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Modeling of No$_x$ Destruction Options for INEEL Sodium-Bearing Waste Vitrification

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ABSTRACT

Off-gas NO_x concentrations in the range of 1 – 5 mol% are expected as a result of the proposed vitrification of sodium-bearing waste at the Idaho National Engineering and Environmental Laboratory. An existing kinetic model for staged combustion (originally developed for NO_x abatement from the calcination process) was updated for application to vitrification offgas. In addition, two new kinetic models were developed to assess the feasibility of using selective non-catalytic reduction (SNCR) or high-temperature alone for NO_x abatement. Each of the models was developed using the Chemkin code. Results indicate that SNCR is a viable option, reducing NO_x levels to below 1000 ppmv. In addition, SNCR may be capable of simultaneously reducing CO emissions to below 100 ppmv. Results for using high-temperature alone were not as promising, indicating that a minimum NO_x concentration of 3950 ppmv is achievable at 3344°F.

EXECUTIVE SUMMARY

Direct vitrification is considered a prime option for treatment of sodium-bearing waste (SBW) currently stored at the Idaho Nuclear Technology and Engineering Center (INTEC) at the Idaho National Engineering Laboratory (INEEL). Abatement of nitrogen oxides (NO_x) has been identified as a necessary step in the off-gas treatment train. To evaluate the feasibility of the NO_x abatement schemes being considered, kinetic modeling of the following technologies was initiated: staged combustion, selective non-catalytic reduction (SNCR), and NO_x abatement using high temperature alone. Following is a brief description of each of these technologies:

- ***Staged Combustion*** **—** In the first stage, excess fuel is added to initiate combustion and create a reducing environment. A number of fuels can be selected, but cleaner-burning fuels such as natural gas and propane are preferred. The operating temperature in this stage is maintained at 1300°C, and NO_x is rapidly destroyed. The offgas is then quenched to 900°C to avoid formation of thermal NO_x in the final combustion stage. In the final stage, excess air is added to promote fuel-lean combustion, thus consuming any residual fuel and destroying any remaining products of incomplete combustion (PICs) such as CO.

- ***SNCR*** **—** Selective catalytic reduction relies on both a reducing agent and elevated temperature to accomplish NO_x destruction. The combustion gas is preheated to 850°C before addition of the reducing agent (typically ammonia or urea). Because the operating window for NO_x destruction is relatively small (~100°C range), and because the reaction of NO_x with ammonia is exothermic, SNCR should be implemented as multiple stages with interstage cooling to be effective in treating a high-NO_x offgas.

- ***High-Temperature NOx Abatement*** **—** For this option, temperature alone is used to generate hydroxyl radicals at very high temperatures (up to 2850°C). These radicals create the reducing environment required to destroy NO_x.

Kinetic models for each of these technologies were developed using the Chemkin code. Because staged combustion has been previously demonstrated for NO_x destruction of calciner offgas, the objective was to update the model for applicability to vitrification off-gas treatment. However, the feasibilities of SNCR and high-temperature NO_x abatement have not been demonstrated for applications similar to the vitrification flowsheet. Therefore, the modeling objective for these technologies was to determine the NO_x destruction feasibility with respect to the vitrification flowsheet.

Staged combustion was modeled as three plug flow reactors in series. Input gas composition was updated to be representative of SBW vitrification off-gas concentrations. Also, an energy balance was performed for each stage of the combustor. Predicted outlet temperatures for the reduction and oxidation stages are 1,268°C and 954°C, respectively. An outlet NO_x concentration of 530 ppmv is predicted.

The SNCR process was modeled as a plug-flow reactor. The optimal operating temperature range was identified as 850°C – 950°C, with an optimal NH_3/NO_x ratio of 1.2. At 900°C, the NO_x outlet concentration was minimized to 173 ppmv, with a corresponding NH_3 slip concentration of <5 ppmv. Also at this temperature, CO was effectively reduced to <5 ppmv.

The high-temperature NO_x abatement process was also modeled as a plug-flow reactor. The optimal operating temperature was identified as 1840°C, corresponding to an outlet NO_x concentration of 3950 ppmv. Additional modeling was performed to investigate whether increasing residence time or adding small amounts of reductants (NH_3, CH_4, H_2) could improve NO_x destruction at high temperatures. Results indicated that increasing gas residence time was ineffective. In addition, although inclusion of a reductant was marginally effective in some of the modeling cases, none of the high-temperature results proved to be an improvement over the lower-temperature SNCR results.

The general conclusion from this modeling effort is that staged combustion and SNCR are both viable options for NO_x abatement of SBW vitrification offgas. Also, because high-temperature NO_x abatement cannot reduce NO_x concentrations to less than 1000 ppmv, it should not be considered further.

In addition to the conclusions stated above, key uncertainties and knowledge gaps associated with this modeling have been identified and documented. Recommendations for model validation, lab/pilot-scale data needs, and future modeling tasks are also called out in this report.

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ACRONYMS

CFD	computational fluid dynamics
DOE	U.S. Department of Energy
DRE	destruction removal efficiency
HEME	high-efficiency mist eliminator
HEPA	high-efficiency particulate air (filter)
INEEL	Idaho National Engineering and Environmental Laboratory
INTEC	Idaho Nuclear Technology and Engineering Center
IWVF	Idaho Waste Vitrification Facility
MACT	Maximum Achievable Control Technology
NWCF	New Waste Calcination Facility
NO_X	nitrogen oxides (NO, NO_2)
PC	personal computer
PIC	product of incomplete combustion
SBW	sodium-bearing waste
SCO	selective catalytic oxidation
SCR	selective catalytic reduction
SNCR	selective non-catalytic reduction
SVOC	semi-volatile organic compound
THC	total hydrocarbons
VB	Visual Basic
VOC	volatile organic compound

Modeling of NO_x Destruction Options for INEEL Sodium-Bearing Waste Vitrification

1. INTRODUCTION

1.1 Purpose/Objective

Direct vitrification is considered a prime option for the treatment of sodium-bearing waste (SBW) currently stored at the Idaho Nuclear Technology and Engineering Center (INTEC) at the Idaho National Engineering Laboratory (INEEL). Abatement of nitrogen oxides (NO_x) has been identified as a necessary step in the off-gas treatment train for the following reasons:

- NO_x abatement simplifies compliance monitoring for volatile organic compounds (VOCs), semi-volatile organic compounds (SVOCs), and toxic metals (especially mercury) that will be required because the vitrification facility will be regulated as a RCRA waste treatment unit.

