MINIMIZATION OF CARBON LOSS IN
COAL REBURNING

Draft Final Report

Period of Performance

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Abstract

This project develops Fuel-Flexible Reburning (FFR) technology that is an improved version of conventional reburning. In FFR solid fuel is partially gasified before injection into the reburning zone of a boiler. Partial gasification of the solid fuel improves efficiency of NO_x reduction and decreases LOI by increasing fuel reactivity. Objectives of this project were to develop engineering and scientific information and know-how needed to improve the cost of reburning via increased efficiency and minimized LOI and move the FFR technology to the demonstration and commercialization stage. All project objectives and technical performance goals have been met, and competitive advantages of FFR have been demonstrated.

The work included a combination of experimental and modeling studies designed to identify optimum process conditions, confirm the process mechanism and to estimate cost effectiveness of the FFR technology. Experimental results demonstrated that partial gasification of a solid fuel prior to injection into the reburning zone improved the efficiency of NO_x reduction and decreased LOI. Several coals with different volatiles content were tested. Testing suggested that incremental increase in the efficiency of NO_x reduction due to coal gasification was more significant for coals with low volatiles content. Up to 14% increase in the efficiency of NO_x reduction in comparison with basic reburning was achieved with coal gasification. Tests also demonstrated that FFR improved efficiency of NO_x reduction for renewable fuels with high fuel-N content.

Modeling efforts focused on the development of the model describing reburning with gaseous gasification products. Modeling predicted that the composition of coal gasification products depended on temperature. Comparison of experimental results and modeling predictions suggested that the heterogeneous NO_x reduction on the surface of char played important role.

Economic analysis confirmed economic benefits of the FFR technology. Two options to gasify coal were considered: one included a common gasifier and another included a gasifier injector at each injection location. Economic analysis suggested that an FFR system with a common gasifier was more economic than a conventional reburning system and had NO_x reduction cost similar to that of the major competing technology, LNB/SOFA system, for all economic scenarios.

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List of Acronyms

AR	- Advanced Reburning
BACT	- Best Available Control Technologies
CAAA	- Clean Air Act Amendment
CEMs	- Continuous Emissions Monitors
COE	- Cost of Electricity
CRF	- Capital Recovery Factor
CRM	- Conventional Coal Reburn with New Dedicated Coal Mill
DOE	- Department of Energy
GCR1	- Coal Reburn with Common Entrained Gasifier
GCR2	- Coal Reburn with Gasifier Injectors
GE EER	- General Electric Energy & Environmental Research Corp.
GR	- Gas Reburning
COE	- Cost of Electricity
FFR	- Fuel-Flexible Reburning
LNB	- Low NO_x burner
LOI	- Loss on Ignition
NASA	- National Aeronautics and Space Administration
NEOTR	- Northeast Ozone Transport Region
NETL	- National Energy Technology Laboratory
NSR	- Nitrogen Stoichiometric Ratio
ODF	- One Dimensional Flame
OFA	- Overfire Air
O&M	- Operating and Maintenance Costs
OTR	- Ozone Transport Region
PFR	- Plug-Flow Reactor
RACT	- Reasonably Available Control Technologies
RCMM	- Reburning Chemistry-Mixing Model
SBIR	- Small Business Innovation Research
SCR	- Selective Catalytic Reduction
SIP	- State Implementation Plans
SNCR	- Selective Non-Catalytic Reduction
SOFA	- Separated Overfire Air
SR	- Stoichiometric Ratio
T_{OFA}	- Flue Gas Temperature at the Location of the Overfire Air Injection
T_{RF}	- Flue Gas Temperature at the Location of the Reburning Fuel Injection
WSR	- Well-Stirred Reactor

Executive Summary

This project develops Fuel-Flexible Reburning (FFR) technology that is an improved version of conventional reburning. In FFR solid fuel is partially gasified before injection into the reburning zone of a boiler. Partial gasification of the solid fuel improves efficiency of NO_x reduction and decreases LOI by increasing fuel reactivity. The FFR can be retrofitted to existing boilers and can be configured in several ways depending on the boiler, fuel characteristics, and NO_x control requirements. Fly ash generated by the technology is a saleable byproduct for use in the cement and construction industries.

Objectives of this project were to develop engineering and scientific information and know-how needed to improve the cost of reburning via increased efficiency and minimized LOI and move the FFR technology to the demonstration and commercialization stage. Specifically, project goals included: (1) optimize FFR with injection of gasified and partially gasified fuels with respect to NO_x and LOI reduction; (2) characterize flue gas emissions; (3) develop a process model to predict FFR performance and (4) complete an engineering and economic analysis of FFR as compared to conventional reburning and other commercial NO_x control technologies.

The work included a combination of experimental and modeling studies designed to identify optimum process conditions, confirm the process mechanism, and to estimate cost effectiveness of the FFR technology. Pilot scale tests were designed to provide key engineering data required for an FFR demonstration and were conducted at the GE EER test site in Irvine, California in 300 kW Boiler Simulator Facility. Coal was gasified in a gasifier which was designed, assembled and tested within scope of this program. The steps of the modeling approach for this project included (1) updating chemistry-mixing reburning model developed by GE EER in previous R&D projects to include soot, (2) development of a coal gasification model, (3) integrating chemistry-mixing reburning model with coal gasification model and (4) applying this model to predicting the performance of gas-phase coal gasification products as a reburning fuel.

The experimental part of the program was conducted in coordination with two other programs: a commercial coal reburning project that GE EER performed for a commercial client, and DOE SBIR Phase II project No. DE-FG03-98ER82573 titled "Clean and Efficient Utilization of Sewage Sludge." In the commercial project GE EER investigated the potential to

apply coal reburning technology to achieve substantial reductions in power plant NO_x emissions. This allowed the FFR technology to be introduced to the commercial client. The client expressed interest in an FFR demonstration in a 200 MW plant if the study showed economic advantages of coal reburning over other approaches to control NO_x emissions. Testing of renewable fuels was conducted in coordination with the DOE SBIR project. These tests demonstrated that renewable fuels with high fuel-N content could be utilized in FFR.

Experimental results demonstrated that partial coal gasification prior to injection into the reburning zone improved the efficiency of NO_x reduction and decreased LOI. Several coals with different volatiles content were tested. Testing suggested that the incremental increase in the efficiency of NO_x reduction due to coal gasification was more significant for coals with low volatiles content. Tests also demonstrated that the efficiency of NO_x reduction in FFR was more significant when air was used as a transport media. Up to 14% increase in the efficiency of NO_x reduction in comparison with basic reburning was achieved with air transport. Efficiency of NO_x reduction in FFR also depended on the residence time in the reburning zone. Benefits of using FFR over basic reburning were more significant at shorter residence times when coal reaction time was limited.

Tests demonstrated that FFR improved efficiency of NO_x reduction for renewable fuels with high fuel-N content and had a small effect on the performance of fuels with low fuel-N content. Fuels with high fuel-N content benefited more from gasification prior to the injection into reburning zone because fuel-N was partially converted to N_2 during gasification, thus reducing negative impact of fuel-N on NO_x reduction in reburning.

Modeling efforts focused on the development of the model predicting NO_x reduction in reburning with gaseous gasification products. Modeling predicted that composition of coal gasification products depended on temperature. Main gasification products were soot, H_2, CO, and CH_4. Modeling predicted that under fast mixing conditions gasification of small particles of bituminous coals at reaction time of 1 s and temperatures higher than 600 K produced enough volume of products to be used as a reburning fuel at heat inputs up to 20% of the total. However, optimum conditions for a specific solid fuel have to be determined based on fuel characteristics and design parameters of a specific gasifier.

Economic analysis confirmed economic benefits of the FFR technology. Two options to gasify coal were considered: one included a common gasifier and another included a gasifier

injector at each injection location. Analysis suggested that utilization of a common gasifier in FFR was a more economic option than having separate gasifiers for each reburn fuel injector. Economic analysis also suggested that FFR system with common gasifier was more economic than conventional reburning and had NO_x reduction cost similar to that of major competing technology, LNB/SOFA system, for all economic scenarios.

All project objectives and technical performance goals were met, and competitive advantages of FFR were demonstrated.

1.0 INTRODUCTION

This project develops Fuel-Flexible Reburning (FFR) technology that is an improved version of conventional coal reburning. In FFR solid fuel is partially gasified before injection into the reburning zone of a boiler. To achieve gasification, fuel can be transported and injected by a recycled flue gas stream. 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 fuel, gaseous products, and char (Option No. 1). Alternatively, solid fuel can be partially gasified in a gasifier prior to the injection into reburning zone, or gasified in a gasifier injector. Gasification increases coal reactivity and results in lower unburned carbon levels, also referred to as loss on ignition (LOI). In the other 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 allows 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 LOI during coal reburning. Splitting off the char fraction and conveying it to the main burner zone provides high fuel combustion efficiency. The N-agent can be injected into one or several zones of a boiler to increase the efficiency of NO_x reduction. FFR especially improves reburning performance of solid fuels with high fuel-N content by partially converting fuel-N to N_2 during gasification.

The project started in August 2000 and was conducted over a two-year period. The work included a combination of experimental and modeling studies designed to identify optimum process conditions, confirm the process mechanism and to estimate cost effectiveness of the FFR technology. This report consists of 6 sections and 5 appendices. *Section 2* describes the GE EER approach to FFR development. *Section 3* presents results of experimental work conducted in a 300 kW combustor. *Section 4* describes modeling activities and *Section 5* presents FFR conceptual design and economics. A project summary is presented in *Section 6*.

1.1 Technologies for Reducing NO_x Emissions from Coal Fired Boilers

Title 1 of the Clean Air Act Amendments (CAAA) of 1990 specifically links NO_x to ozone levels and, accordingly, requires NO_x controls in ozone non-attainment areas. Title 4 regulations, on the other hand, attacks acid rain, and the regulations address the NO_x component of acid rain by mandating the installation of low-NO_x burners (LNB), whose performance levels were characterized as Reasonably Available Control Technologies (RACT). With initial NO_x RACT standards ranging from 0.45 to 0.50 lb/MMBtu and costs for such technologies low, there was little industry demand for higher efficiency and more expensive NO_x controls such as Selective Non-Catalytic Reduction (SNCR), and Selective Catalytic Reduction (SCR).

Over the last ten years, U.S. Environmental Protection Agency (EPA) has developed most of the specific NO_x regulations authorized by the CAAA under Title 1. The most stringent NO_x controls are required in ozone non-attainment areas or areas which transport pollutants into ozone non-attainment areas. In the Northeast, EPA has defined the Northeast Ozone Transport Region (NEOTR) consisting of Pennsylvania and the states North and East. The EPA originally required that the effected States submit State Implementation Plans that would permit them to achieve new control levels by May 1, 2003 (SIP Call), though the May deadline was subsequently extended 13 months by a court decision. The new levels are determined as a function of the NO_x budget allocated for each state. The budget for a given state represents an average NO_x emission rate of 0.15 lb/MMBtu for each boiler affected at a future date, based upon projected power demand. For many units this corresponds to 70-90% NO_x reduction.

As these specific regulations have developed, the trend has been towards cost effective emission controls. Rather than setting specific limits for each plant, in many areas the regulations have been established to provide the flexibility to over-control on some units and under-control on others, if that approach is cost effective. This can be of considerable advantage since the cost of NO_x control for some units (particularly smaller units) may be much higher than for others, on a basis of \$/ton of NO_x removed. This bubbling approach depends on the availability of NO_x control technologies which can achieve NO_x reductions greater than the nominal control levels (70-90%) at low cost.

At present, the only commercial NO_x control technology capable of achieving such deep NO_x control is SCR. With SCR, NO_x is reduced to N_2 by reactions with N-agents on the surface

of a catalyst. The SCR process effectively uses the N-agent. Injection at a Nitrogen Stoichiometric Ratio, NSR (defined as molar ratio of N atoms in N-agent to NO_x) of 1.0 typically achieves about 80% NO_x reduction (i.e., 80% N-agent utilization). SCR is fully commercialized in Europe and Japan and there are several U.S. installations. This is the reason for its extensive use as the basis of NO_x control requirements for post-RACT.

Since the post-RACT NO_x control requirements are largely based on SCR, achieving the required NO_x levels with SCR is relatively easy. However, SCR is far from an ideal utility solution. There are several important problems, and cost leads the list. SCR requires a catalyst in the flue gas exhaust stream. This catalyst, and the associated installation and boiler modifications, are expensive. As SCR technology has advanced over the last decade, the cost has decreased; however, at present, the initial cost of an 80% NO_x control SCR system for a coal-fired boiler is still about a factor of four greater than that of LNB. Increasing the NO_x control to 95% approximately doubles the SCR system cost.

In addition, the SCR catalyst life is limited. Catalyst deactivation, through a number of mechanisms, typically limits catalyst life to about 4 years for coal-fired applications. SCR catalysts are also toxic, and therefore pose disposal problems. Since the catalyst is the major cost element in the SCR system, catalyst replacement and disposal contributes heavily to the total cost of NO_x control.

As an alternative to SCR, Combustion Modification achieves deep NO_x control by integrating several components:

- Low NO_x Burners - LNB (aerodynamic staging) is typically the lowest cost Combustion Modification technique and is usually applied as the first step towards low cost deep NO_x control. At the time of SIP Call compliance, most units will already have LNB to meet the 2000 Title 4 requirements.

- Overfire Air - OFA (air staging) can reduce NO_x by an additional ~25% from LNB.

- Reburning (fuel staging) involves injecting additional fuel above the existing burner zone followed by OFA for burnout and CO control. Reburning can effectively reduce NO_x by up to 60% from LNB levels depending on site-specific factors and the amount of reburn fuel injected. The reburning fuel can be natural gas, oil, micronized coal, biomass, etc.

- Advanced Reburning - AR (integration of reburning with nitrogen agent injection) can reduce NO_x, as suggested by recent GE EER full scale field trials using overfire air as the

agent carrier, by an additional 40%, with a minimum of ammonia slip problems. The N-agent (ammonia or urea) can be injected in a number of configurations selected to optimize overall performance of the reburning and SNCR components at minimum overall cost.

Reburning is a low-cost NO_x control technology. However, reburning alone cannot provide the level of NO_x reduction required by the EPA regulations. Integration of reburning with other low cost NO_x control technologies (for example, LNB) can achieve the target 0.15 lb/MMBtu NO_x emissions in many cases. Therefore, even a small increase in reburning efficiency due to optimized conditions of reburning would be very important. It would allow low cost NO_x control technologies to provide the required level of control in many units. *Results of this project demonstrated that an increase in reburning efficiency could be achieved by partially gasifying solid fuel prior to the injection into reburning zone.*

1.2 The Problem of Ash Utilization Associated with NO_x Reduction Technologies

Many combustion modification techniques can cause LOI to increase to unacceptable levels. In numerous examples the retrofit of LNB to existing boilers has resulted in LOI increase and consequently combustion efficiency losses. The unburned carbon represents a few percent of total fuel consumption (1% loss at $40/ton represents $400,000 per million tons of coal). Additionally, productive uses of carbon-enriched fly ash are limited and high carbon ash is more expensive to dispose of. A typical use for fly ash is as an additive in concrete. Fly ash can react with lime providing improved concrete properties, such as additional strength, lower water content, lower heat of hydration, and lower cost. However, high carbon ash is not usable in concrete. The standard specifications call for less than 6% carbon in ash, although some specific projects require as low as 3%.

The challenge today is to minimize carbon loss while also minimizing NO_x emissions. Two methods have been demonstrated for reducing LOI under low NO_x conditions. The first method is the reduction of coal particle size, and the second is natural gas reburning (GR). Although particle size reduction is an effective method of reducing carbon loss in low NO_x systems, this usually requires expensive modifications or complete replacement of the pulverizing equipment.

Utilizing GR is another method of operating a combustion system with low carbon losses and NO_x emissions. For example, at Public Service of Colorado's Cherokee Station on a 173

MWe wall-fired unit, the initial baseline LOI was approximately 4.0% at full load. Retrofit of LNB resulted in NO_x reduction of about 40% with an increase in LOI to 6.0%. The addition of GR resulted in further 65% NO_x reduction and, at the same time, reduced LOI to 4.5%.

Although gas reburning is a proven technology for effective NO_x reduction and reducing carbon losses, the cost of gas, about $2.5-3.5/MMBtu, is significantly higher than the cost of the main fuel, coal (typically, $1.0-1.5/MMBtu). When reburning or AR are applied using natural gas, the differential cost of the reburn fuel is a key cost element, often comprising more than half of the total cost of NO_x control. The differential cost of the reburning fuel can be eliminated by reburning with the same fuel normally fired in the boiler - coal. Unfortunately, it is difficult to achieve complete burnout of the reburn coal due to the lack of oxygen in the reburning zone and the low temperature in the burnout zone once OFA is injected. Thus, while the differential cost of the reburn fuel is eliminated, there is a reduction in combustion efficiency and the resulting high carbon ash cannot be sold and must be disposed at additional cost. *Results of this project demonstrated that FFR reduces LOI in comparison with basic reburning.*

1.3 Fuel-Flexible Reburning

The FFR technology is an improved version of coal reburning targeted to minimize LOI while providing high efficiency NO_x control. As was noted earlier, if coal reburning is applied, LOI can increase to unacceptable levels, precluding utilization of the ash by the cement industry. To address these problems, the FFR technology allows inexpensive reburn fuels to be utilized under conditions that minimize LOI. Results presented in this report demonstrated that partial solid fuel gasification decreased LOI and improved fuel reactivity by forming reactive gas-phase species.

The FFR technology is particularly effective for fuels with high fuel-N content. Coal typically contains about 1% fuel-N, some renewable fuels (for example, sewage sludge) can contain up to 3% fuel-N. Significant fraction of the fuel-N is released into the gas-phase during combustion. When injected in the reburning zone, N-containing species are partially reduced to N_2 and partially oxidized by excess air coming from the main combustion zone to form NO_x coursing reduction in NO_x removal efficiency. In FFR, part of the fuel-N is converted to N_2 in the fuel-rich environment of the gasification zone. Pilot-scale tests conducted within scope of this program confirmed this.

Figure 1-1 shows how the FFR technology can be applied to a coal fired power plant. A wall-fired boiler is illustrated, but the technology is equally applicable to all firing configurations. Different approaches to partially gasify coal before injecting into reburning zone can be used. One approach includes utilization of a common coal gasifier for all reburning injectors (Figure 1-1a).

a
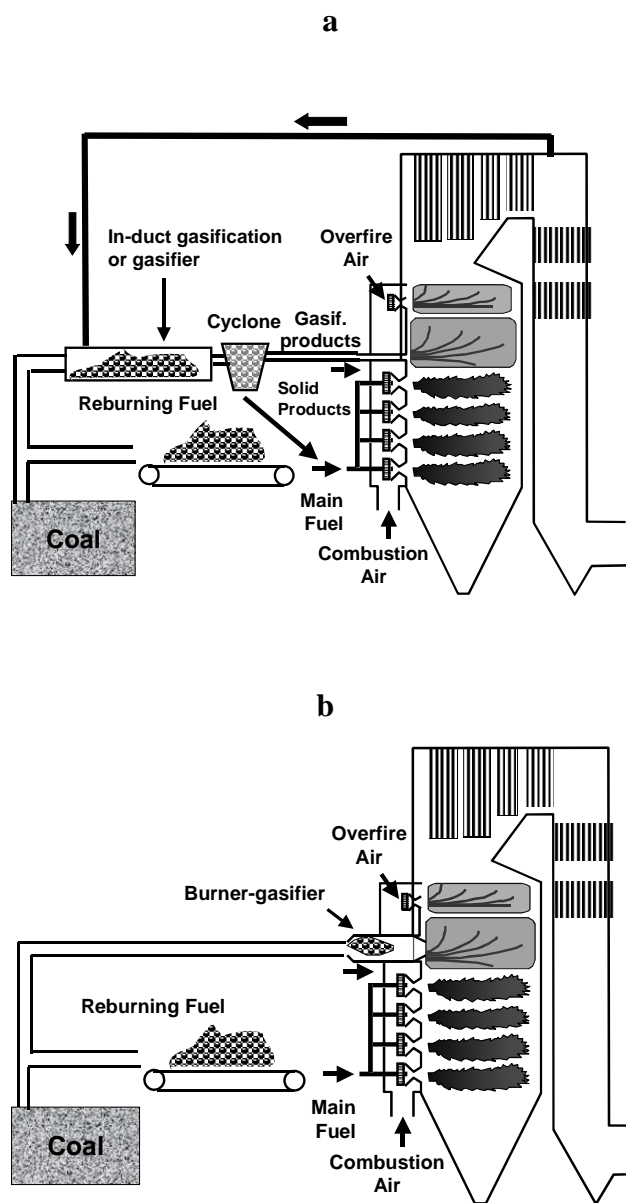
Figure 1-1. FFR application to coal-fired boiler. a - common gasifier/in-duct gasification of the reburning fuel, b – gasifier injector at each injection location.

b

Such a gasifier can consist of a conventional coal pipe and utilizes partial coal combustion to generate heat required for coal gasification. Alternatively, hot recirculated flue gas can be used to

partially gasify coal. In this approach coal is injected into the duct and conveyed to the furnace by hot flue gas. Char can be separated from gas-phase products using a cyclone and then injected along with coal into the main combustion zone. Gas-phase gasification products are injected into reburning zone. Another approach to gasify coal includes utilization of a gasifier injector at each injection location (Figure 1-1b). In this approach each reburning fuel injector has extended length to provide enough residence time to allow coal gasification. Limited amount of air is supplied for coal combustion and coal is gasified at relatively high temperatures and short residence times within reburn fuel injector.

The components of the FFR process depend on the specific configuration chosen for coal gasification and may include:

- <u>Reburning fuel injection system</u> - similar to a conventional reburning fuel injection system.
- <u>Overfire air ports</u> - similar to those used for conventional OFA.
- <u>Coal partial gasification system</u> - This system can include a common gasifier, in-duct gasification using recycled flue gas, or a gasifier injector.

