperatures lower than approximately 600 K heat value of gasification products formed from coal after 1 s in the gasification zone is not enough (arrow in Figure 4-3 indicates heat input of 20%) for the reburning process. At temperatures higher than 600 K gasification of bituminous coals produces enough combustible gaseous products to be used as a reburning fuel.

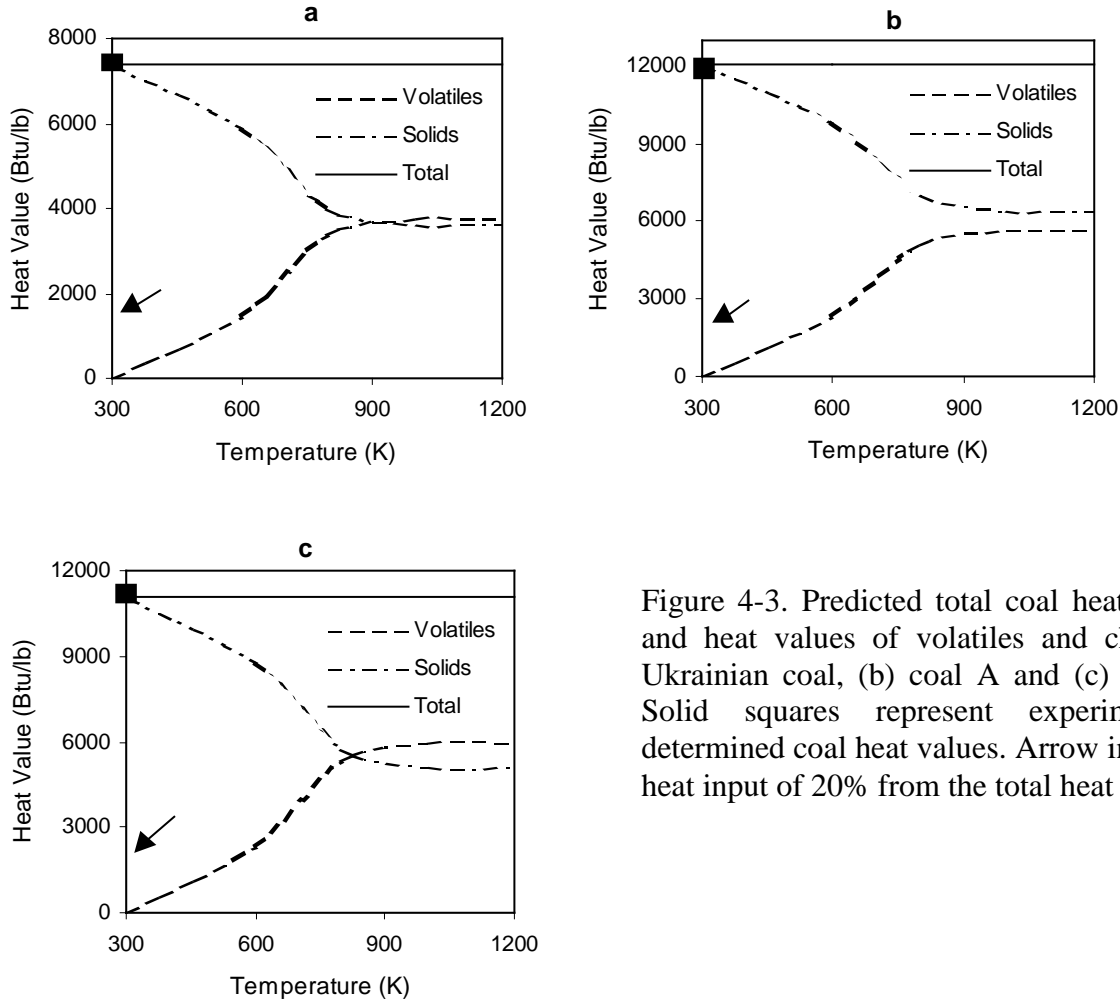


Figure 4-3. Predicted total coal heat values and heat values of volatiles and char: (a) Ukrainian coal, (b) coal A and (c) coal B. Solid squares represent experimentally determined coal heat values. Arrow indicates heat input of 20% from the total heat input.

4.2 Performance of Coal Gasification Products as Reburning Fuel

4.2.1 Updating the Natural Gas RCMM

Coupling of chemical kinetics and gas dynamics is recognized to be important for modeling of the reburning process. The approach⁹ adopted by GE EER to model reburning process includes a combination of a detailed kinetic mechanism with a simplified representation of mixing and utilizes well-stirred (WSR) and plug-flow (PFR) reactors to describe processes that occur in the boiler: combustion in the main combustion zone, mixing of the reburning fuel with flue gas, NO_x reduction in the reburning zone, addition of OFA, and reactions in the burnout zone. This approach was successfully used to describe natural gas basic reburning⁹ and

Advanced Reburning¹⁰ (Advanced Reburning is a combination of basic reburning with injection of a N-agent in one or several zones of a boiler). This model is referred here as the reburning chemistry-mixing model (RCMM).

The characteristic feature of RCMM is utilization of the integrated approach to describe the reburning process. This approach includes (1) evaluation of mixing characteristics of the combustion facility under investigation using model of single jet in crossflow, (2) utilization of PFR to describe processes that occur in the boiler, (3) the distributed addition of reagents, and (4) the inverse mixing approach. The mixing is described by using Zwietering approach¹¹ (the secondary stream is distributed along the primary stream in a continuous fashion over a certain period of time). It is assumed that composition of products, except for NO_x, exiting the primary combustion zone corresponds to equilibrium conditions at the experimental values of temperature.

The kinetic mechanism¹² used in RCMM to describe natural gas reburning included 447 reactions of 65 C-H-O-N gas phase species. Since soot and char reactions were not included in this mechanism, it could not be used to describe reburning by coal and gasification products. Recently Østberg et al.⁸ suggested a mechanism of Coal Reburn which was evaluated⁸ against bench- and pilot-scale data and showed a good description of reburning with bituminous coals. The mechanism⁸ includes 499 reactions of 90 species and has a sub-model to describe reactions that occur during reburning of natural gas and coal gasification products. This mechanism was combined with the mixing model developed as part of RCMM and applied to the description of FFR. However, the updated RCMM first had to be validated against experimental data on natural gas reburning to make sure that RCMM performance has not changed when the gas-phase reaction mechanism¹² was replaced with coal mechanism⁸. The chemical kinetic code ODF (for “One Dimensional Flame”)¹³ was employed to execute model calculations for comparison with experimental data.

Data on NO_x reduction in natural gas reburning were obtained by GE EER within the scope of previous R&D projects. Figure 4-4 shows comparison of predictions of the updated RCMM model with experimental data on natural gas reburning obtained in the BSF. The updated RCMM correctly describes the reburning efficiency at different amounts of the reburning fuel. Thus, performance of the RCMM has not changed when kinetic mechanism of natural gas combustion was replaced with that of coal.

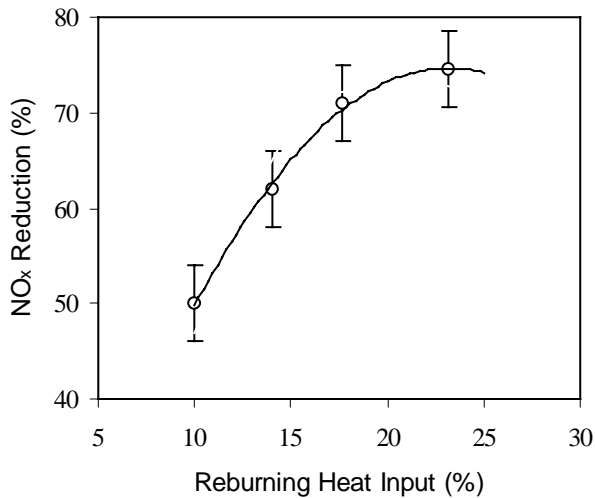


Figure 4-4. Comparison of updated RCMM predictions with experimental data on natural gas reburning obtained in the BSF at the initial NO_x = 600 ppm.

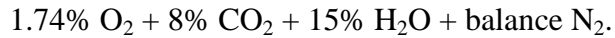
The updated RCMM currently is used only for the description of reburning by natural gas and coal gasification products. Limitations of the model in application to Coal Reburn and plans for development of the Coal Reburn model are discussed in *Section 6.0*.

4.2.2 FFR Model Setup

Results presented in previous sections suggest that gasification products have high content of soot, CH₄, H₂ and CO and thus can be utilized as a reburning fuel. The updated RCMM was used to predict performance of reburning by gasification products. The chemical kinetic code ODF¹³ was employed in modeling. ODF treats a system as a series of one-dimensional reactors. Each reactor may be perfectly mixed (WSR) or unmixed (PFR). 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 many different chemical processes to be simulated in a variety of mixing regimes.

For FFR modeling, the reburning process was treated as series of five reactors (Figure 4-5). Each reactor described one of the physical and chemical processes occurring in a boiler: combustion of the main portion of fuel, addition of the reburning fuel, NO_x reduction as a result of the reaction with the reburning fuel, addition of OFA, and completion of oxidation in the burnout zone.

Modeling was done for natural gas used as a primary fuel. The mixture entering the second reactor corresponds to products of natural gas combustion in air at $SR_1 = 1.1$ (first reactor). Assuming that the combustion process in the primary zone is complete, the mixture with $SR_1 = 1.1$ 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. Therefore, the premixed reactants entering the second reactor can be described as:



The gasification products were added to the main stream of reactants in the second reactor. The third reactor described the continued process of NO removal in the reburning zone after the reburning fuel and flue gas are mixed. The fourth reactor described the process of OFA mixing with flue gas. The fifth reactor described oxidation of the products of incomplete combustion.

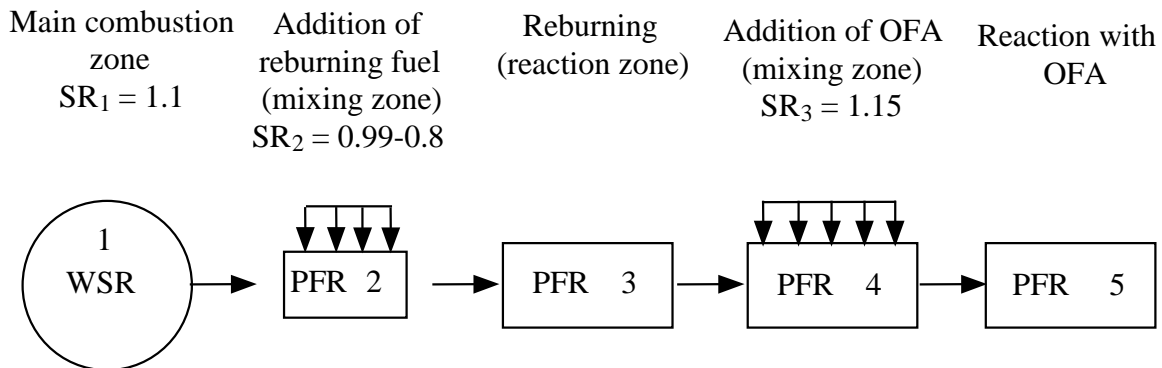


Figure 4-5. Reactor diagram of model setup.

The following parameters are inputs for RCMM:

- Relative amounts of the reburning fuel, OFA, and primary flue gas. Compositions in the main, reburning and burnout zones in modeling corresponded to $SR_1 = 1.1$, $SR_2 = 0.99-0.8$, and $SR_3 = 1.15$.
- Temperatures of the flue gas at the point where reburning fuel and OFA are injected 1700 K and 1450 K, respectively (the same temperatures as those in experiments).
- Initial temperatures of the reburning fuel and OFA. Temperature of gasification products was a variable and was the same as temperature in the gasification reactor; OFA temperature was 300 K.