- NO_x abatement reduces the concern over mercury sorbent degradation that can occur in a high-NO_x environment.

- Previous INEEL facility air permits with the State of Idaho have included NO_x emission limits. It is almost certain that similar (or more stringent) limits will be imposed on the Idaho Waste Vitrification Facility (IWVF). Implementation of NO_x abatement will greatly simplify facility permitting in this regard.

- Nitrogen dioxide (NO_2) is a brown gas that poses health hazards at levels above 15 ppm. Additionally, the presence of NO_2 in the stack offgas creates a visible plume. These are issues of serious concern to the Department of Energy (DOE), the INEEL, and other stakeholders. NO_x abatement addresses these concerns.

To evaluate the feasibility of the NO_x abatement schemes being considered for the IWVF, modeling of these technologies was initiated. In addition to evaluating technical feasibility, a secondary objective was to develop and refine models for technologies already deemed suitable for implementation at the IWVF. It is anticipated that the models developed as part of this effort may find broader application to similar problems within the DOE complex.

1.2 Scope

Four technologies were considered as part of this task: staged combustion, selective catalytic reduction (SCR), selective non-catalytic reduction (SNCR), and high-temperature NO_x destruction. The scope of modeling for each of these tasks is briefly summarized in the following sections. It should be noted that modeling results from this study were considered in a broader study to directly compare and down-select IWVF NO_x abatement options. Hence, a more comprehensive comparison of these technologies is documented elsewhere.[1]

1.2.1 Staged Combustion

A kinetic model has previously been developed for staged combustion.[2] In addition, two successful pilot-scale trials have been performed on simulated New Waste Calcination Facility (NWCF) offgas.[3, 4] Therefore, the feasibility of this technology has already been established. Hence, the objective in modeling staged combustion was to update the model for application to the IWVF, including factors such as gas residence time, inlet gas composition, and equipment size.

The model produced from this effort will be suitable for two tasks. First, it can be integrated with the steady-state process model used for design of the facility, thus improving accuracy of that model. Second, the kinetic set produced from this task can be reduced for inclusion in a computational fluid dynamics (CFD) code. Such a code will be required to design an efficient staged combustor.

1.2.2 SCR

Successful pilot-scale testing of a hydrogen mordenite SCR performed on a slipstream at the NWCF in the early 1990s.[5,6] Therefore, the feasibility of this technology has already been established. The objective for SCR modeling in FY-01 had only a limited scope. A survey of existing literature was performed, with the intent of identifying and recommending a suitable modeling approach. If the SCR technology is later considered for implementation at the IWVF, a follow-on study can be initiated rapidly based on the groundwork established in this task.

1.2.3 SNCR

For SNCR, the primary focus was to determine the feasibility of reducing NO_x to required levels.[a] More specifically, a detailed kinetic model was developed for the SNCR process, and key parameters were varied over a wide range. Through this exercise, theoretical feasibility of the SNCR process was assessed, and a valid operating window was identified.

1.2.4 High-Temperature NO_x Destruction

As with SNCR, the primary focus of modeling high-temperature NO_x destruction was to determine the feasibility of reducing NO_x to required levels. A detailed kinetic model was developed, and temperature and residence time were varied over a wide range. In addition, a study was performed to determine the effectiveness of adding small quantities of various reductants to enhance NO_x destruction at high temperatures.

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[a] NO_x reduction requirements have not yet been finalized. However, for the purpose of this task, reasonable limits were considered to be less than 1000 ppm NO and 100 ppm NO_2 in the effluent from the NO_x abatement unit operation.

2. NO$_X$ ABATEMENT TECHNOLOGIES

2.1 Technology Descriptions

2.1.1 Staged Combustion

2.1.1.1 Process Overview. A simplified staged combustion flow diagram for destruction of NO$_x$ and products of incomplete combustion (PICs) is presented below (see Figure 1). The first stage is operated under fuel-rich conditions at 1300°C, while the final stage is cooled to 1000°C and an excess of air is introduced. By operating under fuel-rich conditions in the first stage, a highly reducing environment is created and NO$_x$ is destroyed. By operating under fuel-lean conditions in the second stage, an oxidizing environment is created and PICs are destroyed. Interstage cooling is provided to keep the temperature in the second stage below the point where NO$_x$ will reform.