Adapting any of these gasification systems to specific process conditions will not require substantial development. Boiler temperatures will not be significantly impacted and impacts upon boiler thermal efficiency will be minimal.

The FFR technology is an original concept applicable to utility boilers that burn solid fuel as their primary fuel. FFR can cost-effectively reduce NO_x emissions to required levels, can be readily retrofitted to existing plants, and has high potential for commercial success.

2.0 APPROACH TO THE FFR DEVELOPMENT

This section describes the GE EER approach to the development of the FFR technology. Figure 2-1 presents the task structure and the major milestones of the project. Task 1, Project Management and Reporting, coordinated the efforts of key personnel involved with the project so that the objectives of this project are met on time, on specification, and on budget. Pilot scale tests (Tasks #2 and 3) were designed to provide key engineering data required for the FFR demonstration. Pilot-scale experiments were conducted at the GE EER test site in Irvine, California. The 300 kW Boiler Simulator Facility (BSF) described in *Section 3* was used in tests. Coal was gasified in a gasifier which was designed, assembled and tested within scope of this program. The steps of the modeling approach for this project included (1) updating chemistry-mixing reburning model developed by GE EER in previous R&D projects to include soot and char reactions, (2) development of coal gasification model, (3) integrating chemistry-mixing reburning model with coal gasification model (Task # 4) and applying this model to predicting the performance of gas-phase coal gasification products as a reburning fuel. Based on previous experience with reburning modeling, such a model could predict process performance for the FFR Option No. 2. A conceptual FFR process design was developed in Task 5. Two options to gasify coal were considered: one included a common gasifier and another included a gasifier injector at each injection location. Cost estimate demonstrated cost effectiveness of the FFR technology.
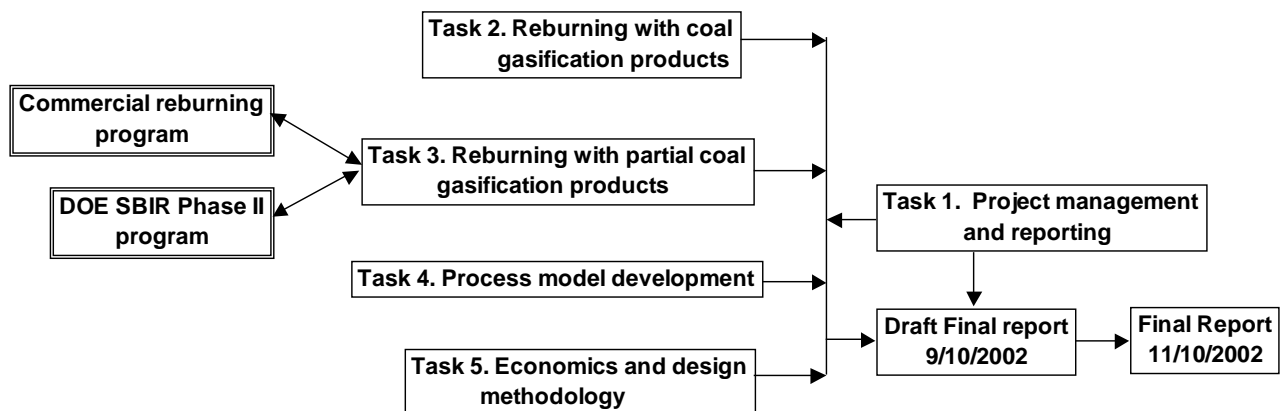
Figure 2-1. Project task structure.

The experimental part of the program was conducted in coordination with two other programs: a commercial coal reburning project that GE EER performed for a commercial client, and DOE SBIR Phase II project No. DE-FG03-98ER82573 titled "Clean and Efficient Utilization of Sewage Sludge." Specifically, basic coal reburning tests were conducted in the scope of the commercial project. In the commercial project GE EER investigated the potential to apply coal reburning technology to achieve substantial reductions in power plant NO_x emissions. This allowed to introduce the commercial client to the FFR technology. The client expressed interest in FFR demonstration in 200 MW plant, if the study showed economic advantages of coal reburning over other approaches to control NO_x emissions. Testing of renewable fuels was conducted in coordination with the DOE SBIR project. Because of their high fuel-N content, these fuels are not considered as promising reburning fuels. FFR tests demonstrated new application for renewable fuels with high fuel-N content.

Significant efforts were undertaken to advertise FFR technology to make it visible to potential users. Project results were presented at the following conferences:

1. DOE NETL sponsored Conference on Unburned Carbon on Utility Fly Ash, Pittsburgh, PA, May 2001.

2. DOE NETL sponsored Conference on Selective Catalytic Reduction and Selective Non-Catalytic Reduction for NO_x Control, Pittsburgh, PA, May 2002.

3. 2002 Spring Meeting of the Western States Section of the Combustion Institute, University of California at San Diego, La Jolla, CA, March 2002.

The following papers were published:

1. V. Lissianski, L. Ho, P. Maly and V. Zamansky, "Minimization of Carbon Loss in Coal Reburning", 2[d] Joint Meeting of the U.S. Sections of the Combustion Institute, Oakland, CA, March 27, 2001.

2. V. Lissianski, L. Ho, P. Maly and V. Zamansky, "*Integration of Coal Gasification and Reburning*", 2002 Spring Meeting of the Western States Section of the Combustion Institute, University of California at San Diego, La Jolla, CA, March 2002.

All project objectives and technical performance goals have been met, and it was demonstrated that FFR technology can increase efficiency of NO_x reduction and decrease LOI in comparison with basic reburning.

3.0 PILOT-SCALE TESTS

3.1 Experimental Facilities

Two test facilities were utilized in the experimental work: Boiler Simulator Facility (BSF) and a gasifier. Both facilities are located at GE EER's test site in Irvine, CA. A schematic of the experimental setup is shown in Figure 3-1. The BSF was utilized in basic reburning tests while an integrated gasifier-BSF setup was used in FFR tests. In all tests natural gas was main fuel. In basic reburning tests solid fuel was injected directly into BSF reburning zone. In gasification tests solid fuel was injected in the gasifier and partially gasified. Gas-phase products of the gasification and char were delivered to the BSF through stainless steel duct.

The following sub-sections describe BSF, solid fuel gasifier and its shakedown.
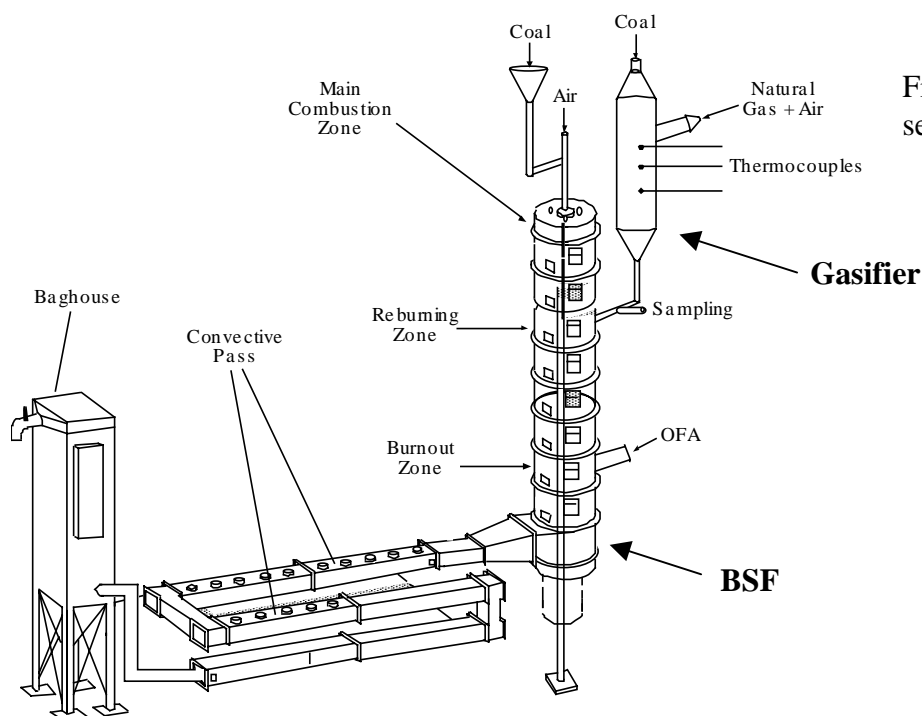
Figure 3-1. Experimental setup.

3.1.1 Boiler Simulator Facility (BSF)

The Boiler Simulator Facility (BSF) is a down-fired combustion research facility with a nominal firing rate of 300 kW. It is designed to simulate the thermal characteristics of a utility boiler. As shown in Figure 3-1, the BSF consists of a burner, vertical radiant furnace, and horizontal convective pass. The facility's variable swirl diffusion burner is equipped to fire coal, oil, or natural gas. The furnace is constructed of eight modular refractory lined spool sections

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with access ports. The furnace has an inside diameter of 0.55 m and a height of 5.4 m. The radiant section is equipped with adjustable heat removal panels. Configuration of these panels is adjusted such that the BSF matches the residence time-temperature profile and furnace exit gas temperature of a specific full-scale boiler. The convective pass is equipped with air-cooled tube bundles designed to simulate the superheater and economizer sections of a coal-fired boiler. The facility has a baghouse at the end of the convective pass to control fly ash emissions. Because it accurately simulates the thermal environment of a full-scale boiler, the BSF is ideally suited to process optimization studies leading to utility boiler application.

Figure 3-2 shows a typical axial temperature profile for the BSF. Temperature gradient was adjusted to simulate environment in a typical large-scale boiler.
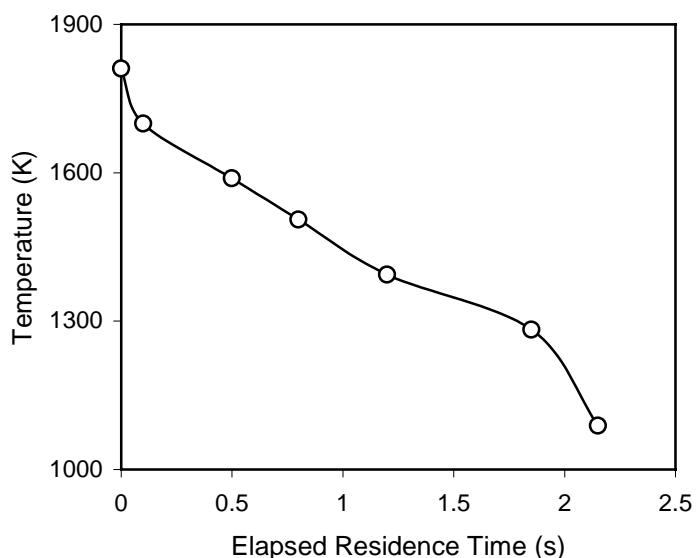
Figure 3-2. Axial temperature profile in BSF. Elapsed time corresponds to the time after injection of the reburning fuel.

Process performance was characterized by continuous emissions monitors (CEMs), which provided an online analysis of flue gas composition. The CEMs consisted of a water-cooled sample probe, sample conditioning system (to remove water and particulate), and gas analyzers. Species analyzed, detection principles, and detection limits were as follows:

- O_2: paramagnetism, 0.1%
- NO_x: chemiluminescence, 1 ppm
- CO: nondispersive infrared, 1 ppm
- CO_2: nondispersive infrared, 0.1%
- N_2O: nondispersive infrared, 1 ppm

Manual method sampling was also performed for NH_3 using SCAQMD Method 207 (sampling, Nessler reagent, colorimetry), with 1 ppm precision.

       High purity dry nitrogen was used to zero the analyzers. Certified span gases were used to calibrate and check linearity of the analyzers. A chart recorder was used to obtain a hard copy of analyzer outputs. A personal computer based data acquisition system (LabTech Notebook) was used for storage and analysis of test data. Furnace gas temperatures were periodically measured using a calibrated suction pyrometer.

3.1.2 Solid Fuel Gasifier Design and Shakedown

       Schematic of the solid fuel gasifier is shown in Figure 3-3. The gasifier was constructed from stainless steel and its inner walls were refractory lined. Heat required for solid fuel gasification was supplied by the combustion of natural gas in air. The auxiliary section of the gasifier had an internal diameter of 20 cm. Solid fuel was injected into the gasification section that had an internal diameter of 30 cm. Nitrogen or air was used as a transport media for solid fuel. Temperature profile in the gasification zone was measured using several thermocouples located along the zone. Ports located near the exit of the gasifier allowed gas and solid samples to be taken and analyzed.

       After the gasifier was designed, assembled and installed, shakedown tests with coal were conducted to characterize its performance. Goals of these tests were to determine the dependence of the extent of coal gasification on the value of auxiliary heat, coal transport media, temperature and residence time in the gasifier. During shakedown tests, the auxiliary natural gas burner heat input varied from 70,000 to 80,000 Btu/hr. Kittanning coal (see Table 3-1 for coal composition) was used in shakedown tests. Figure 3-4 shows measured temperature profile in the gasification zone at 70,000 Btu/hr auxiliary heat input at 16% and 26% heat inputs of the reburning fuel. Here heat input of the reburning fuel is defined as percent from the total BSF heat input.

Table 3-1. Test fuel analyses.

		Units	Coal A	Coal B	Kittanning	Sewage sludge	Utah	WKE-C	Almond shell	Walnut shells	Willow wood
As received						Ultimate Analysis					
	C	wt %	68.92	63.11	72.40	33.03	66.94	66.77	-	-	-
	H	wt %	4.07	4.00	4.20	4.81	4.74	4.35	-	-	-
	N	wt %	1.30	1.02	1.21	3.81	1.32	1.49	-	-	-
	S	wt %	0.84	5.77	1.22	1.25	0.63	3.15	-	-	-
	Ash	wt %	14.89	17.58	10.85	34.05	7.17	9.17	-	-	-
	O	wt %	4.04	4.07	7.02	16.5	10.52	5.10	-	-	-
	H_2O	wt %	5.94	4.45	3.10	6.55	8.68	9.97	-	-	-
	HV	Btu/lb	11,912	11,269	12,390	6,251	11,806	11,848	-	-	-
Dry	C	wt %	73.27	66.05	74.72	35.35	73.30	74.16	36.27	51	51.15
	H	wt %	4.33	4.19	4.33	5.15	5.19	4.83	3.94	5.72	3.4
	N	wt %	1.38	1.07	1.25	4.08	1.45	1.66	0.79	0.32	0.35
	S	wt %	0.89	6.04	1.26	1.34	0.69	3.50	0.05	0	0.05
	Ash	wt %	15.83	18.40	11.20	36.44	7.85	10.19	26.57	1.93	2.68
	O	wt %	4.30	4.26	7.24	17.66	11.52	5.66	32.38	41.03	42.37
	HV	Btu/lb	12,664	11,794	12,786	6,689	12,928	13,160	Not Determined		
						Proximate Analysis					
	Volatiles	wt%	38.21	45.59	33.78	Not Determined	46.44	44.13	Not Determined		
	Fixed C	wt%	61.79	54.41	66.22	Determined	53.56	55.87			
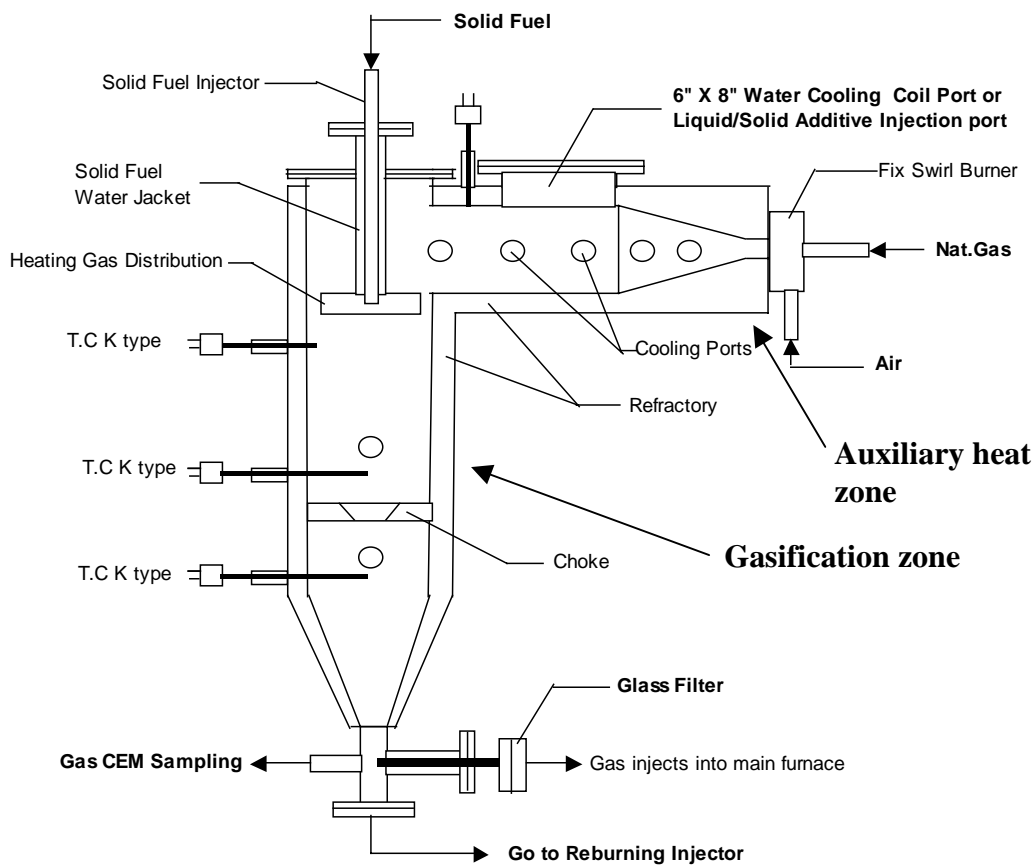
Figure 3-3. Solid fuel gasifier.
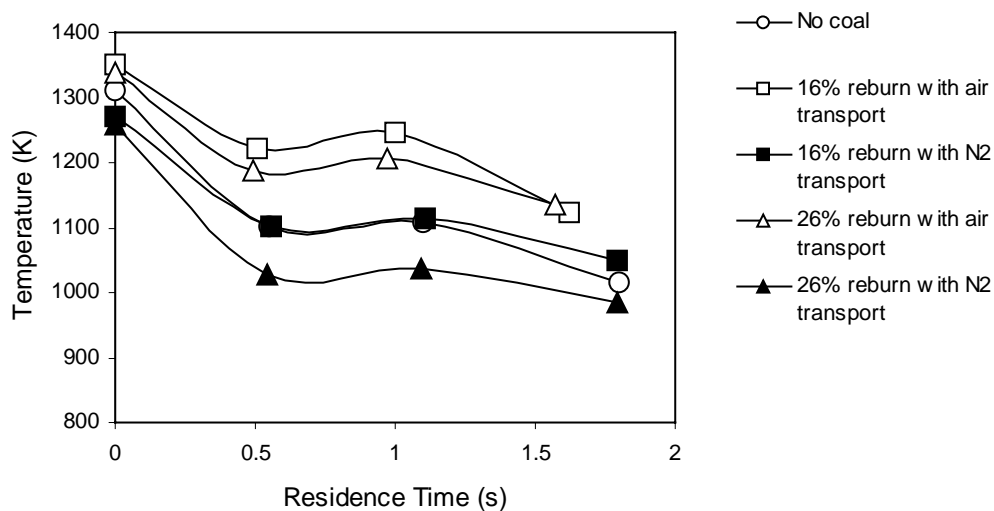
Figure 3-4. Temperature profiles in the gasification zone at 16% and 26% heat inputs of the reburning fuel. Auxiliary heat input is 70,000 Btu/hr.

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Figure 3-4 demonstrates that temperature in the middle of the gasification zone is about 1100 K without coal injection and decreases when nitrogen is used as a transport media for coal injection. The decrease is most likely caused by coal gasification, which is an endothermic process. This conclusion is supported by the observation that the temperature decrease becomes more significant when a larger amount of coal is injected into gasification zone. When air is used as a coal transport media, temperature in the gasification zone increases due to the partial coal oxidation by oxygen from air. This temperature increase is more significant for a larger amount of coal injected.

Figure 3-5 shows temperature profiles in the gasification zone at 80,000 Btu/hr auxiliary heat input and different heat inputs of the reburning fuel. As for 70,000 Btu/hr auxiliary heat input, the temperature in the gasifier decreases with nitrogen transport and increases with air transport. Comparison of Figures 3-4 and 3-5 demonstrates that temperature in the gasification zone increases as auxiliary heat input increases. During the test program, auxiliary heat was set at 80,000 Btu/hr.
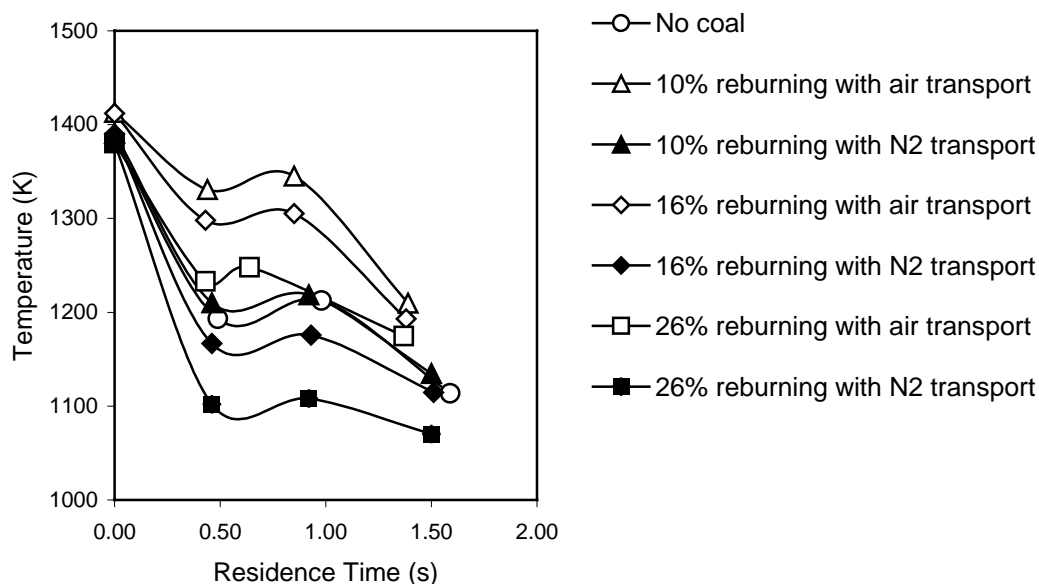
Figure 3-5. Temperature profiles in the gasification zone at different heat inputs of the reburning fuel. Auxiliary heat input is 80,000 Btu/hr.