- Initial NO_x concentration in the primary zone was 600 ppm.
- Mixing times in the reburning and burnout zones of the BSF were estimated in the previous study⁹ to be 120 ms.
- Temperature profile in mixing area was the same as estimated⁹ for natural gas reburning.

The use of some of the mixing parameters estimated for the natural gas reburning in the gasification products reburning was justified, since the BSF reburning jet consists of N₂ at about 70% (large flow of N₂ is used to keep constant mixing conditions as the amount of the reburning fuel changes).

4.2.3 Initial Modeling Results

Figure 4-6 shows comparison of NO_x reduction efficiencies in reburning while firing natural gas, coal, mixture of gasification products and char, and gasification products alone for Ukrainian coal as function of gasification temperature. Square in Figure 4-6 represents experimentally determined efficiency of NO_x reduction by injection of a mixture of gasification products and char in the reburning zone at gasification temperature of 550 K and gasification residence time of 1 s. The model predicts (line) that as gasification temperature increases, efficiency of NO_x reduction decreases. This decrease is caused by the decrease in concentration of methane and increase in concentrations of H₂ and CO (see Figure 4-1) at higher temperatures. The efficiency of NO_x reduction by gasification products is less than that of natural gas at all temperatures and is higher than that of coal at gasification temperatures lower than 850 K. As gasification temperature decreases below 600 K, the heat value of gasification products becomes too low to satisfy the requirement for the 20% heat input of the reburning fuel from total heat input. As a result, the efficiency of NO_x reduction at gasification temperatures below 600 K decreases. This suggests that separation of gasification products from char for utilization as a reburning fuel can result in an increase in the efficiency of NO_x reduction in comparison with Coal Reburn, if coal is gasified at temperatures in the range of 600 K - 850 K.

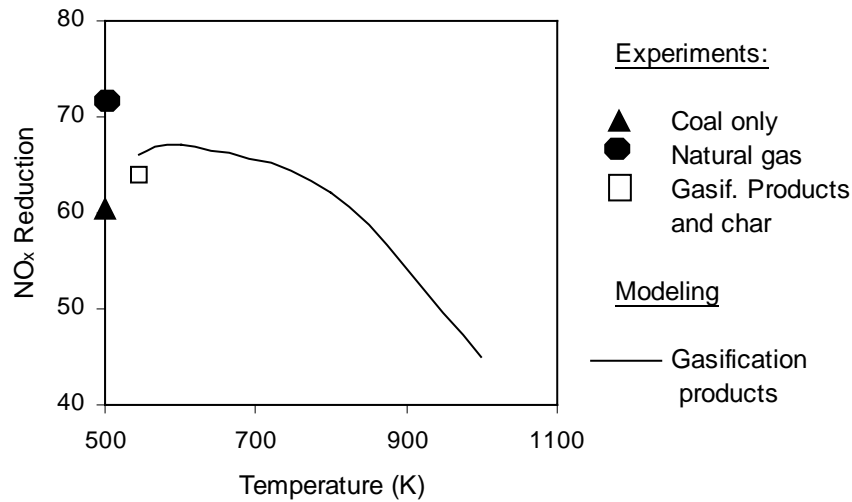


Figure 4-6. Predicted performance of reburning as a function of gasification temperature at 20% reburning from total heat input for Ukrainian coal. Symbols represent experimental data, line modeling predictions.

Figure 4-6 demonstrates that predicted maximum increase in efficiency of NO_x reduction by a mixture of gasification products and char over level provided by coal alone is about 6%. This projected increase should be considered as an estimate since it was obtained from comparison of modeling prediction for the efficiency of gasification products and experimental data for the efficiency of coal reburning. Further development of the Coal Reburn model and more experimental data are needed for more reliable conclusions on the effect of coal gasification on NO_x reduction.

5.0 CONCLUSIONS

The following conclusions can be drawn from experimental and modeling work:

- Pilot-scale tests in a 300 kW facility demonstrated that coal is an effective reburning fuel. Efficiency of NO_x reduction depends on process conditions, coal composition, and initial NO_x.
- Modeling predicted that separation of gasification products from char and utilization of gasification products as a reburning fuel while burning char in the main combustion zone could improve efficiency of reburning. The results are being used in on-going experiments for benchmarking the performance of FFR technology.

- The composition of coal gasification products depends on temperature. It is more beneficial to gasify coal at lower temperatures (600 - 800 K) since yield of hydrocarbons decreases with temperature. Main gasification products at these temperatures are soot and CH₄, while soot, H₂ and CO are main gasification products at higher temperatures.
- Modeling predicted that gasification of bituminous coals at reaction time 1 s and temperatures higher than 600 K produce enough volume of products to be used as a reburning fuel at heat inputs up to 20% from total. These results, however, were obtained for small coal particle size. Gasification of large coal particles may take longer time and may not produce enough gasification products under these conditions.

6.0 FUTURE WORK

Work during the second year will develop tools required to move the technology to a demonstration stage. The work will focus on the development of the following elements of the FFR technology:

- More pilot-scale tests will be conducted to characterize and optimize FFR. In particular, tests will be conducted with coals with different volatile content to determine the effect of coal reactivity on FFR performance. After optimum FFR conditions are identified, test will be conducted to determine the effect of N-agent injection on NO_x reduction. Goal of these tests is to achieve 85% or more NO_x control in FFR.
- Model of Coal Reburn will be refined to include effect of the coal particle size on coal gasification and combustion. This will allow to predict (1) the effect of coal particles on the efficiency of reburning and (2) amount of unburned carbon in ash.
- Model will be improved to be able to be applied to other than bituminous coals. More work will be done on char reactivity as well as on tar and soot formation reactions to improve the reliability of the model.
- Sulfur sub-model will be included in the Coal Reburn mechanism to describe reburning and gasification of coals with high sulfur content.
- The demonstration site will be identified and secured. Potential demonstration sites include Ladyzhin Power Station in Ukraine and a 200 MW power plant operated by commercial client of GE EER. Currently GE EER investigates the potential to apply Coal Reburn technology to achieve substantial reductions in NO_x emissions on one of its

power plants.

7.0 BIBLIOGRAPHY

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Appendix A. Reaction Mechanism of C-H-O-N Species in Chemkin Format

ELEMENTS

H O C N AR

END

SPECIES

NO O2 CO CO2 CH4 NH3 C2H6 NO2 N2O

H2O C2H4 C2H2 HCN N2

H O OH HO2 H2 H2O2 CH2O HCO

CH3 CH2 CH2(S) CH C

CH3OH CH3O CH2OH

C2H5 C2H3 C2H C2

CH3HCO CH2HCO CH3CO C2H2OH OCHCHO CH2CO HCCOH HCCO C2O

C2H5CHO C2H5CO

NO3 HNO HONO H2NO

NH2 NH N N2H2 NNH

HCN CN NCO HNCO HOCN HCNO C2N2 NCN CH3CN CH2CN H2CN

AR VOL VOL* O2* NO*

H* O* OH* HO2* N*

CHAR CHAR* CHARN

VOLS VOL1* VOL2*

SOOT SOOTH SOOTB S*

O# O2# O4 O8 O16 O32

END

REACTIONS

! k = A×Tⁿ exp(-E/RT)

! Units: A mole-cm-sec-K; E cal/mole

!

! Reactions

	A	n	E	
VOL=>38CO+VOL*+38CH4	2.0E16	0.00	59962	! DATA FROM NIKSA & LAU 1993
VOL*=>97C2H4+4HCN	1.0E14	0.00	0	! Help reaction
VOLS=>38CO+VOL1*+99H2	2.0E16	0.00	59962	! DATA FROM NIKSA & LAU 1993
VOL1*=>SOOT+VOL2*+4HCN	1.0E14	0.00	0	! Help reaction
VOL2*=>73H2+32CH4+17C2H4	1.0E14	0.00	0	! Help reaction
SOOT(+O2)=>83S*(+O2)	1.1E07	0.00	34097	! Nagle and Stickland-Constable
(ka/kz/166)				
LOW	/2.0E10	1.00	30004/	! Nagle and Stickland-Constable
(ka/166)				
S*+O2=>2CO+2O#	1.0E14	0.00	0	! Help reaction
SOOT=>SOOTB	3.0E14	0.00	96966	! Nagle and Stickland-Constable
(kT)				
SOOTB+O2=>83S*+O2	4.4E06	1.00	15181	! Nagle and Stickland-Constable
(kb/166)				
SOOTB+O2=>SOOT+O2	7.3E08	1.00	15181	! Nagle and Stickland-Constable
(kb)				
SOOT+H=>SOOTH	7.2E12	0.50	0	! 1.02E-13 [m3/s/K^@]
SOOTB+H=>SOOTH	7.2E12	0.50	0	! 1.02E-13 [m3/s/K^@]
SOOT+O=>SOOT+O#	4.2E11	0.50	0	! 5.91E-15 [m3/s/K^@]
SOOTH+O=>SOOTH+O#	4.2E11	0.50	0	! 5.91E-15 [m3/s/K^@]
SOOTB+O=>SOOT+O#	4.2E11	0.50	0	! 5.91E-15 [m3/s/K^@]
SOOT+O=>99CO+67CO+O	2.5E09	0.50	0	! 5.91E-15/166 [m3/s/K^@]
SOOTH+O=>99CO+67CO+OH	2.5E09	0.50	0	! 5.91E-15/166 [m3/s/K^@]
SOOTB+O=>99CO+67CO+O	2.5E09	0.50	0	! 5.91E-15/166 [m3/s/K^@]