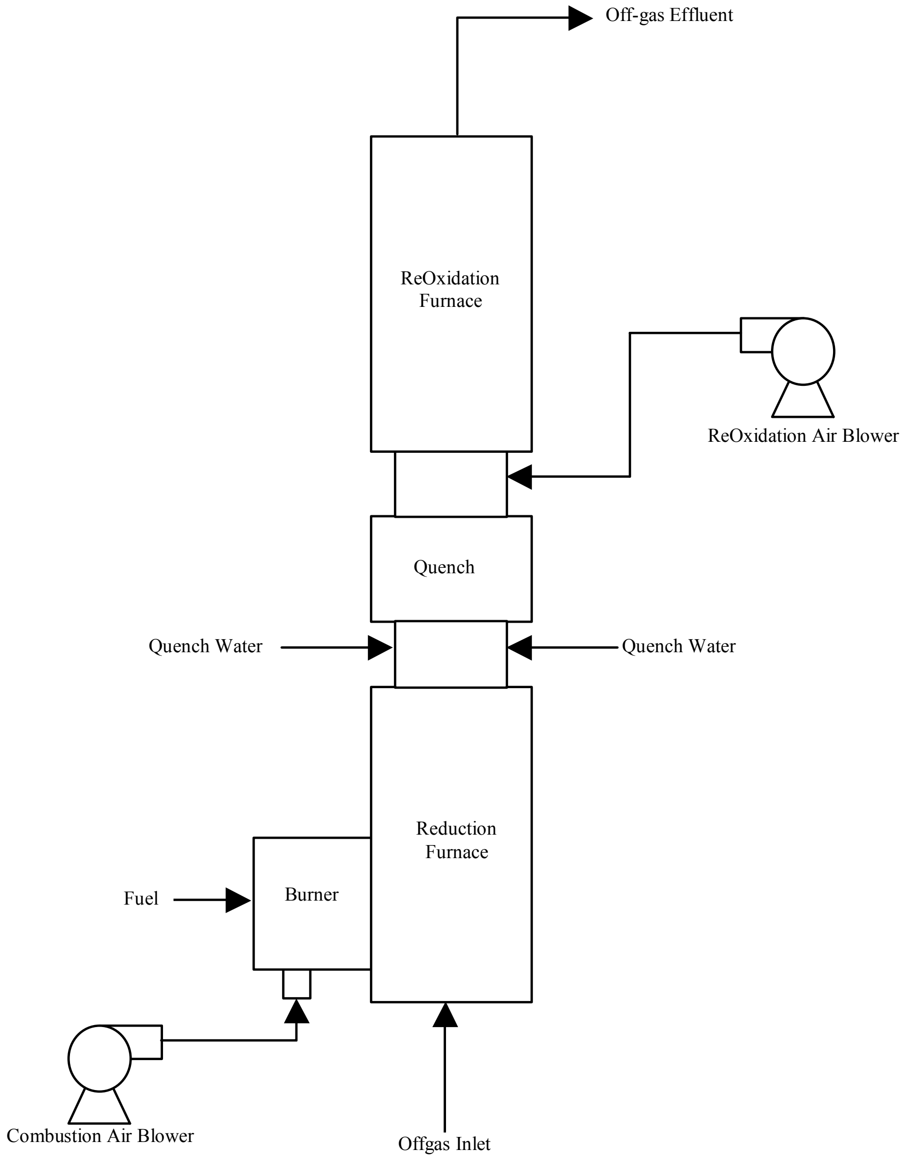

Figure 1. Simplified multistage combustion flow diagram.

Major equipment required to implement staged combustion includes: the staged-combustion vessel and combustion chamber, a combustion air blower, a reoxidation air blower, cooling water injection nozzles, a propane storage and delivery system, inlet/outlet NO_x analyzers, and an outlet CO analyzer.

2.1.1.2 Reaction Chemistry. The reaction chemistry associated with staged combustion is quite complex, and involves free radical reactions. However, kinetic modeling has been performed in an attempt to better understand the predominant reactions for NO_2 destruction. Results of this modeling indicate that NO_2 is quickly destroyed in the combustion chamber via the following reactions at 1300°C:[2]

$$NO_2 + HCO \rightarrow H + CO_2 + NO \tag{1}$$

$$NO_2 + HCO \rightarrow HONO + CO \tag{2}$$

$$NO_2 + CH_3 \rightarrow CH_3O + NO \tag{3}$$

$$NO_2 + H \rightarrow OH + NO \tag{4}$$

$$NO_2 + CH_2O \rightarrow HCO + HONO \tag{5}$$

It should be noted that test results indicate that NO_2 will be converted to NO at this temperature regardless of whether the mixture is fuel-rich or fuel-lean.[b] Therefore, in the event of less-than-adequate control of the combustion process, it is still likely that NO_2 (and the associated yellow/brown plume) will be destroyed.

Reaction chemistry for the destruction of NO has been studied in depth, and is better understood. The overall reactions for NO reduction by methane (and similarly for other hydrocarbons) can be written as:

$$2NO + 2CH_4 \rightarrow 2HCN + 2H_2O + H_2 \tag{6}$$

$$6NO + 2CH_4 \rightarrow 2CO + 4H_2O + 3N_2 \tag{7}$$

In the reoxidizing stage, CO and H_2 are destroyed according to following reactions:

$$2CO(g) + O_2(g) \rightarrow 2CO_2(g) \tag{8}$$

$$2H_2(g) + O_2(g) \rightarrow 2H_2O(g) \tag{9}$$

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[b] This statement is based on discussions with MSE personnel in regard to testing performed during March through May of 2000. The standard startup procedure for the staged combustion unit calls for lining out operation under oxidizing conditions prior to switching the reduction stage to fuel-rich conditions. During these times, offgas exiting the stack was colorless, indicating the lack of NO_2 in the exit gas. In another instance, a severe fluctuation in natural gas header pressure caused a large fuel surge to the staged combustor, resulting in overly fuel-rich conditions. In this instance, some soot was observed in the stack offgas, but the yellow-brown plume associated with NO_2 emissions was not observed. Hence, it appears that temperature alone is sufficient to reduce NO_2 to NO over a wide range of the equivalence ratio.

2.1.1.3 Technical Maturity. NO_x reburning technology was initially developed in the 1960s, and is a fairly mature technology. Staged combustion has been used successfully to perform NO_x reburning in a wide variety of applications involving nitrogen-containing wastes, including treatment of amines, nitriles, nitroaromatics, ammonia, HCN, and NO_x. The majority of commercial installations are on large-scale boilers. Although commercial use is common, staged combustion has not yet been implemented in a radioactive environment. However, testing has been performed on simple non-radioactive NWCF off-gas simulants, achieving destruction efficiencies in excess of 92%. To date, both natural gas and propane have been used as the fuel for these tests with similar success.

Based on industry experience and NWCF off-gas simulant testing, staged combustion is a technically viable option for treatment of SBW vitrification offgas.

2.1.1.4 Suitability to SBW Vitrification Off-Gas Treatment. The following list highlights benefits and advantages of staged combustion in regard to treating SBW vitrification offgas:

- Staged combustion can destroy NO_x, CO, H_2, and PICs in a single unit operation
- Staged combustion is relatively insensitive to variations in inlet NO_x concentration
- Staged combustion has been demonstrated to achieve greater than 92% NO_x destruction efficiency
- Due to temperature alone, NO_2 entering the combustion zone will be destroyed, thus eliminating plume visibility caused by NO_2.