To determine the extent of coal gasification, gas and solid samples were taken at the gasifier exit. Gas samples were sent to an outside lab and analyzed to determine content of hydrocarbons, CO, and H_2. Solid samples were analyzed to determine unburned fuel (LOI).

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Figures 3-6 and 3-7 show the effect of the residence time and stoichiometric ratio (SR) in the gasification zone on gasification products LOI. Gasifier SR was varied by varying the amount of coal and by changing gas carrier from air to nitrogen. Moving the coal injector deeper into the gasification zone varied residence time. Figures 3-6 and 3-7 demonstrate that the extent of gasification increases as residence time and SR increase.
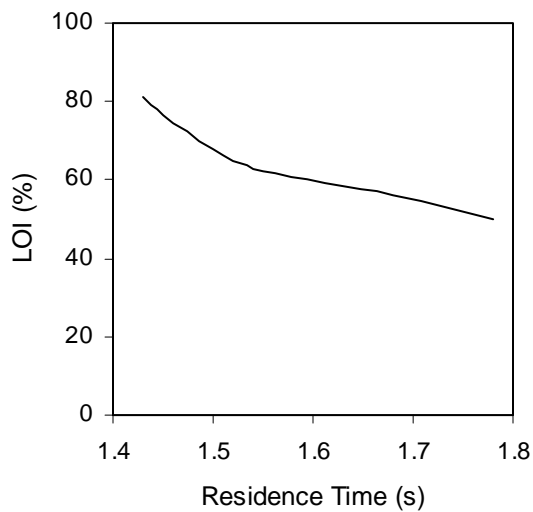
Figure 3-6. Effect of the gasifier residence time on carbon content in gasification products.
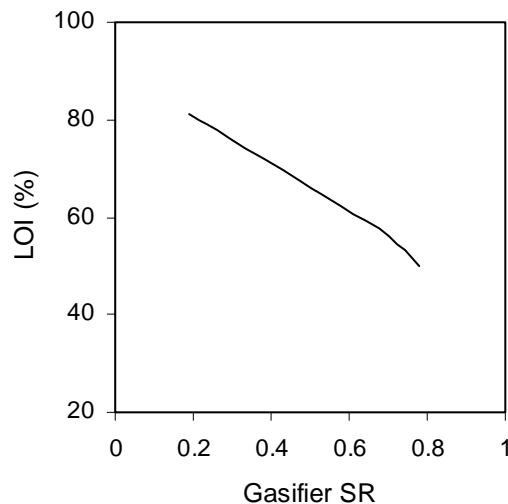
Figure 3-7. Effect of the stoichiometric ratio in the gasification zone on carbon content in gasification products.

Figure 3-8 shows composition of coal gasification products. Samples were collected only with nitrogen as a transport media. Sample analysis did not show heavy hydrocarbons, most likely because they condensed in the sampling line which was maintained at room temperature. Data presented in Figure 3-8 were obtained at 10% and 20% of the reburning fuel heat input. Comparison of data at 10% and 20% reburning shows that concentrations of combustible species increase as the amount of coal increases. Predominant combustible gasification products are H_2 followed by CO and CH_4.
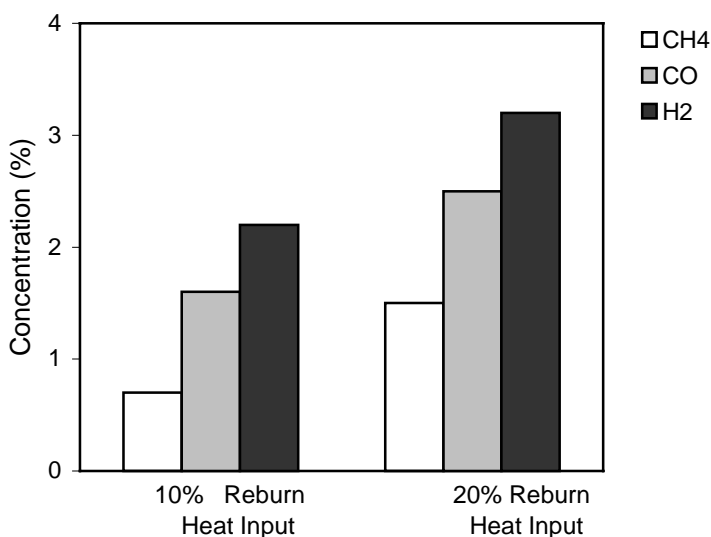
Figure 3-8. Composition of gasification products at 10% and 20% reburning fuel heat input.

3.2 Basic Coal Reburn Tests

Studies conducted by GE EER have shown that a number of solid fuels can be used effectively in the reburning process. However, due to the heterogeneous nature of solid fuel, it is difficult to predict how a specific fuel will perform as a reburning fuel based upon easily characterized fuel properties. Therefore, combustion tests were performed to evaluate the basic reburning performance of several solid fuels including coals A and B, Kittanning coal and sewage sludge. The goals were to characterize their performance as a benchmark for gasification tests. Fuel characteristics are shown in Table 3-1.

Coals A and B were tested in the scope of the commercial coal reburning project that GE EER performed for a commercial client. In that project GE EER investigated the potential to apply coal reburning technology to achieve substantial reductions in power plant NO_x emissions.

Kittanning is a bituminous coal similar in composition to a significant portion of coals used by the US power industry. It has been used in previous pilot-scale studies involving coal combustion and its performance is well characterized.

Sewage sludge is produced as a byproduct of the treatment of raw sewage. Sewage sludge is used as a fertilizer or landfilled, with a small percentage incinerated. However, recently concerns were raised about its use as fertilizer or disposal in landfills. These concerns focused on the potential for contamination of water and land resources from the migration of sewage sludge toxic constituents. Thus, alternative approaches to utilize sewage sludge are needed.

Because of the high fuel-N content, sewage sludge is not considered as a promising reburning fuel. It was expected, however, that sewage sludge performance would be acceptable in FFR.

Tests were performed to characterize the impacts of reburning process parameters on NO_x reduction at conditions typical for the full-scale boilers. These tests provided baseline data that were used for benchmarking FFR.

For the basic reburning experiments, the main burner was fired with natural gas. Ammonia was premixed with the combustion air to provide a controlled initial NO_x level. Each fuel was pulverized in a CE-Raymond deep bowl mill such that 70% passed through a 200 mesh sieve.

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) or air. The range of parameters investigated in the study represented the range of conditions available at the 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 furnace heat input. The 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 for coals A and B, and at 400 ppm for Kittanning coal and sewage sludge.

Figure 3-9 shows reburning performance of the coal A at initial NO_x = 430 ppm. Figure 3-10 compares performances of coals A and B at initial 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.

It is believed that the observed trends are related to 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. Another 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.
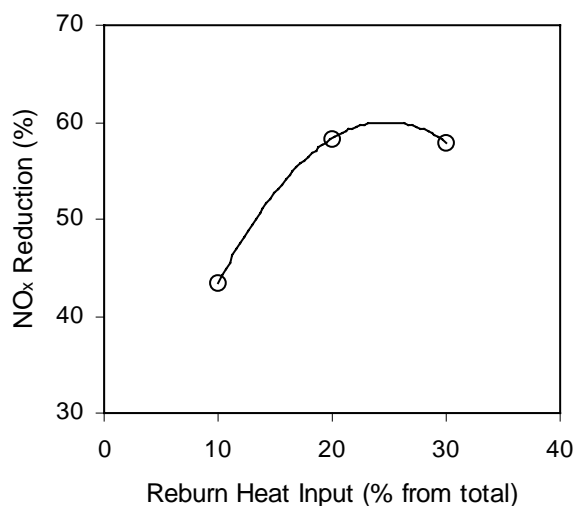
Figure 3-9. Basic coal reburning performance of coal A at initial NO_x = 430 ppm with N_2 transport.
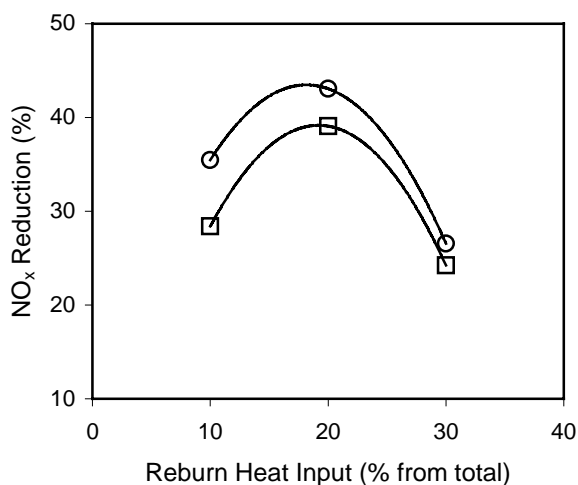
Figure 3-10. Basic coal reburning performance of coals A (rectangles) and B (circles) at initial NO_x = 230 ppm with N_2 transport.

Figure 3-11 shows performance of a blend of coals A and B at initial NO_i = 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 NO_i = 230 ppm.

Figure 3-12 shows basic coal reburn performance of Kittanning coal. Maximum NO_x reduction provided by Kittanning coal was about 40% with N_2 transport. Reburn performance of sewage sludge (Figure 3-13), on the other hand, was much worse than that of coal. As expected, tests demonstrated that sewage sludge was not a promising reburning fuel. Because of the high fuel-N content of the fuel, at some conditions injection of sewage sludge resulted in NO_x formation rather than reduction.

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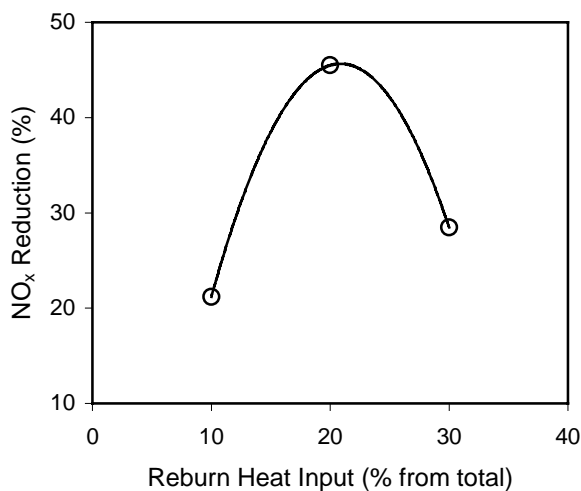
Figure 3-11. Basic coal reburn performance of coal blend (70% Coal A/30% Coal B) at initial NOx = 230 ppm with N_2 transport.
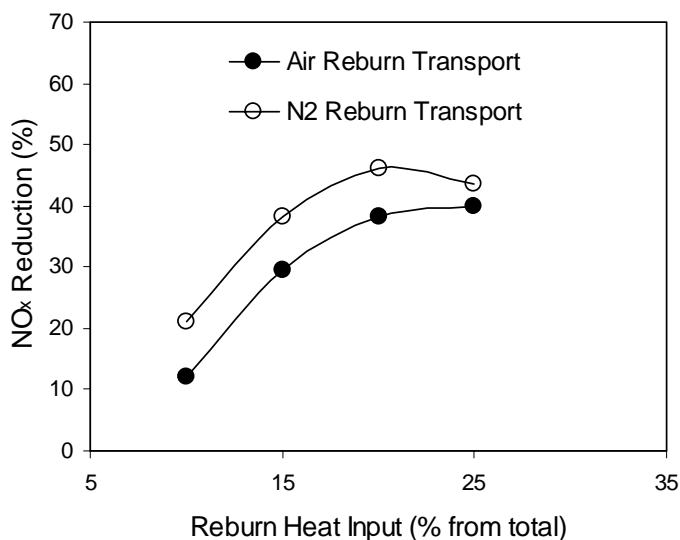
Figure 3-12. Basic Kittanning coal reburn performance at initial NO_x=400 ppm.

The following conclusions can be drawn from basic reburning tests:

- Coal can be an effective reburning fuel. Efficiency of NO_x reduction in coal reburning depends on process conditions and coal type.

- Efficiency of NO_x reduction decreases with the decrease in the initial NO_x concentration.

- Up to 60% NO_x reduction was achieved for coal A at 20-30% heat input of the reburning fuel.

- Because of the high fuel-N content, sewage sludge is not a promising reburn fuel at typical reburn conditions of coal-fired boilers.

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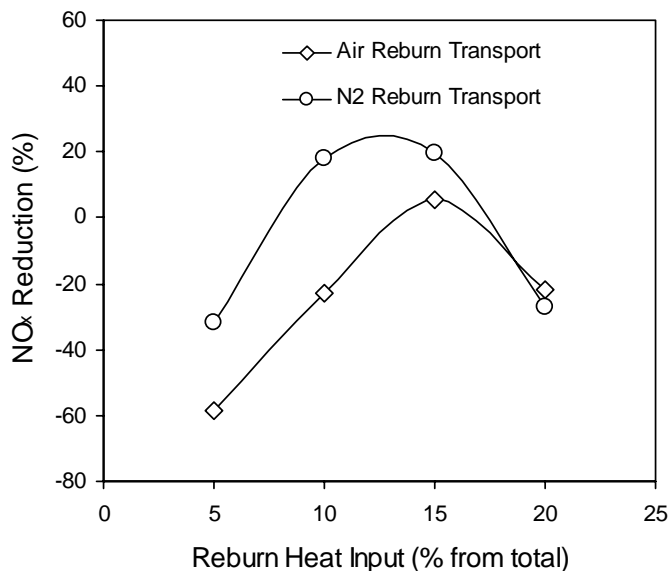
Figure 3-13. Basic sewage sludge reburn performance at initial NO_x=400 ppm.

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3.3 FFR Tests

3.3.1 Coal Gasification

Tests were conducted to determine the effect of partial coal gasification on the efficiency of NO_x reduction in FFR. Figure 3-14 shows a schematic of the injector that was used to inject gasification products into the BSF reburning zone. Walls of the injector were water-cooled to prevent their damage by hot gases coming from the BSF main combustion zone. Walls of the injector were also refractory lined from inside to maintain high temperature of gasification products and prevent condensation of heavy hydrocarbons.
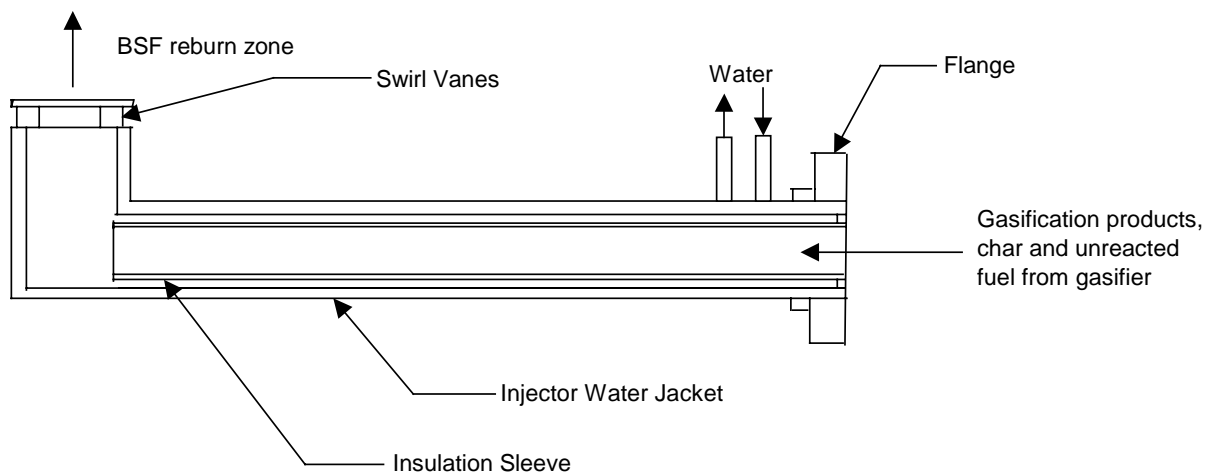
Figure 3-14. Schematic of solid fuel injector.

　　　　Sections 3.3.2 and *3.3.3* describe coal screening and FFR optimization tests and *Section 3.3.4* describes FFR tests with renewable fuels.

3.3.2 Coal Screening Tests

　　　　Coal screening tests were first conducted with several coals to determine the effect of coal composition on the efficiency of NO_x reduction in FFR and to select a coal for FFR optimization. Besides A, B, and Kittanning coals, Utah and WKE-C coals were also tested to broaden base of the screening tests. Compositions of tested coals are presented in Tables 3-1.

　　　　Figures 3-15 compares efficiencies of NO_x reduction of coals and gasified coals. The amount of the reburning fuel was 20% for Kittanning, Utah and WKE-C coals, 10% for coal A and 15% for coal B. Residence time in the reburning zone was 0.6 s. Reburning fuel was injected at a flue gas temperature T_{RF} of 1750 K and OFA was injected at flue gas temperature T_{OFA} of 1640 K. Initial NO_i was 370 ppm at 0%O_2. Figure 3-15 demonstrates that coal gasification improves the efficiency of NO_x reduction for all five tested fuels. The largest improvement in the efficiency of NO_x reduction was achieved for Kittanning coal, while improvements for coals A, B, and Utah were smaller.
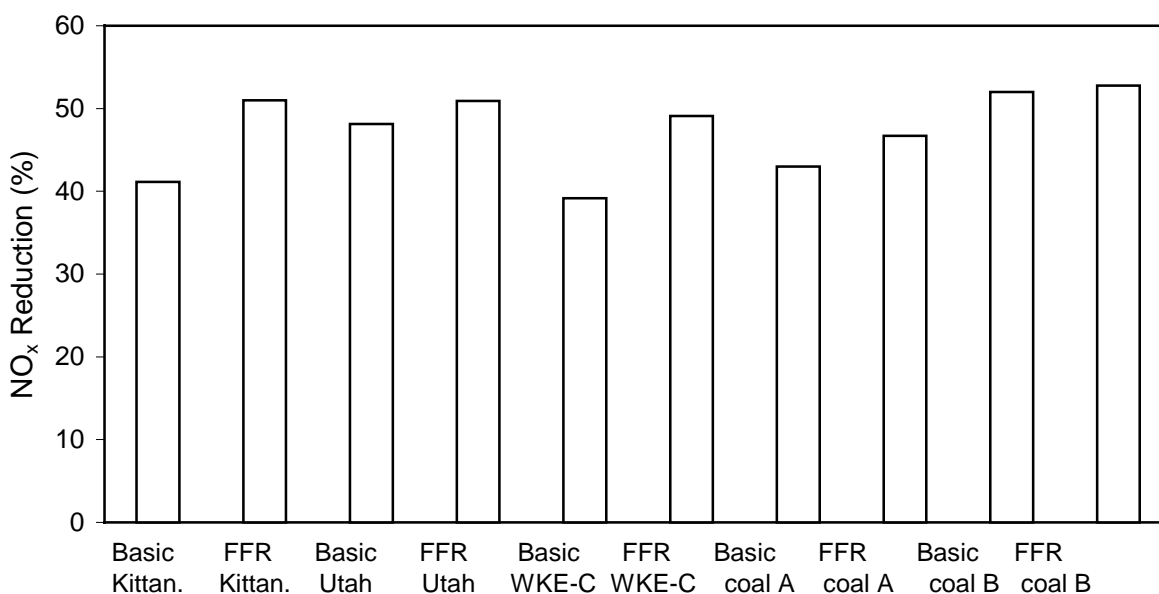
Figure 3-15. Comparison of basic reburn and FFR performances at 20% reburn for Kittanning, Utah, WKE-C coals, at 10% reburn for coal A, and 15% reburn for coal B.

　　　　Figure 3-16 demonstrates the dependence of the relative NO_x reduction on coal volatiles

content. Relative NO_x reduction is defined as a difference between NO_x reduction by gasified and un-gasified coal (basic reburn). In other words, it is the incremental increase in NO_x reduction due to coal gasification. With air and nitrogen transport, relative NO_x reduction decreases when volatiles content increases above 45%.
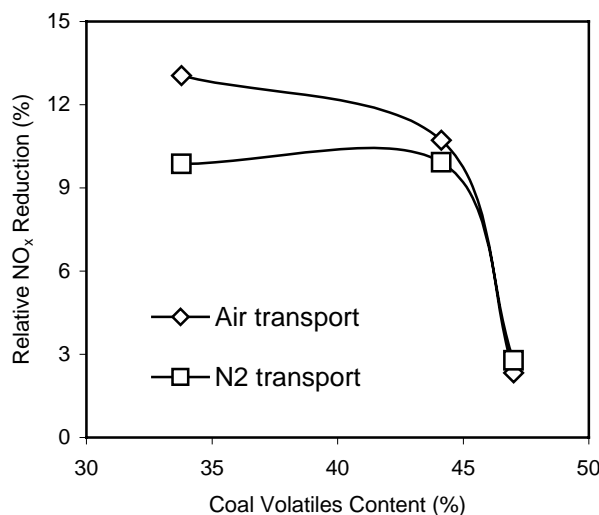
Figure 3-16. Effect of coal volatiles content on relative NO_x reduction.

Since screening tests demonstrated that increase in relative NOx reduction was the most significant for Kittanning coal, this coal was selected for optimization tests.

3.3.3 FFR Optimization Tests

Optimization tests were conducted with Kittanning coal to determine the effect of process parameters on the efficiency of NO_x reduction in FFR. Process parameters varied in these tests included T_{RF}, initial NO_x, residence times in the reburning and gasification zones, and auxiliary heat input.