! Reactions	A	n	E	
SOOT+OH=>SOOTH+O#	2.3E11	0.50	0	! 3.24E-15 [m3/s/K^@]
SOOTB+OH=>SOOTH+O#	2.3E11	0.50	0	! 3.24E-15 [m3/s/K^@]
SOOT+OH=>99CO+67CO+OH	1.4E09	0.50	0	! 3.24E-15/166 [m3/s/K^@]
SOOTB+OH=>99CO+67CO+OH	1.4E09	0.50	0	! 3.24E-15/166 [m3/s/K^@]
SOOTH+H=>SOOT+H2	1.4E12	0.50	2301	! 1.94E-14*exp(-1158/T)
SOOTH+OH=>SOOT+H2O	1.13E12	0.50	0	! 5*"SOOT+OH"
SOOT+NO=>SOOT+N*+O#	2.4E12	0.50	29805	! 3.42E-14*exp(-15000/T)
SOOTH+NO=>SOOTH+N*+O#	2.4E12	0.50	29805	! 3.42E-14*exp(-15000/T)
SOOTB+NO=>SOOTB+N*+O#	2.4E12	0.50	29805	! 3.42E-14*exp(-15000/T)
SOOT+NO=>99CO+67CO+NO	1.4E10	0.50	29805	! 3.42E-14*exp(-15000/T)/166
SOOTH+NO=>99CO+67CO+HNO	1.4E10	0.50	29805	! 3.42E-14*exp(-15000/T)/166
SOOTB+NO=>99CO+67CO+NO	1.4E10	0.50	29805	! 3.42E-14*exp(-15000/T)/166
O#+O#=>O2#	1.0E14	0.00	0	! Sink for O producing CO
O2#+O2#=>O4	1.0E14	0.00	0	! Sink for O producing CO
O4+O4=>O8	1.0E14	0.00	0	! Sink for O producing CO
O8+O8=>O16	1.0E14	0.00	0	! Sink for O producing CO
O16+O16=>O32	1.0E14	0.00	0	! Sink for O producing CO
CHAR + H => CHAR + H*	1.17E11	-0.50	0	! q = 0.3
CHAR + O => CHAR + O*	4.93E10	-0.50	0	! q = 0.5
CHAR + OH => CHAR + OH*	2.87E10	-0.50	0	! q = 0.3
CHAR + HO2 => CHAR + HO2*	2.05E10	-0.50	0	! q = 0.3
CHAR + N => CHAR + N*	3.16E10	-0.50	0	! q = 0.3
H* + OH* => H2O	1.00E14	0.00	0	! Help reaction
OH* + OH* => H2O + O*	1.00E14	0.00	0	! Help reaction
H* + H* => H2	1.00E14	0.00	0	! Help reaction
H* + O* => OH*	1.00E14	0.00	0	! Help reaction
HO2* => O* + OH*	1.00E14	0.00	0	! Help reaction
N* + N* => N2	1.00E14	0.00	0	! Help reaction
CHAR+NO=>CHAR+N*+O*	2.26E09	1.00	32688	! Data from Song et al. 1981
CHAR+O2=>99S*+CHAR*+O2#	5.77E09	1.00	21508	! Data from Field 1970 for 451 C
CHAR*=>99S*+27S*+CHARN	1.00E14	0.00	0	! Help Reaction
CHARN=>NO+5N*+CO	1.00E14	0.00	0	! Help Reaction
O+OH=O2+H	2.0E14	-0.40	0	
O+H2=OH+H	5.0E04	2.67	6290	
OH+H2=H2O+H	2.1E08	1.52	3450	
2OH=O+H2O	4.3E03	2.70	-2486	
H+H+M=H2+M	1.0E18	-1.00	0	
H2O/0/				
H+H+H2O=H2+H2O	6.0E19	-1.25	0	
H+O+M=OH+M	6.2E16	-0.60	0	
H2O/5/				
H+OH+M=H2O+M	1.6E22	-2.00	0	
H2O/5/				
O+O+M=O2+M	1.9E13	0.00	-1788	
H2O/5/				
H+O2+M=HO2+M	2.1E18	-1.00	0	! *
H2O/10/ N2/0/				
H+O2+N2 = HO2+N2	6.7E19	-1.42	0	! *
H+HO2=H2+O2	4.3E13	0.00	1411	
H+HO2=2OH	1.7E14	0.00	874	
H+HO2=O+H2O	3.0E13	0.0	1721	
O+HO2=O2+OH	3.3E13	0.0	0	
OH+HO2=H2O+O2	1.9E16	-1.0	0	
!OH+HO2=H2O+O2	2.9E13	0.0	-497	
HO2+HO2=H2O2+O2	4.2E14	0.0	11982	
DUP				

```

! Reactions
H2O2+HO2=H2O2+O2      1.3E11  0.0  -1629
  DUP
H2O2+M=OH+OH+M        1.3E17  0.0  45500
  H2O/5/
H2O2+H=HO2+H2         1.7E12  0.0   3755
H2O2+H=OH+H2O         1.0E13  0.0   3576
H2O2+O=OH+HO2         6.6E11  0.0   3974
H2O2+OH=H2O+HO2       7.8E12  0.0   1330
  DUP
H2O2+OH=H2O+HO2       5.8E14  0.0   9560 ! +
  DUP
!
! *****
! *   CO Subset   *
! *****
!
CO+O+M=CO2+M          6.2E14  0.0   3000 ! nbs86
  H2O/5/
CO+OH=CO2+H           1.5E07  1.3   -758 ! gla86
CO+O2=CO2+O           2.5E12  0.0  47700 ! nbs86
HO2+CO=CO2+OH         5.8E13  0.0  22934 ! gla86
!
! *****
! *   CH2O/HCO Subset   *
! *****
!
CH2O+M=HCO+H+M        3.3E16  0.0   81000 ! gla86
  H2O/5/
CH2O+H = HCO+H2       1.3E08  1.62  2166 ! CEC94 *change*
!CH2O+H=HCO+H2       2.2E08  1.77   3000 ! nbs86
CH2O+O=HCO+OH         1.8E13  0.00   3080 ! nbs86
CH2O+OH=HCO+H2O       3.4E09  1.18  -447 ! nbs86
CH2O+HO2 = HCO+H2O2   3.0E12  0.00  13000 !+cec92
CH2O+O2 = HCO+HO2     6.0E13  0.00  40660 !+cec92
HCO+M=H+CO+M          1.9E17 -1.0   17000 ! tim87
  H2O/5/
HCO+H=CO+H2           1.2E13  0.25    0 ! lrev (harding,21st)
HCO+O=CO+OH           3.0E13  0.000    0 ! cec92
HCO+O=CO2+H           3.0E13  0.000    0 ! cec92
HCO+OH=H2O+CO         1.0E14  0.00    0 ! cec92
HCO+O2=HO2+CO         7.6E12  0.0    406 ! tim88
!
! *****
! *   CH4/CH3/CH2/CH/C Subset   *
! *****
!
CH3+H(+M)=CH4(+M)     1.3E16 -0.63   383 ! GRI-MECH2.11
  LOW/1.75E33  -4.76 2440.0/
  TROE/0.783  74.0 2941.0 6964.0/
  H2O/8.57/ N2/1.43/
CH4+H=CH3+H2          2.2E04  3.00   8750 ! nbs86
CH4+O=CH3+OH          1.0E09  1.5    8604 ! nbs86
CH4+OH=CH3+H2O        1.6E06  2.10   2460 ! war84
CH4+HO2=CH3+H2O2      1.8E11  0.00  18700 ! nbs86
CH4+O2=CH3+HO2        7.9E13  0.00  56000 ! ski72
CH3+H=CH2+H2          9.0E13  0.00  15100 ! gla86

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! Reactions	A	n	E
CH2(S)+H2=CH3+H	7.2E13	0.0	0 ! cec92
CH3+O=CH2O+H	8.4E13	0.0	0 ! cec92
CH3+OH=CH2+H2O	7.5E06	2.0	5000 ! m
CH2(S)+H2O=CH3+OH	3.0E15	-0.6	0 ! car/wag95,hack/hggw 88
CH2OH+H=CH3+OH	1.0E14	0.0	0 ! m
CH3O+H=CH3+OH	1.0E14	0.0	0 ! m
CH3+OH(+M)=CH3OH(+M)	6.3E13	0.0	0 ! GRI2.11
LOW/1.89E38 -6.3 3100/			
TROE/0.2105 83.5 5398 8370/			
N2/1.43/ H2O/8.58/			
CH3+HO2 = CH3O+OH	8.0E12	0.00	0 ! TRO92 *change*
!CH3+HO2=CH3O+OH	2.0E13	0.0	0 ! nbs86
CH3+O2=CH3O+O	2.9E13	0.0	30481 ! yu/fre95
CH3+O2=CH2O+OH	1.9E12	0.0	20315 ! yu/fre95
CH3+CH3(+M)=C2H6(+M)	2.1E16	-0.97	620 ! GRI2.11
LOW /1.26E50 -9.67 6220/			
TROE/ 0.5325 151 1038 4970 /			
N2/1.43/ H2O/8.59/ H2/2/ CO/2/ CO2/3/			
CH3+CH2O = CH4+HCO	7.8E-8	6.10	1967 !+cec94
CH3+HCO = CH4+CO	1.2E14	0.00	0 !+nbs86
CH2+H=CH+H2	1.0E18	-1.56	0 ! gla86
CH2+O=CO+H+H	5.0E13	0.0	0 ! lrev
CH2+O=CO+H2	3.0E13	0.0	0 ! lrev
CH2+OH=CH+H2O	1.1E07	2.0	3000 ! m
CH2+OH=CH2O+H	2.5E13	0.0	0 ! m
CH2+O2=CO+H2O	2.2E22	-3.3	2867 ! dom92,m
CH2+O2=CO2+H+H	3.3E21	-3.3	2867 ! dom92,m
CH2+O2=CH2O+O	3.3E21	-3.3	2867 ! dom92,m
CH2+O2=CO2+H2	2.6E21	-3.3	2867 ! dom92,m
CH2+O2=CO+OH+H	1.6E21	-3.3	2867 ! dom92,m
CH2+CO2=CH2O+CO	1.1E12	0.0	1000 ! gla86
CH2+CH4 = CH3+CH3	4.3E12	0.0	10030 ! boh85
CH2+CH3=C2H4+H	4.2E13	0.0	0 ! cec92
CH2+CH2=C2H2+H+H	4.0E13	0.0	0 ! BRAUN,ET AL
CH2+HCCO=C2H3+CO	3.0E13	0.00	0 ! m
CH2(S)+M=CH2+M	1.0E13	0.0	0 ! m
H/0/ H2O/0/ N2/0/ AR/0/			
CH2(S)+N2=CH2+N2	1.3E13	0.0	430 ! Hayes, 1996
CH2(S)+AR=CH2+AR	1.5E13	0.0	884 ! Hayes, 1996
CH2(S)+H=CH2+H	2.0E14	0.0	0 ! m
CH2(S)+H2O=CH2+H2O	3.0E13	0.0	0 ! WAGNER
CH2(S)+H=CH+H2	3.0E13	0.0	0 ! nbs86
CH2(S)+O=CO+H+H	3.0E13	0.0	0 ! nbs86
CH2(S)+OH=CH2O+H	3.0E13	0.0	0 ! nbs86
CH2(S)+O2=CO+OH+H	7.0E13	0.0	0 ! CBM/ADJ
CH2(S)+CO2=CH2O+CO	3.0E12	0.0	0 ! nbs86
CH2(S)+CH4=CH3+CH3	4.3E13	0.0	0 ! nbs86
CH2(S)+CH3=C2H4+H	2.0E13	0.0	0 ! nbs86
CH2(S)+CH2CO=C2H4+CO	1.6E14	0.0	0 ! WAGNER
CH2(S)+C2H6=CH3+C2H5	1.2E+14	0.0	0 ! nbs86