Technical uncertainties and potential areas of concern for implementation of staged combustion are:

- Current testing indicates that staged combustion will result in an off-gas volume dilution of four to six times the original off-gas flow rate. Further testing is required to determine if the volume increase can be reduced.
- Staged combustion may be perceived negatively by stakeholders due to the thermal nature of the process.

2.1.2 SCR

2.1.2.1 Process Overview. Selective catalytic reduction employs both a catalyst and reducing additive to accomplish NO_x destruction at relatively low temperatures. A potential SCR flow diagram is presented below (see Figure 2). Note that this flowsheet includes two stages with interstage cooling. This is required for the IWVF flowsheet because the temperature rise in a single stage could be excessive due to the large amounts of NO_x and the associated exothermic reactions for NO_x destruction. Major equipment required to implement SCR includes: a preheater, a minimum of two catalyst beds, interstage cooler(s), a reductant storage and delivery system, and inlet/interstage/outlet NO_x analyzers.

SCR catalyst units come in honeycomb, pellet, and plate designs. Additionally, numerous types of catalysts are currently used. Performance for the major catalyst types is shown below (see Figure 3) From this figure, it can be seen that zeolite catalysts offer the widest temperature window in which >90% destruction of NO_x can be achieved. This is a significant advantage due to the large temperature rise expected during NO_x abatement of SBW vitrification offgas. However, it may be feasible to use a vanadium/titanium-based catalyst as the first bed in series, followed directly by a second zeolite bed. In this configuration, it may be possible to eliminate the need for interstage cooling. Additional factors must also be considered when selecting the optimal catalyst(s), including the potential for catalyst poisoning, expected catalyst life, catalyst cost and availability, and the disposal path for spent catalyst.

Another important parameter for the SCR process is the selection of a reducing agent. Various reducing agents are currently used, with the most common being ammonia, urea, or various hydrocarbons such as CH_4. For most commercial SCR installations, either ammonia or urea is used.

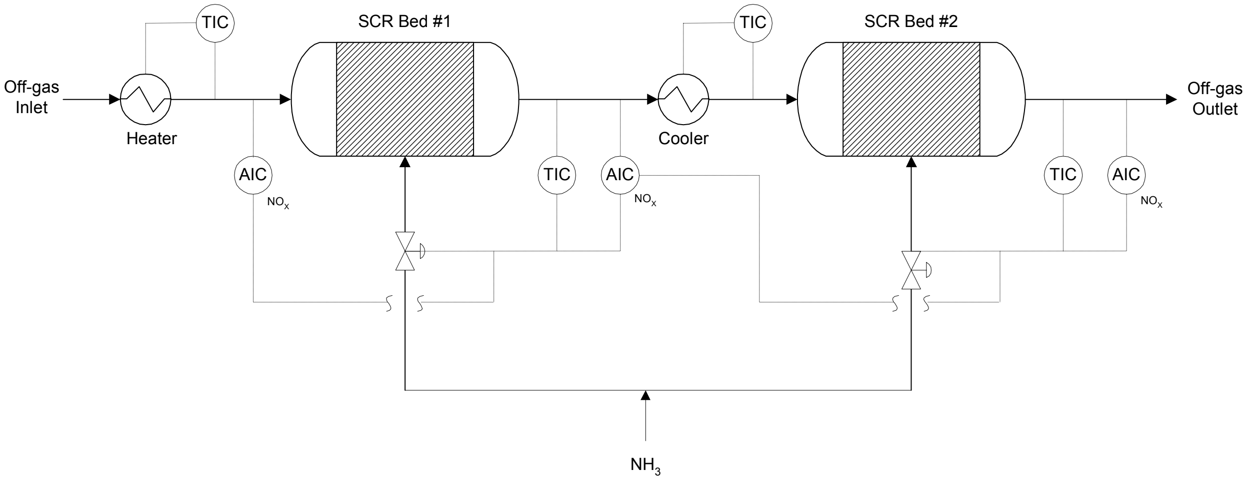
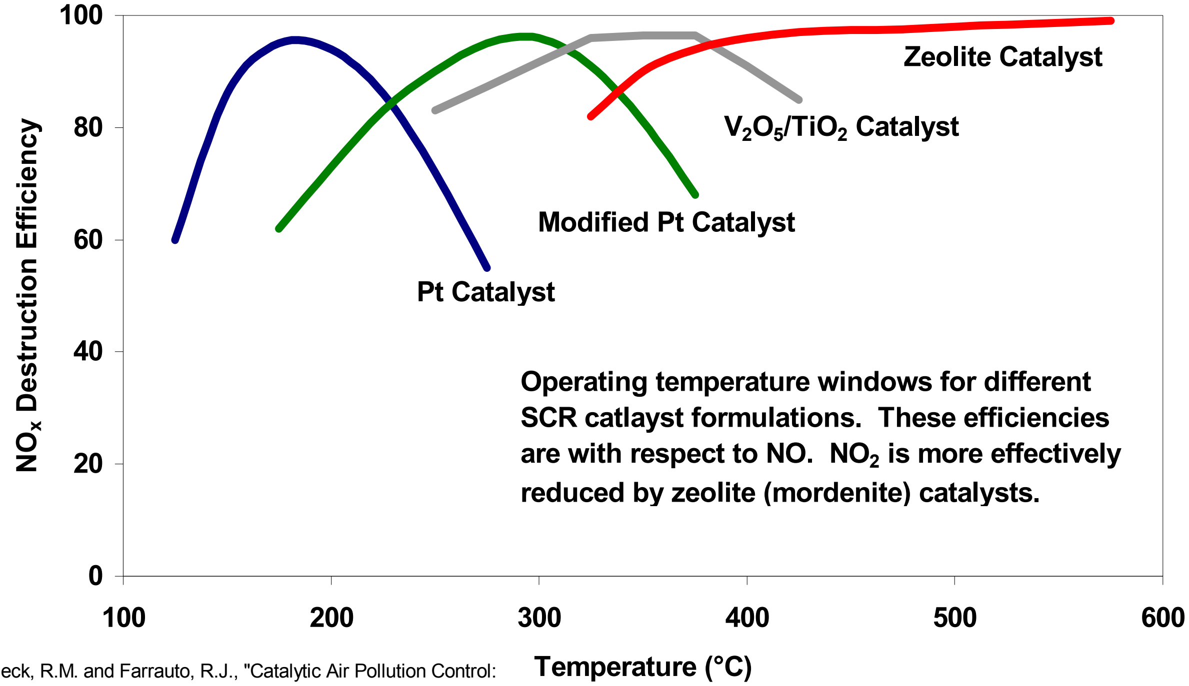


Figure 2. Potential NO_x SCR configuration.



