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SECOND GENERATION ADVANCED REBURNING FOR HIGH EFFICIENCY NOx CONTROL

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1.0 Introduction

Title 1 of the Clean Air Act Amendment (CAAA) of 1990 requires NO_x controls in ozone non-attainment areas. The initial Title 1 regulations, implemented over the last few years, required Reasonably Available Control Technologies (RACT). In most areas, the NO_x levels for RACT are based on Low NO_x Burners (LNB) and are in the range of 0.4 to 0.5 $lb/10^6$ Btu. As a result, there has been little industry demand for higher efficiency and more expensive NO_x controls such as reburning, Selective Non-Catalytic Reduction (SNCR), and Selective Catalytic Reduction (SCR). However, the current RACT requirements will not be the end of NO_x regulations. Much more stringent NO_x control will be required to bring many of the ozone non-attainment areas into compliance, particularly in the Northeast.

The post-RACT requirements are being based, to a large extent, on SCR, the commercial technology with the highest NO_x control efficiency. 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 large catalyst, and its related 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.

Low NO_x burners and overfire air (OFA) provide only modest NO_x control, but their capital costs are low and, since no reagents are required, their operating costs are near zero. This has made them the technologies of choice for the modest NO_x control required under Title 4 and the initial RACT under Title 1 of the CAAA. However, alone, they cannot approach the NO_x control required for post-RACT or the 90-95% NO_x control goal of the near future.

For deeper NO_x control, reburning, SNCR or SCR can be added to low NO_x burners and OFA, or installed as stand alone systems. Reburning controls NO_x via fuel staging. The main portion of the fuel is fired through the conventional burners with a small portion of the fuel injected into the furnace above the burners. The result is a slightly fuel rich "reburning zone" where NO_x is reduced by reactions with hydrocarbons. The reburning fuel can be coal or gas. Reburning alone can achieve only 50-70% NO_x control and, hence, may not be a candidate for most post-RACT applications.

The reaction of N-Agents with NO_x can proceed without a catalyst at high temperatures. This is the SNCR process. It is effective over a narrow "temperature window" centered about 1700°F where the N-Agent forms NH_2 radicals which react with NO. Under ideal laboratory conditions, deep NO_x control can be achieved; however, in practical, full scale installations, the non-uniformity of the temperature profile, difficulties of mixing the N-Agent across the full boiler cross section, limited residence time for reactions, and ammonia slip, limit SNCR's effectiveness. In most applications, NO_x control is limited to 40-50%.

In summary, the NO_x control technologies listed above all have limitations which may prevent them from successfully achieving cost effective post-RACT compliance. Thus, there is a need for a high efficiency, low cost NO_x control which utilities could apply to meet post-RACT NO_x control requirements. This project develops such a technology, Second Generation Advanced Reburning (SGAR), which has a potential to achieve 90+% NO_x control at a significantly lower cost than SCR.

1.1 Advanced Reburning and Second Generation Advanced Reburning

The conventional Advanced Reburning (AR) process is a synergetic integration of basic reburning and N-Agent injection, an adaptation of SNCR. With AR, a N-Agent is injected along with the OFA and the reburning system is adjusted to optimize the NO_x reduction due to the N-Agent. By adjusting the reburning fuel injection rate to achieve near stoichiometric conditions (instead of the fuel rich conditions normally used for reburning), the CO level is controlled and the temperature window for selective NO_x reduction is considerably broadened and deepened. The reburning fuel is reduced from about 20 to about 10% which has considerable economic benefits (the incremental cost of gas for gas reburning and the cost of the coal pulverization equipment for coal reburning). With AR, the NO_x control due to reburning is somewhat reduced, however, this reduction is offset by the significant enhancement of the N-Agent NO_x control.

The AR process was developed by EER as part of a DOE program (Chen et al., 1989) focusing on the optimization of basic reburning. Tests were conducted over a range of scales (up to 10 MBtu/hr) and an AR design methodology was developed by extending EER's reburning design methodology.

This project develops improved versions of AR for post-RACT applications. The SGAR systems have the potential to achieve 90+% NO_x control on all types of coal fired boilers without massive hardware changes, without increasing air toxic and toxic waste problems, and at a cost for NO_x control on the order of half that of SCR. These systems will provide flexible installations that allow NO_x levels to be lowered as new elements of the technology become available. The SGAR systems will incorporate several improvements over conventional AR, such as:

- N-agent injection into the reburning zone; and
- Promoter additives which enhance the effectiveness of the N-agent.

By integrating these improvements with AR, NO_x control can be increased to 90-95% for cyclone units and even higher for pulverized coal fired units (wall and tangentially fired) where AR can be further integrated with low NO_x burners and overfire air. The SGAR systems are intended for post-RACT applications in ozone non-attainment areas where NO_x control in excess of 80% is required. The SGAR systems will comprise a family of high efficiency NO_x control technologies which include:

- Promoted Advanced Reburning (PAR) - conventional AR (N-agent injected with the OFA) with a promoter added to the agent.
- Promoted Advanced Reburning Rich (PAR-Rich) - N-agent injection along with a promoter into the reburning zone.
- Multiple Injection Advanced Reburning (MIAR) - N-agents with promoters injected in two locations: within the reburning zone and with the OFA.

1.2 Objectives of the Program

The overall objective of Phase I is to demonstrate the effectiveness of the SGAR technologies at bench and pilot scale over a sufficiently broad range of conditions to provide all of the information needed for process optimization and scale up. The Phase I program will be conducted over a two year period. The program will:

1. Develop an understanding of the mechanisms through which promoter additives improve N-agent effectiveness;

2. Develop a kinetic analytical model of the Promoted and Multiple Injection AR technologies;

3. Optimize the SGAR processes using the analytical model and bench and pilot scale experiments under controlled mixing conditions; and

4. Upgrade EER's AR design methodology to include the second generation advances.

Phase I will determine the ability of the SGAR technologies to meet the following technical performance goals:

- NO_x emissions from the 1 MBtu/hr coal fired Boiler Simulator Facility controlled to less than the requirements for post-RACT NO_x control in the NESCAUM area for the year 2003;

- Total estimated cost of controlling NO_x emissions based on the 1 MBtu/hr coal fired tests less than that currently projected for SCR NO_x control systems; and

- No significant reduction in boiler efficiency or significant adverse environmental impacts when compared to current reburning and SNCR technologies.

2.0 Fundamentals of the SGAR Process

2.1 Reburning

Reburning, a fuel staging method for NO_x control, was suggested by Wendt et al., 1973. This is a three stage method which involves combustion of a fuel in two stages (Figure 2-1a). In the main combustion zone 80-90% of the fuel is burned with normal amount of air (about 10% excess). The combustion process forms a definite amount of NO_x. Then, on the second stage, the rest of the fuel (reburning fuel) is added at temperatures of about 2000-2600°F into the secondary combustion zone, called the reburning zone, to maintain a fuel-rich environment. In this reducing atmosphere both NO_x formation and NO_x removal reactions occur. Experimental results indicate that in a specific range of conditions (equivalence ratio in the reburning zone, temperature and residence time in the reburning zone) the NO_x concentrations can typically be reduced by 50-70%. In the third stage the OFA is injected at a lower temperature to complete combustion. Addition of the reburning fuel leads to the rapid oxidation of a portion of the fuel by oxygen to CO and hydrogen. The reburning fuel provides a fuel-rich mixture with certain concentrations of carbon containing radicals: CH_3, CH_2, CH, C, HCCO, etc. These active species can participate either in formation of NO precursors in reactions with molecular nitrogen or in reactions with NO. Many elementary steps can share responsibility for NO reduction, and there is no commonly accepted opinion about their importance. Miller and Bowman, 1989 suggest that the main reaction paths converting NO to N_2 include NO reactions with C and CH:

$$C + NO \rightarrow CN + O$$

$$CH + NO \rightarrow HCN + O$$

and CN and HCN are oxidized to NCO. A diagram of what seem to be the main reactions in the reburning zone is presented in Figure 2-1b. The carbon containing radicals (CH_i) formed in the reburning zone are capable of reducing NO concentrations by converting it to various intermediate species with C-N bonds. These species are reduced in reactions with different radicals into NH_i species (NH_2, NH, and N) which react with NO to form molecular nitrogen.

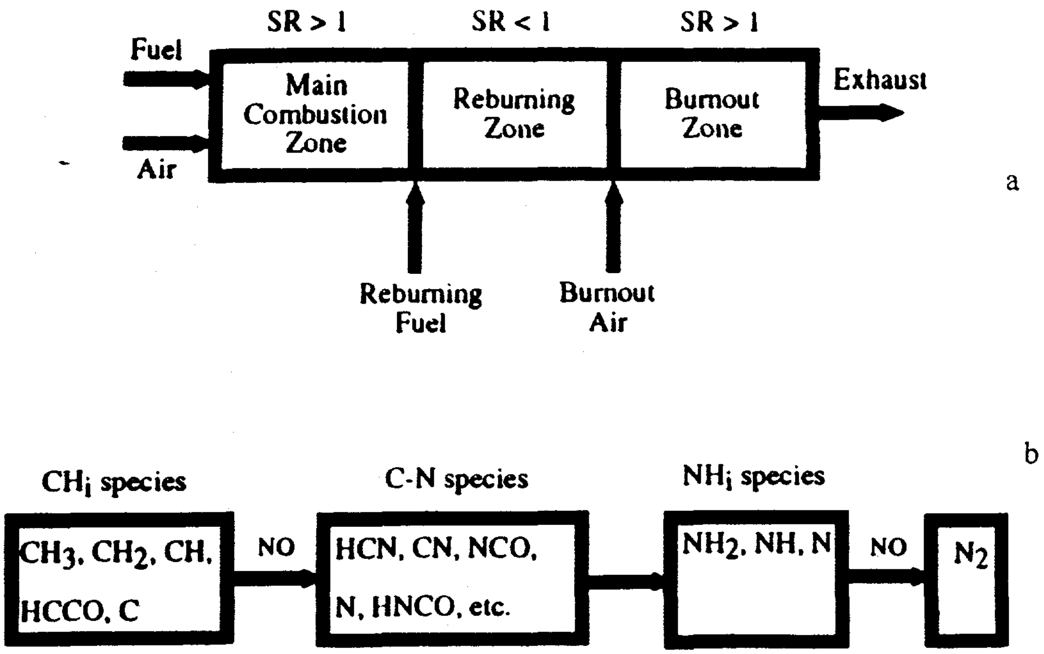

Figure 2-1. Diagram of the reburning process (a) and main reaction paths in the reburning zone (b).

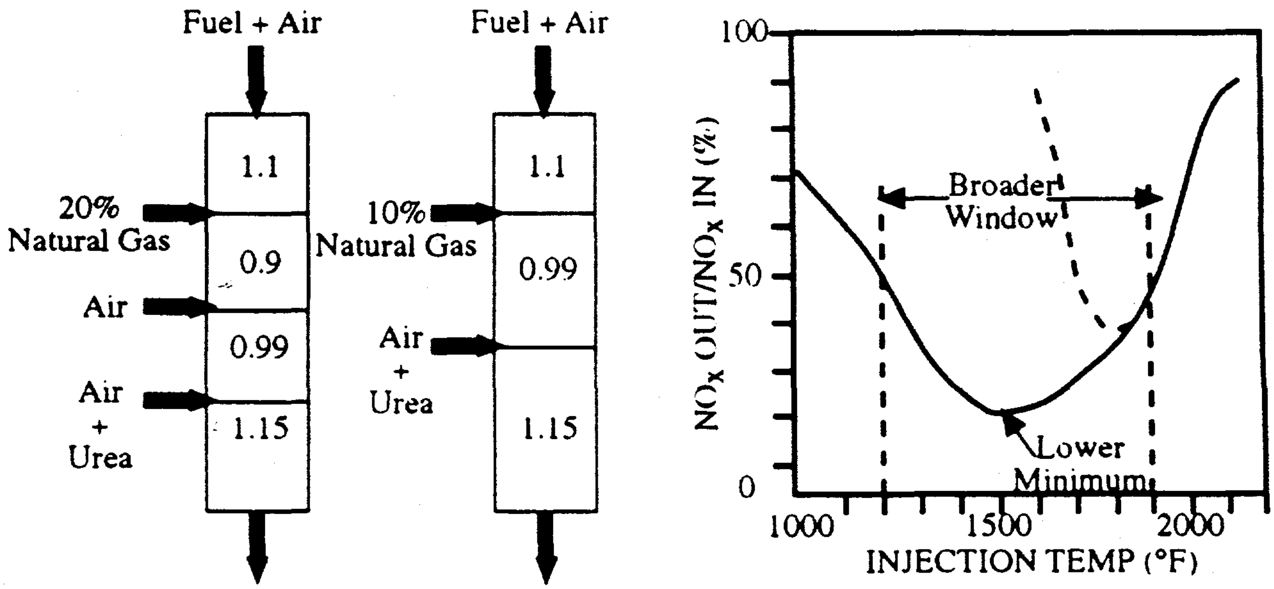

Figure 2-2. Schematic and performance of advanced reburning.

Thus, there are two types of chemical reactions of NO removal: with CH_i and with NH_i radicals. The OFA added on the last stage of the process oxidizes existing CO, H_2, HCN, and NH_3.