CH+H=C+H2	1.5E14	0.0	0 ! m
CH+O=CO+H	5.7E13	0.0	0 ! gla86
CH+OH=HCO+H	3.0E13	0.0	0 ! m
CH+OH=C+H2O	4.0E7	2.0	3000 ! m
CH+O2=HCO+O	3.3E13	0.0	0 ! cec92
CH+H2O=CH2O+H	5.7E12	0.0	-751 ! cec92

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! Reactions
CH+CO2=HCO+CO      3.4E12  0.0    690 ! cec92
CH+CH4=C2H4+H      6.0E13  0.0     0 ! gla86
CH+CH3=C2H3+H      3.0E13  0.0     0 ! m
CH+CH2=C2H2+H      4.0E13  0.0     0 ! m
CH+CH2O=CH2CO+H    9.5E13  0.00    -515 ! cec92
CH+HCCO=C2H2+CO    5.0E13  0.00     0 ! m
C+OH=CO+H          5.0E13  0.00     0 ! m
C+O2=CO+O          2.0E13  0.00     0 ! gla86
C+CH3=C2H2+H       5.0E13  0.00     0 ! m
C+CH2=C2H+H        5.0E13  0.00     0 ! m
!
! *****
! *   CH3OH/CH2OH/CH2O subset   *
! *****
!
CH3OH+H=CH2OH+H2   1.7E7   2.1    4868 ! nbs87
CH3OH+H=CH3O+H2    4.2E6   2.1    4868 ! nbs87
CH3OH+O=CH2OH+OH   3.9E5   2.5    3080 ! nbs87
CH3OH+OH=CH2OH+H2O 5.30E4  2.53    960 ! nbs87
CH3OH+OH=CH3O+H2O 1.32E4  2.53    960 ! nbs87
CH3OH+HO2=CH2OH+H2O2 9.6E10  0.0    12578 ! nbs87
CH2O+H(+M)=CH3O(+M) 5.4E11  0.454   2600 ! GRI2.11
  LOW/1.54E30  -4.8  5560 /
  TROE/ 0.758  94 1555 4200/
  N2/1.43/  H2O/8.58/
CH3O+H=CH2O+H2    2.0E13  0.00     0 ! nbs86
CH3O+O=CH2O+OH    1.0E13  0.00     0 ! m
CH3O+OH=CH2O+H2O  1.0E13  0.00     0 ! m
CH3O+O2=CH2O+HO2  6.3E10  0.00    2600 ! nbs86
H+CH2O(+M)=CH2OH(+M) 5.4E11  0.454   3600 ! GRI2.11
  LOW/.91E32  -4.82 6530/
  TROE/0.7187 103 1291 4160/
  N2/1.43/  H2O/8.58/  CO/2/  CO2/3/  H2/2/
CH2OH+H=CH2O+H2   2.0E13  0.00     0 ! m
CH2OH+O=CH2O+OH   1.0E13  0.00     0 ! m
CH2OH+OH=CH2O+H2O 1.0E13  0.00     0 ! m
CH2OH+O2=CH2O+HO2 1.6E15  -1.0     0 ! cec92
  DUP
CH2OH+O2=CH2O+HO2 7.2E13  0.0    3577 !
  DUP
!
! *****
! *   C2H6/C2H5/C2H4/C2H3/C2H2/C2H/C2 subset *
! *****
!
C2H6+H=C2H5+H2     5.4E02  3.50    5210 ! nbs86
C2H6+O=C2H5+OH     3.0E07  2.00    5115 ! war84
C2H6+OH=C2H5+H2O   7.2E6   2.0     864 ! cec92
C2H6+HO2 = C2H5+H2O2 1.3E13  0.00   20460 ! cec92 +
C2H6+O2=C2H5+HO2   5.0E13  0.0    55000 ! m,ben96
C2H6+CH3=C2H5+CH4  5.5E-1  4.00    8300 ! nbs86
C2H4+H(+M)=C2H5(+M) 1.1E12  0.454   1822 ! mar95
  LOW/1.112E34  -5.0  4448.0/
  TROE/0.5  95.0  95.0  200./
  H2O/5/

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! Reactions
C2H5+H(+M) = C2H6(+M)      5.2E17 -0.99  1580 ! GRI2.11 *add*
  LOW / 2.0E41 -7.08 6685/
  TROE/ 0.8422 125 2219 6882 /
  N2/1.0/ H2O/6/ AR/0.7/
C2H5+H=CH3+CH3            4.9E12  0.35    0 ! lrev
C2H5+O = CH3+CH2O          4.2E13  0.00    0 ! SLA/GUT/MIL88 *add*
C2H5+O = CH3HCO+H          5.3E13  0.00    0 ! SLA/GUT/MIL88 *add*
C2H5+O = C2H4+OH           3.0E13  0.00    0 ! SLA/GUT/MIL88 *add*
C2H5+OH = C2H4+H2O         2.4E13  0.00    0 ! NBS86 *add*
C2H5+O2 = C2H4+HO2         1.0E10  0.00 -2190 ! CEC92 *change*
!*****
!C2H5+O2 = C2H5O2          5.2E35 -7.63   6033 ! boz93 **2.5**!
!C2H5O2+NO = CH3CH2O+NO2   5.4E12  0.00    0 ! ATK92 **2.5**!
!CH3CH2O = CH3+CH2O        8.0E13  0.00  21500 ! CEC92 **2.5**!
!CH3CH2O+O2 = CH3HCO+HO2   6.0E10  0.00   1650 ! CEC92 **2.5**!
!CH3CH2O+NO = CH3HCO+HNO   7.8E12  0.00    0 ! ATK92 **2.5**!
!*****
C2H5+CH2O = C2H6+HCO       5.5E03  2.81   5860 ! NBS86 *add*
C2H5+HCO = C2H6+CO         1.2E14  0.00    0 ! NBS86 *add*
C2H5+CH3 = C2H4+CH4        1.1E12  0.00    0 ! CEC94 *add*
C2H5+C2H5 = C2H6+C2H4      1.5E12  0.00    0 ! cec92 *add*
C2H3+H(+M)=C2H4(+M)        6.1E12  0.27   280 ! GRI2.11
  LOW /0.98E30 -3.86 3320./
  TROE /0.7820 207.50 2663.00 6095.00/
  H2/2.85/ CO/2.1/ CO2/2.85/ H2O/7.14/ CH4/2.85/ C2H6/4.29/ N2/1.43/
C2H4+M=C2H2+H2+M          3.5E16  0.0   71500 ! cec92
  N2/1.5/ H2O/10/
C2H4+H=C2H3+H2            5.4E14  0.0   14900 ! cec92
C2H4+O = CH2HCO+H          4.7E06  1.88   180 ! cec94
C2H4+O = CH3+HCO           8.1E06  1.88   180 ! cec94
C2H4+O = CH2CO+H2          6.8E05  1.88   180 ! cec94
C2H4+OH=C2H3+H2O          2.0E13  0.00   5940 ! cec92
C2H4+HO2=CH3HCO+OH        2.2E12  0.0   17200 ! cec94,PRD JAM
C2H4+O2=CH2HCO+OH         2.0E8   1.5   39000 ! m,ben96
C2H4+CH3 = C2H3+CH4        5.0E11  0.00  15000 ! zha90 ** add **
H+C2H2(+M)=C2H3(+M)       3.1E11  0.58   2590 ! mar96 *
  LOW/2.254E40 -7.269 6577./
  TROE/0.5 675. 675./
  H2/2/ CO/2/ CO2/3/ H2O/5/
C2H3+H=C2H2+H2            4.0E13  0.00    0 ! mrev
C2H3+O=CH2CO+H            3.0E13  0.000   0 ! cec92
C2H3+OH=C2H2+H2O         2.0E13  0.0     0 ! m
C2H3+O2 = CH2O+HCO         1.1E23 -3.29  3890 ! boz93 *change*
C2H3+O2 = CH2HCO+O         2.5E15 -0.78  3135 ! boz93 *change*
C2H3+O2=C2H2+HO2          5.2E15 -1.26  3310 ! boz93 *change*
C2H3+CH2O = C2H4+HCO       5.4E03  2.81   5860 ! nbs86 *add*
C2H3+HCO = C2H4+CO         9.0E13  0.00    0 ! nbs86 *add*
C2H3+CH3 = C2H2+CH4        2.1E13  0.00    0 ! Fahr 91 (*add*)
C2H3+C2H3 = C2H4+C2H2     1.5E13  0.00    0 ! Fahr 91 *add*
C2H2+M=C2H+H+M            9.1E30 -3.7  127138 ! nbs86?
  H2/2/ CO/2/ CO2/3/ H2O/5/
H2+C2H=C2H2+H             4.1E05  2.39   864 ! gla86
C2H2+O=CH2+CO             6.1E6   2.00  1900 ! JAM,FONT,PEETERS
C2H2+O=HCCO+H            1.4E7   2.00  1900 ! JAM,FONT,PEETERS
C2H2+O=C2H+OH            3.2E15 -0.60  15000 ! gla86
OH+C2H2=C2H+H2O          3.4E7   2.0   14000 ! mil88

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! Reactions
OH+C2H2=HCCOH+H      5.0E5  2.3  13500 ! mil88
OH+C2H2=CH2CO+H      2.2E-4  4.5  -1000 ! mil88
OH+C2H2=CH3+CO       4.8E-4  4.0  -2000 ! mil88
OH+C2H2(+M)=C2H2OH(+M) 1.5E8  1.7  1000 ! mil88,cec92
  LOW/1.81E23  -2.0  0.0 /
  H2/2/ CO/2/ CO2/3/ H2O/5/
HO2+C2H2=CH2HCO+O    1.0E12  0.0  10000 ! m
HO2+C2H2=CH2O+HCO    1.0E12  0.0  10000 ! m
C2H2+O2=HCO+HCO     2.0E08  1.5  30100 ! m,ben96
C2+H2=C2H+H         4.0E5  2.4  1000 ! m
C2H+O=CH+CO        5.0E13  0.00  0 ! gla86
C2H+OH=HCCO+H      2.0E13  0.00  0 ! m
C2H+OH=C2+H2O       4.0E7  2.0  8000 ! m
C2H+O2=CO+CO+H     2.5E13  0.0  0 ! mrev
C2H+CH4=CH3+C2H2    7.2E12  0.0  976 ! Leone JPC 1996
C2+OH=C2O+H        5.0E13  0.0  0 ! m
C2+O2=CO+CO        5.0E13  0.0  0 ! m
!
! *****
! * CH3HCO/CH2HCO/CH3CO/CH2CO/HCCOH/HCCO/C2O subset *
! *****
!
CH3HCO = CH3+HCO     7.1E15  0.00  81280 ! cec94
CH3HCO+H = CH3CO+H2  4.1E09  1.16  2400 ! cec94
CH3HCO+O = CH3CO+OH  5.8E12  0.00  1800 ! cec94
CH3HCO+OH=CH3CO+H2O  2.3E10  0.73  -1110 ! cec94