Operating temperature windows for different SCR catlayst formulations. These efficiencies are with respect to NO. NO_2 is more effectively reduced by zeolite (mordenite) catalysts.

Heck, R.M. and Farrauto, R.J., "Catalytic Air Pollution Control: Commercial Technology", VanNostr and Reinhold, 1995.

Figure 3. Typical performance of SCR catalyst types.

2.1.2.2 Reaction Chemistry. The primary reactions responsible for NO_x destruction in the SCR reactors are shown below:[7, 8, 9, 10]

$$4NO(g) + 4NH_3(g) + O_2(g) \xrightarrow{catalyst} 4N_2(g) + 6H_2O(g) \tag{10}$$

$$6NO(g) + 4NH_3(g) \xrightarrow{catalyst} 5N_2(g) + 6H_2O(g) \tag{11}$$

$$2NO_2(g) + 4NH_3(g) + O_2(g) \xrightarrow{catalyst} 3N_2(g) + 6H_2O(g) \tag{12}$$

$$6NO_2(g) + 8NH_3(g) \xrightarrow{catalyst} 7N_2(g) + 12H_2O(g) \tag{13}$$

$$NO(g) + NO_2(g) + 2NH_3(g) \xrightarrow{catalyst} 2N_2(g) + 3H_2O(g) \tag{14}$$

$$4NO(g) + 4NH_3(g) + 3O_2(g) \xrightarrow{catalyst} 4N_2O(g) + 6H_2O(g) \tag{15}$$

$$8NO_2(g) + 6NH_3(g) \xrightarrow{catalyst} 7N_2O(g) + 9H_2O(g) \tag{16}$$

It is generally accepted that in most SCR systems, reactions 10 and 13 predominate. Note that equations 15 and 16 produce an undesired product, N_2O. In addition to the NO_x destruction reactions listed above, O_2 also competes with NO_x to consume NH_3 according to the following reaction:

$$4NH_3(g) + 3O_2(g) \xrightarrow{catalyst} 2N_2(g) + 6H_2O(g) \tag{17}$$

Reaction 17 is sometimes referred to as selective catalytic oxidation (SCO) of ammonia. Fortunately, at elevated temperature in the presence of water vapor, this reaction is impeded and NH_3 requirements are reduced.

The SCR process chemistry presents some concerns. First, the NH_3/NO_x ratio must be carefully controlled to minimize NH_3 slip. Excessive NH_3 slip is a concern because of the potential to form NH_4NO_3 according to the homogenous reaction shown below:

$$2NO_2(g) + 2NH_3(g) \rightarrow NH_4NO_3(s) + N_2(g) + H_2O(g) \tag{18}$$

Ammonium nitrate formation presents two principal concerns. First, upon cooling in subsequent downstream off-gas treatment operations, NH_4NO_3 could plate out on cool spots in the equipment and piping, resulting in plugging. Second, the presence of an energetic salt could increase the risk for an explosion. Fortunately, SCR operating temperatures are greater than the decomposition temperature of NH_4NO_3. In addition, the associated reaction kinetics are not favorable when the temperature is increased beyond room temperature. However, in order to mitigate off-gas plugging and potential safety concerns, NH_3 slip must be minimized. Additionally, minimizing NH_3 slip will correspondingly reduce NH_3 emissions to the environment. One potential means of eliminating this concern is to locate a catalytic oxidizer immediately downstream of the SCR process, thus rapidly oxidizing any NH_3 exiting the SCR process.[c] In addition, as previously discussed, temperature control within the prescribed reaction

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[c] Due to the potential necessity for CO and total hydrocarbon (THC) destruction to comply with MACT standards, a catalytic oxidation reactor would be placed in the off-gas train if SCR were implemented for NO_x abatement.

temperature range is necessary due to the exothermic nature of the reactions. This could be accomplished either by carefully selecting the catalysts for each stage, or through implementation of interstage cooling.

2.1.2.3 Technical Maturity.

The SCR process is used widely throughout the world in many commercial applications. Additionally, there is considerable past experience in the use of SCR for NO_X abatement in offgas produced in nuclear fuel reprocessing waste management. Two such implementations are summarized below.[11]

West Valley Nuclear Services Company (WVNSCO) operates a nuclear waste vitrification melter similar to the one planned for the IWVF. The WVNSCO vitrification melter offgas has a NO_X composition of 5,000 ppm, with spikes as high as 20,000 ppm. An SCR system with NH_3 as the reductant has been operating successfully for over 5 years. The WVNSCO configuration consists of two reactors in parallel (one in service, the other in standby). The catalyst (Norton NC-300, a hydrogen mordenite zeolite catalyst) was designed to operate through 52 operating cycles per year for 2 years. However, WVNSCO has yet to observe any degradation in catalyst performance in the operational reactor through 5 years of operation. To date, use of the standby reactor has not been required. The catalyst absorbs up to 5 wt % NH_3. Therefore, during minor mismatches between the amount of NO_X in the offgas and the amount of NH_3 injected, the excess NH_3 held by the catalyst will make up the NH_3 deficit, and the NO_X abatement system functions acceptably.