Figure 3-17 compares performances of natural gas, coal and gasified coal in reburning. It is known that the efficiency of NO_x reduction can be affected by mixing conditions in the reburning zone. Precautions were taken to preserve the same mixing conditions in the reburning zone for all three fuels. In basic reburning tests natural gas or coal were injected into BSF reburning zone through the duct connecting gasifier with the BSF. Gasifier auxiliary natural gas flame in basic reburning tests was operating at the same conditions as in gasification tests. The same injector that was used in gasification tests was used to inject natural gas and coal. This allowed direct comparison of NO_x reduction by different fuels under similar mixing conditions in

the reburning zone. The auxiliary natural gas was fired at 80,000 Btu/hr, and the main fuel in BSF was natural gas. Initial NO_i was 370 ppm at $0\%O_2$ and was controlled by adding ammonia to the air in the main combustion zone. Reburning fuel and OFA were injected at T_{RF} of 1640 K and T_{OFA} of 1450 K, respectively, and the residence time in the reburning zone was 0.7 s.
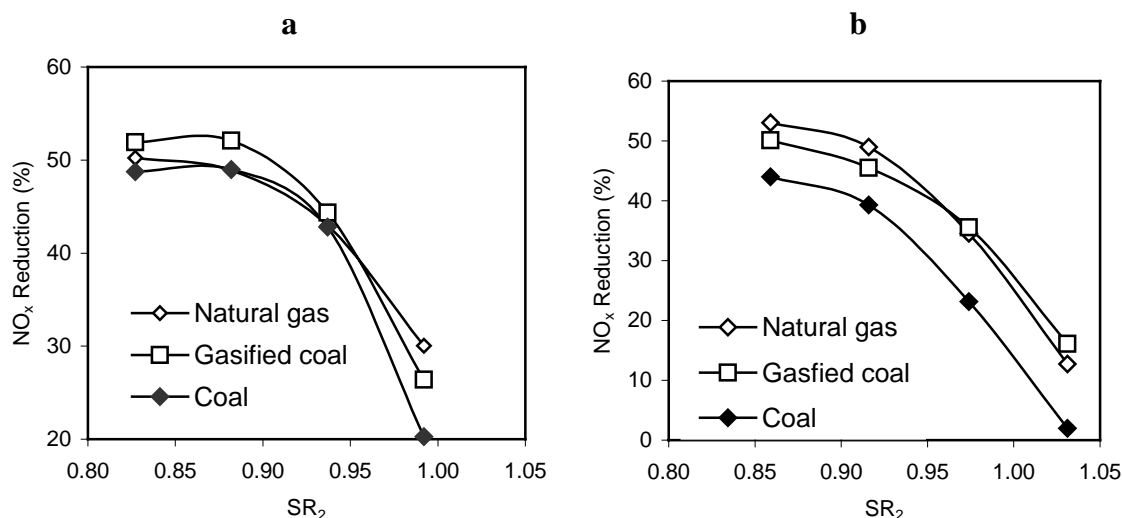
Figure 3-17. Effect of fuel type and SR in the reburning zone on
NO_x reduction with nitrogen (a) and air (b) transport.

Figure 3-17a demonstrates that reburning efficiencies of coal, natural gas and coal gasification products are similar. Differences in performances of these fuels were more significant when air was used as a transport media (Figure 3-17b). Efficiency of NO_x reduction by coal gasification products was almost the same as that of natural gas and was 5-12% higher than that of coal. Differences in the performances of coal and gasification products were less significant at large heat inputs of the reburning fuel possibly because of the decrease in the temperature in the gasification zone at large heat input of the reburning fuel (Figure 3-5).

   Figures 3-18 and 3-19 show the effect of the residence time in the reburning zone on NO_x reduction at 20% reburning fuel heat input. Initial NO_i concentration was 370 ppm at 0% O_2. T_{RF} and T_{OFA} were 1640 K and 1450 K, respectively. Figures 3-18 and 3-19 demonstrate that benefits of coal gasification are more significant when reburning fuel has less time to react in the reburning zone. This is because gasification products contain gas-phase combustible species which are more reactive than char. Efficiency of NO_x reduction decreases as the residence time in the reburning zone decreases since coal requires more time to react.
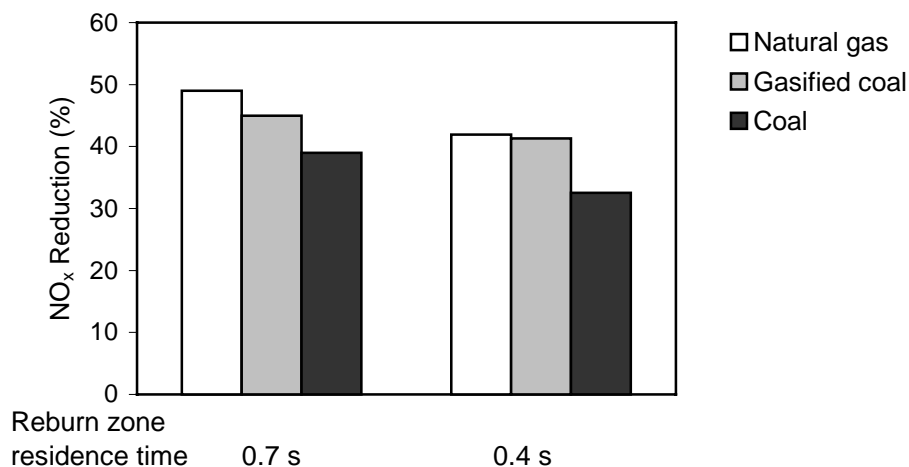
Figure 3-18. Effect of the residence time in the reburning zone on NO_x reduction with air transport.

Figure 3-19 demonstrates that at some conditions reburning efficiency of gasified coal can be even higher than that of natural gas.
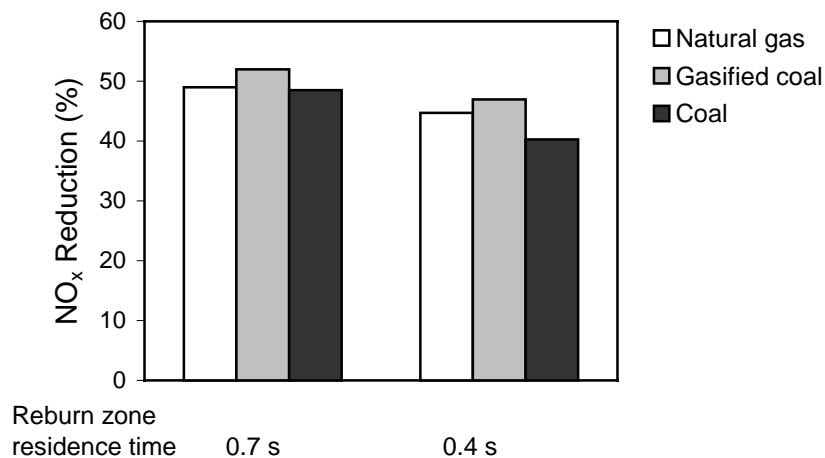
Figure 3-19. Effect of the residence time in the reburning zone on NO_x reduction with nitrogen transport.

Figures 3-20 and 3-21 demonstrate the effect of initial NO_x concentration (NO_i) on NO_x reduction with air and nitrogen transport. Reburning fuel was injected at T_{RF} of 1750 K and OFA at T_{OFA} of 1640 K, residence time in the reburning zone was 0.6 s. The amount of reburning fuel was 20% of the total heat input. Figures 3-20 and 3-21 demonstrate that efficiencies of NO_x reduction for all fuels decrease to about the same extend with a decrease in NO_i.

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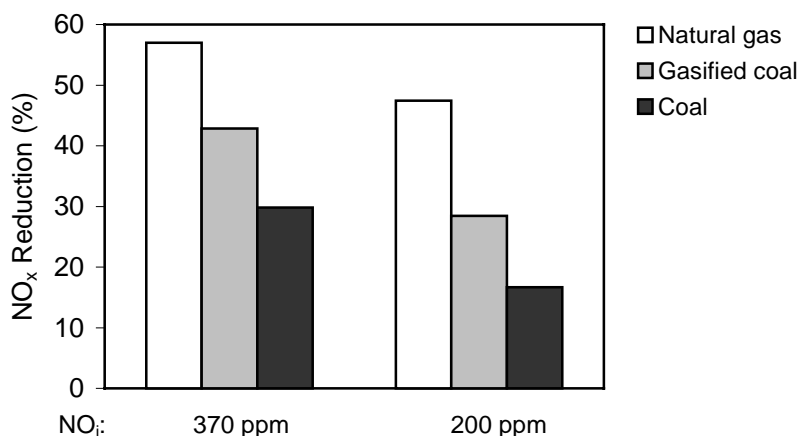
Figure 3-20. Effect of NO_i on NO_x reduction with air transport.
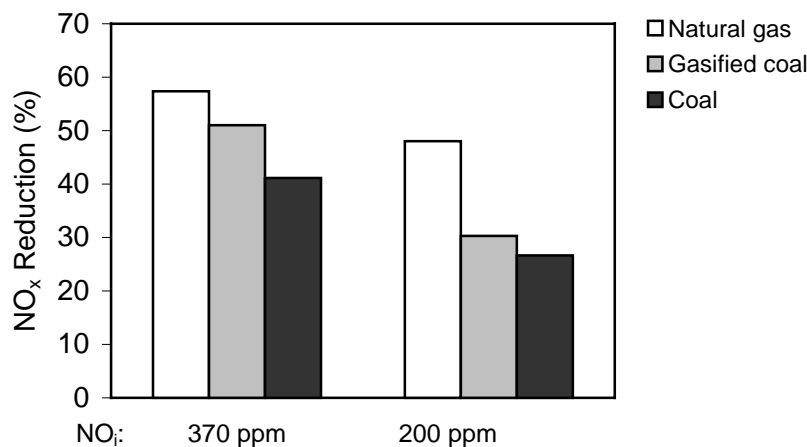
Figure 3-21. Effect of NO_i on NO_x reduction with nitrogen transport.

Coal residence time in the gasification zone is an important parameter that can affect the FFR efficiency. On the one hand, long residence time gives more time for coal to be gasified thus producing more gas-phase products. On the other hand, hydrocarbons which are more effective as NO_x reducing agents than CO and H_2, can be partially converted to CO and H_2 at long residence times. Figure 3-22 shows the effect of the residence time in the gasification zone on the efficiency of NO_x reduction. The amount of the reburning fuel was 20% from total heat input, T_{RF} and T_{OFA} were 1750 K and 1640 K, respectively. Residence time in the reburning zone was 0.6 s. Figure 3-22 demonstrates that efficiency of NO_x reduction improves as residence time decreases from 1.6 s to 1 s. Physical limitations in the gasifier did not allow to decrease

residence time to below 1 s. However, data presented in Figure 3-22 indicate that a decrease in the residence time to below 1 s will unlikely result in significant further improvement of NO_x reduction.
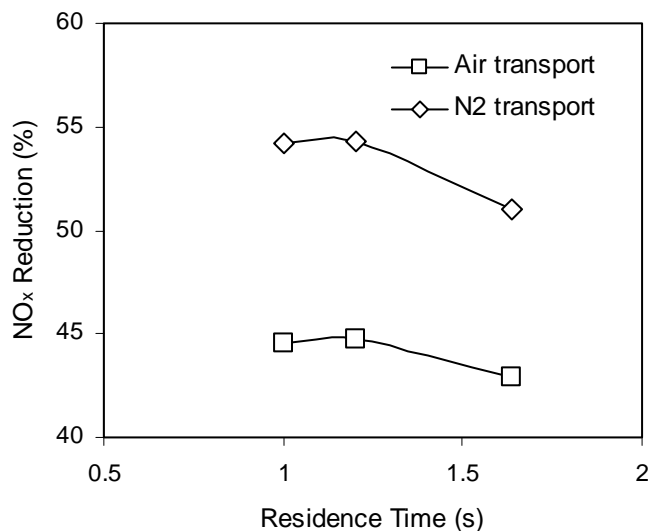
Figure 3-22. Effect of the residence time in the gasification zone on NO_x reduction.

Tests were also conducted to determine the effect of the auxiliary heat input in the gasifier on the efficiency of NO_x removal. Tests were conducted at 10% and 20% reburning heat input for auxiliary heat inputs of 80,000 Btu/hr and 95,000 Btu/hr. Reburn fuel was injected at 1750 K, NO_i was 370 ppm. Tests demonstrated that for the tested range of auxiliary heat inputs, the effect of the heat input was marginal. It should be noted, however, that auxiliary heat input has to be high enough to generate temperatures in the gasifier that result in solid fuel gasification. If auxiliary heat input is too small, the extent of the solid fuel gasification will be small, resulting in FFR efficiency similar to that of basic coal reburning.

Due to the fuel-rich environment and relatively short residence time in the reburning zone, reburn fuel may not burn completely in basic reburn, resulting in increased levels of unburned carbon (LOI). It was expected that combustion of solid fuel in FFR would be more complete than in basic reburn. Figure 3-23 compares values of LOI for basic reburn and FFR. Figure 3-23 demonstrates that LOI values are significantly smaller for FFR, especially at large heat input of the reburn fuel.
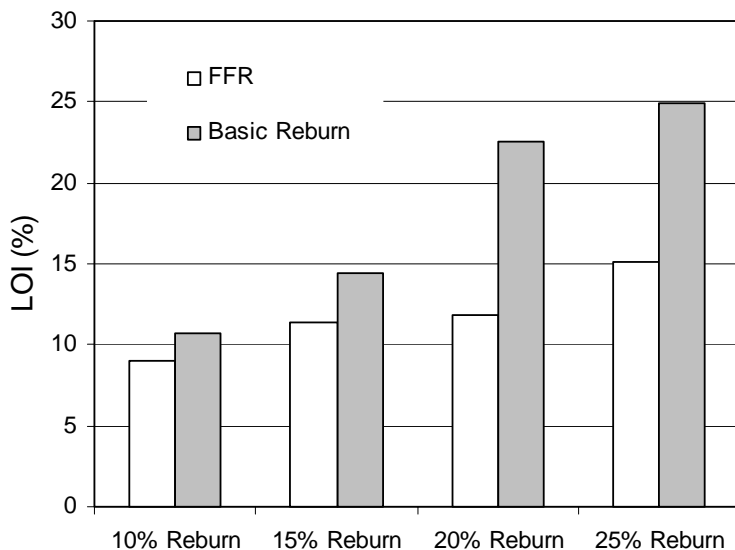
Figure 3-23. Effect of reburn heat input on LOI for basic reburn and FFR.

3.3.4 Performance of Renewable Fuels in FFR

Effect of solid fuel gasification on NO_x reduction was tested for two renewable fuels: almond shells and sewage sludge. Compositions of sewage sludge and almond shells are presented in Table 3-1. One of the most significant differences between compositions of sewage sludge and almond shells is that sewage sludge has much higher content of fuel-N. As a result, it was expected that performances of sewage sludge and almond shells in FFR would be different.

Because of the limited amount of almond shells available for tests, only gasification tests were performed with almond shells. Figure 3-24 compares performances of almond shells in FFR with that of walnut shells and willow wood in basic reburning. Composition of walnut shells and willow wood is presented in Table 3-1.

Figure 3-27 demonstrates that almond shell performance in FFR, and willow wood and walnut shells in basic reburning are similar. Since biomass fuels typically have high volatile content and are easily gasified, gasification of these fuel before injection into reburning zone may not offer additional benefits in comparison with basic reburning. Figure 3-24 demonstrates that this is the case.
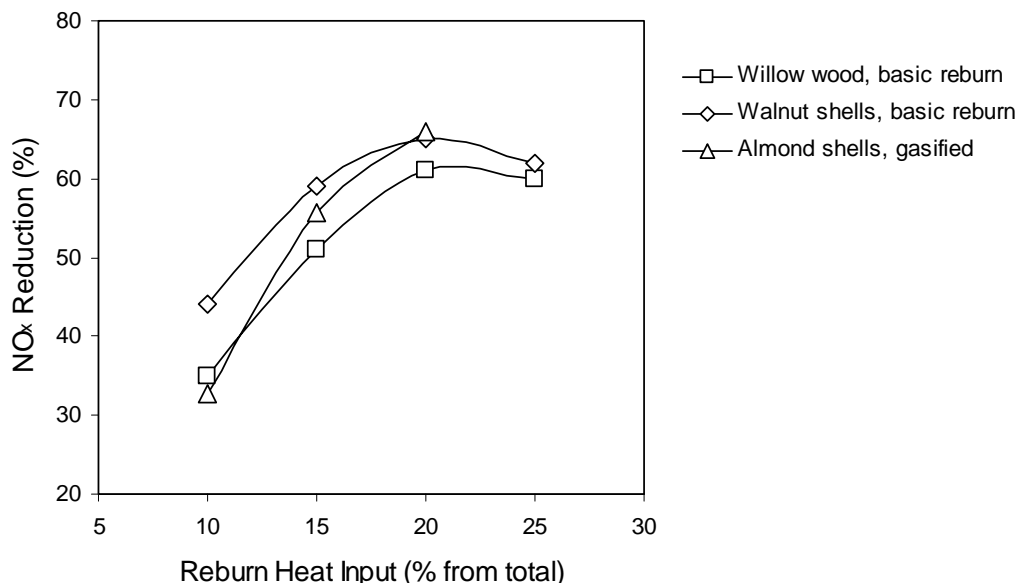
Figure 3-24. Comparison of willow wood and walnut shells basic reburn performance and almond shells FFR performance.

Gasification of renewable fuel prior to the injection into reburning zone, however, can be beneficial for fuels with high fuel-N content. Fuel-N in the gasification zone can be partially converted to N_2 thus reducing negative impact of fuel-N on NO_x reduction in reburning. Sewage sludge is an example of such a fuel. Fuel-N content in sewage sludge is high (3.8%, Table 3-1) making it poor reburning fuel (Figure 3-13). Figure 3-25 compares performances of sewage sludge in basic reburn and FFR.

Figure 3-25 demonstrates that sewage sludge gasification significantly improves efficiency of NO_x reduction. Efficiency of NO_x reduction increased from about 20% to about 60% for N_2 and from about 5% to about 60% for air as a transport media. These improvements are believed to be due to the partial conversion of fuel-N to N_2 during gasification. Typically, most fuel-N is converted to NH_3 or HCN at combustion conditions. These species are partially oxidized to form NO even in the fuel-rich combustion of the reburning zone. In FFR, these species are mainly converted to N_2 prior to the injection into reburning zone. Figure 3-26 demonstrates that most of fuel-N (86% at 20% reburn heat input) in FFR is converted to N_2 before gasification products are injected into reburning zone.
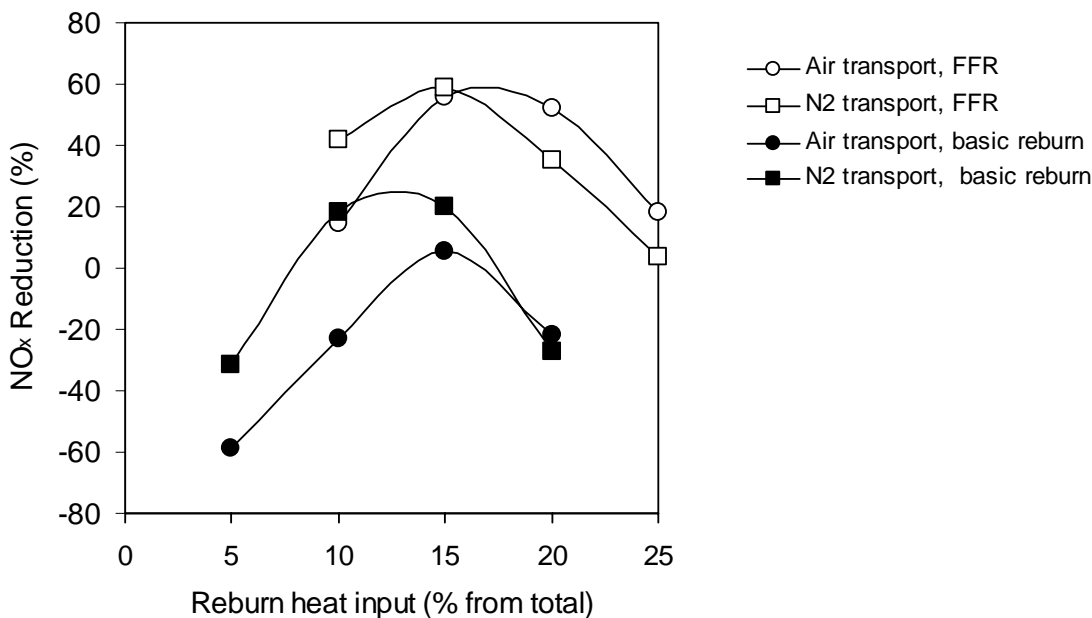
Figure 3-25. Comparison of sewage sludge performance in FFR and basic reburning.
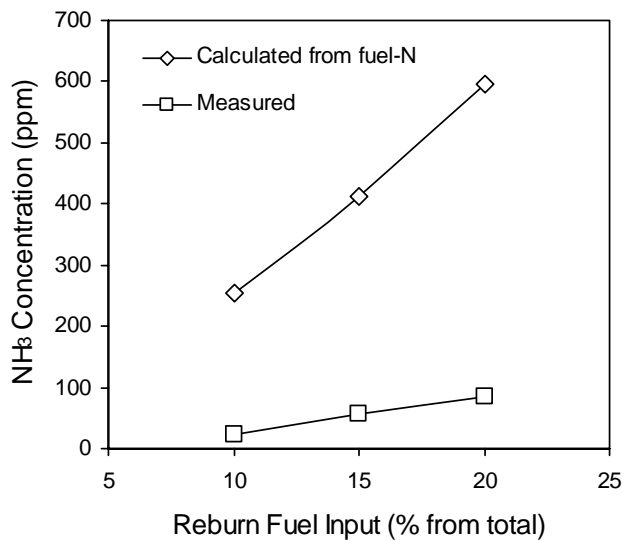
Figure 3-26. Calculated (from fuel-N) and measured NH_3 concentrations in sewage sludge gasification products.