2.2 Selective Non-Catalytic Reduction

SNCR methods provide NO_x reduction by injection of various nitrogen compounds capable of reacting with NO in flue gas. The most common SNCR agents are ammonia and urea. The corresponding methods are called Thermal $DeNO_x$ and NO_xOUT processes. The Thermal $DeNO_x$ process was invented by Lyon, 1975 and described in detail by Lyon and Hardy, 1986. If ammonia is injected into combustion flue gas containing NO and oxygen at temperatures between 1500 and 2000°F, a chemical reaction between these compounds occurs and NO is converted to molecular nitrogen. The reaction starts with formation of NH_2 radicals:

$$NH_3 + OH \rightarrow NH_2 + H_2O$$

which can be also formed in reactions with O and H atoms:

$$NH_3 + O \rightarrow NH_2 + OH \text{ and}$$
$$NH_3 + H \rightarrow NH_2 + H_2.$$

The main elementary reaction of NO to N_2 conversion is:

$$NH_2 + NO \rightarrow N_2 + H_2O.$$

Another SNCR additive is urea, $(NH_2)_2CO$, which was suggested by Arand et al., 1980 and is used in the NO_xOUT process. The mechanism of urea injection includes the important features of the NH_3 and HNCO reactions with NO, because urea is rapidly converted to NH_3 and HNCO at high temperatures:

$$(NH_2)_2CO \rightarrow NH_3 + HNCO.$$

The most important HNCO reactions with radicals are:

$$HNCO + H \rightarrow NH_2 + CO \text{ and}$$
$$HNCO + OH \rightarrow NCO + H_2O.$$

As in the Thermal $DeNO_x$ process, NH_2 radicals can either remove NO:

$$NH_2 + NO \rightarrow N_2 + H_2O$$

or form NO via HNO radicals. NCO radicals can remove NO to form N_2O:

$$NCO + NO \rightarrow N_2O + CO$$

and then CO and N_2O molecules are oxidized by OH and H:

$$CO+OH \rightarrow CO_2+H \text{ and}$$
$$N_2O+H \rightarrow N_2+OH.$$

Thus, the process has a similar narrow temperature window, as NH_3 injection, but can be complicated by N_2O formation. The SNCR temperature window could be broadened to lower temperatures if an alternative source of OH radicals could be found. Attempts to do this include addition of hydrogen or hydrogen peroxide to ammonia, alcohols to urea, etc. However, the action of the additives is to shift the temperature at which the de-NO_x reactions are optimum, rather than to broaden the de-NO_x temperature window.

2.3 Advanced Reburning

EER's Advanced Reburning process provides an ideal approach for increasing the OH concentration. It incorporates the chain branching reaction of CO oxidation into the process. When CO reacts with oxygen, it initiates many free radicals. Thus, if a controlled amount of CO from the reburning zone can be introduced at the point of N-agent injection, the low temperature limitation of the window can be broadened and the NO_x reduction enhanced.

EER experimental studies (Seeker, 1990; Chen et al., 1991) demonstrated two approaches, presented in Figure 2-2, for addition of OFA in reburning to prepare specific SNCR conditions. One approach was to split the OFA addition so that the bulk of the oxidation is completed at the conventional OFA injection point while a moderate amount of CO is left for burnout at a second injection point at lower temperature where conditions are more favorable for $DeNO_x$ reactions. In subsequent studies, an alternative approach was adopted in which the reburning zone was deliberately de-tuned by increasing the stoichiometry to about 0.98 - 1.0. This allows a significant reduction in the natural gas flow, and eliminates one of the air injection stages. The general AR approach is illustrated in Figure 2-2 which compares also experimental data for SNCR and CO-promoted N-Agent injection. Figure 2-2 shows that the temperature window can be broadened and NO removal efficiency increased, if both CO and the O_2 concentrations are controlled to fairly low values (CO at the order of 1000 ppm and O_2 at less than 0.5 percent). At the point of air addition, CO and O_2 are both at low values because of the close approach to SR=1.0.

How does AR chemistry work? The chemistry of AR is no different than that for basic reburning and SNCR, and the reactions discussed above proceed. The critical difference is how the two sets of chemical reactions are synergistically integrated together. The final OFA initiates the oxidation of CO from the reburning zone:

$$CO + OH \rightarrow CO_2 + H$$
$$H + O_2 \rightarrow OH + O \quad \text{and}$$
$$O + H_2O \rightarrow OH + OH.$$

This chain branching sequence provides additional OH radicals to initiate the NH_3 oxidation sequence:

$$NH_3 + OH \rightarrow NH_2 + H_2O \quad \text{and}$$
$$NH_2 + NO \rightarrow N_2 + H_2O.$$

2.4 Second Generation Improvements to Advanced Reburning

Based on kinetic modeling and experimental studies, EER has recently developed concepts for using small amounts of promoter species and delayed ammonia injection into reburning zone to further improve upon the AR process. Extensive optimization and development of these concepts is the subject of the current project.

As discussed above, one constraint with SNCR processes is that the temperature window over which N-Agents are effective is relatively narrow. If the temperature of the flue gas is too low at the point where the N-Agent is injected, the efficiency of NO_x reduction is low and ammonia slip may occur. If the temperature is too high, the reducing agent tends to be oxidized to produce NO_x, and the net reduction of NO_x is poor. In addition, injection of urea or cyanuric acid often produces high emissions of N_2O, a potential greenhouse gas which can lead to degradation of the stratospheric ozone.

An experimental study was conducted at EER to investigate the promotion of SNCR processes. EER patented inorganic salt promoters (Ho et al., 1993) were tested in a 1 MBtu/hr Boiler Simulator Furnace (BSF) to determine their influence on the performance of SNCR with urea and ammonia. The BSF is one of the test units to be used in the current test program. The addition of sodium carbonate significantly extended the temperature window of NO control to lower temperatures and enhanced the NO_x reduction efficiencies with both ammonia and urea. Close to 90% NO_x reduction was achieved at 1700°F with the addition of only 10 ppm Na_2CO_3. An increase in the promoter concentration to 30 ppm does not affect the NO reduction. Furthermore, sodium also dramatically reduced N_2O emissions from both urea and ammonia injection. Although the promotion mechanisms are not fully understood, there exists the potential of using promoters to further widen the temperature window, enhance NO_x reductions, and control N_2O emissions.

A preliminary series of promoted AR with fuel rich side N-agent tests was also conducted at BSF. The studies were performed with natural gas as the main and reburn fuels. The reburn fuel accounted for 10% of total facility heat input, corresponding to a reburn zone stoichiometry of 0.99. N-agents, including urea or aqueous ammonia, were injected into the fuel rich reburn zone. The promotion tests were conducted only with Na_2CO_3 concentration of 100 ppm in flue gas. Test variables included N-agent stoichiometric ratio and delay time between the reburn fuel and N-agent injection locations. The delay time was varied from 0 to 0.5 s. The NO control performance was significantly enhanced by delaying N-agent injection. Maximum overall NO_x reduction with the N-agent and Na_2CO_3 promoter was about 85% for the combined process.

Preliminary kinetic modeling data show that addition of a small amount of ammonia into the reburning zone significantly improves NO_x reduction if the NH_i species precursors are produced shortly after introduction of the reburning fuel. When fuel is added to the reburning zone, the oxygen disappears very fast in the reaction with the fuel. If NH_i precursors are injected into the reburning zone, then they can react either with O_2 into NO or with NO into N_2. The NO reduction process is effective if the NH_i precursors appear in the gas mixture when concentration of oxygen has been significantly depleted by the reburning fuel, thus preventing oxidation into NO. Calculated characteristic times for O_2 disappearance after the injection of the reburning fuel are less than 0.01 s at 2500°F and about 0.1 s at 2150°F. This means that the delay between injection of a reburning fuel and the formation of NH_i species should exceed these times for effective NO reduction.

The delayed introduction of N-agent can be accomplished either by physically separating the injection of NH_i precursors (ammonia, urea, etc.) from that of the reburning fuel, or by utilizing an aqueous solution of urea or aqueous ammonia which is injected in the form of a droplet cloud together with the reburning fuel. The evaporation time of the aqueous droplets and N-agent decomposition time can provide the delay time necessary for the consumption of oxygen in the reburning zone. This delay time can be controlled by adjusting the droplet size to vary the rate of evaporation of the droplets.

As follows from EER's experimental data with salt promoters, Na_2CO_3 can promote the effect of N-agents, broaden the temperature window, and reduce the NO concentration under both fuel-rich and fuel-lean conditions. Available to date modeling results involve hypothetical sodium reactions and qualitatively explain the experimental results obtained under SNCR conditions.

3.0 Phase I Program Description

Initial parametric screening tests at a bench scale facility, followed by pilot scale developmental studies will be conducted in Phase I. The experimental work will be paralleled by kinetic modeling work which will provide a scientific understanding of the process, including the activity of N-agent promoters. The modeling will use experimental data to define key process parameters, culminating in a design methodology for the eventual scale-up and implementation of the technologies.

Phase I consists of six tasks:

Task 1.1 Project Coordination and Reporting/Deliverables
Task 1.2 Kinetics of Na_2CO_3 Reactions with Flue Gas Components
Task 1.3 0.1×10^6 Btu/hr Optimization Studies
Task 1.4 1.0×10^6 Btu/hr Process Development Tests
Task 1.5 Mechanism Development and Modeling
Task 1.6 Design Methodology and Application

The initial Task 1.1, Project Coordination and Reporting/Deliverables, will efficiently coordinate the efforts of the Key Personnel involved with the project so that the objectives of this project are met: on time, on specification, and on budget. Task 1.2, Kinetics of Na_2CO_3 Reactions with Flue Gas Components, will be performed at the University of Texas at Austin. Under this task, the reactions of sodium carbonate with simulated flue gas will be studied to develop an understanding of the promotion effect. The results will be used for updating kinetic models and for evaluating other prospective additives in Phase II. Tasks 1.3 and 1.4 will include bench and pilot scale studies to optimize the SGAR processes. The Phase I program will utilize two existing EER test facilities providing nominal thermal capacities of 0.1 and 1.0 MBtu/hr. All kinetic modeling work will be carried out in Task 1.5 in parallel with the experimental program. A detailed reaction mechanism of the SGAR processes will be developed based on available combustion chemistry data. Existing kinetic codes will be extensively used to apply the model for process optimization. Phase I will culminate in upgrading EER's existing design methodology for conventional AR to include the second generation improvements (Task 1.6).

Activities during the reporting period included 1) preparation of the Project Management Plan which was approved in November, 1995; 2) performing the project Kick-off meeting at PETC, December 15, 1995; 3) preparation of the 0.1 MBtu/hr bench-scale facility to the experimental program; and 4) selection of mechanisms for modeling. The results of experimental and modeling activities are presented below.

4.0 Task 1.3: 0.1 MBtu/hr Optimization Studies

The SGAR process involves injection of six reagents into the post-combustion zone:

- reburning fuel;
- N-agent rich-side;
- promoter rich-side;
- N-agent lean-side;
- promoter lean-side;
- OFA.

Under Task 1.3, bench scale tests will be performed to isolate and optimize each injection process individually via parametric testing. Combined optimization tests will be conducted later at pilot scale.

The bench scale tests will be conducted at EER's Controlled Temperature Tower (CTT). The CTT is a vertically downfired combustor with a nominal firing rate of 0.1 x 10^6 Btu/hr (Figure 4-1). Because of the relatively small size of the facility, it is possible to use bottled gases (e.g. O_2, N_2, SO_2) to control furnace gas composition. In addition, characteristic mixing times in the CTT furnace are on the order of 100 ms, making it easy to separate zones and characterize individual processes.

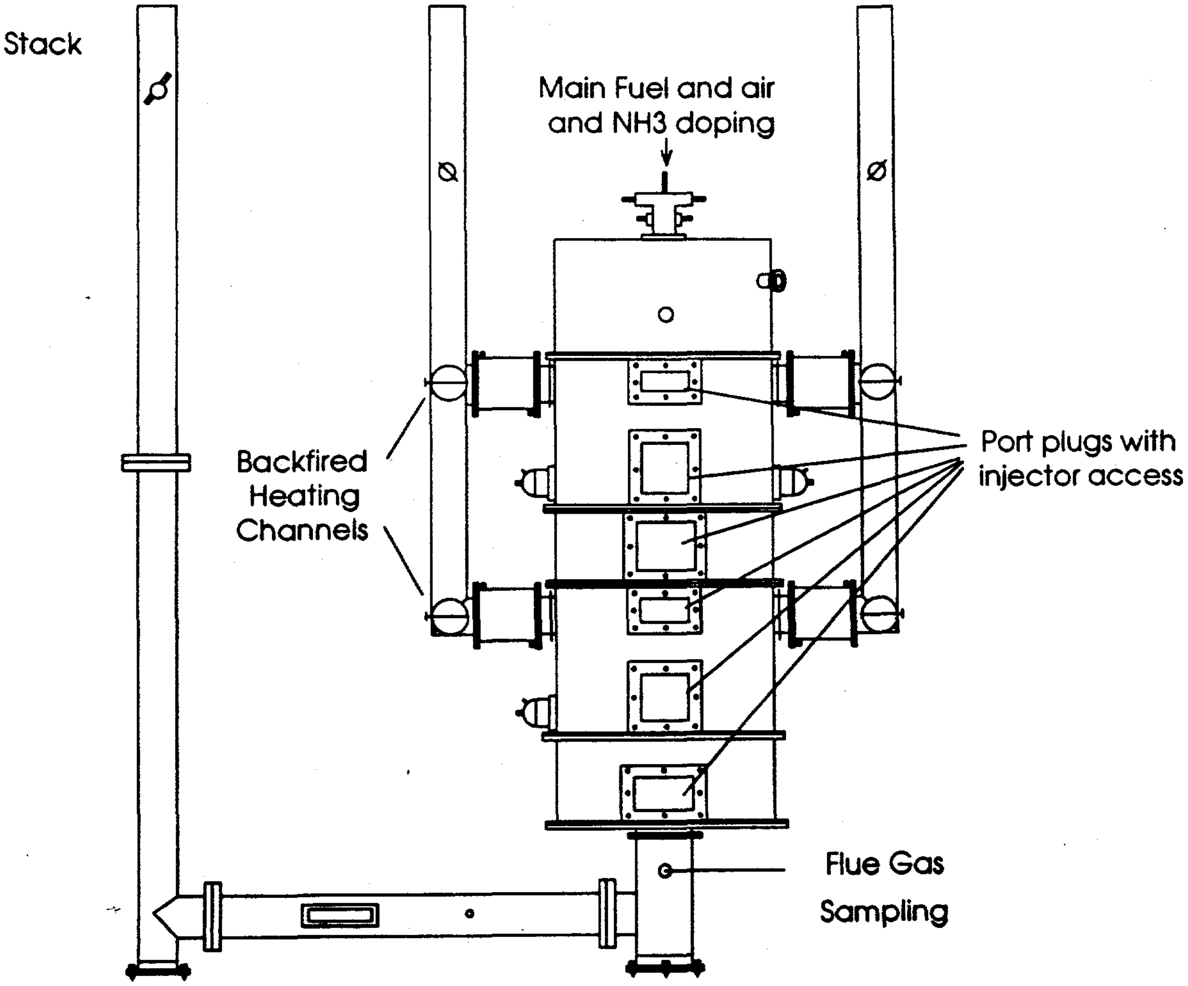

Figure 4-1. Controlled Temperature Tower (CTT) setup.