CH3HCO+HO2 = CH3CO+H2O2  3.0E12  0.00  12000 ! cec94
CH3HCO+O2 = CH3CO+HO2  3.0E13  0.00  39000 ! cec94
CH3HCO+CH3=CH3CO+CH4  2.0E-6  5.6  2464 ! cec94
CH2HCO=CH3+CO       1.0E13  0.0  42000 ! m **change**
!CH2HCO+M=CH3+CO+M  2.0E16  0.0  42000 ! m
! H2/2/ CO/2/ CO2/3/ H2O/5/
CH2HCO+H=CH3+HCO    1.0E14  0.0  0 ! m
CH2HCO+H=CH3CO+H    3.0E13  0.0  0 ! m
CH2HCO+O=CH2O + HCO  5.0E13  0.0  0 ! m
CH2HCO+OH=CH2CO+H2O  2.0E13  0.0  0 ! m
CH2HCO+OH=CH2OH+HCO  1.0E13  0.0  0 ! m
CH2HCO+O2 = CH2O+CO+OH  2.2E11  0.0  1500 ! ** change p**
!CH2HCO+O2=OH+OCHCHO  2.2E11  0.0  1500 ! CEC 1992/JAM
CH2HCO+CH3=C2H5CHO  5.0E13  0.0  0 ! **change p**
!CH2HCO+CH3=C2H5+HCO  5.0E13  0.0  0 ! m
CH2HCO+CH2=C2H4+HCO  5.0E13  0.0  0 ! m
CH2HCO+CH =C2H3+HCO  1.0E14  0.0  0 ! m
C2H5+HCO = C2H5CHO  1.8E13  0.0  0 ! ** add **
C2H5CHO+H = C2H5CO+H2  8.0E13  0.0  0 ! ** add **
C2H5CHO+O = C2H5CO+OH  7.8E12  0.0  1730 ! ** add **
C2H5CHO+OH = C2H5CO+H2O  1.2E13  0.0  0 ! ** add **
C2H5+CO = C2H5CO    1.5E11  0.0  4800 ! ** add **
C2H2OH+H=CH2HCO+H   5.0E13  0.0  0 ! m
C2H2OH+O=OCHCHO+H   5.0E13  0.0  0.0 ! m
C2H2OH+O2=OCHCHO+OH  1.0E12  0.0  5000 ! m
CH3CO(+M)=CH3+CO(+M) 2.8E13  0.0  17100 ! cec94 *
  LOW/2.1E15  0.0  14000./
  TROE/ 0.5 1.0E-30 1.0E30 /
  H2/2/ CO/2/ CO2/3/ H2O/5/
CH3CO+H = CH3+HCO    2.1E13  0.00  0 ! bar91,ohm90 +

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! Reactions
CH3CO+H = CH2CO+H2      1.2E13  0.00    0 ! bar91,ohm90 +
CH3CO+O = CH3+CO2       1.5E14  0.00    0 ! cec94 +
CH3CO+O = CH2CO+OH      4.0E13  0.00    0 ! cec94 +
CH3CO+OH = CH2CO+H2O    1.2E13  0.00    0 ! nbs86 +
CH2+CO(+M)=CH2CO(+M)    8.1E11  0.5     4510 ! GRI2.11
  LOW/ 1.88E33 -5.11 7095./
  TROE/ 0.5907 275 1226 5185/
    H2/2/ CO/2/ CO2/3/ H2O/8.58/ N2/1.43/
CH2CO+H=CH3+CO          5.9E6   2.0     1300 ! cec92,m
CH2CO+H=HCCO+H2        3.0E7   2.0    10000 ! m
CH2CO+O=CO2+CH2        1.8E12  0.0     1350 ! mrev
CH2CO+O=HCCO+OH        2.0E7   2.0    10000 ! m
CH2CO+OH=HCCO+H2O      1.0E7   2.0     3000 ! m
CH2CO+OH=CH2OH+CO      7.2E12  0.0      0 ! gru94
CH2CO+OH=CH3+CO2       3.0E12  0.0      0 ! gru94 *add*
HCCOH+H=HCCO +H2       3.0E7   2.0     1000 ! m
HCCOH+OH=HCCO+H2O      1.0E7   2.0     1000 ! m
HCCOH+O=HCCO+OH        2.0E7   3.0     1900 ! m
OCHCHO+M=HCO+HCO+M     1.0E17  0.0    58000 ! m
OCHCHO+H=CH2O+HCO      3.0E13  0.0      0 ! m
CH+CO(+M)=HCCO(+M)     5.0E13  0.0      0 ! GRI2.11
  LOW/ 1.88E28 -3.74 1936 /
  TROE/ 0.5757 237 1652 5069 /
    N2/1.43/ H2O/8.58/ CO/2/ CO2/3/ H2/2/
H+HCCO=CH2(S)+CO       1.0E14  0.0      0 ! mrev
O+HCCO=H+CO+CO         1.0E14  0.0      0 ! mrev
HCCO+OH=C2O+H2O        6.0E13  0.0      0 ! m
HCCO+O2=CO2+CO+H       1.4E7   1.7     1000 ! mrev
HCCO+O2=CO +CO +OH     2.9E7   1.7     1000 ! mrev
HCCO+HCCO=C2H2+CO+CO   1.0E13  0.00     0 ! m
C2O+H=CH+CO            1.0E13  0.0      0 ! m
C2O+O=CO+CO            5.0E13  0.0      0 ! m
C2O+OH=CO+CO+H        2.0E13  0.0      0 ! m
C2O+O2=CO+CO+O        2.0E13  0.0      0 ! m
!
! *****
! * H/N/O subset *
! * taken from [nh2no2] except where noted *
! *****
!
H+NO+M=HNO+M           2.7E15  0.0    -600 ! bau73
  H2O/10/ O2/1.5/ H2/2/ CO2/3/ N2/0.0/
H+NO+N2=HNO+N2         2.4E18 -1.0      0 ! see text
NO+O+M=NO2+M           7.5E19 -1.41     0 !
  N2/1.7/ O2/1.5/ H2O/10/
OH+NO+M=HONO+M         5.1E23 -2.51    -68 !
  H2O/5/
HO2+NO=NO2+OH          2.1E12  0.00   -479 !
NO2+H=NO+OH            8.4E13  0.0      0 !
NO2+O=NO+O2            3.9E12  0.0    -238 !
NO2+O(+M)=NO3(+M)      1.3E13  0.0      0 !
  LOW/1.0E28 -4.08 2470./
  N2/1.5/ O2/1.5/ H2O/18.6/
NO2+NO2=NO+NO+O2       1.6E12  0.0    26123 !
NO2+NO2=NO3+NO         9.6E09  0.73   20900 !
NO3+H=NO2+OH           6.0E13  0.0      0 !

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! Reactions	A	n	E
NO3+O=NO2+O2	1.0E13	0.0	0 !
NO3+OH=NO2+HO2	1.4E13	0.0	0 !
NO3+HO2=NO2+O2+OH	1.5E12	0.0	0 !
NO3+NO2=NO+NO2+O2	5.0E10	0.0	2940 !
HNO+H=H2+NO	4.5E11	0.72	655 !
HNO+O=NO+OH	1.0E13	0.0	0 ! +
HNO+OH=NO+H2O	3.6E13	0.0	0 !
HNO+O2=HO2+NO	1.0E13	0.0	25000 !
HNO+NO2=HONO+NO	6.0E11	0.0	2000 !
HNO+HNO=N2O+H2O	9.0E08	0.0	3100 ! *
HNO+NH2=NH3+NO	3.63E6	1.63	-1252 ! lin96
H2NO+M=HNO+H+M	2.5E15	0.0	50000 ! see text
H2O/5/ N2/2/			
H2NO+H=HNO+H2	3.0E7	2.0	2000 !
H2NO+H=NH2+OH	5.0E13	0.0	0 !
H2NO+O=HNO+OH	3.0E7	2.0	2000 !
H2NO+O = NH2+O2	2.0E14	0	0 ! snr96
H2NO+OH=HNO+H2O	2.0E7	2.0	1000 !
H2NO+NO=HNO+HNO	2.0E04	2.0	13000 ! * k/1000 !
H2NO+NO2=HNO+HONO	6.0E11	0.0	2000 !
HONO+H=H2+NO2	1.2E13	0.0	7352 !
HONO+O=OH+NO2	1.2E13	0.0	5961 !
HONO+OH=H2O+NO2	4.0E12	0.0	0 !
NH3+M = NH2+H+M	2.2E16	0	93470 ! +
NH3+H=NH2+H2	6.4E05	2.39	10171 !
NH3+O=NH2+OH	9.4E06	1.90	6460 ! *
NH3+OH=NH2+H2O	2.0E06	2.04	566 !
NH3+HO2=NH2+H2O2	3.0E11	0.0	22000 !
NH2+H=NH+H2	4.0E13	0.00	3650 !
NH2+O=HNO+H	6.6E14	-0.50	0 !
NH2+O=NH+OH	6.8E12	0.	0 !
NH2+OH=NH+H2O	4.0E06	2.	1000 !
NH2+HO2=H2NO+OH	5.0E13	0.0	0 !
NH2+HO2=NH3+O2	1.0E13	0.0	0 !
NH2+NO=NNH+OH	8.9E12	-0.35	0 ! bodenstein
NH2+NO=N2+H2O	1.3E16	-1.25	0 ! bodenstein
DUP			
NH2+NO=N2+H2O	-8.9E12	-0.35	0 !
DUP			
NH2+NO2=N2O+H2O	3.2E18	-2.2	0 !
NH2+NO2=H2NO+NO	3.5E12	0.	0 !
NH2+H2NO=NH3+HNO	3.0E12	0.0	1000 !
HONO+NH2=NO2+NH3	71.1	3.02	-4941 ! lin96
NH2+NH2=N2H2+H2	8.5E11	0.	0 !
NH2+NH=N2H2+H	5.0E13	0.	0 !
NH2+N=N2+H+H	7.2E13	0.	0 !
NH+H=N+H2	3.0E13	0.	0
NH+O=NO+H	9.2E13	0.	0
NH+OH=HNO+H	2.0E13	0.	0
NH+OH=N+H2O	5.0E11	0.50	2000
NH+O2=HNO+O	4.6E05	2.	6500 !
NH+O2=NO+OH	1.3E06	1.5	100 !
NH+NO=N2O+H	2.9E14	-0.4	0 !
DUP			
NH+NO=N2O+H	-2.2E13	-0.23	0
DUP			

! Reactions	A	n	E	
NH+NO=N2+OH	2.2E13	-0.23	0	
NH+NO2=N2O+OH	1.0E13	0.	0	
NH+NH=N2+H+H	2.5E13	0.	0	
NH+N=N2+H	3.0E13	0.	0	
N+OH=NO+H	3.8E13	0.	0	
N+O2=NO+O	6.4E09	1.	6280	
N+NO=N2+O	3.3E12	0.30	0	
N2H2+M=NNH+H+M	5.0E16	0.	50000	
H2O/15/ O2/2/ N2/2/ H2/2/				
N2H2+H=NNH+H2	5.0E13	0.	1000	
N2H2+O=NH2+NO	1.0E13	0.	0	
N2H2+O=NNH+OH	2.0E13	0.	1000	
N2H2+OH=NNH+H2O	1.0E13	0.	1000	
N2H2+NO=N2O+NH2	3.0E12	0.	0	
N2H2+NH2=NH3+NNH	1.0E13	0.	1000	
N2H2+NH=NNH+NH2	1.0E13	0.	1000	
NNH=N2+H	1.0E7	0.	0	! bodenstein
NNH+H=N2+H2	1.0E14	0.	0	
NNH+O=N2+OH	8.0E13	0.	0	
NNH+O=N2O+H	1.0E14	0.	0	
NNH+O=NH+NO	5.0E13	0.	0	
NNH+OH=N2+H2O	5.0E13	0.	0	
NNH+O2=N2+HO2	2.0E14	0.	0	! bodenstein
NNH+O2=N2+O2+H	5.0E13	0.	0	! bodenstein