The calculation of NH_3 concentrations was conducted under assumption that all fuel-N was converted to NH_3.

3.4 Summary of Test Results

Tests demonstrated that partial coal gasification prior to the injection into the reburning

zone improved the efficiency of NO_x reduction. The following conclusions can be made from the analysis of experimental data:

- Several coals with different volatiles content were tested. Data suggested that incremental increase in the efficiency of NO_x reduction due to coal gasification was more significant for coals with low volatiles content. Coals with low volatiles content are usually less reactive in basic reburning. Coal gasification improves their reactivity by producing gas-phase combustible species prior to the injection into the reburning zone. Coals with high volatile content are easily gasified in the reburning zone and thus benefit less from gasification prior to the injection.

- Up to 14% increase in the efficiency of NO_x reduction in comparison with basic reburning was achieved in FFR.

- Efficiency of NO_x reduction in FFR depended on the residence time in the reburning zone. Benefits of using FFR over basic reburning become were more significant at smaller residence times when coal did not have enough time to react.

- Temperature and residence time in the gasification zone affected the efficiency of NO_x reduction in FFR. Coal gasification in the temperature range of 1000 – 1150 K resulted in production of hydrocarbons, CO, H_2, and char. Tests demonstrated that NO_x reduction was maximum at residence time of about 1 s.

- FFR improved efficiency of NO_x reduction for renewable fuels with high fuel-N content and had a small effect on the performance of fuels with relatively low fuel-N content. Since renewable fuels are usually more reactive than coal, the increase in fuel reactivity due to fuel gasification is not as significant for renewable fuels as for coal. Renewable fuels with high fuel-N content benefit more from gasification prior to the injection into reburning zone because fuel-N is mainly converted to N_2 during gasification thus reducing negative impact of fuel-N on NO_x reduction in reburning.

3.0 MODEL DEVELOPMENT

The objective of the modeling task was to develop a model for predicting NO_x control performance in reburning with gaseous gasification products. This model can be used to predict composition of coal gasification products and to optimize FFR Option 2 which includes separation of gaseous and solid gasification products. Specific objectives of modeling were to:

(1) Predict performance of FFR in Option No. 2. Since experimental data were obtain for combined injection of gasification products, char and un-reacted coal into reburning zone (data presented in *Section 3*), prediction of NO_x reduction efficiency in Option 2 was done using modeling. Previous GE EER experience demonstrated high reliability of the gas-phase reburning model. Modeling of NO_x reduction by char and coal, on the other hand, can be done only if kinetic parameters of specific chars and coals are well defined.

(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.

Sections 4.1 and *4.2* describe the 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

Model was developed for the temperature range of 300 – 1400 K to address other options to gasify coal than that used in FFR tests (see *Section 3*). While coal gasification using partial coal combustion or auxiliary heat results in relatively high temperatures in the gasification zone (1100 - 1400 K), coal gasification using recycled flue gas may result in lower gasification temperatures.

Composition of coal gasification products was predicted using coal proximate and

ultimate analyses and CET93 equilibrium code[1]. Gasification of coals A, B, and Kittanning were considered in modeling. The 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.

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

- C, H, O, and N content of the volatile matter were determined using coal ultimate and proximate analyses.

- All hydrogen and oxygen were assumed to be released as volatiles.

- These data were used to calculate equilibrium composition of gasification products, except for N-containing species.

- For fuel-N containing species, the coal nitrogen was assumed to be distributed mainly as nitrogen bound in char (char-N) and hydrogen cyanide[2]. An increasing fraction of the char-N was converted to HCN with increasing temperature[3].

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

Modeling predicted that composition of gasification products depended on temperature: soot and methane were the main components at low temperatures and soot, H_2, and CO were the main components at high temperatures. This finding agreed with experimental data[4] suggesting that yield of hydrocarbons in coal gasification was larger at low temperatures. Since it was known[5,6] that hydrocarbons were more effective reburning fuels than H_2 and CO, these results suggested that coal gasification at lower temperatures produced more effective reburning fuel than coal gasification at higher temperatures.

1. McBride, B. and Gordon, S. *Chemical Equilibrium with Thermal Transport Properties*, Lewis Research Center, Cleveland, Ohio, 1993.
2. Niksa, S. and Cho, S. *Energy Fuels* 10:463 (1966).
3. Chen, J.C., Castagnoli, C., and Niksa, S. *Energy Fuels* 6:264 (1992).
4. Rűdiger, H., Greul, U., Spliethoff, H., and Hein, K.R.G. *3d International Conference Combustion Technologies for a Clean Environment*, Lisbon, Portugal, 1995, Vol. 2, p. 9.
5. Glarborg, P., Kristensen, P.G., Dam-Johansen, K., Alzueta, M.U., Millera, A. and Bilbao, R. *Energy Fuels* 14:828 (2000).

Table 4-1. 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_2O	0.094	0.064	0.015	0.001	0.000
	N_2	0.006	0.005	0.004	0.004	0.004
	C(gr)	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_2O	0.090	0.055	0.013	0.001	0.000
	N_2	0.006	0.005	0.004	0.004	0.004
	C(gr)	0.612	0.593	0.542	0.533	0.524
Kittanning coal	CH_4	0.280	0.210	0.100	0.007	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	0.390	0.454	0.460
	H_2O	0.136	0.091	0.022	0.002	0.000
	N_2	0.007	0.006	0.005	0.005	0.005
	C(gr)	0.531	0.448	0.404	0.433	0.433

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

Modeling predictions also agree with experimental data presented in *Section 3*. These data (Figure 3-8) suggest that H_2 and CO are main gaseous products at coal gasification temperatures of 1100 – 1400 K.

6.   Chen, S.L., McCarthy, J.M., Clark, W.D., Heap, M.P., Seeker, W.R., and Pershing, D.W. *Proc. Combust. Inst.* 21:1159 (1986).
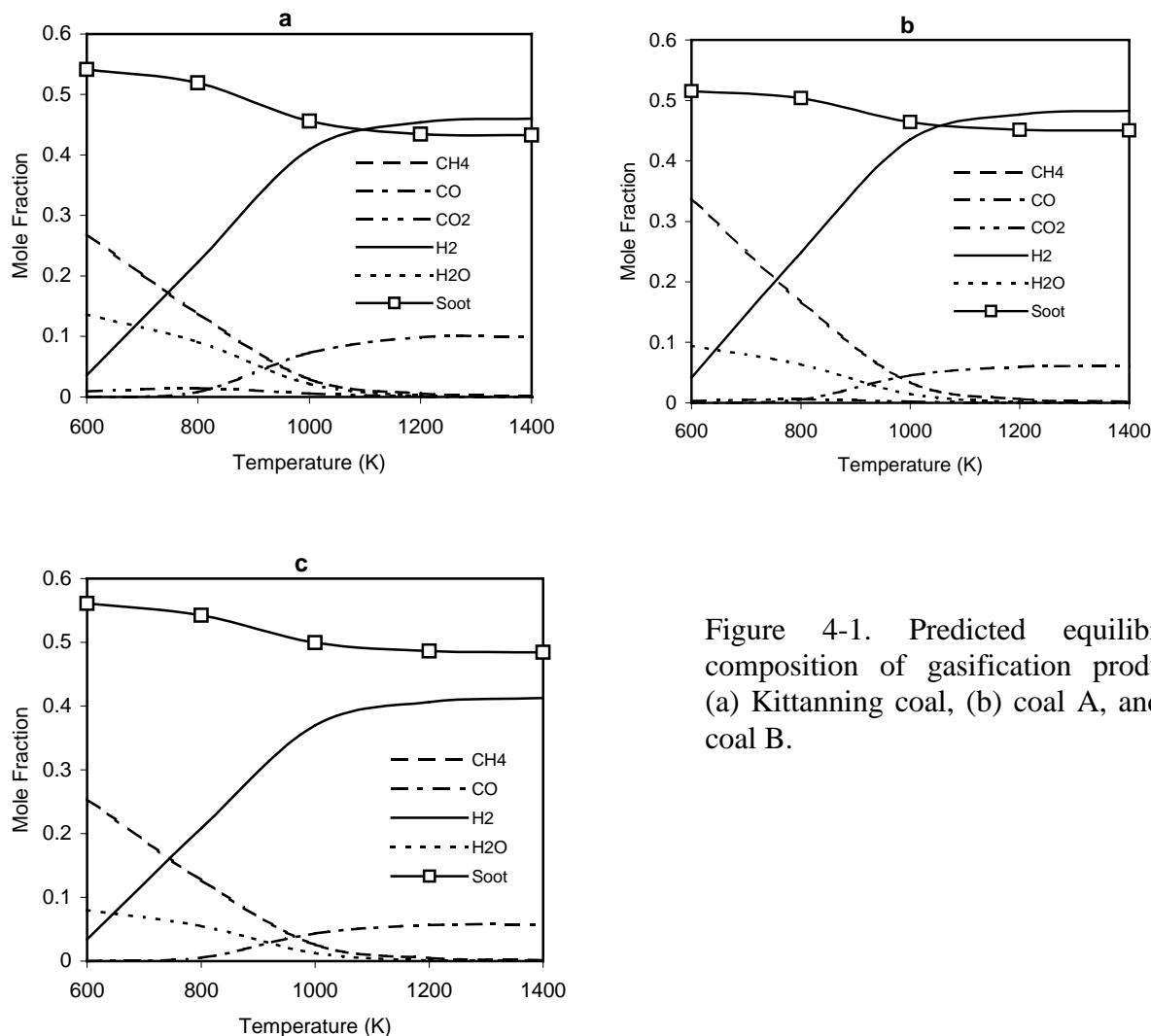
Figure 4-1. Predicted equilibrium composition of gasification products: (a) Kittanning coal, (b) coal A, and (c) coal B.

4.1.2 Rate of Coal Gasification

The rate of coal gasification 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 may 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% of 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 cannot be used for other coals. Recently Østenberg et al.[7] developed a model for reburning with coal. The model provides a good description of reburning with gasification products and with bituminous coals. Since Kittanning 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. Coal combustion mechanism and thermo data are presented in *Appendices A* and *B*.

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 is chosen because this time is expected to be a 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 suggests that coal gasification is complete at FFR conditions described in *Section 3*.
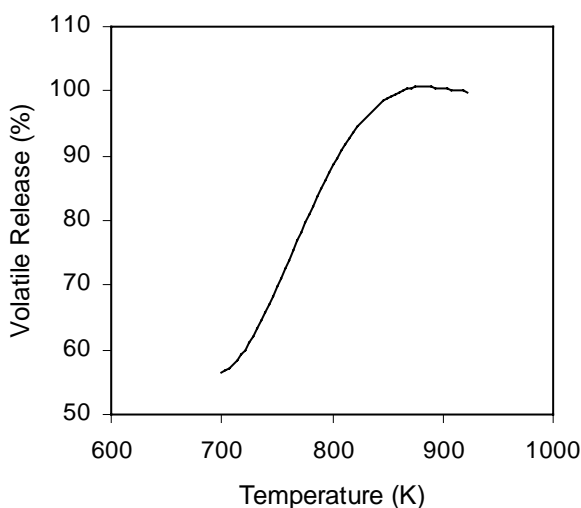
Figure 4-2. Predicted temperature dependence of the volatile matter release in gasification of bituminous coal at 1 s reaction time.

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 gaseous products also depends on these parameters. The heat value of gaseous products has to satisfy requirement of 15-20% heat input typical for reburning installations.

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7. Østberg, M., Glarborg, P., Jensen, A., Johnsson, J.E., Pedersen, L.S., and Dam-Johansson, J.E. *Proc. Combust. Inst.* 27:3027 (1998).

The following procedure was used to estimate the heat value of gasification products at different gasification temperatures. Table 4-2 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. The ΔH_0^{298} values from Table 4-2 and compositions of gasification products from Table 4-1 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 Table 3-1 and ΔH_0^{298} for the reaction of elemental carbon oxidation from Table 4-2. 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 Kittanning coal and coals A and B at different temperatures at a gasification residence time of 1 s. Experimental coal heat values (Tables 3-1) 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). This agreement suggests that assumptions made to estimate heat value of gasification and solid products at different gasification temperatures were reasonable.

Table 4-2. Enthalpies for combustion of gasification products.

Reactions of Gasification Products	ΔH_0^{298}, Btu/lb
$CO+0.5O_2=CO_2$	0.05
$H_2+0.5O_2=H_2O$	0.255
$CH_4+2O_2=CO_2+2H_2O$	0.106
$C+O_2=CO_2$ (soot)	0.069
$C+O_2=CO_2$ (char)	0.069

Data presented in Figure 4-3 suggest that at temperatures lower than approximately 600 K the heat value of gasification products formed from coal after 1 s in the gasification zone is not

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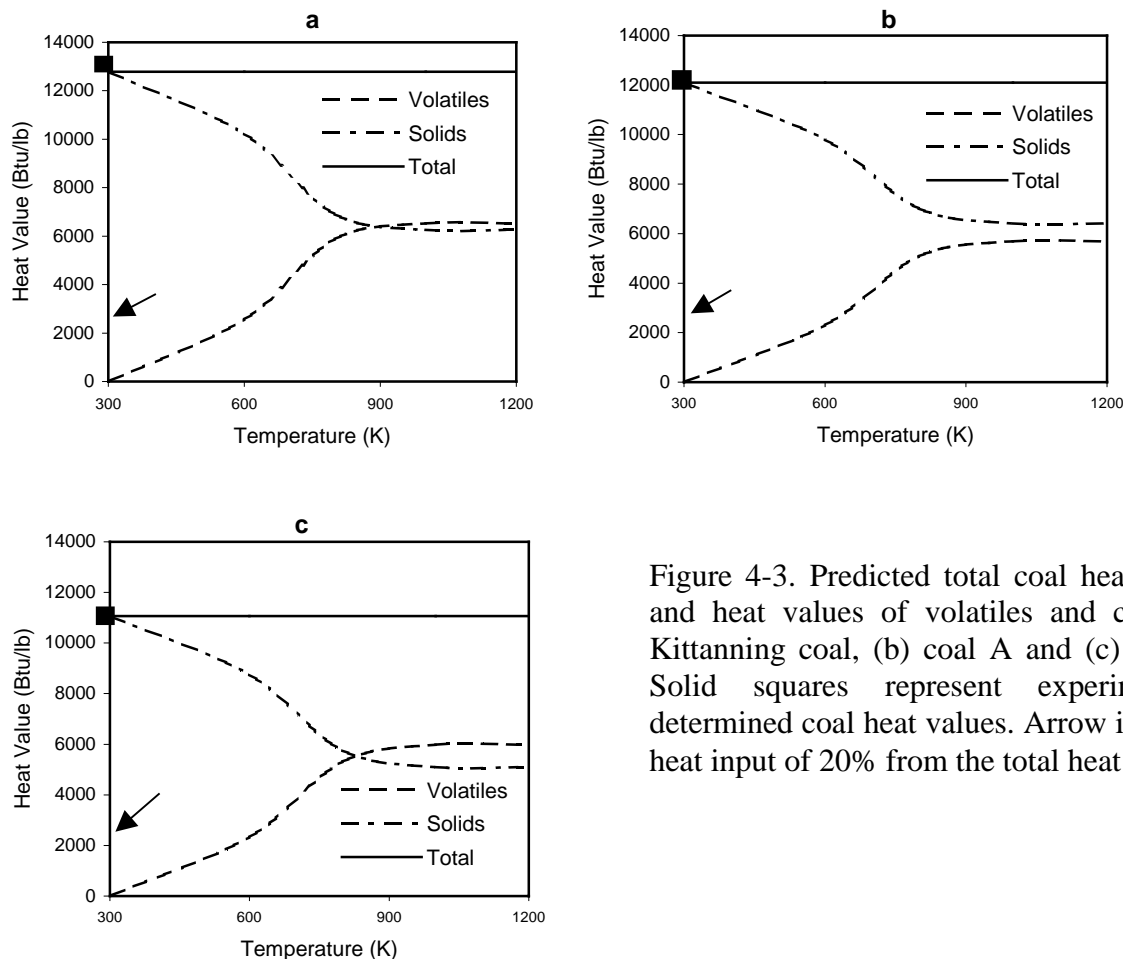
Figure 4-3. Predicted total coal heat values and heat values of volatiles and char: (a) Kittanning coal, (b) coal A and (c) coal B. Solid squares represent experimentally determined coal heat values. Arrow indicates heat input of 20% from the total heat input.

4.2 Performance of Coal Gasification Products as Reburning Fuel

4.2.1 Reburning Model

Coupling of chemical kinetics and gas dynamics is recognized to be important for modeling of the reburning process. The approach[8] 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 reburning[8] and Advanced Reburning[9]. This model is referred to 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 cross flow, (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 approach[10] (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 mechanism[11] 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.[7] suggested a mechanism of coal reburn which was evaluated against bench- and pilot-scale data and showed a good description of reburning with bituminous coals. The mechanism[7] 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. The mechanism and appropriate thermo data are presented in *Appendices A* and *B*. 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 mechanism[11] was replaced with coal mechanism[7]. The chemical kinetic code ODF (for "One

8. Lissianski, V.V., Zamansky, V.M., Maly, P.M. and Sheldon, M.S., *Combust. Flame* 125:1310 (2001).
9. Lissianski, V.V., Zamansky, V.M., Maly, P.M. and Sheldon, M.S., *Proc. Combust. Inst.* 28:2475 (2000).
10. Zwietering, T.N., *Chem. Eng. Scie.* 11:1 (1959).
11. Glarborg, P., Alzueta, M.U., Dam-Johansen, K., and Miller, J.A., *Combust. Flame* 115:1 (1998).

Dimensional Flame")[12] was employed to execute model calculations for comparison with experimental data.

Data on NO_x reduction in natural gas reburning are presented in Figure 3-17. Figure 4-4 shows comparison of the updated RCMM model predictions 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.
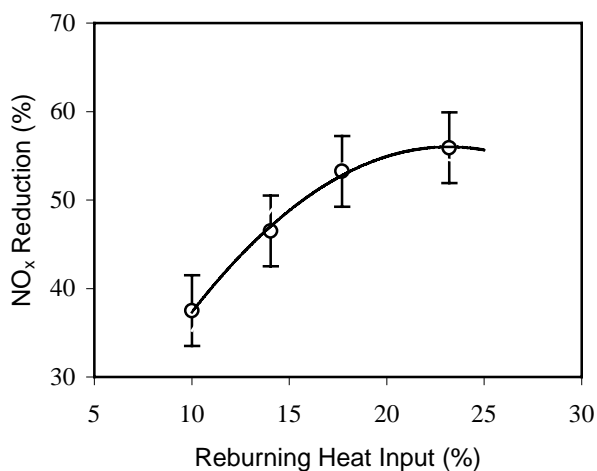
Figure 4-4. Comparison of updated RCMM predictions with experimental data on natural gas reburning obtained in the BSF at conditions of Figure 3-17b. $NO_i = 370$ ppm.

4.2.2 FFR Model Setup

Results presented in previous sections suggest that gasification products have a high content of soot, CH_4, H_2 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 ODF^{12} 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.

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12. Kau, C. J., Heap, M. P., Seeker, W. R., and Tyson, T. J., Fundamental Combustion Research Applied to Pollution Formation. *U.S. Environmental Protection Agency Report No. EPA-6000/7-87-027*, *Volume IV: Engineering Analysis,* 1987.

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:

$$1.74\% \ O_2 + 8\% \ CO_2 + 15\% \ H_2O + \text{balance } N_2.$$
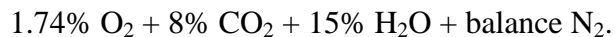
The gasification products were added to the main stream of reactants in the second reactor. The third reactor described the continued process of NO removal in the reburning zone after the reburning fuel and flue gas are mixed. The forth reactor described the process of OFA mixing with flue gas. The fifth reactor described oxidation of the products of incomplete combustion.
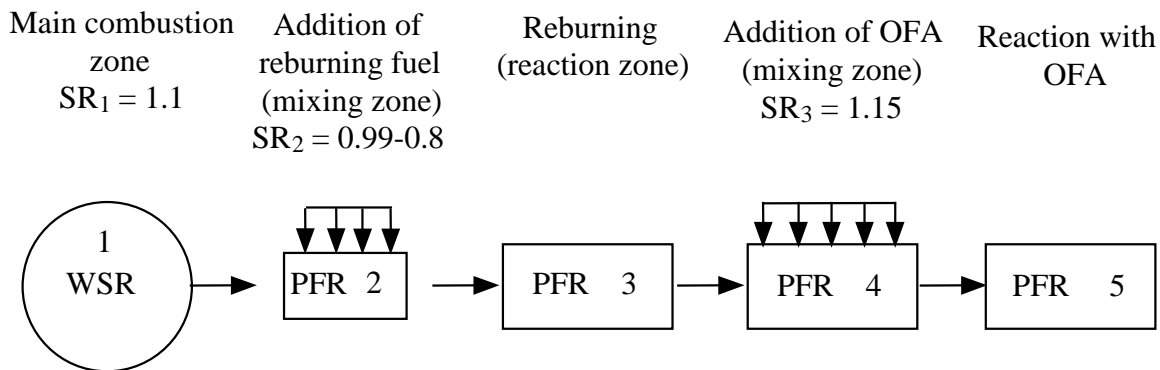
Figure 4-5. Reactor diagram of model setup.

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 of the reburning fuel and OFA injection were 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 370 ppm.

- Mixing times in the reburning and burnout zones of the BSF were estimated in the previous study[8] to be 120 ms. For the FFR modeling, this time was increased to 160 ms to take into account changes in the reburn fuel injector design.

- Temperature profile in mixing area was the same as estimated[8] for natural gas reburning.

The use of some of the mixing parameters estimated for the natural gas reburning in FFR was justified, since the BSF reburning jet consists of N_2 at about 70% (a large flow of N_2 is used to keep constant mixing conditions as the amount of the reburning fuel changes).