4.1 Setup of the Bench-Scale Test Facility

The CTT was configured for the test program. The approach for the bench scale studies is to configure the CTT to provide furnace access at the temperatures of interest for advanced reburning. Natural gas will be used as the main and reburn fuels for all tests, with coal studies being conducted later at pilot scale. Injectors were constructed to facilitate injection of reburn fuel, promoted advanced reburning additives, overfire air, and promoted lean side additives. Spray nozzles were ordered from Delavan Corp. and Sonotec Corp. for aqueous additives. For twin fluid nozzles, the test system is able to use either compressed air or bottled dry nitrogen as the atomizing medium. Additive assemblies, consisting of nozzles, injectors, compressed air/nitrogen lines, liquid lines, and liquid pumps, were constructed and tested. All injectors are inserted into the CTT through axial ports along the furnace. Refractory port plugs were made which were designed to sit flush with the furnace wall while providing access holes for the injectors. The inside of the furnace was inspected and any minor cracks were repaired using castable refractory. A system was installed to allow ammonia injection into the main burner, providing control over initial NO_x concentrations. System instrumentation was installed and verified, including thermocouples, pressure gauges, and the flue gas sample system.

Continuous emissions monitors (CEMs) for O_2, CO, CO_2, NO/NO_x, N_2O, and SO_2 were prepared for characterization of the process performance. The CEM system consists of a water cooled sample probes, sample conditioning system (to remove water and particulate), and gas analyzers. Species to be analyzed, detection principles, and detection limits are as follows:

- O_2: paramagnetism, 0.1%
- NO_x: chemiluminescence, 1 ppm
- CO: nondispersive infrared, 1 ppm
- CO_2: nondispersive infrared, 0.1%
- SO_2: nondispersive ultraviolet, 1 ppm
- N_2O: nondispersive infrared, 1 ppm
- NH_3: SCAQMD Method 207 (sampling, Nessler reagent, colorimetry), 1 ppm

- HCN: sampling, ion-specific electrode, 1 ppm

Certified span gases were used to calibrate and check the linearity of the analyzers. A chart recorder was installed to obtain a hard copy of analyzer outputs. A personal computer based data acquisition system (LabTech Notebook) was adjusted for storage and analysis of test data. Furnace temperature profile was measured using a calibrated suction pyrometer. Calibration curves were checked for the natural gas and air rotameters. A firing rate check was performed in which the CTT was fired at full load and proper operation of all facility subsystems and instrumentation was verified.

4.2 Test Matrix

As was mentioned above, the six main components of the system include the reburn fuel, N-agent rich side (in the reburning zone), N-agent lean side (with OFA), promoter rich side, promoter lean side, and OFA. A test matrix was developed to characterize and optimize each of these components individually. Specific test parameters and ranges of variation are as follows:

- Reburn fuel: 10-20% of heat input (reburn zone stoichiometry of 0.99 - 0.90);
- N-agents injection temperatures: 1800-2700° F;
- N-agent type: urea, aqueous ammonia;
- N-agent stoichiometric ratio: 0.5 - 3.0;
- Promoter compound type: Na_2CO_3, $NaHCO_3$, NaOH;
- Promoter amount: 0 - 100 ppm in furnace gas;
- Promoter injection mode: separate injection or premixing with the N-agent (urea/ammonia);
- OFA injection temperature: 1800 - 2400°F;
- Initial NO_x concentration: 200 - 1000 ppm; and
- SO_2 concentration: 0 - 2000 ppm

The maximum achievable NO control will be of primary importance in these experiments.

Figure 4-2 presents the nomenclature to refer to the various regions of the furnace and parameters of these regions. The region upstream of the reburning fuel injection is referred to as the "primary zone". The primary zone stoichiometry is maintained at $SR_1=1.1$ for all tests and the initial NO concentration in this zone is referred to by a single subscript "i". The region between the reburning fuel and overfire air (OFA) injection is referred to as the "reburning zone". The first N-agent (A_1) is introduced with a Nitrogen Stoichiometric molar Ratio $NSR_1=A_1/NO_{ii}$ into the reburn zone, this zone is divided into two fuel rich zones with SR_2. NO concentration upstream of the first N-agent injection is referred to as "ii". NO reduction from NO_i to NO_{ii} is caused by reburning only. The first N-agent is injected with or without promoters (Pr_1) with a t_1 delay time after injection of the reburning fuel. NO concentration downstream of the A_1 injection is called NO_{iii}, and NO reduction from NO_{ii} to NO_{iii} is caused by the first N-agent. Overfire air is injected with a t_2 delay time after injection of the reburning fuel. OFA is a career gas for injecting the second N-agent (A_2) which is injected with or without promoters (Pr_2). A_2 is injected with $NSR_2=A_2/NO_{iii}$. The downstream region is referred to as the "burnout zone". Stoichiometric ratio in this zone is SR_f, and the final NO concentration is NO_f.

5.0 Task 1.5: Mechanism Development and Modeling

In this Task, a high temperature kinetic mechanism should be developed and tested to model the SGAR process. The mechanism should include reactions of C-H-O species, as well as reactions of N-, S-, and Na-containing compounds. During the reporting period, a mechanism for modeling the C-H-O-N system was selected.

5.1 Selection of the C-H-O-N Mechanism

The performed analysis of available kinetic information resulted in preliminary selection of two reaction mechanisms for modeling the chemical behavior in the C-H-O-N system. Both mechanisms are based on the recently issued Version 2.11 of GRI-Mech (Bowman et al., 1995). GRI-Mech-2.11 does not include SNCR reactions, and they had to be added from other sources.

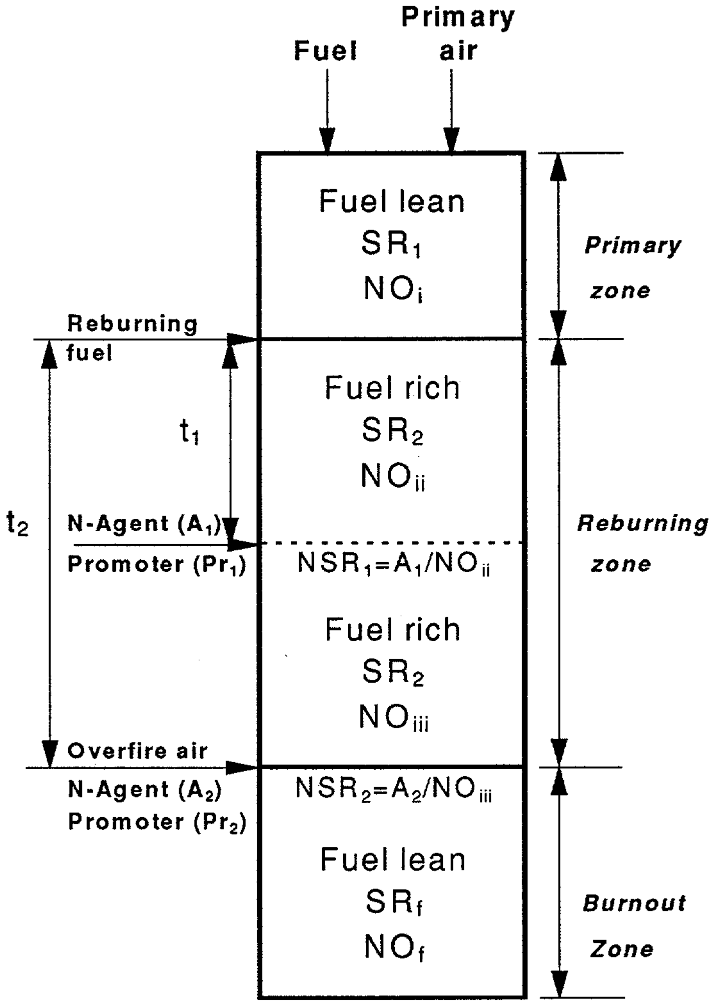

Figure 4.2 SGAR schematic - definitions.

Figure 5-1 presents a general schematic for mechanism development. The total mechanism should include sub-mechanisms of C-H-O, N-, S-, and Na-reactions. The S-reactions will be selected later from the literature. The Na-mechanism should be developed in the scope of this project by a joint effort of EER and the University of Texas (UT). Two variants of the C-H-O-N mechanism were considered: A and B. Mechanism A includes all GRI-Mech-2.11 reactions and reactions selected from the SNCR scheme suggested by Bowman, 1995. Mechanism B consists of GRI-Mech-1.2 (which describes the C-H-O system), N-chemistry reactions proposed by Glarborg et al., 1993, and reactions of CH_i radicals with nitrogenous species ("C-N chemistry" - selected from GRI-Mech-2.11). Both schemes seems to be a state of the art for C-H-O-N chemistry modeling. The mechanisms A and B are presented in Appendixes 1 and 2, respectively.

5.2 Thermal DeNOx Calculations

Two selected mechanisms include the complete GRI-Mech-1.2 scheme which was verified by its authors against multiple C-H-O experimental data from various sources. The N-chemistry from GRI-Mech-2.11 and the Glarborg's N-mechanism were also verified against experimental data on reburning. However, both mechanisms were broaden to include SNCR sub-mechanisms. Therefore the total schemes needed some verification associated with SNCR nitrogen chemistry. Calculations were performed by the use of available experimental data on the Thermal DeNOx process. Two sets of experiments were selected for comparison with modeling:

1. Laboratory-scale data presented by Lyon and Hardy, 1986. Conditions: flow system tests, variation of reactor temperature, residence time 0.1 s. Mixture composition: 225 ppm NO - 450 ppm NH_3 - balance He.

2. EER's recent pilot-scale experimental data. Conditions: BSF natural gas combustion tests, variation of NH_3 injection temperature, quenching rate 167 K/s. Flue gas composition: 200 ppm NO - 300 ppm NH_3 - 3.8% O_2 (dry measure) - 8% CO_2 - 15% H_2O - balance N_2.

The CHEMKIN-II kinetic program developed at the Sandia National Laboratories (Kee et al., 1989) was used for modeling. Figure 5-2 demonstrates comparison of the experimental results and

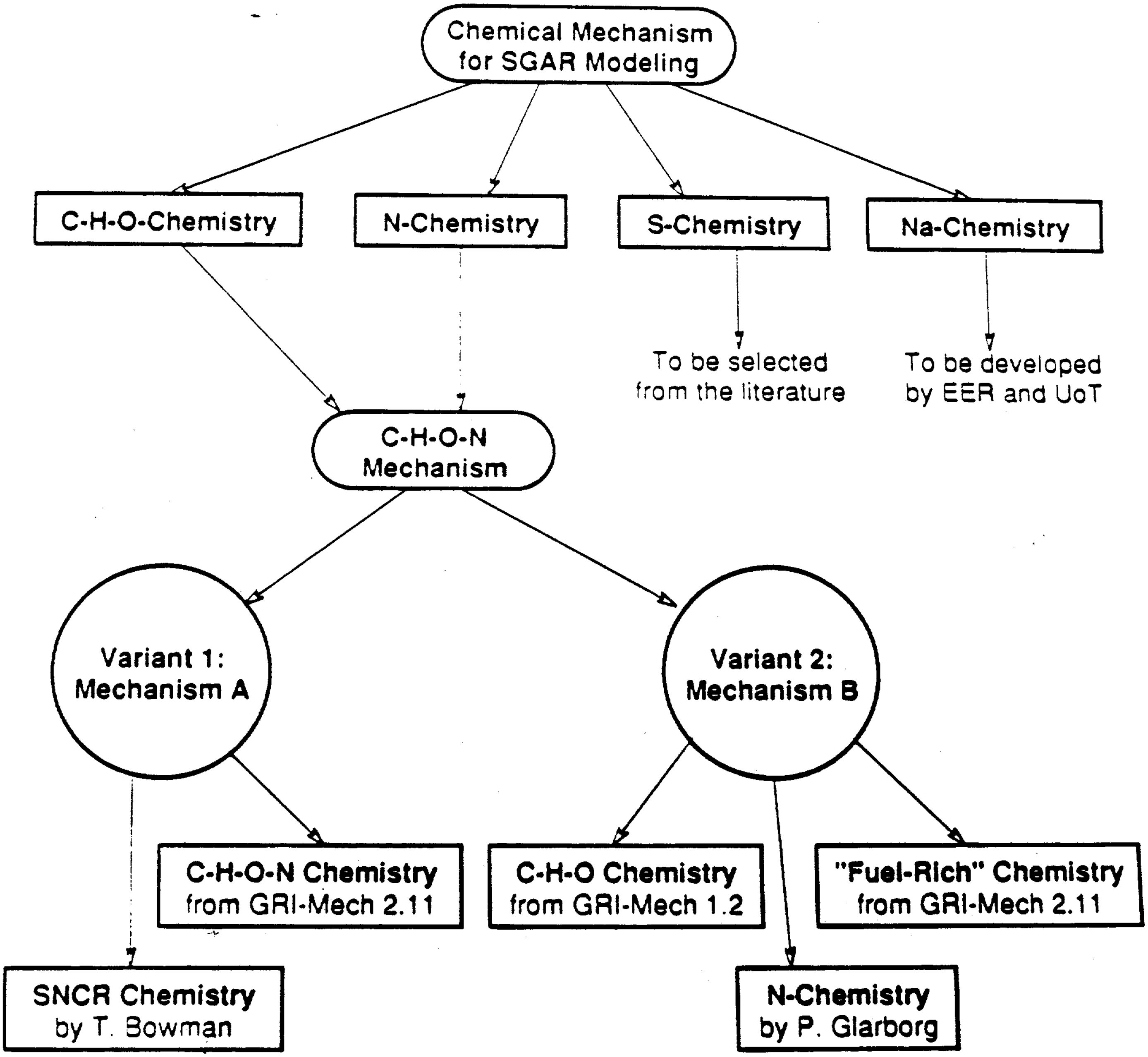

Figure 5-1. Schematic of mechanism development.