SCR pilot plant tests for NO_X abatement in the NWCF off-gas stream were conducted in the early 1990s at INTEC. These studies were conducted on an off-gas stream containing 15,000 ppm NO_X using a hydrogen mordenite zeolite catalyst.[d] Conversion efficiencies of 95% were demonstrated with minimal NH_3 slip. These results strongly indicate that a similar SCR configuration may be suitable for inclusion in the IWVF off-gas train. Catalyst deactivation was not observed during this 90-day test. Information concerning the primary reactions was well documented, including reaction time, heats of reaction, the effect of humidity and temperature on NO_X conversion efficiency, and other useful design information.

2.1.2.4 Suitability to SBW Vitrification Off-Gas Treatment.

Overall, SCR technology appears well suited for treatment of SBW vitrification offgas. The following list highlights benefits and advantages of the SCR technology:

- SCR processes have been successfully used not only in commercial industry, but also in the DOE complex for treatment of vitrification offgas
- The SCR process operates at moderate temperatures (<600°C)
- NO_x destruction efficiency in excess of 95% can be achieved with minimal NH_3 slip
- Minor process upsets will not result in decreased efficiency due to the ability of the catalyst to absorb NH_3
- Implementation of the SCR process results in negligible dilution of the off-gas stream.

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[d] A zeolite catalyst was selected over noble and precious metal-based catalysts after extensive testing. Hydrogen mordenite and copper zeolite were found to be the most effective for reducing NO_2. Other considerations included cost, catalyst poisoning potential, and catalyst configuration. The zeolite catalysts are more readily extruded into forms that can be used in a packed bed, thus providing easier ways of remotely handling the catalysts for change out and disposal. In addition, the zeolite catalysts likely are easier to immobilize and dispose as a secondary waste form because they contain no additional heavy metals and they have a natural-earth mineral base (except for iron and/or copper that is added to enhance catalyst activity).

Technical uncertainties and potential areas of concern for implementation of SCR technology are:

- A rapid-response NO_x analyzer and control system is required to ensure high efficiency during more severe process upsets.
- NH_3 handling, transportation, and storage, although performed safely at similar installations, introduces additional safety hazards and concerns.
- Catalyst deactivation due to poisoning by mercury, iodine, halogens, or other trace species needs to be further investigated for this specific application and waste stream.
- Hydrothermal sintering is a concern for mordenite-based zeolite when temperature excursions occur. This requires accurate temperature limit control and efficient mixing of NH_3 in the influent of the reactors.
- Because SCR technology is implemented as a packed bed unit operation, it is susceptible to plugging if the inlet stream is particulate-laden. Therefore, this technology is suitable for implementation only downstream of a particulate removal unit operation.
- Precautionary steps must be taken to mitigate the potential for NH_4NO_3 formation downstream of the SCR unit operation because of concerns related to the potential for an explosion as well as off-gas pipe plugging.

2.1.3 SNCR

2.1.3.1 Process Overview. Selective non-catalytic reduction is similar to SCR in that it employs a reducing additive to accomplish NO_x reduction. However, SNCR uses elevated temperatures rather than a catalyst to promote reaction. A potential SNCR flow diagram is presented below (see Figure 4). Major equipment required to implement SNCR includes: a preheater, a minimum of two reaction vessels or stages, interstage cooler(s), a reductant storage and delivery system, and inlet/interstage/outlet NO_x analyzers.

As with SCR, various reducing agents can also be used with SNCR. Ammonia is the most common reducing agent selected, but considerable work has also been done using urea.

For a successful implementation of the SCNR technology, the off-gas temperature window of operation must be maintained between 850°C and 950°C. Below 850°C, the rate of reaction is too slow, resulting in incomplete NO_x destruction and excessive NH_3 slip. Above 950°C, the reverse reactions are significant, thus resulting in reformation of NO_x. This likely necessitates implementation of SNCR using at least two stages. Therefore, as with the SCR process, accurate temperature control is essential for SNCR to be effectively implemented. However, the window of operation for SNCR is significantly smaller than for SCR, thus elevating the importance of precise temperature control.

Another key to successful implementation of the SNCR technology is to ensure adequate mixing of the offgas and reductant in the reactors. With SCR, the catalyst beds promote mixing of the offgas and reductant. With SNCR, mixing considerations must be carefully considered in the equipment design. One potential method to enhance mixing is to insert baffles into the reaction vessels. A second method is to inject the reductant using distribution grids into several locations along the length of the reactors.

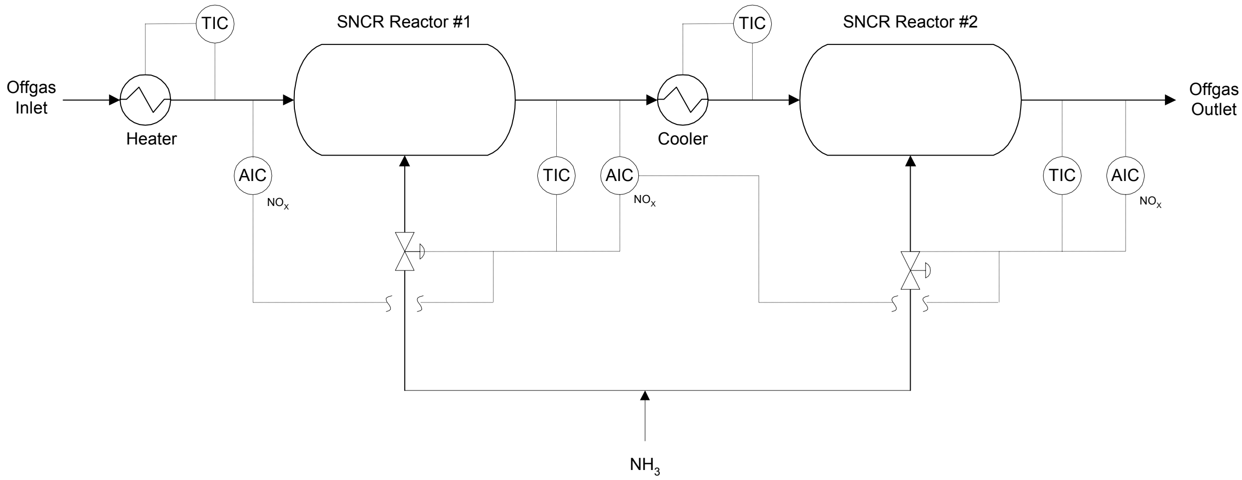

Figure 4. Potential NO_x SNCR configuration.