4.2.3 NO$_x$ Reduction by Coal Gasification Products

Figure 4-6 shows a comparison of experimental data (*Section 3*) on NO_x reduction efficiencies in reburning with natural gas, coal, and gasification products with modeling predictions for gaseous gasification products. All data shown are for Kittanning coal. The amount of the reburning fuel is 20%, reburning fuel and OFA are injected at 1750 and 1640 K, respectively. Initial NO_x is 370 ppm and N_2 is used as transport media. Coal is gasified at 1150 K.

The model predicts that the efficiency of NO_x reduction by gaseous products is similar to that of coal and lower than that of gasified coal. This suggests that separation of gaseous products from char for utilization as a reburning fuel (FFR Option 2) is not as effective of a method to reduce NOx as utilization of gaseous products and char (FFR Option 1). This also implies that NO_x reduction on the surface of char is significant and makes an important contribution to the total NO_x reduction in reburning. Thus, while Option 2 provides more complete coal combustion and reduced LOI by diverting char and un-reacted coal from the reburning zone to the main combustion zone, Option 1 provides more significant NO_x reduction by injecting char into reburning zone. As shown in *Section 3* (Figure 3-24), Option 1 also reduces LOI in comparison with basic reburning.
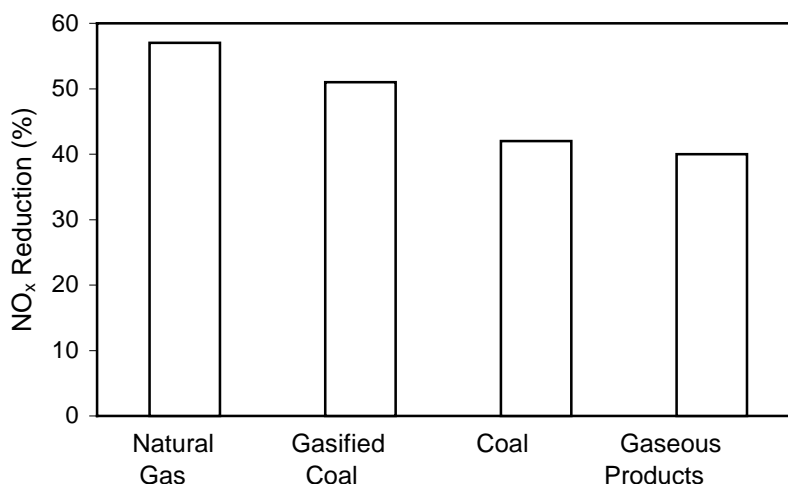
Figure 4-6. Efficiency of NO_x reduction in reburning with different fuels.

4.3 Summary of Modeling Efforts

A model predicting NO_x reduction in reburning with gaseous gasification products has been developed. Composition of gaseous products was predicted for temperature range of 300 – 1400 K. Modeling predicted that composition of coal gasification products depends on temperature. Modeling suggested that it was more beneficial to gasify coal at lower temperatures (600 - 800 K) since yield of hydrocarbons decreased with temperature. Main gasification products at these temperatures are soot and CH_4, while soot, H_2 and CO are main gasification products at higher temperatures. However, gasification at these temperatures may require long residence time.

Comparison of experimental results and modeling predictions suggests that separation of gaseous products from char and utilization of gaseous products as a reburning fuel while burning char in the main combustion zone provides less NO_x reduction then injection of gaseous products and char into reburning zone. This suggests important role of the heterogeneous NO_x reduction on the surface of char.

Modeling predicts that under fast mixing conditions gasification of small particles of bituminous coals at reaction time 1 s and temperatures higher than 600 K produces enough volume of products to be used as a reburning fuel at heat inputs up to 20% from total. Gasification of large coal particles may take longer time and may not produce enough

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gasification products under these conditions. Longer mixing times in the gasification zone also can decrease extent of coal gasification. Thus, optimum conditions for solid fuel gasification have to be determined based on fuel characteristics and design parameters of a specific gasifier.

5.0 FFR CONCEPT DESIGN AND ECONOMICS

While experimental and modeling data demonstrated that FFR results in increase in NO_x reduction, more complete coal combustion and decrease in LOI, FFR can be commercialized only if it is cost effective. Objectives of the design and economic study were to (1) line up FFR equipment, (2) determine cost of NO_x reduction via FFR, and (3) compare this cost with cost of competitive technologies. The FFR technology has to provide cost effective performance improvements over both conventional coal reburn and the best competing technologies if it is to capture a significant market share.

5.1 Approach

Typically, coal gasification requires expensive, large, refractory structures which are very scale dependent. Therefore, the following were applied in the selection of a reference plant against which to draw comparative conclusions as to FFR economic viability:

- The reference boiler application should be large, preferably over 350 MW.
- Low volatility Eastern bituminous coals were considered. These are typical bituminous coals used by the U.S. power industry.

5.1.1 Reference Plant

The reference plant was selected after reviewing past GE EER studies, boiler demographics, and coal reburn commercial offerings. The 386 MW Wateree opposed wall, PC fired boiler located in South Carolina with a steam rate of 2,567,000 lb/hr satisfied the study requirements. Opposed wall fired boilers are typical in this size range and larger, and usually have an odd number of mills. Because of this, no single mill can carry the reburn fuel load, thus requiring a new, larger mill. Further, the furnace cross sections tend to be large in the firing direction, requiring additional boost air for good reburn fuel penetration at reasonable primary fan pressures. A mill classifier is typically added to improve the coal grind, which will also be advantageous relative to obtaining acceptable gasifier residence times and, therefore, equipment size. A conventional 386 MW coal reburn system has the following characteristics:

- Reburn fuel, 24% of the total heat input or 80,600 lb/hr to achieve a reburn SR = 0.9.
- Coal transport air, Air/Fuel = 2 or 161,000 lb/hr.
- Boost air from primary fan, Air/Fuel = 2 or 161,000 lb/hr.

- Stoichiometric air to fuel ratio, 9.6.

- 10% ash in coal.

- About 45% NO_x reduction with air transport from a 0.52 lb/MMBtu baseline.

5.1.2 Gasifier Concepts

A coal reburn conceptual design and cost estimate has been developed for the reference plant and is the basis for the comparative performance assessment discussed below. Two in-duct gasification configurations have been studied:

- Option 1, common gasifier serving a reburn injection system.
- Option 2, gasifier injector at each injection location.

Gasifier operating conditions have been established using a combination of pilot plant process data and computational models (*Appendix C*). Process conditions (gasifier stoichiometry) have been developed which achieve a product gas temperature of between 1150 K and 1260 K while generating a reactive reburn product gas under partial combustion conditions. This requires residence times of 0.6 to 1.0 seconds resulting in between 20% and 30% of the coal being unburned.

5.2 Process Design

The above conditions were used to first develop an estimate of gasifier stoichiometry which then set the amount of combustion air required relative to reburn coal flow. Two limit case calculations based on mass balances and adiabatic conditions were used, Figure 5-1:

- Equilibrium calculations to develop an operating curve of temperature vs. gasifier stoichiometry for the pilot plant Eastern bituminous (Kittanning) reburn coal.
- Simple chemical reaction balances assuming 25% (mass) coal uncombusted and product gas is primarily H_2 and CO.

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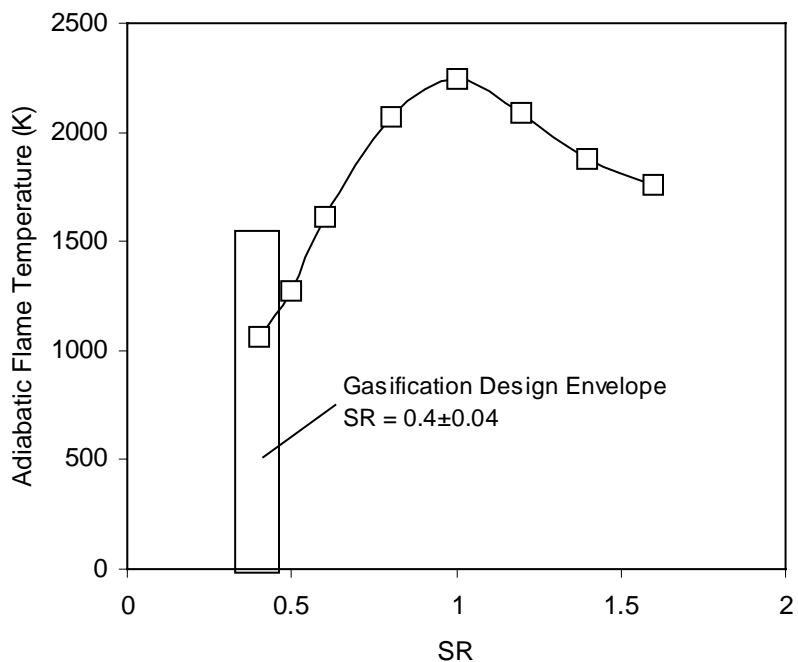
Figure 5-1. Adiabatic flame temperature of Kittanning coal.

Product gas composition and molecular weight were also estimated. Both calculations suggested that a stoichiometry of about 0.4±0.04 was required to achieve the required process conditions. Simplified calculations estimated higher temperatures than equilibrium at the design stoichiometry assuming 75% coal conversion. This was the result of operating with a greater effective air to fuel ratio since not all of the coal was combusted, the remaining char passed through the gasifier as an inert much like the fly ash. Design residence times for each gasifier configuration were selected based on the following assumptions:

- The large central gasifier is designed for an operating temperature of 1150 K and a residence time of one second to provide adequate time for lower temperature gasification kinetics.

- The gasifier injector is designed to operate at higher temperature (1260 K) and a shorter residence time for close-coupled operation in a more confined space.

5.2.1 Centralized Gasifier Design

The centralized gasifier design velocity was selected to reflect the pulverized coal size distribution (grind) and the "in-duct" concept. A design velocity of 21 m/s is consistent with conventional coal pipe deliver and results in a gasifier height of 21 m to achieve a one second

residence time. The actual volumetric flow is estimated from the gasifier stoichiometry (0.36), operating temperature (1150 K), and reburn coal flow (80,600 lb/hr), Figure 5-2.
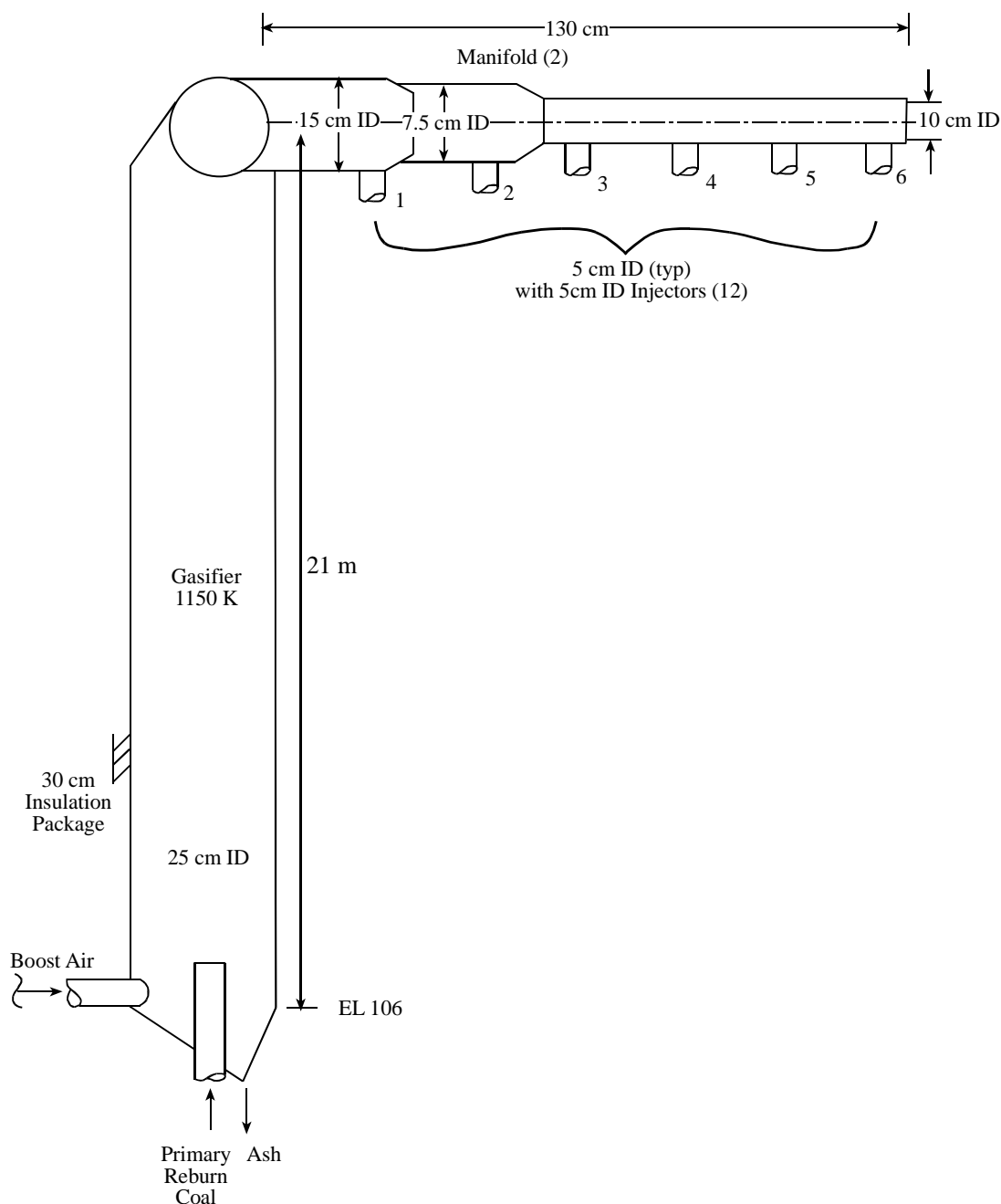
Figure 5-2. Common-entrained gasifier.

A 25 cm ID gasifier duct is required to satisfy the residence time (1 sec), height (21 m) and calculated volumetric flow (5711 acfs) requirements. The gasifier aspect ratio (l/d) of 7 achieves good cylinder structural stability to buckling, Figure 5-3.
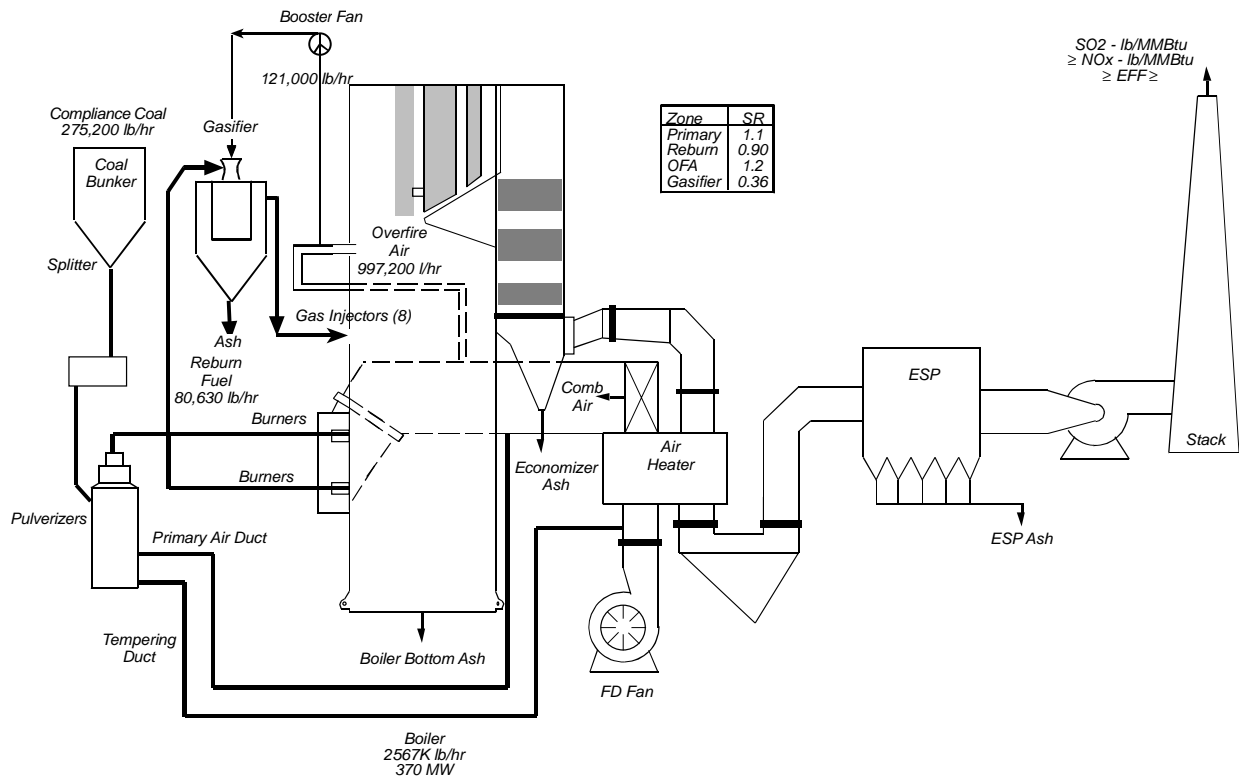
Figure 5-3. Option 1 design process flow diagram for common coal duct partial combustion gasifier.

The gasifier is elevated to a position (106 El) where the discharge manifolds are at or slightly below the elevation of the reburn injectors (168 El) which minimizes the expensive high temperature product gas manifold and duct runs to the injector locations. The gasifier is located along one of the non-firing sides of the boiler and the horizontal manifolds are routed from its top to the back and front firing walls. The boiler width is 18 m, therefore, two, 15 m manifolds are required to distribute the product gas to each of 6 injectors per side. Product gas ducts are short and the design velocity selected to provide the same jet momentum as the conventional boosted coal reburn injectors. This requires tube wall penetrations that are twice as large (5 cm ID) as the conventional coal injectors with boost air (Air/Fuel = 4). The gasifier is fed from a single, 7.5 cm ID bottom inlet coal pipe operating at an Air/Fuel = 2. Additional preheated air (Air/Fuel = 1.5) is added to the gasifier to achieve the design stoichiometry (0.36). Where boost air is required for conventional coal reburn, both streams can be taken from a mill primary air fan sized for the total flow and split accordingly. All ducts and components containing hot product gas will require insulation packages to minimize heat loss. For the large surface, low velocity

gasifier components a 30 cm insulation package will be required, high alumina internal layer backed by a low density/conductivity outer layer, all contained in a carbon steel shell. For the product gas distribution ducting and manifolds this might be relaxed to 25 cm of insulation. Note that the low temperature operation and long residence time might require limestone injection to catalyze the tar reactions to avoid fouling. This has not been considered in the conceptual design, but limestone could be added to the mill coal.

5.2.2 Gasifier Injector

Individual injector gasifiers replace the conventional air boosted coal reburn system injectors. Gasification chambers (12) are attached directly to the tube wall opening (60 cm ID) and operate under partial combustion. They are sized for a shorter residence time (0.6 sec) and a higher operating temperature (1260 K) to improve reactivity, Figure 5-4.
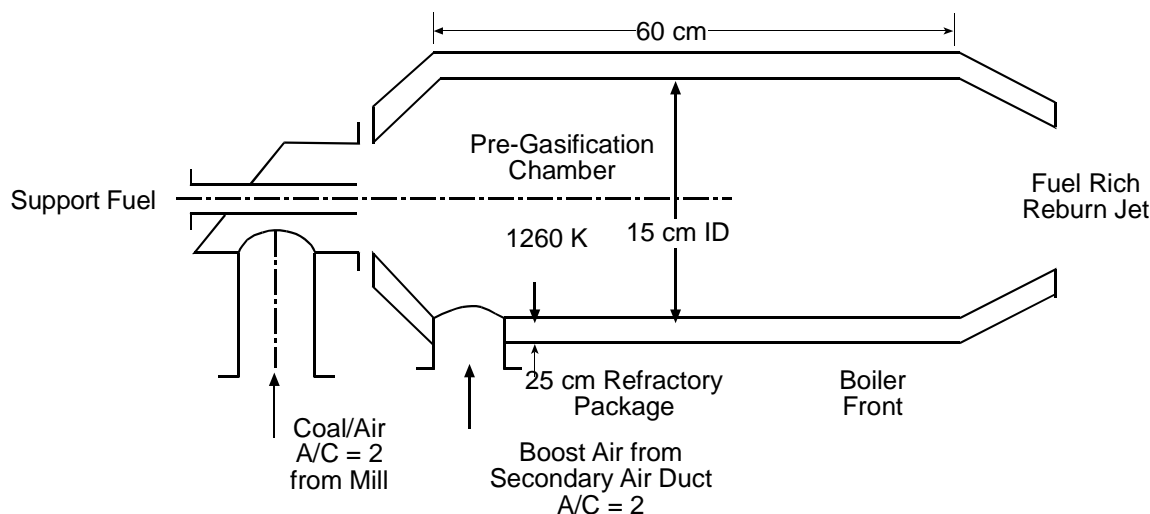
Figure 5-4. Rich partial combustion burner chamber conceptual design.