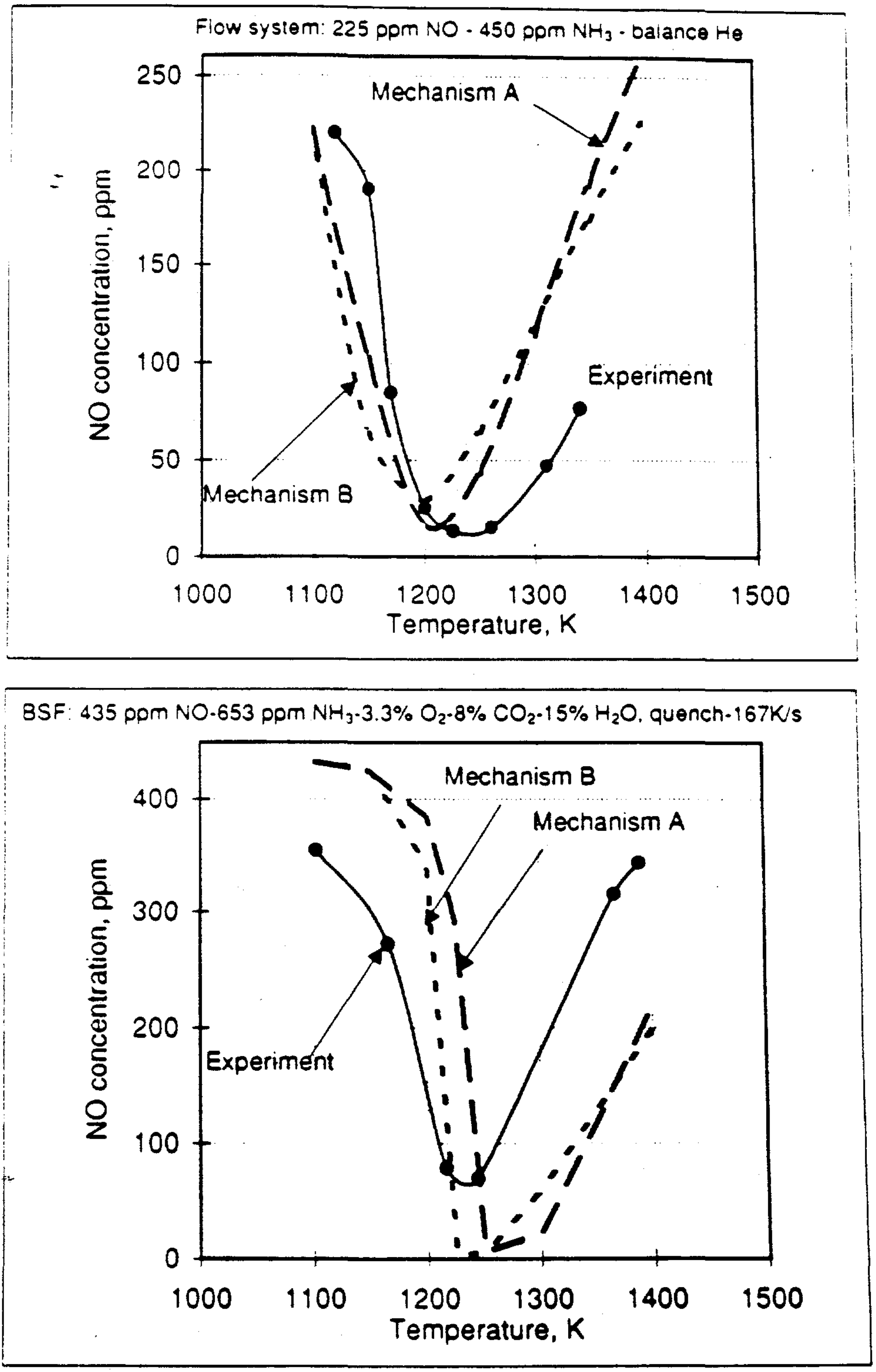

Figure 5-2. Comparison of experimental data and modeling with mechanisms A and B for the Thermal DeNOx process.

modeling by the use of the mechanisms A and B. Although both mechanisms show some difference from the experimental data and there is shift in temperature, they both qualitatively model the temperature window of the Thermal DeNOx process. The differences can be explained by the values of rate constants, by errors in experimental temperature measurements, and by influence of mixing effects on NO removal. Calculations with both mechanisms were performed without any adjustments in rate constants taking into account an actual BSF temperature profile. One can see that both models at least qualitatively described the most substantial feature of the SNCR process: the temperature window of NO reduction. However, differences in quantitative comparison of modeling and future SGAR experiments will be not surprising.

Both mechanisms show about the same performance in modeling experimental data, and therefore, it is difficult to prefer one of them. Mechanism A was selected for further calculations since it includes less constituent parts (sub-mechanisms) and all of them were suggested by the same group of authors.

6.0 Future Plans

Modeling activities will be continued in the next few months with the use of the selected C-H-O-N mechanism. The following issues will be addressed:

- modeling of reburning with various stoichiometric ratios in the reburning zone;
- variation of reburning fuel injection temperature;
- ammonia injection into the reburning zone with different delay times;
- injection of ammonia with OFA;
- preliminary selection of the sodium mechanism;
- direct comparison of experimental observations with model predictions.

Experimental program at the University of Texas will start during the second quarter of the project. Details of this program were discussed at UT during a project initiation meeting attended by V. Zamansky, W. Gardiner and V. Lissianski. The initial work to be done at UT will focus on the following specific tasks:

1. Experimental characterization of the process of injecting droplets of a sodium carbonate solution into high temperature gas streams. This will involve construction and testing of a laboratory-scale apparatus and characterizing the results of the injection process by analytical methods such as gas chromatography and mass spectrometry.

2. Evaluation of the thermochemistry of sodium-carbon-oxygen-hydrogen systems as required for understanding and modeling the physical and chemical processes expected to dominate the dynamics of the NO reduction process enhanced in the presence of sodium. It is anticipated that most of this task comprises literature survey and evaluation, but that molecular electronic structure calculations may be needed for some species.

Once the above tasks are accomplished it will be possible to select specific shock tube, flow tube and spectroscopic experiments described in the Statement of Work. In particular, it will become possible to isolate reaction conditions and diagnostics that will lead most efficiently to kinetic characterization of critical steps of the promoted NO reduction process.

Experimental results with the use of the bench-scale 0.1 MBtu/hr combustion facility will be obtained and reduced during the next quarter.

7.0 References

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Appendix 1. Mechanism A (GRI-Mech/Bowman) in CHEMKIN format