NNH+NO=N2+HNO	5.0E13	0.	0	
NNH+NH2=N2+NH3	5.0E13	0.	0	
NNH+NH=N2+NH2	5.0E13	0.	0	
N2O+M=N2+O+M	4.0E14	0.	56100	
N2/1.7/ O2/1.4/ H2O/12/ CO/1.5/ CO2/3/				
N2O+H=N2+OH	3.3E10	0.	4729	
DUP				
N2O+H=N2+OH	4.4E14	0.	19254	
DUP				
N2O+O=NO+NO	6.6E13	0.	26630	! nbs91
N2O+O=N2+O2	1.0E14	0.	28000	! nbs91
N2O+OH=N2+HO2	1.3E-2	4.72	36561	! Mebel,Lin IJCK 1996
N2O+OH=HNO+NO	1.2E-4	4.33	25081	! Mebel,Lin IJCK 1996
!HNO+NO = N2O+OH	2.0E12	0.0	26000	!
N2O+NO=NO2+N2	5.3E05	2.23	46281	! Mebel,Lin IJCK 1996
!				
! *****				
! * cyanide subset *				
! * taken from [hcn,hnco] except where noted *				
! *****				
!				
CN+H2=HCN+H	3.0E05	2.45	2237	! woo96
HCN+O=NCO+H	1.4E04	2.64	4980	
HCN+O=NH+CO	3.5E03	2.64	4980	
HCN+O=CN+OH	2.7E09	1.58	29200	
HCN+OH = CN+H2O	3.9E06	1.83	10300	! woo95
HCN+OH=HOCN+H	5.9E04	2.40	12500	
HCN+OH=HNCO+H	2.0E-3	4.	1000	
HCN+OH=NH2+CO	7.8E-4	4.	4000	
HCN+CN=C2N2+H	1.5E07	1.71	1530	!
CN+O=CO+N	7.7E13	0.	0	!
CN+OH=NCO+H	4.0E13	0.	0	! Woo96

! Reactions	A	n	E	
CN+O2=NCO+O	7.5E12	0.	-389	!
CN+CO2=NCO+CO	3.7E06	2.2	26884	!
CN+NO2=NCO+NO	5.3E15	-0.752	344	! WOOLD. (HTGL) , PARK&HERSH
CN+NO2=CO+N2O	4.9E14	-0.752	344	! WOOLD. (HTGL) , PARK&HERSH.
CN+NO2=N2+CO2	3.7E14	-0.752	344	! WOOLD. (HTGL) , PARK&HERSH.
CN+HNO=HCN+NO	1.8E13	0.00	0	
CN+HONO=HCN+NO2	1.2E13	0.00	0	
CN+N2O=NCN+NO	3.9E03	2.6	3696	!
CN+HNCO=HCN+NCO	1.5E13	0.	0	!
CN+NCO=NCN+CO	1.8E13	0.	0	!
HNCO+M=NH+CO	1.1E16	0.	86000	!
HNCO+H=NH2+CO	2.2E07	1.	3800	!
HNCO+O=HNO+CO	1.5E08	1.57	44012	!
HNCO+O=NH+CO2	9.8E7	1.41	8524	!
HNCO+O=NCO+OH	2.2E6	2.11	11425	!
HNCO+OH=NCO+H2O	6.4E05	2.	2563	!
HNCO+HO2=NCO+H2O2	3.0E11	0.	22000	!
HNCO+O2=HNO+CO2	1.0E12	0.	35000	!
HNCO+NH2=NH3+NCO	5.0E12	0.	6200	!
HNCO+NH=NH2+NCO	3.0E13	0.	23700	!
HOCN+H=NCO+H2	2.0E07	2.	2000	!
HOCN+O=NCO+OH	1.5E04	2.64	4000	!
HOCN+OH=NCO+H2O	6.4E05	2.	2563	!
HCNO+H=HCN+OH	1.0E14	0	12000	!
HCNO+O=HCO+NO	2.0E14	0.	0	! JAM
HCNO+OH=CH2O+NO	4.0E13	0.	0	! JAM
NCO+M=N+CO+M	3.1E16	-0.50	48000	!
NCO+H=NH+CO	5.0E13	0.	0	!
NCO+O=NO+CO	4.7E13	0.	0	!
NCO+OH=NO+HCO	5.0E12	0.	15000	! MILLER&BOWMAN IJCK
NCO+O2=NO+CO2	2.0E12	0.	20000	! MILLER&BOWMAN IJCK
NCO+H2=HNCO+H	7.6E02	3.	4000	! JAM&CFM IJCK 1992
NCO+HCO=HNCO+CO	3.6E13	0.	0	! TSANG&HERRON
NCO+NO=N2O+CO	6.2E17	-1.73	763	!MERTENS ,ATAKAN ,HERSHBERGER
NCO+NO=N2+CO2	7.8E17	-1.73	763	!MERTENS ,ATAKAN ,HERSHBERGER
NCO+NO2=CO+NO+NO	2.5E11	0.	-707	!WOOLD. ,HERSH. (JAM)
NCO+NO2=CO2+N2O	3.0E12	0.	-707	!WOOLD. ,HERSH. (JAM)
NCO+HNO=HNCO+NO	1.8E13	0.	0	! TSANG&HERRON
NCO+HONO=HNCO+NO2	3.6E12	0.	0	! TSANG&HERRON
NCO+N=N2+CO	2.0E13	0.	0	! JAM, LIF\$FRENK
NCO+NCO=N2+CO+CO	1.8E13	0.	0	! TSANG&HERRON
C2N2+O=NCO+CN	4.6E12	0.	8880	! STANFORD
C2N2+OH=HOCN+CN	1.9E11	0.	2900	! PHILLIPS
NCN+O=CN+NO	1.0E14	0.	0	! JAM
NCN+OH=HCN+NO	5.0E13	0.	0	! JAM
NCN+H=HCN+N	1.0E14	0.	0	! JAM
NCN+O2=NO+NCO	1.0E13	0.	0	! JAM
H+CH3CN=HCN+CH3	4.0E7	2.	2000.	! JAM
H+CH3CN=CH2CN+H2	3.0E7	2.	1000.	! JAM
O+CH3CN=NCO+CH3	1.5E4	2.64	4980	!JAM(O+HCN)
OH+CH3CN=CH2CN+H2O	2.0E7	2.	2000.	! JAM
CH2CN+O=CH2O+CN	1.0E14	0.	0.	! JAM
CN+CH2OH=CH2CN+OH	5.0E13	0.	0	!
H2CN+M=HCN+H+M	3.0E14	0.	22000	! JAM
! * subset for CxHyOz+nitrogen species reactions				*
CO+NO2 = CO2+NO	9.0E13	0.	33779	!

! Reactions	A	n	E
CO+N2O=N2+CO2	3.2E11	0.	20237 !
CO2+N=NO+CO	1.9E11	0.	3400 !
CH2O+NCO=HNCO+HCO	6.0E12	0.	0 !
CH2O+NO2 = HCO+HONO	8.0E02	2.77	13730 !
HCO+NO=HNO+CO	7.2E12	0.	0 !
HCO+NO2 = CO+HONO	1.2E23	-3.29	2355 !
HCO+NO2 = H+CO2+NO	8.4E15	-0.75	1930 !
HCO+HNO=CH2O+NO	6.0E11	0.	2000 !
CH4+CN=CH3+HCN	6.2E04	2.64	-437 !
NCO+CH4 = CH3+HNCO	9.8E12	0.00	8120 !
CH3+NO=HCN+H2O	1.5E-1	3.523	3950 !
CH3+NO=H2CN+OH	1.5E-1	3.523	3950 !
CH3+NO2=CH3O+NO	1.4E13	0.	0 !
CH3+N=H2CN+H	7.1E13	0.	0 !
CH3+CN=CH2CN+H	1.0E14	0.	0 !
CH3+HOCN=CH3CN+OH	5.0E12	0.	2000 !
CH2+NO=HCN+OH	2.2E12	0.	-378 !
CH2+NO=HCNO+H	1.3E12	0.	-378 !
CH2+NO2=CH2O+NO	5.9E13	0.	0 !
CH2+N=HCN+H	5.0E13	0.	0 !
CH2+N2=HCN+NH	1.0E13	0.	74000 !
H2CN+N=N2+CH2	2.0E13	0.	0 !
CH2(S)+NO=HCN+OH	2.0E13	0.	0 !
CH2(S)+NO=CH2+NO	1.0E14	0.	0 !
CH2(S)+HCN=CH3+CN	5.0E13	0.	0 !
CH+NO2=HCO+NO	1.0E14	0.	0 !
CH+NO = HCN+O	4.8E13	0.00	0 !
CH+NO = HCO+N	3.4E13	0.00	0 !
CH+NO = NCO+H	1.9E13	0.00	0 !
CH+N=CN+H	1.3E13	0.	0 !
CH+N2=HCN+N	3.7E07	1.42	20723 !
CH+N2O=HCN+NO	1.9E13	0.	-511 !
!CH+HCN=CH2+CN	3.0E13	0.	-994 !
! sink for ch2 and cn (1E18!)			
C+NO=CN+O	2.0E13	0.	0 !
C+NO=CO+N	2.8E13	0.	0 !
C+N2=CN+N	6.3E13	0.	46019 !
C+N2O=CN+NO	5.1E12	0.	0 !
C2H6+CN=C2H5+HCN	1.2E05	2.77	-1788 !
C2H6+NCO = C2H5+HNCO	1.5E-9	6.89	-2910 !
C2H4+CN = C2H3+HCN	5.9E14	-0.24	0 !
C2H3+NO=C2H2+HNO	1.0E12	0.	1000 !
C2H3+N=HCN+CH2	2.0E13	0.	0 !
C2H2+NCO = HCCO+HCN	1.4E12	0.00	1815 !
C2H+NO=CN+HCO	2.1E13	0.	0 !
CH2CO+CN=HCCO+HCN	2.0E13	0.	0 !
HCCO+NO=HCNO+CO	7.2E12	0.	0 !
HCCO+NO=HCN+CO2	1.6E13	0.	0 !
HCCO+NO2=HCNO+CO2	1.6E13	0.	0 !
HCCO+N=HCN+CO	5.0E13	0.	0 !
END			

Appendix B. Thermodynamic Database for C-H-O-N Species in Chemkin Format

Thermodynamic properties for each species are calculated from polynomial fits to the specific heat at constant pressure:

$$C_p^o/R = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4$$

$$H^o/RT = a_1 + (a_2/2)T + (a_3/3)T^2 + (a_4/4)T^3 + (a_5/5)T^4 + (a_6/T)$$

$$S/R = a_1 \ln(T) + a_2T + (a_3/2)T^2 + (a_4/3)T^3 + (a_5/4)T^4 + a_7$$

These coefficients are stored for two temperature intervals, one between a low temperature and a common temperature, the second between the common temperature and the high temperature. The second line of the database (before any species data) contains the lowest, highest, and default common temperatures. The data for each species occupies four lines (with the line number at the right margin, in column 80) and contains the following information:

Line 1: Species Name

Date (not used in the code)
up to four atomic symbols and formula
phase of species (S, L, or G for solid, liquid, or gas, respectively)
low temperature
high temperature
common temperature (or blank for default)
fifth atomic symbols and formula (if needed)

Line 2: Coefficients a_1 through a_5 , for the upper temperature interval

Line 3: Coefficients a_6 , a_7 for the upper temperature interval and a_1 , a_2 , a_3 for the lower temperature interval

Line 4: Coefficients a_4 , a_5 , a_6 , a_7 for the lower temperature interval