2.1.3.2 Reaction Chemistry. The primary reactions responsible for NO_x destruction in the SNCR process are the same as in SCR. However, because the process takes place at higher temperatures, the detailed chemistry is quite complex and involves free radical reactions. Additionally, it is likely that NO_2 will be rapidly reduced to NO in the preheater according to the following reaction:

$$2NO_2(g) \leftrightarrow 2NO(g) + O_2(g) \tag{19}$$

Therefore, primary destruction of NO_x in the SNCR reactors will be due to decomposition of NO, not NO_2. In the case of urea as the reductant, the overall reaction for NO is given as:[10]

$$4NO(g) + 2H_2NCONH_2(g) + O_2(g) \xrightarrow{850°-950°C} 4N_2(g) + 2CO_2(g) + 4H_2O(g) \tag{20}$$

Optionally, urea can be used to generate ammonia, which can subsequently be used as the reductant in the SNCR. This may be desirable because urea presents reduced transportation and storage risks, as compared with anhydrous ammonia. The corresponding reaction is:

$$H_2NCONH_2(g) + H_2O \rightarrow 2NH_3(g) + CO_2(g) \tag{21}$$

NH_3 is then used to reduce NO_x to N_2 via similar reactions presented for SCR NO_x destruction (albeit using temperature rather than a catalyst to promote reaction). At Hanford, current plans are to generate NH_3 from urea for use in SCR NO_x abatement. One disadvantage of using urea as the reductant is the undesirable possibility of forming N_2O as a byproduct.[e]

As with the SCR process, it is also possible for NH_3 to react with oxygen via the SCO reaction of ammonia in Equation 17. In addition, formation of NH_4NO_3 in the downstream equipment raises concerns of an explosion or plugging in the off-gas piping if excessive NH_3 slip occurs. One potential means of eliminating this concern is to locate a thermal oxidizer immediately downstream of the SNCR

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[e] When using urea as a reductant, as much as 25% can be converted to N_2O.

process, thus rapidly oxidizing any NH_3 exiting the SNCR process.[f] In the thermal oxidizer, O_2 would be injected while maintaining temperature around 800°C, thus promoting the SCO reaction of ammonia to N_2 via Equation 17 (albeit using temperature rather than a catalyst to promote reaction).

2.1.3.3 Technical Maturity. The SNCR process is used widely throughout the world in commercial applications (>300 installations as of 1997).[12] However, the majority of these installations are for coal-fired utility boilers. In most of these installations, NH_3 or urea is injected directly into the boiler. Because boiler temperatures are not optimal for NO_x reduction, and because of highly inefficient mixing, NO_x destruction efficiencies of only 30-70% are typically achieved. In some instances, a NO_x destruction efficiency of 80% has been reported. The destruction removal efficiency (DRE) is likely to be limited by the low NO_x concentrations in these systems. In the case of SBW vitrification offgas, NO_x concentration will be much higher, and hence the anticipated NO_x DRE is anticipated to improve.

2.1.3.4 Suitability to SBW Vitrification Off-Gas Treatment. The viability of SNCR for NO_x abatement of SBW vitrification offgas is uncertain. However, the following list highlights potential benefits and advantages if SNCR can be successfully implemented:

- The SNCR process reactors are simple and can be designed to minimize plugging/fouling
- The SNCR process will result in only minimal dilution of the off-gas stream
- Due to temperature alone, NO_2 entering the combustor will be destroyed, thus eliminating plume visibility.

Technical uncertainties and potential areas of concern for implementation of SNCR technology are:

- A rapid-response NO_x analyzer and control system is required to ensure high efficiency during more severe process upsets.
- Current SNCR installations do not achieve the efficiency required for the IWVF. Development work is required to confirm the feasibility of achieving higher efficiencies.
- Because the SNCR process operates between 850–950°C, materials of construction must be selected to tolerate the extreme temperatures. Ceramic lined vessels and heaters will most likely be required.
- Precautionary steps must be taken to mitigate the potential for NH_4NO_3 formation downstream of the SNCR unit operation.
- The SNCR technology has yet to be demonstrated in an application similar to SBW vitrification off-gas treatment. Additionally, SNCR use has not been demonstrated in a radioactive environment.
- NH_3 handling, transportation, and storage, although performed safely at similar installations, introduces additional safety hazards.

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[f] Due to the potential necessity for CO and THC destruction to comply with MACT standards, a thermal oxidation reactor would be placed in the off-gas train if SNCR were implemented for NO_x abatement.

- SNCR may be perceived negatively by stakeholders due to the thermal nature of this treatment.

2.1.4 High-Temperature NO_x Destruction

2.1.4.1 Process Overview. High-temperature NO_x destruction refers to the ability to decompose NO_x using thermal means alone. No known implementation of this technology exists on an industrial scale. In order to destroy NO_x, it is hypothesized that temperatures in excess of 1300°C will be required. Above this temperature, it is thought that free radicals will be present in sufficient concentration to facilitate NO_x decomposition. A potential high-temperature NO_x destruction flow diagram is presented below (see Figure 5). Due to the pre-developmental nature of this technology, gas residence time requirements are not known, although at elevated temperatures the kinetics of NO_x decomposition are expected to be very rapid.