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!This is a combination of GRI-Mech2.11 and additional reactions (selected
!from T. Bowman's SNCR.dat mechanism) which are absent in GRI-Mech 2.11
!Removed "-" in activation energy for the reaction H+NH3 and OH+NH3
! (in GRI-Mech2.1)
! GRI-Mech Version 2.1  released 9/6/95  CHEMKIN-II format
! See README21 file at anonymous FTP site unix.sri.com, directory gri;
! WorldWideWeb home page through http://www.gri.org , under 'Basic
! Research', for additional information, contacts, and disclaimer
ELEMENTS
O  H  C  N  AR
END
SPECIES
H2      H       O       O2      OH      H2O     HO2     H2O2
C       CH      CH2     CH2(S)  CH3     CH4     CO      CO2
HCO     CH2O    CH2OH   CH3O    CH3OH   C2H     C2H2    C2H3
C2H4    C2H5    C2H6    HCCO    CH2CO   HCCOH   N       NH
NH2     NH3     NNH     NO      NO2     N2O     HNO     CN
HCN     H2CN    HCNN    HCNO    HOCN    HNCO    NCO     N2
AR      N2H2
END
!THERMO
! Insert GRI-Mech thermodynamics here or use in default file
!END
REACTIONS
2O+M<=>O2+M                              1.200E+17    -1.000        .00
H2/ 2.40/ H2O/15.40/ CH4/ 2.00/ CO/ 1.75/ CO2/ 3.60/ C2H6/ 3.00/ AR/ .83/
O+H+M<=>OH+M                             5.000E+17    -1.000        .00
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
O+H2<=>H+OH                              5.000E+04     2.670    6290.00
O+HO2<=>OH+O2                            2.000E+13      .000        .00
O+H2O2<=>OH+HO2                          9.630E+06     2.000    4000.00
O+CH<=>H+CO                              5.700E+13      .000        .00
O+CH2<=>H+HCO                            8.000E+13      .000        .00
O+CH2(S)<=>H2+CO                         1.500E+13      .000        .00
O+CH2(S)<=>H+HCO                         1.500E+13      .000        .00
O+CH3<=>H+CH2O                           8.430E+13      .000        .00
O+CH4<=>OH+CH3                           1.020E+09     1.500    8600.00
O+CO+M<=>CO2+M                           6.020E+14      .000    3000.00
H2/2.00/ O2/6.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/3.50/ C2H6/3.00/ AR/ .50/
O+HCO<=>OH+CO                            3.000E+13      .000        .00
O+HCO<=>H+CO2                            3.000E+13      .000        .00
O+CH2O<=>OH+HCO                          3.900E+13      .000    3540.00
O+CH2OH<=>OH+CH2O                        1.000E+13      .000        .00
O+CH3O<=>OH+CH2O                         1.000E+13      .000        .00
O+CH3OH<=>OH+CH2OH                       3.880E+05     2.500    3100.00
O+CH3OH<=>OH+CH3O                        1.300E+05     2.500    5000.00
O+C2H<=>CH+CO                            5.000E+13      .000        .00
O+C2H2<=>H+HCCO                          1.020E+07     2.000    1900.00
O+C2H2<=>OH+C2H                          4.600E+19    -1.410   28950.00
O+C2H2<=>CO+CH2                          1.020E+07     2.000    1900.00
O+C2H3<=>H+CH2CO                         3.000E+13      .000        .00
O+C2H4<=>CH3+HCO                         1.920E+07     1.830     220.00
O+C2H5<=>CH3+CH2O                        1.320E+14      .000        .00
O+C2H6<=>OH+C2H5                         8.980E+07     1.920    5690.00
O+HCCO<=>H+2CO                           1.000E+14      .000        .00
O+CH2CO<=>OH+HCCO                        1.000E+13      .000    8000.00
O+CH2CO<=>CH2+CO2                        1.750E+12      .000    1350.00
O2+CO<=>O+CO2                            2.500E+12      .000   47800.00
O2+CH2O<=>HO2+HCO                        1.000E+14      .000   40000.00
H+O2+M<=>HO2+M                           2.800E+18     -.860        .00
O2/ .00/ H2O/ .00/ CO/ .75/ CO2/1.50/ C2H6/1.50/ N2/ .00/ AR/ .00/
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H+2O2<=>HO2+O2                              3.000E+20   -1.720        .00
H+O2+H2O<=>HO2+H2O                          9.380E+18    -.760        .00
H+O2+N2<=>HO2+N2                            3.750E+20   -1.720        .00
H+O2+AR<=>HO2+AR                            7.000E+17    -.800        .00
H+O2<=>O+OH                                 8.300E+13     .000   14413.00
2H+M<=>H2+M                                 1.000E+18   -1.000        .00
H2/ .00/ H2O/ .00/ CH4/2.00/ CO2/ .00/ C2H6/3.00/ AR/ .63/
2H+H2<=>2H2                                 9.000E+16    -.600        .00
2H+H2O<=>H2+H2O                             6.000E+19   -1.250        .00
2H+CO2<=>H2+CO2                             5.500E+20   -2.000        .00
H+OH+M<=>H2O+M                              2.200E+22   -2.000        .00
H2/ .73/ H2O/3.65/ CH4/2.00/ C2H6/3.00/ AR/ .38/
H+HO2<=>O+H2O                               3.970E+12     .000     671.00
H+HO2<=>O2+H2                               2.800E+13     .000    1068.00
H+HO2<=>2OH                                 1.340E+14     .000     635.00
H+H2O2<=>HO2+H2                             1.210E+07    2.000    5200.00
H+H2O2<=>OH+H2O                             1.000E+13     .000    3600.00
H+CH<=>C+H2                                 1.100E+14     .000        .00
H+CH2(+M)<=>CH3(+M)                         2.500E+16    -.800        .00
     LOW  /  3.200E+27   -3.140   1230.00/
     TROE/    .6800   78.00  1995.00  5590.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
H+CH2(S)<=>CH+H2                            3.000E+13     .000        .00
H+CH3(+M)<=>CH4(+M)                         1.270E+16    -.630     383.00
     LOW  /  2.477E+33   -4.760   2440.00/
     TROE/    .7830   74.00  2941.00  6964.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
H+CH4<=>CH3+H2                              6.600E+08    1.620   10840.00
H+HCO(+M)<=>CH2O(+M)                        1.090E+12     .480    -260.00
     LOW  /  1.350E+24   -2.570   1425.00/
     TROE/    .7824  271.00  2755.00  6570.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
H+HCO<=>H2+CO                               7.340E+13     .000        .00
H+CH2O(+M)<=>CH2OH(+M)                      5.400E+11     .454    3600.00
     LOW  /  1.270E+32   -4.820   6530.00/
     TROE/    .7187  103.00  1291.00  4160.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
H+CH2O(+M)<=>CH3O(+M)                       5.400E+11     .454    2600.00
     LOW  /  2.200E+30   -4.800   5560.00/
     TROE/    .7580   94.00  1555.00  4200.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
H+CH2O<=>HCO+H2                             2.300E+10    1.050    3275.00
H+CH2OH(+M)<=>CH3OH(+M)                     1.800E+13     .000        .00
     LOW  /  3.000E+31   -4.800   3300.00/
     TROE/    .7679  338.00  1812.00  5081.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
H+CH2OH<=>H2+CH2O                           2.000E+13     .000        .00
H+CH2OH<=>OH+CH3                            1.200E+13     .000        .00
H+CH2OH<=>CH2(S)+H2O                        6.000E+12     .000        .00
H+CH3O(+M)<=>CH3OH(+M)                      5.000E+13     .000        .00
     LOW  /  8.600E+28   -4.000   3025.00/
     TROE/    .8902  144.00  2838.00 45569.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
H+CH3O<=>H+CH2OH                            3.400E+06    1.600        .00
H+CH3O<=>H2+CH2O                            2.000E+13     .000        .00
H+CH3O<=>OH+CH3                             3.200E+13     .000        .00
H+CH3O<=>CH2(S)+H2O                         1.600E+13     .000        .00
H+CH3OH<=>CH2OH+H2                          1.700E+07    2.100    4870.00
H+CH3OH<=>CH3O+H2                           4.200E+06    2.100    4870.00
H+C2H(+M)<=>C2H2(+M)                        1.000E+17   -1.000        .00
     LOW  /  3.750E+33   -4.800   1900.00/
     TROE/    .6464  132.00  1315.00  5566.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
H+C2H2(+M)<=>C2H3(+M)                       5.600E+12     .000    2400.00
     LOW  /  3.800E+40   -7.270   7220.00/
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     TROE/   .7507   98.50  1302.00   4167.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
H+C2H3(+M)<=>C2H4(+M)                        6.080E+12     .270     280.00
     LOW  /  1.400E+30   -3.860   3320.00/
     TROE/   .7820  207.50  2663.00   6095.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
H+C2H3<=>H2+C2H2                             3.000E+13     .000        .00
H+C2H4(+M)<=>C2H5(+M)                        1.080E+12     .454    1820.00
     LOW  /  1.200E+42   -7.620   6970.00/
     TROE/   .9753  210.00   984.00   4374.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
H+C2H4<=>C2H3+H2                             1.325E+06    2.530   12240.00
H+C2H5(+M)<=>C2H6(+M)                        5.210E+17    -.990    1580.00
     LOW  /  1.990E+41   -7.080   6685.00/
     TROE/   .8422  125.00  2219.00   6882.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
H+C2H5<=>H2+C2H4                             2.000E+12     .000        .00
H+C2H6<=>C2H5+H2                             1.150E+08    1.900    7530.00
H+HCCO<=>CH2(S)+CO                           1.000E+14     .000        .00
H+CH2CO<=>HCCO+H2                            5.000E+13     .000    8000.00
H+CH2CO<=>CH3+CO                             1.130E+13     .000    3428.00
H+HCCOH<=>H+CH2CO                            1.000E+13     .000        .00
H2+CO(+M)<=>CH2O(+M)                         4.300E+07    1.500   79600.00
     LOW  /  5.070E+27   -3.420  84350.00/
     TROE/   .9320  197.00  1540.00 10300.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
OH+H2<=>H+H2O                                2.160E+08    1.510    3430.00
2OH(+M)<=>H2O2(+M)                           7.400E+13    -.370        .00
     LOW  /  2.300E+18    -.900  -1700.00/
     TROE/   .7346   94.00  1756.00   5182.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
2OH<=>O+H2O                                  3.570E+04    2.400   -2110.00
OH+HO2<=>O2+H2O                              2.900E+13     .000    -500.00
OH+H2O2<=>HO2+H2O                            1.750E+12     .000     320.00
 DUPLICATE
OH+H2O2<=>HO2+H2O                            5.800E+14     .000    9560.00
 DUPLICATE
OH+C<=>H+CO                                  5.000E+13     .000        .00
OH+CH<=>H+HCO                                3.000E+13     .000        .00
OH+CH2<=>H+CH2O                              2.000E+13     .000        .00
OH+CH2<=>CH+H2O                              1.130E+07    2.000    3000.00
OH+CH2(S)<=>H+CH2O                           3.000E+13     .000        .00
OH+CH3(+M)<=>CH3OH(+M)                       6.300E+13     .000        .00
     LOW  /  2.700E+38   -6.300   3100.00/
     TROE/   .2105   83.50  5398.00   8370.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
OH+CH3<=>CH2+H2O                             5.600E+07    1.600    5420.00
OH+CH3<=>CH2(S)+H2O                          2.501E+13     .000        .00
OH+CH4<=>CH3+H2O                             1.000E+08    1.600    3120.00
OH+CO<=>H+CO2                                4.760E+07    1.228      70.00
OH+HCO<=>H2O+CO                              5.000E+13     .000        .00
OH+CH2O<=>HCO+H2O                            3.430E+09    1.180    -447.00
OH+CH2OH<=>H2O+CH2O                          5.000E+12     .000        .00
OH+CH3O<=>H2O+CH2O                           5.000E+12     .000        .00
OH+CH3OH<=>CH2OH+H2O                         1.440E+06    2.000    -840.00
OH+CH3OH<=>CH3O+H2O                          6.300E+06    2.000    1500.00
OH+C2H<=>H+HCCO                              2.000E+13     .000        .00
OH+C2H2<=>H+CH2CO                            2.180E-04    4.500   -1000.00
OH+C2H2<=>H+HCCOH                            5.040E+05    2.300   13500.00
OH+C2H2<=>C2H+H2O                            3.370E+07    2.000   14000.00
OH+C2H2<=>CH3+CO                             4.830E-04    4.000   -2000.00
OH+C2H3<=>H2O+C2H2                           5.000E+12     .000        .00
OH+C2H4<=>C2H3+H2O                           3.600E+06    2.000    2500.00
OH+C2H6<=>C2H5+H2O                           3.540E+06    2.120     870.00
OH+CH2CO<=>HCCO+H2O                          7.500E+12     .000    2000.00
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2HO2<=>O2+H2O2                           1.300E+11     .000    -1630.00
 DUPLICATE
2HO2<=>O2+H2O2                           4.200E+14     .000    12000.00
 DUPLICATE
HO2+CH2<=>OH+CH2O                        2.000E+13     .000         .00
HO2+CH3<=>O2+CH4                         1.000E+12     .000         .00
HO2+CH3<=>OH+CH3O                        2.000E+13     .000         .00
HO2+CO<=>OH+CO2                          1.500E+14     .000    23600.00
HO2+CH2O<=>HCO+H2O2                      1.000E+12     .000     8000.00
C+O2<=>O+CO                              5.800E+13     .000      576.00
C+CH2<=>H+C2H                            5.000E+13     .000         .00
C+CH3<=>H+C2H2                           5.000E+13     .000         .00
CH+O2<=>O+HCO                            3.300E+13     .000         .00
CH+H2<=>H+CH2                            1.107E+08    1.790     1670.00
CH+H2O<=>H+CH2O                          1.713E+13     .000     -755.00
CH+CH2<=>H+C2H2                          4.000E+13     .000         .00
CH+CH3<=>H+C2H3                          3.000E+13     .000         .00
CH+CH4<=>H+C2H4                          6.000E+13     .000         .00
CH+CO(+M)<=>HCCO(+M)                     5.000E+13     .000         .00
     LOW  /  2.690E+28   -3.740   1936.00/
     TROE/   .5757  237.00  1652.00  5069.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
CH+CO2<=>HCO+CO                          3.400E+12     .000      690.00
CH+CH2O<=>H+CH2CO                        9.460E+13     .000     -515.00
CH+HCCO<=>CO+C2H2                        5.000E+13     .000         .00
CH2+O2<=>OH+HCO                          1.320E+13     .000     1500.00
CH2+H2<=>H+CH3                           5.000E+05    2.000     7230.00
2CH2<=>H2+C2H2                           3.200E+13     .000         .00