```

THERMO
  200.000  1500.000  6000.000
C2H5      83194H  5C  2  0  0G  300.000  4000.000  1400.00  0  1
  0.87349157E+01  0.54537677E-02-0.37647177E-06-0.31297920E-09  0.52844000E-13  2
  0.10265269E+05-0.23104086E+02  0.24398923E+01  0.13747212E-01-0.85500653E-06  3
-0.31469924E-08  0.93754355E-12  0.13158588E+05  0.13099146E+02  4
C2H3      83194H  3C  2  0  0G  300.000  4000.000  1400.00  0  1
  0.71861677E+01  0.34552682E-02-0.29435373E-06-0.20681942E-09  0.36797774E-13  2
  0.32229627E+05-0.15977573E+02  0.24955740E+01  0.10269993E-01-0.10226917E-05  3
-0.27594382E-08  0.96919825E-12  0.34232813E+05  0.10614626E+02  4
C2H       83194H  1C  2  0  0G  300.000  4000.000  1400.00  0  1
  0.52086663E+01  0.12875765E-02-0.10398387E-06-0.67526325E-10  0.11751871E-13  2
  0.64697773E+05-0.53721781E+01  0.39396334E+01  0.32114412E-02-0.39412765E-06  3
-0.74782530E-09  0.27493521E-12  0.65224684E+05  0.17814000E+01  4
CH2(S)    83194H  2C  1  0  0G  300.000  4000.000  1400.00  0  1
  0.40752106E+01  0.15779120E-02-0.10806129E-06-0.84592437E-10  0.14033284E-13  2
  0.50007492E+05-0.15480316E+01  0.35932946E+01  0.13151238E-02  0.30756846E-06  3
  0.42637904E-09-0.34178712E-12  0.50451547E+05  0.17780241E+01  4
CH2       83194H  2C  1  0  0G  300.000  4000.000  1400.00  0  1
  0.39737520E+01  0.16097502E-02-0.10785119E-06-0.86399922E-10  0.14301196E-13  2
  0.45608973E+05  0.75549729E-01  0.36872995E+01  0.15066403E-02  0.69679857E-07  3
  0.23537297E-09-0.19397147E-12  0.45863672E+05  0.20267601E+01  4
CH3CN     111596H  3C  2N  1  0G  300.000  3000.000  1000.00  0  1
  0.23924046E+01  0.15618873E-01-0.79120497E-05  0.19372333E-08-0.18611956E-12  2
  0.84999377E+04  0.11145236E+02  0.25197531E+01  0.13567523E-01-0.25764077E-05  3
-0.30893967E-08  0.14288692E-11  0.85533762E+04  0.10920868E+02  4
CH2CN     111596H  2C  2N  1  0G  300.000  3000.000  1000.00  0  1
  0.46058146E+01  0.94485160E-02-0.47116329E-05  0.11389957E-08-0.10828942E-12  2
  0.29171486E+05  0.10084415E+01  0.25296724E+01  0.18114138E-01-0.18960575E-04  3
  0.11944583E-07-0.32544142E-11  0.29592293E+05  0.10993441E+02  4

```

OCHCHO	120596H	2C	2O	2	OG	300.000	3000.000	1000.00	0	1
0.49087462E+01	0.13182673E-01	-0.71416730E-05	0.18461316E-08	-0.18525858E-12						2
-0.27116386E+05	0.59148768E+00	0.25068862E+01	0.18899139E-01	-0.10302623E-04						3
0.62607508E-09	0.88114253E-12	0.26427374E+05	0.13187043E+02							4
C2H2OH HCCO TRAN	121196H	3C	2O	1	OG	300.000	3000.000	1000.00	0	1
0.57206843E+01	0.10704185E-01	-0.50358494E-05	0.11324499E-08	-0.10086621E-12						2
0.12849424E+05	-0.47081776E+01	0.81498282E-01	0.31640644E-01	-0.34085361E-04						3
0.18978838E-07	-0.41950165E-11	0.14060783E+05	0.22908977E+02							4
C2H5CO burcat	T 9/92C	3H	5O	1	OG	298.150	5000.000	1000.00		1
0.30445698E+01	0.23236429E-01	-0.86317936E-05	0.14799550E-08	-0.96860829E-13						2
-0.61787211E+04	0.13122302E+02	0.67368294E+01	-0.26945299E-02	0.49927017E-04						3
-0.50025808E-07	0.15011503E-10	-0.65703366E+04	-0.23398732E+01	-0.43321855E+04						4
C2H5CHO burcat	T 9/92C	3H	6O	1	OG	273.150	5000.000	1000.00		1
0.33137982E+01	0.26619606E-01	-0.10475596E-04	0.18815334E-08	-0.12761310E-12						2
-0.25459603E+05	0.96608447E+01	0.76044596E+01	-0.86403564E-02	0.73930097E-04						3
-0.79687398E-07	0.28004927E-10	-0.25489789E+05	-0.67643691E+01	-0.23097645E+05						4
CH3CN	111596H	3C	2N	1	OG	300.000	3000.000	1000.00	0	1
0.23924046E+01	0.15618873E-01	-0.79120497E-05	0.19372333E-08	-0.18611956E-12						2
0.84999377E+04	0.11145236E+02	0.25197531E+01	0.13567523E-01	-0.25764077E-05						3
-0.30893967E-08	0.14288692E-11	0.85533762E+04	0.10920868E+02							4
CH2CN	111596H	2C	2N	1	OG	300.000	3000.000	1000.00	0	1
0.46058146E+01	0.94485160E-02	-0.47116329E-05	0.11389957E-08	-0.10828942E-12						2
0.29171486E+05	0.10084415E+01	0.25296724E+01	0.18114138E-01	-0.18960575E-04						3
0.11944583E-07	-0.32544142E-11	0.29592293E+05	0.10993441E+02							4
HNO	pg9601H	1N	1O	1	G	0300.00	5000.00	1000.00		1
0.03615144E+02	0.03212486E-01	-0.01260337E-04	0.02267298E-08	-0.01536236E-12						2
0.11769108E+05	0.04810264E+02	0.02784403E+02	0.06609646E-01	-0.09300223E-04						3
0.09437980E-07	-0.03753146E-10	0.12025976E+05	0.09035629E+02							4
HCN	110193H	1C	1N	1	G	0300.00	4000.00	1000.00		1
0.03426457E+02	0.03924190E-01	-0.01601138E-04	0.03161966E-08	-0.02432850E-12						2
0.01485552E+06	0.03607795E+02	0.02417787E+02	0.09031856E-01	-0.01107727E-03						3
0.07980141E-07	-0.02311141E-10	0.01501044E+06	0.08222891E+02							4
HNCO	110193H	1C	1N	1O	1G	0300.00	4000.00	1400.00		1
0.06545307E+02	0.01965760E-01	-0.01562664E-05	-0.01074318E-08	0.01874680E-12						2
-0.01664773E+06	-0.01003880E+03	0.03858467E+02	0.06390342E-01	-0.09016628E-05						3
-0.01898224E-07	0.07651380E-11	-0.01562343E+06	0.04882493E+02							4
HOCN	110193H	1C	1N	1O	1G	0300.00	4000.00	1400.00		1
0.06022112E+02	0.01929530E-01	-0.01455029E-05	-0.01045811E-08	0.01794814E-12						2
-0.04040321E+05	-0.05866433E+02	0.03789424E+02	0.05387981E-01	-0.06518270E-05						3
-0.01420164E-07	0.05367969E-11	-0.03135335E+05	0.06667052E+02							4
NCO	110193C	1N	1O	1	G	0300.00	4000.00	1400.00		1
0.06072346E+02	0.09227829E-02	-0.09845574E-06	-0.04764123E-09	0.09090445E-13						2
0.01359820E+06	-0.08507293E+02	0.03359593E+02	0.05393239E-01	-0.08144585E-05						3
-0.01912868E-07	0.07836794E-11	0.01462809E+06	0.06549694E+02							4
NO	J 6/63N	1O	1	0	OG	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
NO2	J 9/64N	1O	2	0	OG	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
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
N2	J 9/65N	2	0	0	OG	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

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
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
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
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
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
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
O	L 1/90O	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
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
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
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
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
HCO	LL2/89H	1C	1O	1	OG	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	OG	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

CH3	L11/89C	1H	3	00	OG	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	
C	L11/88C	1	00	00	OG	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	OG	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	
CH2OH	GUNL93C	1H	30	1	OG	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	30	1	OG	300.000	3000.000	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	40	1	OG	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	
CH2CO	L 5/90C	2H	20	1	OG	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	OG	300.000	4000.000	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	2O	1H	2	OG	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	
NO3	121286N	1O	3		G	0300.000	5000.000	1000.000	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	
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	
N	J 3/61N	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	
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	OG	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	
NH2	L 9/81N	1H	2	0	OG	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	
H2NO	M/JB86	N	1H	20	1	OG	300.000	5000.000	1398.000	01
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	10	2	OG	300.000	5000.000	1377.000	11
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	

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	
HCN	L12/69H	1C	1N	1	OG	300.000	5000.000	1394.000	01	
4.14927783E+00	2.75915264E-03	-9.32137186E-07	1.43421227E-10	-8.26578641E-15					2	
1.47264307E+04	-5.23695997E-01	2.85596121E+00	6.10771304E-03	-4.55238121E-06					3	
2.02415417E-09	-3.88077841E-13	1.51690915E+04	6.34976764E+00						4	
H2CN	MELIUS 88	H	2C	1N	1	OG	300.000	5000.000	1447.000	01
5.10020023E+00	4.02780465E-03	-1.36439689E-06	2.10725393E-10	-1.21898915E-14					2	
2.75503210E+04	-4.27685930E+00	2.45567293E+00	7.78048141E-13	-1.59463967E-06					3	
-1.33785611E-09	5.32582054E-13	2.86868686E+04	1.07457988E+01						4	
AR	120186AR	1			G	300.000	5000.000	1000.000	1	
0.02500000E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00					2	
-0.07453750E+04	0.04366000E+02	0.02500000E+02	0.00000000E+00	0.00000000E+00					3	
0.00000000E+00	0.00000000E+00	-0.07453750E+04	0.04366000E+02						4	
CN	J 6/69C	1N	1	0	OG	300.000	5000.000	1417.000	01	
3.11872424E+00	1.21876263E-03	-3.73455811E-07	5.23704641E-11	-2.79895164E-15					2	
5.13563933E+04	6.24339093E+00	3.15725686E+00	1.05392231E-03	-1.60373461E-07					3	
-5.86681004E-11	1.78191482E-14	5.13535562E+04	6.06796978E+00						4	
C2	RUS 79C	2	0	0	OG	200.000	6000.000	1000.000	1	
0.37913706E+01	0.51650473E-03	-0.25486960E-07	-0.82263554E-11	0.10086168E-14					2	
0.99023059E+05	0.28151802E+01	0.86470550E+00	0.39353120E-01	-0.11981818E-03					3	
0.13908103E-06	-0.55205503E-10	0.98731303E+05	0.11530141E+02	0.99928438E+05					4	
CH3HCO	L 8/88C	2H	40	1	OG	200.000	6000.000	1000.000	1	
0.54041108E+01	0.11723059E-01	-0.42263137E-05	0.68372451E-09	-0.40984863E-13					2	
-0.22593122E+05	-0.34807917E+01	0.47294595E+01	-0.31932858E-02	0.47534921E-04					3	
-0.57458611E-07	0.21931112E-10	-0.21572878E+05	0.41030159E+01	-0.19987949E+05					4	
CH3CO	T 9/92C	2H	30	1	OG	200.000	6000.000	1000.000	1	
0.59447731E+01	0.78667205E-02	-0.28865882E-05	0.47270875E-09	-0.28599861E-13					2	
-0.37873075E+04	-0.50136751E+01	0.41634257E+01	-0.23261610E-03	0.34267820E-04					3	
-0.44105227E-07	0.17275612E-10	-0.26574529E+04	0.73468280E+01	-0.12027167E+04					4	
CH2HCO	T04/830	1H	3C	2	OG	300.	5000.	1000.000	1	
0.59756699E+01	0.81305914E-02	-0.27436245E-05	0.40703041E-09	-0.21760171E-13					2	
0.49032178E+03	-0.50320879E+01	0.34090624E+01	0.10738574E-01	0.18914925E-05					3	
0.71585831E-08	0.28673851E-11	0.15214766E+04	0.95714535E+01	0.30474436E+04					4	
C2O	RUS 79C	2O	1	0	OG	200.000	6000.000	1000.000	1	