The higher temperature requires operation at a higher gasifier stoichiometry (0.42) and results in a somewhat higher level of unburned coal. Supporting infrastructure (coal pipes, boost air and associated manifolds) to the burner location is identical to conventional boosted coal reburn, Figure 5-5.
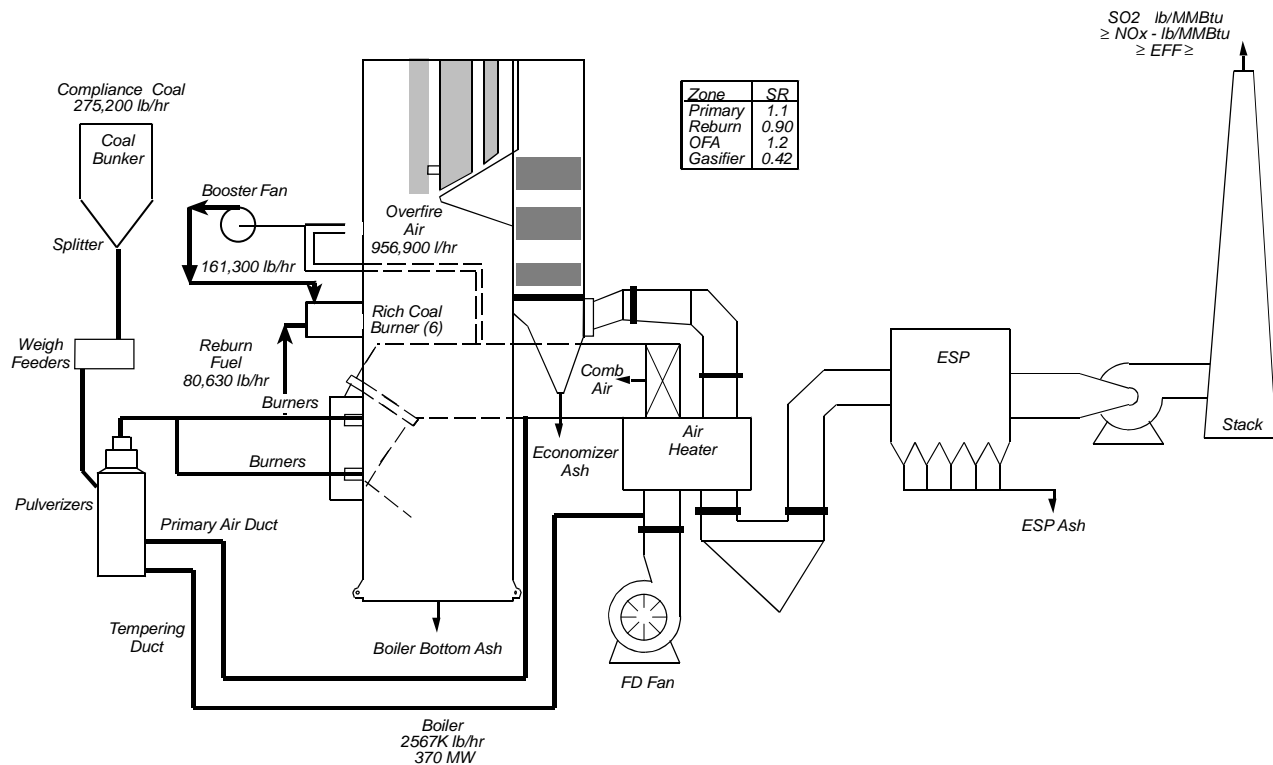
Figure 5-5. Option 2 design process flow diagram for rich coal gasification injectors.

However, the gasifier design envelope is constrained by the width of the boiler. Six injectors matched to the primary coal burner spacing (20 cm centers) are constrained to an inside diameter of 1.8 m (assuming a 25 cm insulation package). This defines the length (7.2 m) required to achieve the design residence time. Although space in the boiler house may be an issue at this elevation, no major structural modifications are assumed other than additional support steel for the gasifier deck.

5.3 FFR Economics

The economics of the three coal reburn technology configurations as previously described have been evaluated:

- Conventional coal reburn with new dedicated coal mill and primary air fan (CRM).

- Configuration 1, coal reburn with common entrained gasifier and product gas manifold (GCR1).

- Configuration 2, coal reburn with gasifier injectors close coupled to injection point (GCR2).

Comparisons are also made relative to their next best alternative commercially available control technology, low NO_x burner (LNB)/separated over fire air (SOFA). Two application venues have been investigated:

- Large coal fired boiler in the Ozone Transport Region (OTR) firing Eastern bituminous coal, target stack NO_x is 0.15 lb/MMBtu.

- Large coal fired boiler in a Western venue firing Western bituminous coal and under a regional haze consent decree, target NO_x is most cost effective ($/ton) technology capable of achieving less than 0.25 lb/MMBtu.

5.3.1 Assumptions

Major assumptions affecting the economics are summarized in Table 5-1 and have been inputted into the NO_x Technology Assessment code. Since all coal reburn projects are relatively capital intensive, the method of capital amortization can significantly affect the economics. A capital recovery approach based on 7% equivalent interest and a 15-year asset has been assumed (capital recovery factor (CRF) = 11% of capital/yr). Boilers in this size range typically operate at high capacity factor and are usually base loaded since they are the most efficient and lowest cost of electricity (COE) boilers on the grid. Therefore, a high load factor of 85% is assumed. Although LOI is a potential issue with any of the evaluated technologies, sufficient equipment (mill classifiers) has been added to levelize this effect. For SOFA, all five existing primary mills are assumed to require classifiers, only the new reburn mill needs a classifier for the coal reburn technologies. It should be appreciated that conventional coal reburn and LNB/SOFA might avoid the incremental cost of a classifier. A fuel penalty due to increased LOI (2 to 6%) will result in a fuel penalty of about 0.75%. This is equivalent to $31.3/hr or $233 k/yr and $96 k/yr in additional coal cost for base loaded Western and OTR venues, respectively. Since classifiers cost about $300k/mill, simple payback would favor their use for all reburn applications assuming ash is landfilled.

Table 5-1. Basic economic assumptions[a].

Item	Description	Units	Selected Value	Potential Range	Reference/Comment
1	Utility Costs				
	- Power, annual	$/MW hr	40		Wholesale power costs
	ozone season				
2	Capital Recovery				
	- Equipment Life	yrs	15	10 to 20	Consistent with IRS depreciation schedules
	- Real Interest[b]	%	7	5 to 8	Recent historical
3	Load Factor, Annual	%	85	65 to 90	Western Base Loaded
	ozone season	%	85	80 to 90	5 Months/yr or 3283 FL hrs
4	Baseline NOx	ppmvd@3%			Calculated from mass rate
		lb/MMBtu	0.52		Per RFP
	Baseline SO_2	lb/MMBtu	5		E. Bituminous
			1.5		W. Bituminous
5	Coal cost, compliance	$/MMBtu	1.23		Typical, but site specific
	high S		1.23		
6	Emissions Allowances				
	- SO_2	$/ton	175		Typical
	- NOx		2000	2000 to 3000	Will depend on how much boiler capacity converted to SCR
7	Steam Generation[c]				B&W performance
	- Design, capital cost	Mlb/hr	2600		Specification sheets, steam generated at
	- MCR, operations		2600		3735 psia, 815 K
8	Plant Energy				
	- Coal heating value	HHV Btu/lb	12000		All coals
	- Boiler efficiency	%	88		
	- Heat rate	Btu/kW-hr	9060		
	- LOI	%C	2	1 to 3	
9	O&M Costs		2	1 to 3	EPRI TAG
	- Supervisory	%			
	- Maintenance	Capital			
	- Operators				
10	Fly Ash				
	- Coal fraction	%	8	6 to 12	70% to fly ash
	- Land fill cost	$/ton	10	3 to 20	Typical
11	Chemical Reagents				
	- Anhydrous NH_3	Cost per	300	250 to 300	Quotes from La Roche and Agrium, indexed
	- Aqueous NH_3	contained	350	300 to 350	to NG
	- Urea	ton of NH_3	500	400 to 600	

Notes: a. Technology specific costs may be found in *Appendix C*

b. Real interest assuming no inflation, otherwise capital paid with inflated dollars

c. Design load used to size equipment, % of MCR for operating costs

Since all five mills require classifiers for SOFA, the payback stretches out to about 6 years and may not be considered cost-effective. If ash is sold as a pozzilon additive for cement, all of the applications can cost effectively use classifiers since ash sales (at $20/ton) could bring in additional revenue of up to $680 k/yr to $1638 k/yr for OTR and Western venues, respectively.

None of the technologies achieve the required NO_x reduction performance in the OTR and will require trading credit purchases. Costs of the credits are anticipated to range between $2000 and $3000/ton NO_x. The value of $2000/ton is typical of the cost of SCR operations where trading credits can be generated by over design and was the value used to achieve regulatory limits. Credits are purchased to achieve either:

- The OTR level of 0.15 lb/MMBtu.

- 0.25 lb/MMBtu, Western consent decrees vary widely, but are usually pegged to the most cost effective control technology.

5.3.2 Capital Costs

Capital costs have been developed for the process conditions presented in Tables 5-2 and 5-3 using a cost estimating code and proprietary data. Internal cross technology consistency is the primary objective of the cost estimates. Commercial OM and risk margins have been assumed for all applications. Detailed scopes of supply and developed cost estimates may be found in *Appendix C*.

The centralized gasifier capital cost was estimated at $15,851,000, slightly higher than the conventional coal reburn with boost air, a new mill and primary air fan with classifier. The primary reason for the small cost difference reflects expanded duct approach where the major cost trade is between a single coal pipe feeding a common gasifier (with limited distribution manifolding at the reburn deck) and a complex coal and boost air distribution system. Although the gasifier duct requires more expensive insulation, there are significant returns to scale relative to 12 coal pipes and a separate boost air system feeding 12 injectors. The gasifier injector is the most expensive, $18,543,000, since twelve large, heavy reactors must be placed at the reburn deck elevation. It is problematical that space can be cleared without major structural modifications. Only sufficient structural steel was considered in the estimate to support the equipment.

Table 5-2. Common gasifier: cost impacts relative to conventional coal reburn.

Item	Subsystem	Gasifier	Conventional	Comments
1	Coal Transport			
1.1	Coal A/C	2	2	No change
1.2	Grind	New Pulverizer	New Pulverizer	No change
1.3	Coal Pipe Runs, m	33	56	Less piping
	, no	1, 7.5 cm ID	12, 2.5 cm ID	and complexity
2	Gasifier			
2.1	Gasifier (1)	25 cm ID x 23 m	Not Required	New
2.2	Product Gas Pipe (12)	5 cm ID x 17 m	Not Required	New
2.3	Hot Gas Manifold (2)	3.75 cm ID x 130 cm	Not Required	New
3	Reburn Injectors			
	Number	2 x 6	2 x 6	No change
	Penetration ID, m	0.6 ID	0.3 ID	Increased tube wall diameters
4	Primary Air Fan	New	New	
4.1	Fan - Flow Mlb/hr	282	322	Flow decrease, fan
	- Pressure, in wc	50	50	HP slightly lower
4.2	Boost Air, Mlb/hr	33 m, 1 m ID	60 m	Less piping
4.3	Boost Air Manifold (2)	Not required	16 m	Delete manifold
5	OFA (6)	Dual Register	Dual Register	No change

Table 5-3. Gasifier injector: cost impacts relative to conventional coal reburn.

Item	Subsystem	Gasifier	Conventional	Comments
1	Coal Transport			
1.1	Coal A/C	2	2	No change
1.2	Grind	New Pulverizer	New Pulverizer	No change
1.3	Coal Pipe Runs (12)	56 m	56 m	No change
2	Gasifier			
2.1	Gasifier (12)	1.8 m ID x 8 m	Not Required	New
2.2				
3	Reburn Injectors			
	Number	Not Required	2x6	
	Penetration ID, m	0.6 ID	0.3 ID	Increased tube wall diameters
4	Primary Air			
4.1	Fan - Flow Mlb/hr	322	322	No change
	- Pressure, in wc	60	50	Small HP increase
4.2	Boost Air Manifold (2)	16 m	16 m	No change
5	OFA (6)	Dual Register	Dual Register	No change

The cost of LNB and SOFA systems were developed scaling an earlier study. Adding classifiers to all five existing mills to control LOI results in an adjusted price for this technology of $7,430,000.

5.3.3 Economics

The primary cost effectiveness parameter evaluated is the annualized cost per ton of NO_x removed ($/ton). All major system operating costs were considered including additional mill power for classifiers, fuel efficiency penalties due to LOI increases (if any), and O&M costs for new mills and additional instrumentation and control (I&C). Since the fuel input to the boiler is not significantly different from baseline, additional operator and control room supervision is not required or budgeted. Significant parameters from the cost and performance estimations are summarized in Tables 5-4 and 5-5. The economics are dominated by the annualized capital cost and the reduction efficiency. Other operating costs are a small fraction (6% to 15%) of the annualized cost. Clearly, the most cost effective solution in both venues before trading credit purchases is a combination of LNB/SOFA, although a significant NO_x control short fall occurs. This is probably the reason why most Western power plant consent decrees are written around this technology.

OTR Economics-The more capital intensive, higher performing gasifier technologies require fewer trading credit purchases and, therefore, have lower compliance costs after trading credit purchases, Table 5-4. The common gasifier configuration is preferred over the gasifier injector because it is less complex and about 12% more cost effective. This configuration has almost identical cost effectiveness ($1416/ton) to LNB/SOFA ($1400/ton) for the NO_x credit purchase price of $2000/ton. A trading credit price of $3000/ton results in about a 12% higher cost for the GCR1 ($1660/ton) over LNB/SOFA ($1894/ton) configuration.

Western Region Economics-Western region economics are more difficult to assess because of absence of uniform regulatory requirement for NO_x emission reductions. Two approaches have been evaluated, Table 5-5:

- Treat the economics as a trading credit issue.
- Assume the station owner will evaluate alternative technologies relative to putting SCR or GCR1 on fewer units to offset not controlling smaller, older, dispatched units.

Table 5-4. Coal reburn economics in OTR 370 MW opposed wall unit.

Item	Description	Units	Technology			
			GCR1	GCR2	LNB/SOFA	CRM
1	Configuration					
	- New dedicated mill		X	X		X
	- Classifer		X	X	X(5)	X
	- Primary fan		X	X		X
2	Capital - 1st	kW	15851	18543	7430	15713
	- Recovery	%	11	11	11	11
3	Operations					
	- Utilities	kW	226	226	1009	226
	- Boiler Eff	%	0.19	0.19	0.07	0.19
4	Economics	$k/hr				
	- Utilities		7.93	7.93	35.34[c]	7.93
	- Fuel		8.85	8.85	3.26	8.85
	- O&M		19.5	22.8	9.1	19.3
	- Capital		568	666	267	562
5	Emission Reductions					
	- Reduction efficiency	%	55	54	37	45
	- Annual	tpy	1489	1462	967	1219
6	Cost Effectiveness w/o trading credit purchase	$/ton	1227	1458	1001	1485
7	Cost of Credits[a]					
	- Tons purchased[b]	ton/yr	479	506	967	749
	- Price @ $2000/t	$k/yr	958	1012	1934	1498
	- Cost before credits		1830	2130	820	1810
	- Total cost	$	2780	3142	2754	3308
	- Cost effectiveness	$/tons	1416	1600	1400	1681

Notes: a. To achieve 0.15 lb/MMBtu
          b. Total reduction 1968 t/yr
          c. Additional power for classifers on all mills to achieve low LOI

Treating the economics as a trading issue assuming that regulations will force an emission standard similar to BACT, e.g., at the level achieved with GCR1. The GCR1 ($585/ton) is clearly the technology of choice over LNB/SOFA (($927/ton) under this scenario.

Table 5-5. Coal reburn economics in Western Region 370 MW opposed wall unit.

Item	Description	Units	Technology			
			GCR1	GCR2	LNB/SOFA	CRM
1	Configuration					
	- New dedicated mill		X	X		X
	- Classifer		X	X	X(5)	X
	- Primary fan		X	X		X
2	Capital - 1st	$k	15851	18543	7430	15713
	- Recovery	%	11	11	11	11
3	Operations					
	- Utilities	kW	226	226	1009	226
	- Boiler Eff	%	0.19	0.19	0.07	0.19
4	Economics	$k/hr				
	- Utilities		7.93	7.93	35.34	7.93
	- Fuel		8.85	8.85	3.26	8.85
	- O&M		42.3	55.7	22.2	46.9
	- Capital		233	273	110	232
5	Emission Reductions					
	- Reduction efficiency	%	50	49	37	45
	- Annual	tpy	3289	3223	2430	2960
6	Cost Effectiveness w/o trading credit purchase	$/ton	656	778	414	723
7	Cost of Credits[a]					
	- Tons purchased[b]	ton/yr	0	66	859	329
	- Price @ $2000/t	$k/yr	0	132	1718	658
	- Cost before credits		2160	2510	1010	2140
	- Total cost	$	2160	2642	2728	2798
	- Cost effectiveness	$/tons	656	803	829	851

Notes: a. Realtive to BACT = GCR1, credits purchased at $2000/ton
                b. Total required reduction of 3587 t/yr

SCR on large, base loaded units should achieve a cost effectiveness of about $1000/ton. It is assumed that the control requirement is set by LNB/SOFA. Therefore, any additional reduction obtained with an alternative technology is taken as a credit relative to SCR. The common gasifier configuration (GCR1) performs similarly ($400/ton) to the LNB/SOFA system ($414/ton) and significantly better than the conventional CRM system ($662/ton). GCR1 always performs better than the CRM configuration under all assumptions of venue and economic selection criteria.

Summary of FFR economics is presented in Table 5-6.

Table 5-6. Cost effectiveness summary.

Region	Description	Units	Technology		
			GRC-1	CRM	LNB/OFA
OTR	Capital	$(000)	15851	15713	7430
	NO$_x$ Reduction				
5 mo/yr	- Eff	%	55	45	37
LF=85%	- Annual	TPY	1489	1219	967
	Cost Effectiveness	$/ton			
	- Before TC		1227	1485	1001
	- After TC		1416	1681	1400
Western	Capital	$0	15851	15713	7430
	NO$_x$ Reduction				
12 mo/yr	- Eff	%	50	45	37
LF=85%	- Annual	TPY	3289	2960	2430
	Cost Effectiveness	$/ton			
	- Before TC		656	723	414
	- After TC		656	851	829

Notes: a. GRC-1, Common gasifier with new pulverizer
          b. CRM, conventional coal reburn with new pulverizer
          c. LNB/SOFA, low NO$_x$ burner with over fire air and classifiers on each mill
          d. OTR trading credits, trading credit=$2000/ton referenced to 0.15 lb/MMBtu
          e. Western trading credits, trading credit=$1000/ton, referenced to BACT=GCR-1

5.4 Economic Estimate: Summary

Analysis suggests that utilization of a common gasifier in FFR is more economic option than having separate gasifiers for each reburn fuel injector. Utilization of a common gasifier does not significantly increase capital cost in comparison with basic reburn since gasifier (which is an expanded duct) replaces complex coal and boost air system required for basic reburn. The most expensive FFR option is utilization of separate gasifiers for each reburn fuel injector.

Economic analysis suggests that FFR system with common gasifier is more economic than conventional reburning and has NO$_x$ reduction cost similar to that of major competing technology, LNB/SOFA system, for all economic scenarios.

6.0 SUMMARY AND CONCLUSIONS

This project develops Fuel-Flexible Reburning (FFR) technology that is an improved version of conventional reburning. In FFR solid fuel is partially gasified before injection into the reburning zone of a boiler. Partial gasification of a solid fuel improves efficiency of NO_x reduction and decreases LOI by increasing fuel reactivity. The work included a combination of experimental and modeling studies designed to identify optimum process conditions, confirm the process mechanism and to estimate cost effectiveness of the FFR technology. All project objectives and technical performance goals were met, and competitive advantages of FFR were demonstrated. The following conclusions can be drawn from results of the work:

1. Tests demonstrated that partial coal gasification prior to injection into reburning zone improves the efficiency of NO_x reduction and decreases LOI.

2. Several coals with different volatiles content were tested. Data suggested that incremental increase in the efficiency of NO_x reduction due to coal gasification was more significant for coals with low volatiles content.

3. Up to 14% increase in the efficiency of NO_x reduction in comparison with basic reburning was achieved with coal gasification.

4. Efficiency of NO_x reduction in FFR depends on the residence time in the reburning zone. Benefits of using FFR over basic reburning are more significant at shorter residence times when coal does not have enough time to react.

5. Temperature and residence time in the gasification zone affect the efficiency of NO_x reduction in FFR. Coal gasification in the temperature range of 1000 – 1150 K results in production of hydrocarbons, CO, H_2, and char. Tests demonstrated that NO_x reduction is maximum at residence time of about 1 s.

6. FFR improves efficiency of NO_x reduction for renewable fuels with high fuel-N content and has small effect on the performance of fuels with low fuel-N content. Fuels with high fuel-N content benefit more from gasification prior to the injection into reburning zone because fuel-N is partially converted to N_2 during gasification thus reducing negative impact of fuel-N on NO_x reduction in reburning.

7. Model of reburning with gaseous products has been developed. Modeling predicts that composition of coal gasification products depends on temperature. Coal gasification in the

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temperature range of 600 - 800 K is predicted to be more beneficial since it provides the largest yield of hydrocarbons. Main gasification products at these temperatures are soot and CH_4, while soot, H_2 and CO are main gasification products at higher temperatures. However, coal gasification at these temperatures may require long residence time.

8. Modeling predicts that utilization of coal gasification products as a reburning could result in an improvement in NO_x reduction efficiency in comparison with basic reburning.

9. Modeling predicts that under fast mixing conditions gasification of small particles of bituminous coals at reaction time of 1 s and temperatures higher than 600 K produces enough volume of products to be used as a reburning fuel at heat inputs up to 20% of the total. However, optimum conditions for solid fuel gasification have to be determined based on fuel characteristics and design parameters of a specific gasifier.

10. FFR conceptual design has been developed. The conceptual design includes a common gasifier and gasifier at each reburn fuel injector.

11. Economic analysis confirmed economic benefits of the FFR technology. Analysis suggested that utilization of a common gasifier in FFR is a better option than having separate gasifiers for each reburn fuel injector.

12. Economic analysis also suggests that an FFR system with common gasifier is more economic than conventional reburning and has NO_x reduction cost similar to that of major competing technology, LNB/SOFA system, for all economic scenarios.