CH2+CH3<=>H+C2H4                         4.000E+13     .000         .00
CH2+CH4<=>2CH3                           2.460E+06    2.000     8270.00
CH2+CO(+M)<=>CH2CO(+M)                   8.100E+11     .500     4510.00
     LOW  /  2.690E+33   -5.110   7095.00/
     TROE/   .5907  275.00  1226.00  5185.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
CH2+HCCO<=>C2H3+CO                       3.000E+13     .000         .00
CH2(S)+N2<=>CH2+N2                       1.500E+13     .000      600.00
CH2(S)+AR<=>CH2+AR                       9.000E+12     .000      600.00
CH2(S)+O2<=>H+OH+CO                      2.800E+13     .000         .00
CH2(S)+O2<=>CO+H2O                       1.200E+13     .000         .00
CH2(S)+H2<=>CH3+H                        7.000E+13     .000         .00
CH2(S)+H2O(+M)<=>CH3OH(+M)               2.000E+13     .000         .00
     LOW  /  2.700E+38   -6.300   3100.00/
     TROE/   .1507  134.00  2383.00  7265.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH2(S)+H2O<=>CH2+H2O                     3.000E+13     .000         .00
CH2(S)+CH3<=>H+C2H4                      1.200E+13     .000     -570.00
CH2(S)+CH4<=>2CH3                        1.600E+13     .000     -570.00
CH2(S)+CO<=>CH2+CO                       9.000E+12     .000         .00
CH2(S)+CO2<=>CH2+CO2                     7.000E+12     .000         .00
CH2(S)+CO2<=>CO+CH2O                     1.400E+13     .000         .00
CH2(S)+C2H6<=>CH3+C2H5                   4.000E+13     .000     -550.00
CH3+O2<=>O+CH3O                          2.675E+13     .000    28800.00
CH3+O2<=>OH+CH2O                         3.600E+10     .000     8940.00
CH3+H2O2<=>HO2+CH4                       2.450E+04    2.470     5180.00
2CH3(+M)<=>C2H6(+M)                      2.120E+16    -.970      620.00
     LOW  /  1.770E+50   -9.670   6220.00/
     TROE/   .5325  151.00  1038.00  4970.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
2CH3<=>H+C2H5                            4.990E+12     .100    10600.00
CH3+HCO<=>CH4+CO                         2.648E+13     .000         .00
CH3+CH2O<=>HCO+CH4                       3.320E+03    2.810     5860.00
CH3+CH3OH<=>CH2OH+CH4                    3.000E+07    1.500     9940.00
CH3+CH3OH<=>CH3O+CH4                     1.000E+07    1.500     9940.00
CH3+C2H4<=>C2H3+CH4                      2.270E+05    2.000     9200.00
CH3+C2H6<=>C2H5+CH4                      6.140E+06    1.740    10450.00
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HCO+H2O<=>H+CO+H2O                       2.244E+18   -1.000   17000.00
 DUPLICATE
HCO+M<=>H+CO+M                           1.870E+17   -1.000   17000.00
H2/2.00/ H2O/ .00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
 DUPLICATE
HCO+O2<=>HO2+CO                          7.600E+12     .000     400.00
CH2OH+O2<=>HO2+CH2O                      1.800E+13     .000     900.00
CH3O+O2<=>HO2+CH2O                       4.280E-13    7.600   -3530.00
C2H+O2<=>HCO+CO                          5.000E+13     .000    1500.00
C2H+H2<=>H+C2H2                          4.070E+05    2.400     200.00
C2H3+O2<=>HCO+CH2O                       3.980E+12     .000    -240.00
C2H4(+M)<=>H2+C2H2(+M)                   8.000E+12     .440   88770.00
     LOW  /  7.000E+50   -9.310   99860.00/
     TROE/   .7345  180.00  1035.00  5417.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
C2H5+O2<=>HO2+C2H4                       8.400E+11     .000    3875.00
HCCO+O2<=>OH+2CO                         1.600E+12     .000     854.00
2HCCO<=>2CO+C2H2                         1.000E+13     .000        .00
N+NO<=>N2+O                              3.500E+13     .000     330.00
N+O2<=>NO+O                              2.650E+12     .000    6400.00
N+OH<=>NO+H                              7.333E+13     .000    1120.00
N2O+O<=>N2+O2                            1.400E+12     .000   10810.00
N2O+O<=>2NO                              2.900E+13     .000   23150.00
N2O+H<=>N2+OH                            4.400E+14     .000   18880.00
N2O+OH<=>N2+HO2                          2.000E+12     .000   21060.00
N2O(+M)<=>N2+O(+M)                       1.300E+11     .000   59620.00
     LOW  /  6.200E+14     .000  56100.00/
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
HO2+NO<=>NO2+OH                          2.110E+12     .000    -480.00
NO+O+M<=>NO2+M                           1.060E+20   -1.410        .00
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
NO2+O<=>NO+O2                            3.900E+12     .000    -240.00
NO2+H<=>NO+OH                            1.320E+14     .000     360.00
NH+O<=>NO+H                              5.000E+13     .000        .00
NH+H<=>N+H2                              3.200E+13     .000     330.00
NH+OH<=>HNO+H                            2.000E+13     .000        .00
NH+OH<=>N+H2O                            2.000E+09    1.200        .00
NH+O2<=>HNO+O                            4.610E+05    2.000    6500.00
NH+O2<=>NO+OH                            1.280E+06    1.500     100.00
NH+N<=>N2+H                              1.500E+13     .000        .00
NH+H2O<=>HNO+H2                          2.000E+13     .000   13850.00
NH+NO<=>N2+OH                            2.160E+13    -.230        .00
NH+NO<=>N2O+H                            4.160E+14    -.450        .00
NH2+O<=>OH+NH                            7.000E+12     .000        .00
NH2+O<=>H+HNO                            4.600E+13     .000        .00
NH2+H<=>NH+H2                            4.000E+13     .000    3650.00
NH2+OH<=>NH+H2O                          9.000E+07    1.500    -460.00
NNH<=>N2+H                               3.300E+08     .000        .00
 DUPLICATE
NNH+M<=>N2+H+M                           1.300E+14    -.110    4980.00
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
 DUPLICATE
NNH+O2<=>HO2+N2                          5.000E+12     .000        .00
NNH+O<=>OH+N2                            2.500E+13     .000        .00
NNH+O<=>NH+NO                            7.000E+13     .000        .00
NNH+H<=>H2+N2                            5.000E+13     .000        .00
NNH+OH<=>H2O+N2                          2.000E+13     .000        .00
NNH+CH3<=>CH4+N2                         2.500E+13     .000        .00
H+NO+M<=>HNO+M                           8.950E+19   -1.320     740.00
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
HNO+O<=>NO+OH                            2.500E+13     .000        .00
HNO+H<=>H2+NO                            4.500E+11     .720     660.00
HNO+OH<=>NO+H2O                          1.300E+07    1.900    -950.00
HNO+O2<=>HO2+NO                          1.000E+13     .000   13000.00
CN+O<=>CO+N                              7.700E+13     .000        .00
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CN+OH<=>NCO+H                            4.000E+13     .000        .00
CN+H2O<=>HCN+OH                          8.000E+12     .000    7460.00
CN+O2<=>NCO+O                            6.140E+12     .000    -440.00
CN+H2<=>HCN+H                            2.100E+13     .000    4710.00
NCO+O<=>NO+CO                            2.350E+13     .000        .00
NCO+H<=>NH+CO                            5.400E+13     .000        .00
NCO+OH<=>NO+H+CO                         2.500E+12     .000        .00
NCO+N<=>N2+CO                            2.000E+13     .000        .00
NCO+O2<=>NO+CO2                          2.000E+12     .000   20000.00
NCO+M<=>N+CO+M                           8.800E+16    -.500   48000.00
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
NCO+NO<=>N2O+CO                          2.850E+17   -1.520     740.00
NCO+NO<=>N2+CO2                          5.700E+18   -2.000     800.00
HCN+M<=>H+CN+M                           1.040E+29   -3.300  126600.00
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
HCN+O<=>NCO+H                            1.107E+04    2.640    4980.00
HCN+O<=>NH+CO                            2.767E+03    2.640    4980.00
HCN+O<=>CN+OH                            2.134E+09    1.580   26600.00
HCN+OH<=>HOCN+H                          1.100E+06    2.030   13370.00
HCN+OH<=>HNCO+H                          4.400E+03    2.260    6400.00
HCN+OH<=>NH2+CO                          1.600E+02    2.560    9000.00
H+HCN+M<=>H2CN+M                         1.400E+26   -3.400    1900.00
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
H2CN+N<=>N2+CH2                          6.000E+13     .000     400.00
C+N2<=>CN+N                              6.300E+13     .000   46020.00
CH+N2<=>HCN+N                            2.857E+08    1.100   20400.00
CH+N2(+M)<=>HCNN(+M)                     3.100E+12     .150        .00
     LOW  /  1.300E+25   -3.160    740.00/
     TROE/   .6670  235.00  2117.00  4536.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
CH2+N2<=>HCN+NH                          1.000E+13     .000   74000.00
CH2(S)+N2<=>NH+HCN                       1.000E+11     .000   65000.00
C+NO<=>CN+O                              1.900E+13     .000        .00
C+NO<=>CO+N                              2.900E+13     .000        .00
CH+NO<=>HCN+O                            5.000E+13     .000        .00
CH+NO<=>H+NCO                            2.000E+13     .000        .00
CH+NO<=>N+HCO                            3.000E+13     .000        .00
CH2+NO<=>H+HNCO                          3.100E+17   -1.380    1270.00
CH2+NO<=>OH+HCN                          2.900E+14    -.690     760.00
CH2+NO<=>H+HCNO                          3.800E+13    -.360     580.00
CH2(S)+NO<=>H+HNCO                       3.100E+17   -1.380    1270.00
CH2(S)+NO<=>OH+HCN                       2.900E+14    -.690     760.00
CH2(S)+NO<=>H+HCNO                       3.800E+13    -.360     580.00
CH3+NO<=>HCN+H2O                         9.600E+13     .000   28800.00
CH3+NO<=>H2CN+OH                         1.000E+12     .000   21750.00
HCNN+O<=>CO+H+N2                         2.200E+13     .000        .00
HCNN+O<=>HCN+NO                          2.000E+12     .000        .00
HCNN+O2<=>O+HCO+N2                       1.200E+13     .000        .00
HCNN+OH<=>H+HCO+N2                       1.200E+13     .000        .00
HCNN+H<=>CH2+N2                          1.000E+14     .000        .00
HNCO+O<=>NH+CO2                          9.800E+07    1.410    8500.00
HNCO+O<=>HNO+CO                          1.500E+08    1.570   44000.00
HNCO+O<=>NCO+OH                          2.200E+06    2.110   11400.00
HNCO+H<=>NH2+CO                          2.250E+07    1.700    3800.00
HNCO+H<=>H2+NCO                          1.050E+05    2.500   13300.00
HNCO+OH<=>NCO+H2O                        4.650E+12     .000    6850.00
HNCO+OH<=>NH2+CO2                        1.550E+12     .000    6850.00
HNCO+M<=>NH+CO+M                         1.180E+16     .000   84720.00
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
HCNO+H<=>H+HNCO                          2.100E+15    -.690    2850.00
HCNO+H<=>OH+HCN                          2.700E+11     .180    2120.00
HCNO+H<=>NH2+CO                          1.700E+14    -.750    2890.00
HOCN+H<=>H+HNCO                          2.000E+07    2.000    2000.00
HCCO+NO<=>HCNO+CO                        2.350E+13     .000        .00
CH3+N<=>H2CN+H                           6.100E+14    -.310     290.00
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CH3+N<=>HCN+H2                           3.700E+12     .150     -90.00
NH3+H<=>NH2+H2                           5.400E+05    2.400    9915.00!rem "-"
NH3+OH<=>NH2+H2O                         5.000E+07    1.600     955.00!rem "-"
NH3+O<=>NH2+OH                           9.400E+06    1.940    6460.00
!END of GRI-Mech 2.11
!Reactions selected 11/2/95 from SNCR.dat (T. Bowman's mechanism for
!SNCR, 10/31/95) which are absent in GRI-Mech 2.11
NH2+O=NO+H2                          0.5E13     0.0         0.
NH2+NO=NNH+OH                        0.28E14   -0.55        0.
NH2+NO=N2+H2O                        0.13E17   -1.25        0.
DUPLICATE
NH2+NO=N2+H2O                        -0.28E14  -0.55        0.
DUPLICATE
NNH+NO=N2+HNO                        0.50E14    0.0         0.
NNH+NH2=N2+NH3                       0.50E14    0.0         0.
NNH+NH=N2+NH2                        0.50E14    0.0         0.
NNH+O=N2O+H                          0.10E15    0.0         0.
HNO+NH2=NH3+NO                       0.20E14    0.0      1000.
HNO+HNO=N2O+H2O                      0.395E13   0.0      5000.
HNO+NO=N2O+OH                        0.20E13    0.0     26000.
NH2+NH=N2H2+H                        0.15E16   -0.5         0.
NH+NH=N2+H+H                         0.25E14    0.0         0.
NH2+N=N2+H+H                         0.72E14    0.0         0.
N2H2+M=NNH+H+M                       0.50E17    0.0     50000.
  H2O/15/ O2/2/ N2/2/ H2/2/
N2H2+H=NNH+H2                        0.50E14    0.0      1000.
N2H2+O=NH2+NO                        0.10E14    0.0         0.
N2H2+O=NNH+OH                        0.20E14    0.0      1000.
N2H2+OH=NNH+H2O                      0.10E14    0.0      1000.
N2H2+NO=N2O+NH2                      0.30E13    0.0         0.
N2H2+NH=NNH+NH2                      0.10E14    0.0      1000.
N2H2+NH2=NH3+NNH                     0.10E14    0.0      1000.
NH2+NH2=N2H2+H2                      0.50E12    0.0         0.
NH2+O2=HNO+OH                        0.45E13    0.0     25000.
NCO+NO2=N2O+CO2                      0.58E15   -0.7         0.
NH+HNCO=NH2+NCO                      0.30E14    0.0     23700.
NH2+HNCO=NH3+NCO                     0.10E13    0.0      6955.
HO2+HNCO=NCO+H2O2                    0.3E12     0.0     29000.
NH3+HO2=NH2+H2O2                     0.3E12     0.0     22000.
NH2+NO2=N2O+H2O                      0.284E19  -2.2         0.
NH+NO2=N2O+OH                        0.1E14     0.0         0.
NH2+NH2=NH+NH3                       0.5E14     0.0     10000.
NH2+HO2=NH3+O2                       0.43E14    0.0         0.
END
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Appendix 2. Mechanism B (GRI-Mech/Glarborg)