0.51512722E+01	0.23726722E-02	-0.76135971E-06	0.11706415E-09	-0.70257804E-14					2	
0.33241888E+05	-0.22183135E+01	0.28648610E+01	0.11990216E-01	-0.18362448E-04					3	
0.15769739E-07	-0.53897452E-11	0.33749932E+05	0.88867772E+01	0.35003406E+05					4	
C2N2	RUS 79C	2N	2	0	OG	200.000	6000.000	1000.000	1	
0.67055078E+01	0.36425829E-02	-0.13094063E-05	0.21643797E-09	-0.13121437E-13					2	
0.34860766E+05	-0.10493904E+02	0.23292532E+01	0.26153785E-01	-0.49000399E-04					3	
0.46191748E-07	-0.16432385E-10	0.35668442E+05	0.98501993E+01	0.37175973E+05					4	
HCNO	120186H	1C	1N	10	1G	0250.00	4000.00	1000.00	1	
0.06692412E+02	0.02368360E-01	-0.02371510E-05	-0.12755033E-09	0.02407137E-12					2	
0.01694736E+06	-0.12454345E+02	0.03184858E+02	0.09752316E-01	-0.12802028E-05					3	
-0.06163104E-07	0.03226275E-10	0.01797907E+06	0.06123843E+02						4	
NCN	J12/70C	1N	20	00	OG	300.000	5000.000	1000.000	1	
0.55626268E+01	0.20860606E-02	-0.88123724E-06	0.16505783E-09	-0.11366697E-13					2	
0.54897907E+05	-0.55989355E+01	0.32524003E+01	0.70010737E-02	-0.22653599E-05					3	
-0.28939808E-08	0.18270077E-11	0.55609085E+05	0.66966778E+01	0.56865046E+05					4	
VOL	vol.	H 544C	2740	38N	4G	0300.00	4000.00	1000.00	1	
0.25000000E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00					2	
-0.74540000E+03	0.43660000E+01	0.25000000E+01	0.00000000E+00	0.00000000E+00					3	
0.00000000E+00	0.00000000E+00	-0.74540000E+03	0.43660000E+01						4	
VOL*	dummy H	392C	198N	4	G	0300.00	4000.00	1000.00	1	
0.25000000E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00					2	
-0.74540000E+03	0.43660000E+01	0.25000000E+01	0.00000000E+00	0.00000000E+00					3	
0.00000000E+00	0.00000000E+00	-0.74540000E+03	0.43660000E+01						4	
C*	char	C	1		G	0300.00	4000.00	1000.00	1	
0.25000000E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00					2	
-0.74540000E+03	0.43660000E+01	0.25000000E+01	0.00000000E+00	0.00000000E+00					3	
0.00000000E+00	0.00000000E+00	-0.74540000E+03	0.43660000E+01						4	

CO2*	C	10	2	G	0300.00	5000.00	1000.00	1
0.04453623E+02	0.03140169E-01	-0.01278411E-04	0.02393997E-08	-0.01669033E-12				2
-0.04896696E+06	-0.09553959E+01	0.02275725E+02	0.09922072E-01	-0.01040911E-03				3
0.06866687E-07	-0.02117280E-10	-0.04837314E+06	0.01018849E+03					4
H2O*	H	20	1	G	0300.00	5000.00	1000.00	1
0.02672146E+02	0.03056293E-01	-0.08730260E-05	0.01200996E-08	-0.06391618E-13				2
-0.02989921E+06	0.06862817E+02	0.03386842E+02	0.03474982E-01	-0.06354696E-04				3
0.06968581E-07	-0.02506588E-10	-0.03020811E+06	0.02590233E+02					4
H*	recombH	1		G	0300.00	5000.00	1000.00	1
0.02500000E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00		2
0.02547163E+06	-0.04601176E+01	0.02500000E+02	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00		3
0.00000000E+00	0.00000000E+00	0.02547163E+06	-0.04601176E+01					4
HO2*	recombH	10	2	G	0300.00	5000.00	1000.00	1
0.04072191E+02	0.02131296E-01	-0.05308145E-05	0.06112269E-09	-0.02841165E-13				2
-0.01579727E+04	0.03476029E+02	0.02979963E+02	0.04996697E-01	-0.03790997E-04				3
0.02354192E-07	-0.08089024E-11	0.01762274E+04	0.09222724E+02					4
N*	recombN	1		G	0300.00	5000.00	1000.00	1
0.02450268E+02	0.01066146E-02	-0.07465337E-06	0.01879652E-09	-0.01025984E-13				2
0.05611604E+06	0.04448758E+02	0.02503071E+02	-0.02180018E-03	0.05420529E-06				3
-0.05647560E-09	0.02099904E-12	0.05609890E+06	0.04167566E+02					4
O*	recombO	1		G	0300.00	5000.00	1000.00	1
0.02542060E+02	-0.02755062E-03	-0.03102803E-07	0.04551067E-10	-0.04368052E-14				2
0.02923080E+06	0.04920308E+02	0.02946429E+02	-0.01638166E-01	0.02421032E-04				3
-0.01602843E-07	0.03890696E-11	0.02914764E+06	0.02963995E+02					4
OH*	recombO	1H	1	G	0300.00	5000.00	1000.00	1
0.02882730E+02	0.01013974E-01	-0.02276877E-05	0.02174684E-09	-0.05126305E-14				2
0.03886888E+05	0.05595712E+02	0.03637266E+02	0.01850910E-02	-0.01676165E-04				3
0.02387203E-07	-0.08431442E-11	0.03606782E+05	0.01358860E+02					4
CHAR	char	C 451N	60 452	G	0300.00	4000.00	1000.00	1
0.25000000E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00		2
-0.74540000E+03	0.43660000E+01	0.25000000E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00		3
0.00000000E+00	0.00000000E+00	-0.74540000E+03	0.43660000E+01					4
CHAR*	dummy	C 253N	60 254	G	0300.00	4000.00	1000.00	1
0.25000000E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00		2
-0.74540000E+03	0.43660000E+01	0.25000000E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00		3
0.00000000E+00	0.00000000E+00	-0.74540000E+03	0.43660000E+01					4
CHARN	dummy	C 1N	60 2	G	0300.00	4000.00	1000.00	1
0.25000000E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00		2
-0.74540000E+03	0.43660000E+01	0.25000000E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00		3
0.00000000E+00	0.00000000E+00	-0.74540000E+03	0.43660000E+01					4
VOLS	vol.	H 544C	2740 204N 4G	G	0300.00	4000.00	1000.00	1
0.25000000E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00		2
-0.74540000E+03	0.43660000E+01	0.25000000E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00		3
0.00000000E+00	0.00000000E+00	-0.74540000E+03	0.43660000E+01					4
SOOT	soot	C 166O	166	G	0300.00	4000.00	1000.00	1
0.25000000E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00		2
-0.74540000E+03	0.43660000E+01	0.25000000E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00		3
0.00000000E+00	0.00000000E+00	-0.74540000E+03	0.43660000E+01					4
SOOTB	soot	C 166O	166	G	0300.00	4000.00	1000.00	1
0.25000000E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00		2
-0.74540000E+03	0.43660000E+01	0.25000000E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00		3
0.00000000E+00	0.00000000E+00	-0.74540000E+03	0.43660000E+01					4
SOOTH	sootH	C 166O	166H 1	G	0300.00	4000.00	1000.00	1
0.25000000E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00		2
-0.74540000E+03	0.43660000E+01	0.25000000E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00		3
0.00000000E+00	0.00000000E+00	-0.74540000E+03	0.43660000E+01					4
SOOTO	dummy	C 30O	31	G	0300.00	4000.00	1000.00	1
0.25000000E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00		2
-0.74540000E+03	0.43660000E+01	0.25000000E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00		3
0.00000000E+00	0.00000000E+00	-0.74540000E+03	0.43660000E+01					4
SOOTOH	dummy	C 30O	31H 1	G	0300.00	4000.00	1000.00	1
0.25000000E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00		2
-0.74540000E+03	0.43660000E+01	0.25000000E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00		3
0.00000000E+00	0.00000000E+00	-0.74540000E+03	0.43660000E+01					4

SOOTNO	dummy C 300 31N 1	G	0300.00	4000.00	1000.00	1
0.25000000E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	2
-0.74540000E+03	0.43660000E+01	0.25000000E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	3
0.00000000E+00	0.00000000E+00	-0.74540000E+03	0.43660000E+01			4
SOOTNOH	dummy C 300 31N 1H 1G	G	0300.00	4000.00	1000.00	1
0.25000000E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	2
-0.74540000E+03	0.43660000E+01	0.25000000E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	3
0.00000000E+00	0.00000000E+00	-0.74540000E+03	0.43660000E+01			4
S*	2CO C 20 2	G	0300.00	4000.00	1000.00	1
0.25000000E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	2
-0.74540000E+03	0.43660000E+01	0.25000000E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	3
0.00000000E+00	0.00000000E+00	-0.74540000E+03	0.43660000E+01			4
VOL1*	dummy H 346C 236N 40 166G	G	0300.00	4000.00	1000.00	1
0.25000000E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	2
-0.74540000E+03	0.43660000E+01	0.25000000E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	3
0.00000000E+00	0.00000000E+00	-0.74540000E+03	0.43660000E+01			4
VOL2*	dummy H 342C 66	G	0300.00	4000.00	1000.00	1
0.25000000E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	0.00000000E+00	2
-0.74540000E+03	0.43660000E+01	0.25000000E+01	0.00000000E+00	0.00000000E+00	0.00000000E+00	3
0.00000000E+00	0.00000000E+00	-0.74540000E+03	0.43660000E+01			4
O#	O2sinkO 1	G	0300.00	5000.00	1000.00	1
0.02542060E+02	-0.02755062E-03	-0.03102803E-07	0.04551067E-10	-0.04368052E-14		2
0.02923080E+06	0.04920308E+02	0.02946429E+02	-0.01638166E-01	0.02421032E-04		3
-0.01602843E-07	0.03890696E-11	0.02914764E+06	0.02963995E+02			4
O2#	O2sinkO 2	G	0300.00	5000.00	1000.00	1
0.02542060E+02	-0.02755062E-03	-0.03102803E-07	0.04551067E-10	-0.04368052E-14		2
0.02923080E+06	0.04920308E+02	0.02946429E+02	-0.01638166E-01	0.02421032E-04		3
-0.01602843E-07	0.03890696E-11	0.02914764E+06	0.02963995E+02			4
O4	O2sinkO 4	G	0300.00	5000.00	1000.00	1
0.02542060E+02	-0.02755062E-03	-0.03102803E-07	0.04551067E-10	-0.04368052E-14		2
0.02923080E+06	0.04920308E+02	0.02946429E+02	-0.01638166E-01	0.02421032E-04		3
-0.01602843E-07	0.03890696E-11	0.02914764E+06	0.02963995E+02			4
O8	O2sinkO 8	G	0300.00	5000.00	1000.00	1
0.02542060E+02	-0.02755062E-03	-0.03102803E-07	0.04551067E-10	-0.04368052E-14		2
0.02923080E+06	0.04920308E+02	0.02946429E+02	-0.01638166E-01	0.02421032E-04		3
-0.01602843E-07	0.03890696E-11	0.02914764E+06	0.02963995E+02			4
O16	O2sinkO 16	G	0300.00	5000.00	1000.00	1
0.02542060E+02	-0.02755062E-03	-0.03102803E-07	0.04551067E-10	-0.04368052E-14		2
0.02923080E+06	0.04920308E+02	0.02946429E+02	-0.01638166E-01	0.02421032E-04		3
-0.01602843E-07	0.03890696E-11	0.02914764E+06	0.02963995E+02			4
O32	O2sinkO 32	G	0300.00	5000.00	1000.00	1
0.02542060E+02	-0.02755062E-03	-0.03102803E-07	0.04551067E-10	-0.04368052E-14		2
0.02923080E+06	0.04920308E+02	0.02946429E+02	-0.01638166E-01	0.02421032E-04		3
-0.01602843E-07	0.03890696E-11	0.02914764E+06	0.02963995E+02			4
O2*	1213860 2	G	0300.00	5000.00	1000.00	1
0.03697578E+02	0.06135197E-02	-0.01258842E-05	0.01775281E-09	-0.01136435E-13		2
-0.01233930E+05	0.03189166E+02	0.03212936E+02	0.01127486E-01	-0.05756150E-05		3
0.01313877E-07	-0.08768554E-11	-0.01005249E+05	0.06034738E+02			4
NO*	121286N 10 1	G	0300.00	5000.00	1000.00	1
0.03245435E+02	0.01269138E-01	-0.05015890E-05	0.09169283E-09	-0.06275419E-13		2
0.09800840E+05	0.06417294E+02	0.03376542E+02	0.01253063E-01	-0.03302751E-04		3
0.05217810E-07	-0.02446263E-10	0.09817961E+05	0.05829590E+02			4

END