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×T^n 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                      A      n      E
HO2+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
```

```
! 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
```

```
! Reactions                           A     n        E
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                      A        n      E
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                          A       n       E
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                        A       n       E
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 !
```

```
! 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:

$$C^o_p/R = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4$$
$$H^o/RT = a_1 + (a_2/2)T + (a_3/3)T^2 + (a_4/4)T^3 + (a_5/5)T^4 + (a_6/T)$$
$$S/R = a_1\ln(T) + a_2T + (a_3/2)T^2 + (a_4/3)T^3 + (a_5/4)T^4 + a_7$$

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 a1 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    0G    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    0G    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    0G    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    0G    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    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
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    0G    300.000  5000.000 1397.000      01
 3.30616438E+00 1.05880379E-03-3.35101565E-07 4.84712126E-11-2.66276333E-15    2
 9.80488610E+03 6.14537840E+00 3.18302768E+00 1.26159588E-03-4.40480253E-07    3
 6.32411494E-11-1.29137488E-15 9.85926748E+03 6.84194428E+00                   4
NO2              J 9/64N   1O   2    0    0G    300.000  5000.000 1502.000      01
 5.25702679E+00 1.59120496E-03-5.75149303E-07 9.26518589E-11-5.51558940E-15    2
 1.98171367E+03-2.31252539E+00 2.83832558E+00 6.42094110E-03-3.71675448E-06    3
 7.13464440E-10 2.36187798E-14 2.88065438E+03 1.09303839E+01                   4
N2O              J12/64N   2O   1    0    0G    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    0G    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
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-1.94660247E-09 4.40577561E-13-6.64082103E+03 3.66779173E+00                   4
N2                J 9/65N   2   0   0   0G   300.000  5000.000 1651.000       01
 2.99595342E+00 1.23650804E-03-3.70307892E-07 5.05346628E-11-2.62980307E-15    2
-9.13275945E+02 5.68044094E+00 3.26021755E+00 5.91317615E-04 2.24046981E-07     3
-1.95572855E-10 3.61873253E-14-9.99926028E+02 4.27471775E+00                   4
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               L12/89H   1C   1O   1   0G   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
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-1.33144093E-08 4.33768865E-12 3.83956496E+03 3.39437243E+00 9.98945000E+03    4
CH2O            L 8/88H   2C   1O   1    0G   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    0G   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   0G   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   0G   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   3O   1    0G   200.000  3500.000  1000.000        1
 3.69266569E+00 8.64576797E-03-3.75101120E-06 7.87234636E-10-6.48554201E-14     2
-3.24250627E+03 5.81043215E+00 3.86388918E+00 5.59672304E-03 5.93271791E-06     3
-1.04532012E-08 4.36967278E-12-3.19391367E+03 5.47302243E+00 1.18339080E+04     4
CH3O            121686C   1H   3O   1    0G   300.00   3000.00   1000.000        1
 0.03770799E+02 0.07871497E-01-0.02656384E-04 0.03944431E-08-0.02112616E-12     2
 0.12783252E+03 0.02929575E+02 0.02106204E+02 0.07216595E-01 0.05338472E-04     3
-0.07377636E-07 0.02075610E-10 0.09786011E+04 0.13152177E+02                    4
CH3OH           L 8/88C   1H   4O   1    0G   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   2O   1    0G   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   2O   1    0G   300.00   4000.00   1000.000        1
 0.56282058E+01 0.40853401E-02-0.15934547E-05 0.28626052E-09-0.19407832E-13     2
 0.19327215E+05-0.39302595E+01 0.22517214E+01 0.17655021E-01-0.23729101E-04     3
 0.17275759E-07-0.50664811E-11 0.20059449E+05 0.12490417E+02                    4
HCCOH           SRI91C   2O   1H   2    0G   300.00   5000.00   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 0300.00   5000.00   1000.00           1
 0.07120307E+02 0.03246228E-01-0.14316134E-05 0.02797053E-08-0.02013007E-12     2
 0.05864479E+05-0.12137301E+02 0.12210763E+01 0.01878797E+00-0.13443212E-04     3
 0.12746013E-08 0.13540601E-11 0.07473144E+05 0.01840202E+03                    4
N2H2            J12/65N   2H   2   0    0G   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    0G   300.000  5000.000  1000.000       01
 2.50104420E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00     2
 5.61038356E+04 4.17481974E+00 2.50104420E+00 0.00000000E+00 0.00000000E+00     3
 0.00000000E+00 0.00000000E+00 5.61038356E+04 4.17481974E+00                    4
NH         melius/91 N   1H   1   0    0G   300.000  5000.000 1368.000          01
 2.71207542E+00 1.33555860E-03-3.70230207E-07 4.57845270E-11-2.13216798E-15     2
 4.24170243E+04 6.21142965E+00 3.49617412E+00-2.58512197E-04 8.00229766E-07     3
-3.18729027E-10 3.76580317E-14 4.21181588E+04 1.91107205E+00                    4
NH2             L 9/81N   1H   2   0    0G   300.000  5000.000 1379.000         01
 2.81084081E+00 3.24676780E-03-1.05043681E-06 1.56667098E-10-8.82503591E-15     2
 2.19519093E+04 6.57719920E+00 4.10811911E+00-1.25157496E-03 4.38306028E-06     3
-2.62867774E-09 5.10376771E-13 2.16908327E+04 2.01299833E-01                    4
H2NO       M/JB86     N   1H   2O   1    0G   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
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      1.31067689E-09-1.79413169E-13 6.89825870E+03 1.08768221E+01                4
HONO         NBS         N  1H  1O  2    0G   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    0G   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    0G   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    0G   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-03-1.59463967E-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    0G   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    0G   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  4O  1    0G   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  3O  1    0G   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     T04/83O  1H  3C  2    0G   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    0G   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    0G   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  1O  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  2O  00    0G   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 274O  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
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  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  1O   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  2O   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      2
  0.02547163E+06-0.04601176E+01 0.02500000E+02 0.00000000E+00 0.00000000E+00      3
  0.00000000E+00 0.00000000E+00 0.02547163E+06-0.04601176E+01                    4
HO2*            recombH  1O   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   6O 452      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
CHAR*           dummy C 253N   6O 254      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
CHARN           dummy C   1N   6O   2      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
VOLS            vol.  H 544C 274O 204N   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
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      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
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      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
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      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
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      2
-0.74540000E+03 0.43660000E+01 0.25000000E+01 0.00000000E+00 0.00000000E+00      3
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 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  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
SOOTNO        dummy C  30O  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  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
SOOTNOH       dummy C  30O  31N   1H   1G 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
S*            2CO   C  2O   2      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
VOL1*         dummy H 346C 236N   4O 166G 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
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  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
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*           121386O   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   1O   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
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Appendix C. **Ozone Transport Region Cost Effectiveness for 386 MW Reference Plant**

		Ref. No	1	2	3	4	5	6
			CRM Eff=45	GCR1 Eff = 53%	GCR1 Eff = 55%	GCR2 Eff =52%	GCR2 Eff=54	SOFA/ LNB Eff=37
	Units	Baseline						
Unit capacity (net)	E3 lb/hr	2,600.00	2,600.00	2,600.00	2,600.00	2,600.00	2,600.00	2,600.00
Fuels distribution								
Coal	%							
Burners			0.00	0.00	0.00	0.00	0.00	0.00
Pulverized		100.00	78.00	78.00	78.00	78.00	78.00	0.00
Micronized		0.00	22.00	22.00	22.00	22.00	22.00	100.00
Orimulsion	%	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Gas	%	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Total	%	100.00	100.00	100.00	100.00	100.00	100.00	100.00
Efficiency								
Base efficiency	%	88.20	88.20	88.20	88.20	88.20	88.20	88.20
Enthalpy rise of steam	Btu/lb	1,150.00						
Heat output of steam	E6 Btu/hr	2,990.00						
Base heat input	Btu/hr	3,390.02	3,390.02	3,390.02	3,390.02	3,390.02	3,390.02	3,390.02
Latent Heat Penalties								
Coal								
Burners	%	0.50	0.50	0.50	0.50	0.50	0.50	0.50
Pulverized	%	0.50	0.50	0.50	0.50	0.50	0.50	0.50
Micronized	%	0.33	0.33	0.33	0.33	0.33	0.33	0.33
Orimulsion	%	3.08	3.08	3.08	3.08	3.08	3.08	3.08
Gas	%	5.00	5.00	5.00	5.00	5.00	5.00	5.00
Adjusted heat input	E6 Btu/hr	3,390.02	3,388.75	3,388.75	3,388.75	3,388.75	3,388.75	3,384.22
Additional efficiency impact	%	0.00	0.25	0.25	0.25	0.25	0.25	0.25
Final adjusted heat input	E6 Btu/hr	3,390.02	3,397.22	3,397.22	3,397.22	3,397.22	3,397.22	3,392.68
Final boiler efficiency	%	88.20	88.01	88.01	88.01	88.01	88.01	88.13
Net efficiency reduction	%	0.00	0.19	0.19	0.19	0.19	0.19	0.07
Fuels requirements								
Heat input								
Coal								
Burners	E6 Btu/hr	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Pulverized	E6 Btu/hr	3,390.02	2,649.83	2,649.83	2,649.83	2,649.83	2,649.83	0.00
Micronized	E6 Btu/hr	0.00	747.39	747.39	747.39	747.39	747.39	3,392.68
Orimulsion	E6 Btu/hr	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Gas	E6 Btu/hr	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Total	E6 Btu/hr	3,390.02	3,397.22	3,397.22	3,397.22	3,397.22	3,397.22	3,392.68
Fuel unit costs								
Coal								
Burners	$/E6 btu	1.23	1.23	1.23	1.23	1.23	1.23	1.23
Pulverized	$/E6 btu	1.23	1.23	1.23	1.23	1.23	1.23	1.23
Micronized	$/E6 btu	1.23	1.23	1.23	1.23	1.23	1.23	1.23
Orimulsion	$/E6 btu	2.00	2.00	2.00	2.00	2.00	2.00	2.00
Gas	$/E6 btu	3.06	3.06	3.06	3.06	3.06	3.06	3.06
Fuel total cost								

Coal	$/hr						
Burners	$/hr	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Pulverized	$/hr	4,169.73	3,259.29	3,259.29	3,259.29	3,259.29	3,259.29	0.00
Micronized	$/hr	0.00	919.29	919.29	919.29	919.29	919.29	4,172.99
Orimulsion	$/hr	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Gas	$/hr	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Total	$/hr	4,169.73	4,178.58	4,178.58	4,178.58	4,178.58	4,178.58	4,172.99
Cost increase	$/hr		8.85	8.85	8.85	8.85	8.85	3.26
Auxiliary power								
Pulverization								
Pulverized coal								
Unit pulv. power	Kwh/E6 B	0.63	0.63	0.63	0.63	0.63	0.63	0.63
Pulv. power	Kwh	2,118.76	1,656.14	1,656.14	1,656.14	1,656.14	1,656.14	0.00
Micronized coal								
Unit pulv. power	Kwh/E6 B	0.92	0.92	0.92	0.92	0.92	0.92	0.92
Pulv. power	Kw	0.00	689.19	689.19	689.19	689.19	689.19	3,128.49
Total pulv. power	Kw	2,118.76	2,345.33	2,345.33	2,345.33	2,345.33	2,345.33	3,128.49
Other auxiliary power	Kw	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Total auxiliary power	Kw	2,118.76	2,345.33	2,345.33	2,345.33	2,345.33	2,345.33	3,128.49
Increased aux. power	Kw	0.00	226.57	226.57	226.57	226.57	226.57	1,009.73
Aux. power unit cost	$/kwh	0.04	0.04	0.04	0.04	0.04	0.04	0.04
Increased aux. power cost	$/hr	0.00	7.93	7.93	7.93	7.93	7.93	35.34
NOx								
Percent reductions								
Incremental reductions								
Low NOx Burners	%		0.00	0.00	0.00	0.00	0.00	10.00
Overfire air	%		0.00	0.00	0.00	0.00	0.00	30.00
Reburning	%		45.00	53.00	55.00	52.00	54.00	0.00
Nitrogen agent 1	%		0.00	0.00	0.00	0.00	0.00	0.00
Nitrogen agent 2	%		0.00	0.00	0.00	0.00	0.00	0.00
Total Reduction	%	0.00	45.00	53.00	55.00	52.00	54.00	37.00
Total red from LNB level	%	0.00	45.00	53.00	55.00	52.00	54.00	30.00
Culmulative remaining								
After low NOx burners	%	100.00	100.00	100.00	100.00	100.00	100.00	90.00
After overfire air	%	100.00	100.00	100.00	100.00	100.00	100.00	63.00
After reburning	%	100.00	55.00	47.00	45.00	48.00	46.00	63.00
After nitrogen agent 1	%	100.00	55.00	47.00	45.00	48.00	46.00	63.00
After nitrogen agent 2	%	100.00	55.00	47.00	45.00	48.00	46.00	63.00
Per net heat input								
Initial level	lb/E6 Btu	0.52	0.52	0.52	0.52	0.52	0.52	0.52
After low NOx burners	lb/E6 Btu	0.52	0.52	0.52	0.52	0.52	0.52	0.47
After overfire air	lb/E6 Btu	0.52	0.52	0.52	0.52	0.52	0.52	0.33
After reburning	lb/E6 Btu	0.52	0.29	0.24	0.23	0.25	0.24	0.33
After nitrogen agent 1	lb/E6 Btu	0.52	0.29	0.24	0.23	0.25	0.24	0.33
After nitrogen agent 2	lb/E6 Btu	0.52	0.29	0.24	0.23	0.25	0.24	0.33
Hourly emissions								
Initial level	lb/hr	1,762.81	1,766.55	1,766.55	1,766.55	1,766.55	1,766.55	1,764.19
After low NOx burners	lb/hr	1,762.81	1,766.55	1,766.55	1,766.55	1,766.55	1,766.55	1,587.77
After overfire air	lb/hr	1,762.81	1,766.55	1,766.55	1,766.55	1,766.55	1,766.55	1,111.44
After reburning	lb/hr	1,762.81	971.60	830.28	794.95	847.95	812.61	1,111.44
After nitrogen agent 1	lb/hr	1,762.81	971.60	830.28	794.95	847.95	812.61	1,111.44
After nitrogen agent 2	lb/hr	1,762.81	971.60	830.28	794.95	847.95	812.61	1,111.44
Total NOx emission red.								
Mass	lb/hr	0.00	794.95	936.27	971.60	918.61	953.94	652.75
Percent	%	0.00	45.00	53.00	55.00	52.00	54.00	37.00
Nit. Agents and promoters								
Nitrogen agent 1								
Type			0.00	0.00	0.00	0.00	0.00	0.00
Molecular Weight			16.00	16.00	16.00	16.00	16.00	16.00
Nitrogen atoms/molecule			1.00	1.00	1.00	0.50	1.00	0.50

NSR (N atom ratio)			0.00	0.00	0.00	1.50	0.00	1.50
Flowrate	lb/hr		0.00	0.00	0.00	884.81	0.00	1,159.76
Unit Cost	$/ton		0.00	0.00	0.00	0.00	0.00	0.00
Hourly cost	$/hr		0.00	0.00	0.00	0.00	0.00	0.00
Nitrogen agent 2								
Type			0.00	0.00	0.00	0.00	0.00	0.00
Molecular Weight			16.00	16.00	16.00	16.00	16.00	16.00
Nitrogen atoms/molecule			1.00	1.00	1.00	1.00	1.00	1.00
NSR (N atom ratio)			0.00	0.00	0.00	0.00	0.00	0.00
Flowrate	lb/hr		0.00	0.00	0.00	0.00	0.00	0.00
Unit Cost	$/ton		0.00	0.00	0.00	0.00	0.00	0.00
Hourly cost	$/hr		0.00	0.00	0.00	0.00	0.00	0.00
SO2 Reduction								
Fuel SO2 Potential								
Coal								
Burners	lb/E6 Btu	5.00	5.00	5.00	5.00	5.00	5.00	5.00
Pulverized	lb/E6 Btu	5.00	5.00	5.00	5.00	5.00	5.00	5.00
Micronized	lb/E6 Btu	5.00	5.00	5.00	5.00	5.00	5.00	5.00
Orimulsion	lb/E6 Btu	4.15	4.15	4.15	4.15	4.15	4.15	4.15
Gas	lb/E6 Btu	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Hourly Emissions	lb/hr	16,950.11	16,986.09	16,986.09	16,986.09	16,986.09	16,986.09	16,963.38
Emission reduction	lb/hr		-35.97	-35.97	-35.97	-35.97	-35.97	-13.27
Percent emission reduction	%		-0.21	-0.21	-0.21	-0.21	-0.21	-0.08
Value of SO2 reduction								
Unit value of SO2 red.	$/ton	175.00	175.00	175.00	175.00	175.00	175.00	175.00
Total value of SO2 red.	$/hr		-3.15	-3.15	-3.15	-3.15	-3.15	-1.16
Operation and maintenance								
Capital cost (installed)								
Low NOx Burners	E6$		0.00	0.00	0.00	0.00	0.00	2.66
Overfire air ports	E6$		0.00	0.00	0.00	0.00	0.00	4.77
Reburning	E6$		15.70	15.85	15.85	18.54	18.54	0.00
SNCR-1	E6$		0.00	0.00	0.00	0.00	0.00	0.00
Promotion-1	E6$		0.00	0.00	0.00	0.00	0.00	0.00
SNCR-2	E6$		0.00	0.00	0.00	0.00	0.00	0.00
Promotion-2	E6$		0.00	0.00	0.00	0.00	0.00	0.00
SCR	E6$		0.00	0.00	0.00	0.00	0.00	0.00
Total cost	E6 $	0.00	15.70	15.85	15.85	18.54	18.54	7.43
Maint./cap. (at 65% cf)	%/year		2.00	2.00	2.00	2.00	2.00	2.00
Maintenance cost	$/hr	0.00	19.30	19.49	19.49	22.79	22.79	9.13
Catalyst replacement								
Catalyst Cost								
Relative to SCR cost	%		0.00	0.00	0.00	0.00	0.00	0.00
Total cost	E6 $		0.00	0.00	0.00	0.00	0.00	0.00
Life (@ 65% cap. fac.)	Years		0.00	0.00	0.00	0.00	0.00	0.00
Replacement cost	$/hr		0.00	0.00	0.00	0.00	0.00	0.00
Ash Disposal								
Coal fuels Ash content								
Burners	%	8.00	8.00	8.00	8.00	8.00	8.00	8.00
Pulverized	%	8.00	8.00	8.00	8.00	8.00	8.00	8.00
Micronized	%	8.00	8.00	8.00	8.00	8.00	8.00	8.00
Orimulsion	%	0.25	0.25	0.25	0.25	0.25	0.25	0.25
Coal fuels heating value (coal only)								
Burners	Btu/lb	12,000	12,000	12,000	12,000	12,000	12,000	12,000
Pulverized	Btu/lb	12,000	12,000	12,000	12,000	12,000	12,000	12,000
Micronized	Btu/lb	12,200	12,200	12,200	12,200	12,200	12,200	12,200
Orimulsion	Btu/lb	13,000	13,000	13,000	13,000	13,000	13,000	13,000

Coal ash content								
Burners	lb/E6 Btu	6.67	6.67	6.67	6.67	6.67	6.67	6.67
Pulverized	lb/E6 Btu	6.67	6.67	6.67	6.67	6.67	6.67	6.67
Micronized	lb/E6 Btu	6.56	6.56	6.56	6.56	6.56	6.56	6.56
Orimulsion	lb/E6 Btu	0.19	0.19	0.19	0.19	0.19	0.19	0.19
Ash flowrate	tons/hr	11.30	11.28	11.28	11.28	11.28	11.28	11.12
Unit ash disposal cost	$/ton	10.00	10.00	10.00	10.00	10.00	10.00	10.00
Total ash disposal cost	$/hr	113.00	112.83	112.83	112.83	112.83	112.83	111.24
Incr. ash dispos. cost	$/hr		-0.17	-0.17	-0.17	-0.17	-0.17	-1.77
Hourly summary								
Cost Increase								
Fuels	$/hr		8.85	8.85	8.85	8.85	8.85	3.26
Nitrogen agents	$/hr		0.00	0.00	0.00	0.00	0.00	0.00
Maintenance	$/hr		19.30	19.49	19.49	22.79	22.79	9.13
Catalyst replacement	$/hr		0.00	0.00	0.00	0.00	0.00	0.00
Ash disposal	$/hr		-0.17	-0.17	-0.17	-0.17	-0.17	-1.77
Subtotal	$/hr		28.15	28.33	28.33	31.64	31.64	12.40
Value of SO2 reduction	$/hr		-3.15	-3.15	-3.15	-3.15	-3.15	-1.16
Net cost of NOx control	$/hr		31.30	31.48	31.48	34.79	34.79	13.56
Emission reductions								
NOx	lb/hr		794.95	936.27	971.60	918.61	953.94	652.75
SO2	lb/hr		-35.97	-35.97	-35.97	-35.97	-35.97	-13.27
Annual summary								
Capacity factor	%	35.00	35.00	35.00	35.00	35.00	35.00	35.00
Operating hours	hr	3,066	3,066	3,066	3,066	3,066	3,066	3,066
Annual operating cost								
Without SO2	E6 $/yr		0.09	0.09	0.09	0.10	0.10	0.04
SO2 value	E6 $/yr		-0.01	-0.01	-0.01	-0.01	-0.01	0.00
Net operating cost	E6 $/yr		0.10	0.10	0.10	0.11	0.11	0.04
Annual NOx reduction	tons/yr		1,219	1,435	1,489	1,408	1,462	1,001
Annual SO2 reduction	tons/yr		-55	-55	-55	-55	-55	-20
Annual NOx + SO2 red.	tons/yr		1,164	1,380	1,434	1,353	1,407	980
Levelized cost								
Economic factors								
Levelization factor		1.000	1.00	1.00	1.00	1.00	1.00	1.00
Capital recovery factor			0.110	0.110	0.110	0.094	0.110	0.110
Levelized annual cost								
Op. & maint. component								
Net	E6 $/yr		0.10	0.10	0.10	0.11	0.11	0.04
Capital component	E6 $/yr		1.72	1.74	1.74	1.74	2.04	0.82
Total	E6 $/yr		1.81	1.83	1.83	1.84	2.13	0.85
Cost of NOx control	$/ton NOx		1,485	1,273	1,227	1,306	1,458	853