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!This is a combination of the C-O-H and fuel-rich chemistry parts of the
      !GRI-Mech 2.11 with the
!Glarborg HCN mechanism.  AR, NCN, H2CN and HONO species are removed (for
!reburning)
! See README file at anonymous FTP site GRI_MECH at CRVAX.SRI.COM
!   for additional information, contacts, and disclaimer
ELEMENTS
O  H  C  N  S
END
SPECIES
H2      H       O       O2      OH      H2O     HO2     H2O2
C       CH      CH2     CH2(S)    CH3     CH4     CO      CO2
HCO     CH2O    CH2OH   CH3O    CH3OH   C2H     C2H2    C2H3
C2H4    C2H5    C2H6    HCCO    CH2CO   HCCOH   N2      HCN
HNCO    NO      N2O     CN      C2N2    HOCN    N    NH
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```
NH2     NH3     NO2     HNO     H2NO    N2H2    NNH     NCO
HCNO  HCNN
END
!THERMO
! Insert GRI-Mech thermodynamics here or use in default file
!END
REACTIONS
! Units are cm3, mole, cal; k = A T**n exp(-E/RT)
2O+M<=>O2+M                              1.200E+17   -1.000        .00
H2/ 2.40/ H2O/15.40/ CH4/ 2.00/ CO/ 1.75/ CO2/ 3.60/ C2H6/ 3.00/
O+H+M<=>OH+M                             5.000E+17   -1.000        .00
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
O+H2<=>H+OH                              5.000E+04    2.670    6290.00
O+HO2<=>OH+O2                            2.000E+13     .000        .00
O+H2O2<=>OH+HO2                          9.630E+06    2.000    4000.00
O+CH<=>H+CO                              5.700E+13     .000        .00
O+CH2<=>H+HCO                            8.000E+13     .000        .00
O+CH2(S)<=>H2+CO                         1.500E+13     .000        .00
O+CH2(S)<=>H+HCO                         1.500E+13     .000        .00
O+CH3<=>H+CH2O                           8.430E+13     .000        .00
O+CH4<=>OH+CH3                           1.020E+09    1.500    8600.00
O+CO+M<=>CO2+M                           6.020E+14     .000    3000.00
H2/2.00/ O2/6.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/3.50/ C2H6/3.00/
O+HCO<=>OH+CO                            3.000E+13     .000        .00
O+HCO<=>H+CO2                            3.000E+13     .000        .00
O+CH2O<=>OH+HCO                          3.900E+13     .000    3540.00
O+CH2OH<=>OH+CH2O                        1.000E+13     .000        .00
O+CH3O<=>OH+CH2O                         1.000E+13     .000        .00
O+CH3OH<=>OH+CH2OH                       3.880E+05    2.500    3100.00
O+CH3OH<=>OH+CH3O                        1.300E+05    2.500    5000.00
O+C2H<=>CH+CO                            5.000E+13     .000        .00
O+C2H2<=>H+HCCO                          1.020E+07    2.000    1900.00
O+C2H2<=>OH+C2H                          4.600E+19   -1.410   28950.00
O+C2H2<=>CO+CH2                          1.020E+07    2.000    1900.00
O+C2H3<=>H+CH2CO                         3.000E+13     .000        .00
O+C2H4<=>CH3+HCO                         1.920E+07    1.830     220.00
O+C2H5<=>CH3+CH2O                        1.320E+14     .000        .00
O+C2H6<=>OH+C2H5                         8.980E+07    1.920    5690.00
O+HCCO<=>H+2CO                           1.000E+14     .000        .00
O+CH2CO<=>OH+HCCO                        1.000E+13     .000    8000.00
O+CH2CO<=>CH2+CO2                        1.750E+12     .000    1350.00
O2+CO<=>O+CO2                            2.500E+12     .000   47800.00
O2+CH2O<=>HO2+HCO                        1.000E+14     .000   40000.00
H+O2+M<=>HO2+M                           2.800E+18    -.860        .00
O2/ .00/ H2O/ .00/ CO/ .75/ CO2/1.50/ C2H6/1.50/ N2/ .00/
H+2O2<=>HO2+O2                           3.000E+20   -1.720        .00
H+O2+H2O<=>HO2+H2O                       9.380E+18    -.760        .00
H+O2+N2<=>HO2+N2                         3.750E+20   -1.720        .00
H+O2<=>O+OH                              8.300E+13     .000   14413.00
2H+M<=>H2+M                              1.000E+18   -1.000        .00
H2/ .00/ H2O/ .00/ CH4/2.00/ CO2/ .00/ C2H6/3.00/
2H+H2<=>2H2                              9.000E+16    -.600        .00
2H+H2O<=>H2+H2O                          6.000E+19   -1.250        .00
2H+CO2<=>H2+CO2                          5.500E+20   -2.000        .00
H+OH+M<=>H2O+M                           2.200E+22   -2.000        .00
H2/ .73/ H2O/3.65/ CH4/2.00/ C2H6/3.00/
H+HO2<=>O+H2O                            3.970E+12     .000     671.00
H+HO2<=>O2+H2                            2.800E+13     .000    1068.00
H+HO2<=>2OH                              1.340E+14     .000     635.00
H+H2O2<=>HO2+H2                          1.210E+07    2.000    5200.00
H+H2O2<=>OH+H2O                          1.000E+13     .000    3600.00
H+CH<=>C+H2                              1.100E+14     .000        .00
H+CH2(+M)<=>CH3(+M)                      2.500E+16    -.800        .00
     LOW  /  3.200E+27   -3.140   1230.00/
     TROE/   .6800   78.00  1995.00  5590.00 /
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H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
H+CH2(S)<=>CH+H2                         3.000E+13     .000        .00
H+CH3(+M)<=>CH4(+M)                      1.270E+16    -.630     383.00
     LOW  /  2.477E+33   -4.760   2440.00/
     TROE/   .7830   74.00  2941.00  6964.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
H+CH4<=>CH3+H2                           6.600E+08    1.620   10840.00
H+HCO(+M)<=>CH2O(+M)                     1.090E+12     .480    -260.00
     LOW  /  1.350E+24   -2.570   1425.00/
     TROE/   .7824  271.00  2755.00  6570.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
H+HCO<=>H2+CO                            7.340E+13     .000        .00
H+CH2O(+M)<=>CH2OH(+M)                   5.400E+11     .454    3600.00
     LOW  /  1.270E+32   -4.820   6530.00/
     TROE/   .7187  103.00  1291.00  4160.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
H+CH2O(+M)<=>CH3O(+M)                    5.400E+11     .454    2600.00
     LOW  /  2.200E+30   -4.800   5560.00/
     TROE/   .7580   94.00  1555.00  4200.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
H+CH2O<=>HCO+H2                          2.300E+10    1.050    3275.00
H+CH2OH(+M)<=>CH3OH(+M)                  1.800E+13     .000        .00
     LOW  /  3.000E+31   -4.800   3300.00/
     TROE/   .7679  338.00  1812.00  5081.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
H+CH2OH<=>H2+CH2O                        2.000E+13     .000        .00
H+CH2OH<=>OH+CH3                         1.200E+13     .000        .00
H+CH2OH<=>CH2(S)+H2O                     6.000E+12     .000        .00
H+CH3O(+M)<=>CH3OH(+M)                   5.000E+13     .000        .00
     LOW  /  8.600E+28   -4.000   3025.00/
     TROE/   .8902  144.00  2838.00 45569.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
H+CH3O<=>H+CH2OH                         3.400E+06    1.600        .00
H+CH3O<=>H2+CH2O                         2.000E+13     .000        .00
H+CH3O<=>OH+CH3                          3.200E+13     .000        .00
H+CH3O<=>CH2(S)+H2O                      1.600E+13     .000        .00
H+CH3OH<=>CH2OH+H2                       1.700E+07    2.100    4870.00
H+CH3OH<=>CH3O+H2                        4.200E+06    2.100    4870.00
H+C2H(+M)<=>C2H2(+M)                     1.000E+17   -1.000        .00
     LOW  /  3.750E+33   -4.800   1900.00/
     TROE/   .6464  132.00  1315.00  5566.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
H+C2H2(+M)<=>C2H3(+M)                    5.600E+12     .000    2400.00
     LOW  /  3.800E+40   -7.270   7220.00/
     TROE/   .7507   98.50  1302.00  4167.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
H+C2H3(+M)<=>C2H4(+M)                    6.080E+12     .270     280.00
     LOW  /  1.400E+30   -3.860   3320.00/
     TROE/   .7820  207.50  2663.00  6095.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
H+C2H3<=>H2+C2H2                         3.000E+13     .000        .00
H+C2H4(+M)<=>C2H5(+M)                    1.080E+12     .454    1820.00
     LOW  /  1.200E+42   -7.620   6970.00/
     TROE/   .9753  210.00   984.00  4374.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
H+C2H4<=>C2H3+H2                         1.325E+06    2.530   12240.00
H+C2H5(+M)<=>C2H6(+M)                    5.210E+17    -.990    1580.00
     LOW  /  1.990E+41   -7.080   6685.00/
     TROE/   .8422  125.00  2219.00  6882.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
H+C2H5<=>H2+C2H4                         2.000E+12     .000        .00
H+C2H6<=>C2H5+H2                         1.150E+08    1.900    7530.00
H+HCCO<=>CH2(S)+CO                       1.000E+14     .000        .00
H+CH2CO<=>HCCO+H2                        5.000E+13     .000    8000.00
H+CH2CO<=>CH3+CO                         1.130E+13     .000    3428.00
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H+HCCOH<=>H+CH2CO                        1.000E+13     .000        .00
H2+CO(+M)<=>CH2O(+M)                     4.300E+07    1.500   79600.00
     LOW  /  5.070E+27   -3.420  84350.00/
     TROE/   .9320  197.00  1540.00 10300.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
OH+H2<=>H+H2O                            2.160E+08    1.510    3430.00
2OH(+M)<=>H2O2(+M)                       7.400E+13    -.370        .00
     LOW  /  2.300E+18    -.900  -1700.00/
     TROE/   .7346   94.00  1756.00  5182.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
2OH<=>O+H2O                              3.570E+04    2.400   -2110.00
OH+HO2<=>O2+H2O                          2.900E+13     .000    -500.00
OH+H2O2<=>HO2+H2O                        1.750E+12     .000     320.00
 DUPLICATE
OH+H2O2<=>HO2+H2O                        5.800E+14     .000    9560.00
 DUPLICATE
OH+C<=>H+CO                              5.000E+13     .000        .00
OH+CH<=>H+HCO                            3.000E+13     .000        .00
OH+CH2<=>H+CH2O                          2.000E+13     .000        .00
OH+CH2<=>CH+H2O                          1.130E+07    2.000    3000.00
OH+CH2(S)<=>H+CH2O                       3.000E+13     .000        .00
OH+CH3(+M)<=>CH3OH(+M)                   6.300E+13     .000        .00
     LOW  /  2.700E+38   -6.300   3100.00/
     TROE/   .2105   83.50  5398.00  8370.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
OH+CH3<=>CH2+H2O                         5.600E+07    1.600    5420.00
OH+CH3<=>CH2(S)+H2O                      2.501E+13     .000        .00
OH+CH4<=>CH3+H2O                         1.000E+08    1.600    3120.00
OH+CO<=>H+CO2                            4.760E+07    1.228      70.00
OH+HCO<=>H2O+CO                          5.000E+13     .000        .00
OH+CH2O<=>HCO+H2O                        3.430E+09    1.180    -447.00
OH+CH2OH<=>H2O+CH2O                      5.000E+12     .000        .00
OH+CH3O<=>H2O+CH2O                       5.000E+12     .000        .00
OH+CH3OH<=>CH2OH+H2O                     1.440E+06    2.000    -840.00
OH+CH3OH<=>CH3O+H2O                      6.300E+06    2.000    1500.00
OH+C2H<=>H+HCCO                          2.000E+13     .000        .00
OH+C2H2<=>H+CH2CO                        2.180E-04    4.500   -1000.00
OH+C2H2<=>H+HCCOH                        5.040E+05    2.300   13500.00
OH+C2H2<=>C2H+H2O                        3.370E+07    2.000   14000.00
OH+C2H2<=>CH3+CO                         4.830E-04    4.000   -2000.00
OH+C2H3<=>H2O+C2H2                       5.000E+12     .000        .00
OH+C2H4<=>C2H3+H2O                       3.600E+06    2.000    2500.00
OH+C2H6<=>C2H5+H2O                       3.540E+06    2.120     870.00
OH+CH2CO<=>HCCO+H2O                      7.500E+12     .000    2000.00
2HO2<=>O2+H2O2                           1.300E+11     .000   -1630.00
 DUPLICATE
2HO2<=>O2+H2O2                           4.200E+14     .000   12000.00
 DUPLICATE
HO2+CH2<=>OH+CH2O                        2.000E+13     .000        .00
HO2+CH3<=>O2+CH4                         1.000E+12     .000        .00
HO2+CH3<=>OH+CH3O                        2.000E+13     .000        .00
HO2+CO<=>OH+CO2                          1.500E+14     .000   23600.00
HO2+CH2O<=>HCO+H2O2                      1.000E+12     .000    8000.00
C+O2<=>O+CO                              5.800E+13     .000     576.00
C+CH2<=>H+C2H                            5.000E+13     .000        .00
C+CH3<=>H+C2H2                           5.000E+13     .000        .00
CH+O2<=>O+HCO                            3.300E+13     .000        .00
CH+H2<=>H+CH2                            1.107E+08    1.790    1670.00
CH+H2O<=>H+CH2O                          1.713E+13     .000    -755.00
CH+CH2<=>H+C2H2                          4.000E+13     .000        .00
CH+CH3<=>H+C2H3                          3.000E+13     .000        .00
CH+CH4<=>H+C2H4                          6.000E+13     .000        .00
CH+CO(+M)<=>HCCO(+M)                     5.000E+13     .000        .00
     LOW  /  2.690E+28   -3.740   1936.00/
     TROE/   .5757  237.00  1652.00  5069.00 /
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H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH+CO2<=>HCO+CO                            3.400E+12       .000      690.00
CH+CH2O<=>H+CH2CO                          9.460E+13       .000     -515.00
CH+HCCO<=>CO+C2H2                          5.000E+13       .000         .00
CH2+O2<=>OH+HCO                            1.320E+13       .000     1500.00
CH2+H2<=>H+CH3                             5.000E+05      2.000     7230.00
2CH2<=>H2+C2H2                             3.200E+13       .000         .00
CH2+CH3<=>H+C2H4                           4.000E+13       .000         .00
CH2+CH4<=>2CH3                             2.460E+06      2.000     8270.00
CH2+CO(+M)<=>CH2CO(+M)                     8.100E+11       .500     4510.00
     LOW   /  2.690E+33   -5.110    7095.00/
     TROE/    .5907  275.00   1226.00  5185.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH2+HCCO<=>C2H3+CO                         3.000E+13       .000         .00
CH2(S)+N2<=>CH2+N2                         1.500E+13       .000      600.00
CH2(S)+O2<=>H+OH+CO                        2.800E+13       .000         .00
CH2(S)+O2<=>CO+H2O                         1.200E+13       .000         .00
CH2(S)+H2<=>CH3+H                          7.000E+13       .000         .00
CH2(S)+H2O(+M)<=>CH3OH(+M)                 2.000E+13       .000         .00
     LOW   /  2.700E+38   -6.300    3100.00/
     TROE/    .1507  134.00   2383.00  7265.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH2(S)+H2O<=>CH2+H2O                       3.000E+13       .000         .00
CH2(S)+CH3<=>H+C2H4                        1.200E+13       .000     -570.00
CH2(S)+CH4<=>2CH3                          1.600E+13       .000     -570.00
CH2(S)+CO<=>CH2+CO                         9.000E+12       .000         .00
CH2(S)+CO2<=>CH2+CO2                       7.000E+12       .000         .00
CH2(S)+CO2<=>CO+CH2O                       1.400E+13       .000         .00
CH2(S)+C2H6<=>CH3+C2H5                     4.000E+13       .000     -550.00
CH3+O2<=>O+CH3O                            2.675E+13       .000    28800.00
CH3+O2<=>OH+CH2O                           3.600E+10       .000     8940.00
CH3+H2O2<=>HO2+CH4                         2.450E+04      2.470     5180.00
2CH3(+M)<=>C2H6(+M)                        2.120E+16      -.970      620.00
     LOW   /  1.770E+50   -9.670    6220.00/
     TROE/    .5325  151.00   1038.00  4970.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
2CH3<=>H+C2H5                              4.990E+12       .100    10600.00
CH3+HCO<=>CH4+CO                           2.648E+13       .000         .00
CH3+CH2O<=>HCO+CH4                         3.320E+03      2.810     5860.00
CH3+CH3OH<=>CH2OH+CH4                      3.000E+07      1.500     9940.00
CH3+CH3OH<=>CH3O+CH4                       1.000E+07      1.500     9940.00
CH3+C2H4<=>C2H3+CH4                        2.270E+05      2.000     9200.00
CH3+C2H6<=>C2H5+CH4                        6.140E+06      1.740    10450.00
HCO+H2O<=>H+CO+H2O                         2.244E+18     -1.000    17000.00
 DUPLICATE
HCO+M<=>H+CO+M                             1.870E+17     -1.000    17000.00
H2/2.00/ H2O/ .00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
 DUPLICATE
HCO+O2<=>HO2+CO                            7.600E+12       .000      400.00
CH2OH+O2<=>HO2+CH2O                        1.800E+13       .000      900.00
CH3O+O2<=>HO2+CH2O                         4.280E-13      7.600    -3530.00
C2H+O2<=>HCO+CO                            5.000E+13       .000     1500.00
C2H+H2<=>H+C2H2                            4.070E+05      2.400      200.00
C2H3+O2<=>HCO+CH2O                         3.980E+12       .000     -240.00
C2H4(+M)<=>H2+C2H2(+M)                     8.000E+12       .440    88770.00
     LOW   /  7.000E+50   -9.310   99860.00/
     TROE/    .7345  180.00   1035.00  5417.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
C2H5+O2<=>HO2+C2H4                         8.400E+11       .000     3875.00
HCCO+O2<=>OH+2CO                           1.600E+12       .000      854.00
2HCCO<=>2CO+C2H2                           1.000E+13       .000         .00
!END of GRI-Mech2.1 (C-O-H part)
!Peter Glarborg HCN mechanism; recieved by e-mail
! ********************************************************
! *          HCN oxidation mechanism                     *
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! *         a: Tsang & Herron 1991                        *
! *         b: Tsang 1992                                 *
! *         c: Miller & Bowman 1989                       *
! *         d: Miller & Bowman 1991                       *
! *         e: Glarborg et al 1994 (IJCK)                 *
! *****************************************************
CN+H2=HCN+H              3.6E08  1.55  3000.  ! b
HCN+O=NCO+H              1.4E04  2.64  4980.  ! c
HCN+O=CN+OH              2.7E09  1.58 29200.  ! c
HCN+O=NH+CO              3.5E03  2.64  4980.  ! c
CN+H2O=HCN+OH            8.0E12  0.    7450.  ! Jacobs ea 86
HCN+OH=HOCN+H            5.9E04  2.4  12500.  !c
HCN+OH=HNCO+H            2.0E-03 4.0   1000.  !c
HCN+OH=NH2+CO            7.8E-04 4.0   4000.  !c
HCN+CN=C2N2+H            1.5E07  1.71   153.  !b
C2N2+O=CN+NCO            4.6E12  0.0   8880.  !c
C2N2+OH=CN+HOCN          1.9E11  0.0   2900.  !c
CN+O=CO+N                7.7E13  0.0      0.  !Davidson ea 90
CN+OH=NCO+H              6.0E13  0.0      0.  !c
CN+O2=NCO+O              7.5E12  0.0   -389.  !Durant & Tully 89
CN+CO2=NCO+CO            3.7E06  2.16 26900.  !Wang ea 91
CN+NO=NCO+N              1.0E14  0.0  42100.  !b
CN+NO2=NCO+NO            2.4E13  0.0   -370.  !b
CN+HNO=HCN+NO            1.8E13  0.0      0.  ! b
HOCN+H=HNCO+H            2.0E07  2.0   2000.  !est
HOCN+OH=NCO+H2O          6.4E05  2.0   2560.  !est (HNCO+OH)
HOCN+O=NCO+OH            1.5E04  2.64  4000.  !est (HCN+O)
HNCO+M=CO+NH+M           1.1E16  0.0  86000.  ! d
    N2/1.5/
HNCO+H=NH2+CO            2.2E07  1.7   3800.  !Miller & Melius 92
HNCO+O=NCO+OH            2.2E06  2.11 11430.  !b
HNCO+O=NH+CO2            9.6E07  1.41  8520.  !b
HNCO+O=HNO+CO            1.5E08  1.57 44012.  !b
HNCO+OH=NCO+H2O          6.4E05  2.0   2560.  !b
HNCO+HO2=NCO+H2O2        3.0E11  0.0  29000.  !d
HNCO+O2=HNO+CO2          1.0E12  0.0  35000.  !Glarborg ea 94
HNCO+NH2=NH3+NCO         5.0E12  0.0   6200.  !d
HNCO+NH=NH2+NCO          3.0E13  0.0  23700.  !d
HNCO+CN=HCN+NCO          1.5E13  0.0      0.  !b
NCO+M=N+CO+M             3.1E16 -0.50 48000.  !c
    N2/1.5/
NCO+H=CO+NH              5.0E13  0.0      0.  !b
NCO+O=NO+CO              4.7E13  0.0      0.  !b
NCO+H2=HNCO+H            7.6E02  3.0   4000.  !Miller & Melius 92
NCO+OH=HCO+NO            5.0E12  0.0  15000.  !c
NCO+O2=NO+CO2            2.0E12  0.0  20000.  !d
NCO+HCO=HNCO+CO          3.6E13  0.0      0.  !b
NCO+CH2O=HNCO+HCO        6.0E12  0.0      0.  !b
NCO+N=N2+CO              2.0E13  0.       0.  !c
NCO+NO=N2O+CO            6.2E17 -1.73   763.  !Mertens ea 92, Hershberger 93
NCO+NO=N2+CO2            7.8E17 -1.73   763.  !Mertens ea 92, Hershberger 93
NCO+NO2=CO+NO+NO         1.3E13  0.0      0.  !b
NCO+NO2=CO2+N2O          5.4E12  0.0      0.  !b
NCO+HNO=HNCO+NO          1.8E13  0.0      0.  !b
NCO+NCO=CO+CO+N2         1.8E13  0.0      0.  !b
NH3+M=NH2+H+M            2.2E16  0.0  93470.  !e
NH3+H=NH2+H2             6.4E05  2.39 10171.  !c,e
NH3+O=NH2+OH             9.4E06  1.94  6460.  !e
NH3+OH=NH2+H2O           2.0E06  2.04   566.  !c,e
NH3+HO2=NH2+H2O2         3.0E11  0.0  22000.  !d,e
NH2+H=NH+H2              4.0E13  0.0   3650.  !e
NH2+O=HNO+H              6.6E14 -0.5      0.  !c,e
NH2+O=NH+OH              6.8E12  0.0      0.  !c,e
NH2+OH=NH+H2O            4.0E06  2.0   1000.  !c,e
NH2+HO2=H2NO+OH          5.0E13  0.0      0.  !e
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NH2+HO2=NH3+O2            1.0E13  0.0         0.   !e
H2NO+O=NH2+O2             4.0E13  0.0         0.   !e
NH2+NH2=N2H2+H2           8.5E11  0.0         0.   !e
NH2+NH2=NH3+NH            5.0E13  0.0     10000.   !e
NH2+NH=N2H2+H             5.0E13  0.0         0.   !c,e
NH2+N=N2+2H               7.2E13  0.0         0.   !c,e
NH2+NO=NNH+OH             2.8E13 -0.55        0.   !e
NH2+NO=N2+H2O             1.75E11 0.0     -4500.   !e see glarborg.xls
NH2+NO2=N2O+H2O           3.2E18 -2.2         0.   !e
NH+H=N+H2                 3.0E13  0.0         0.   !e
NH+O=NO+H                 9.2E13  0.0         0.   !e
NH+OH=HNO+H               2.0E13  0.0         0.   !c,e
NH+OH=N+H2O               5.0E11  0.5      2000.   !c,e
NH+O2=HNO+O               4.6E05  2.0      6500.   !e
NH+O2=NO+OH               1.3E06  1.5       100.   !e
NH+N=N2+H                 3.0E13  0.0         0.   !c,e
NH+NH=N2+2H               2.5E13  0.0         0.   !c,e
NH+NO=N2O+H               7.24E12 0.0     -1280.   !e see glarborg.xls
NH+NO=N2+OH               2.2E13 -0.23        0.   !e
NH+NO2=N2O+OH             1.0E13  0.0         0.   !d,e
N+OH=NO+H                 3.8E13  0.0         0.   !c,e
N+O2=NO+O                 6.4E09  1.0      6280.   !c,e
N+NO=N2+O                 3.3E12  0.3         0.   !c,e
N+CO2=NO+CO               1.9E11  0.0      3400.   !c
NO+O+M=NO2+M              7.5E19 -1.41        0.   !Yarwood ea 1991
    N2/1.7/  O2/1.5/  H2O/10/
NO+HO2=NO2+OH             2.1E12  0.0      -480.   !c,e
HCO+NO=CO+HNO             7.2E12  0.0         0.   !a
NO2+H=NO+OH               3.5E14  0.0      1500.   !c,e
NO2+O=NO+O2               1.0E13  0.0       600.   !c,e
NO2+NO2=NO+NO+O2          1.6E12  0.0     26123.   !a
CO+NO2=CO2+NO             9.0E13  0.0     33800.   !a
HCO+NO2=H+CO2+NO          8.4E15 -0.75     1930.   !a
HNO+M=H+NO+M              1.5E16  0.0     48680.   !c,e
    H2O/10/ O2/2/ N2/2/ H2/2/
HNO+H=NO+H2               4.4E11  0.72      650.   !e
HNO+O=NO+OH               1.0E13  0.0         0.   !d,e
HNO+OH=NO+H2O             3.6E13  0.0         0.   !c,e
HNO+O2=NO+HO2             1.0E13  0.0     25000.   !d,e
HNO+NH2=NO+NH3            2.0E13  0.0      1000.   !c,e
HNO+NO=N2O+OH             2.0E12  0.0     26000.   !c,e
HNO+HNO=N2O+H2O           4.0E12  0.0      5000.   !c,e
HCO+HNO=NO+CH2O           6.0E11  0.00     2000.   !a
H2NO+M=HNO+H+M            5.0E16  0.0     50000.   !e
H2NO+H=HNO+H2             3.0E07  2.0      2000.   !e
H2NO+H=NH2+OH             5.0E13  0.0         0.   !e
H2NO+O=HNO+OH             3.0E07  2.0      2000.   !e
H2NO+OH=HNO+H2O           2.0E07  2.0      1000.   !e
H2NO+NO=HNO+HNO           2.0E07  2.0     13000.   !e
H2NO+NH2=HNO+NH3          3.0E12   0.0     1000.   !e
N2H2+M=NNH+H+M            5.0E16   0.0 50000.   !c,e
    H2O/15.0/  H2/2.0/  N2/2.0/  O2/2.0/
N2H2+H=NNH+H2             5.0E13   0.0  1000.   !c,e
N2H2+O=NH2+NO             1.0E13   0.0  1000.   !c,e
N2H2+O=NNH+OH             2.0E13   0.0  1000.   !c,e
N2H2+OH=NNH+H2O           1.0E13   0.0  1000.   !c,e
N2H2+NH=NNH+NH2           1.0E13   0.0  1000.   !c,e
N2H2+NH2=NNH+NH3          1.0E13   0.0  1000.   !c,e
N2H2+NO=N2O+NH2           3.0E12   0.0     0.   !c,e
NNH=N2+H                  1.0E06   0.0     0.   !e
NNH+H=N2+H2               1.0E14   0.0     0.   !c,e
NNH+O=N2O+H               1.0E14   0.0     0.   !c,e
NNH+OH=N2+H2O             5.0E13   0.0     0.   !c,e
NNH+NH=N2+NH2             5.0E13   0.0     0.   !c,e
NNH+NH2=N2+NH3            5.0E13   0.0     0.   !c,e
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NNH+NO=N2+HNO            5.0E13   0.0      0.  !c,e
N2O+M=N2+O+M             4.0E14   0.0 56100.  !e, Glarborg ea 94
    N2/1.7/ O2/1.4/ CO2/3.0/ H2O/12/
N2O+H=N2+OH              3.3E10   0.0  4729.  !Fontijn ea 87
DUP
N2O+H=N2+OH              4.4E14   0.0 19254.  !Fontijn ea 87
DUP
N2O+O=NO+NO              2.9E13   0.0 23150.  !e
N2O+O=N2+O2              1.4E12   0.0 10800.  !e
N2O+OH=N2+HO2            2.0E12   0.0 40000.  !Miller ea 94
N2O+CO=N2+CO2            2.7E11   0.0 20237.  !a
!END of Glarborg's mechanism
!Fuel-rich chemistry from GRI-Mech2.11 (reactions of C-species with N-species)
C+N2<=>CN+N                              6.300E+13     .000   46020.00
CH+N2<=>HCN+N                            2.857E+08    1.100   20400.00
CH+N2(+M)<=>HCNN(+M)                     3.100E+12     .150        .00
     LOW  /  1.300E+25   -3.160    740.00/
     TROE/    .6670  235.00  2117.00  4536.00 /
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/
CH2+N2<=>HCN+NH                          1.000E+13     .000   74000.00
CH2(S)+N2<=>NH+HCN                       1.000E+11     .000   65000.00
C+NO<=>CN+O                              1.900E+13     .000        .00
C+NO<=>CO+N                              2.900E+13     .000        .00
CH+NO<=>HCN+O                            5.000E+13     .000        .00
CH+NO<=>H+NCO                            2.000E+13     .000        .00
CH+NO<=>N+HCO                            3.000E+13     .000        .00
CH2+NO<=>H+HNCO                          3.100E+17   -1.380    1270.00
CH2+NO<=>OH+HCN                          2.900E+14    -.690     760.00
CH2+NO<=>H+HCNO                          3.800E+13    -.360     580.00
CH2(S)+NO<=>H+HNCO                       3.100E+17   -1.380    1270.00
CH2(S)+NO<=>OH+HCN                       2.900E+14    -.690     760.00
CH2(S)+NO<=>H+HCNO                       3.800E+13    -.360     580.00
CH3+NO<=>HCN+H2O                         9.600E+13     .000   28800.00
HCNN+O<=>CO+H+N2                         2.200E+13     .000        .00
HCNN+O<=>HCN+NO                          2.000E+12     .000        .00
HCNN+O2<=>O+HCO+N2                       1.200E+13     .000        .00
HCNN+OH<=>H+HCO+N2                       1.200E+13     .000        .00
HCNN+H<=>CH2+N2                          1.000E+14     .000        .00
HNCO+OH<=>NH2+CO2                        1.550E+12     .000    6850.00
HCNO+H<=>H+HNCO                          2.100E+15    -.690    2850.00
HCNO+H<=>OH+HCN                          2.700E+11     .180    2120.00
HCNO+H<=>NH2+CO                          1.700E+14    -.750    2890.00
HCCO+NO<=>HCNO+CO                        2.350E+13     .000        .00
CH3+N<=>HCN+H2                           3.700E+12     .150     -90.00
END
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