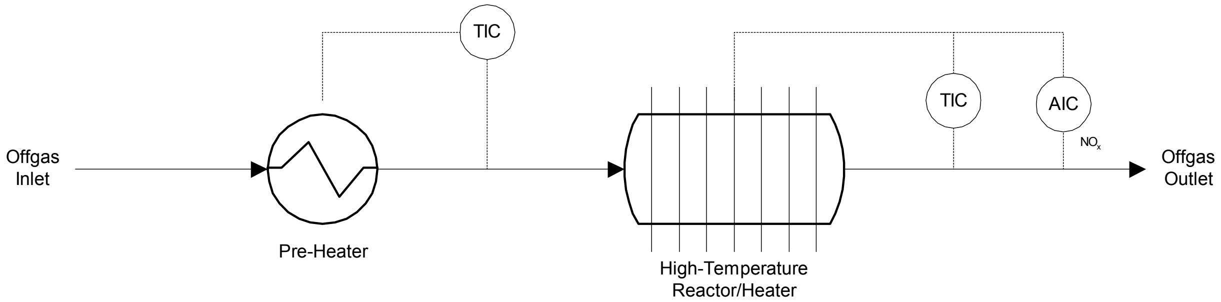

Figure 5. Potential high-temperature NO_x abatement configuration.

One benefit of this approach is the simplicity of the concept. Major equipment required includes: a preheater, a high-temperature heater (which also serves as the reaction vessel), temperature control instrumentation, and an outlet NO_x analyzer.

Two significant hurdles to successful implementation of this process exist. First, a heater must be designed that is capable of heating the off-gas stream to the required temperature. Second, suitable materials of construction must be identified for the high-temperature environment.

2.1.4.2 Reaction Chemistry. As with SNCR, this process takes place at high temperatures. Thus, the detailed chemistry is quite complex and involves free radical reactions. Additionally, it is likely that NO_2 will be rapidly reduced to NO in the preheater according to reaction 19 listed above for SNCR. Therefore, primary destruction of NO_x in the high-temperature reactor will be due to decomposition of NO, not NO_2.

2.1.4.3 Technical Maturity. As discussed above, this technology is pre-developmental. If modeling establishes the feasibility of this approach to NO_x abatement, proof-of-concept testing will be required. Further development will also be required to establish optimal operating conditions and to determine efficiency.

2.1.4.4 Suitability to SBW Vitrification Off-Gas Treatment. The viability of high-temperature NO_x abatement is uncertain. However, the following list highlights potential benefits and advantages if high-temperature NO_x abatement can be successfully implemented:

- The high-temperature NO_x destruction process is simple and can be designed to minimize plugging/fouling

- No appreciable increase in off-gas volume will result from high-temperature NO_x destruction

- High-temperature NO_x destruction is relatively insensitive to variations in inlet NO_x concentration

- Due to temperature alone, NO_2 entering the heaters will be destroyed, thus eliminating plume visibility (unless NO converts to NO_2 in subsequent cooler off-gas treatment equipment, piping, the stack, or the atmosphere)[g]

- A secondary thermal oxidation treatment unit may not be required if high-temperature NO_x destruction is successfully implemented.

Technical uncertainties and potential areas of concern for implementation of high-temperature NO_x abatement are:

- High-temperature NO_x abatement is in a pre-developmental state.

- Because of elevated operating temperatures, materials of construction must be selected to tolerate the extreme temperatures. Ceramic lined vessels and heaters will be required.

- Developing heaters capable of achieving the required temperatures may prove difficult.

- High-temperature NO_x abatement is a thermal process and may be perceived negatively by stakeholders.

2.1.5 Other NO_x Abatement Technologies

As stated previously, only four technologies were modeled as part of this task. Other technologies are also available for NO_x abatement. A brief assessment of the suitability of these technologies for implementation at the IWVF is presented below.

2.1.5.1 NO_x Scrubbing. Wet scrubbing is widely used industrially for NO_x abatement. However, due to the insolubility of NO in water, only NO_2 can be scrubbed efficiently. Therefore, to successfully implement NO_x scrubbing for an offgas containing both NO and NO_2, addition of an oxidizing agent would likely be required to convert NO to NO_2.[h] In addition to this complication, multiple scrubbers are typically employed to achieve high scrubbing efficiencies. This could significantly increase the number of wet process operations in the off-gas train. NO_x scrubbing will also lead to nitrate salt accumulation in the scrub solution, thus requiring an increase in the blowdown amount. There are two possible scenarios for dealing with the increased blowdown solution, neither of which is desirable. First, the additional blowdown could be treated and disposed of as secondary waste. Second, the additional blowdown could

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[g] Even if NO_2 is converted to NO, elevated NO emissions are undesirable because of the potential to contribute to regional haze.

[h] Studies have also shown that pressurization can boost the efficiency of NO scrubbing. However, due to the need for radioactive containment in the system, operation under a slight vacuum pressure is desirable in the off-gas train. Therefore, pressurization is not an acceptable method for improving NO scrubbing efficiency in a radioactive environment.

be recycled to the melter, thus decreasing the net throughput of waste processing. However, in this scenario, excessive nitrate accumulation in the system may become problematic.

Due to the undesirable secondary waste implications associated with NO_x scrubbing, this technology has not been seriously considered for inclusion in the IWVF flowsheet. However, due to the maturity of this technology, it is recommended that NO_x scrubbing scenarios be included in an upcoming steady-state process model evaluation to select the IWVF wet scrubbing configuration.

2.1.5.2 Steam Reforming. Steam reforming is commonly employed industrially for various purposes. It has even been used to treat low-level radioactive waste within the DOE complex (Studsvik Processing Facility at Erwin Tennessee). However, steam reforming as an off-gas treatment method for NO_x abatement has not been previously demonstrated nor tested.

In a recent study,[13] steam reforming was investigated and determined to be a technically viable method for NO_x abatement in the SBW direct vitrification process. However, in this same study, steam reforming was evaluated against staged combustion, SCR, an SNCR, and it was concluded that steam reforming did not compare favorably for this application.

2.1.5.3 Plasma-Enhanced Wet Electrostatic Precipitation. Another approach for NO_x abatement is plasma-enhanced electrostatic precipitation (PEESP).[14] The basic concepts of this technology are:

1. O_2 and steam are charged for use as the reagent gas
2. Ozone is formed due to the charging of the reagent gas
3. Ozone reacts with water to form hydroxyl radicals
4. Hydroxyl radicals react with NO, oxidizing it to NO_2
5. NO_2 is further reacted to NO_3^- and subsequently scrubbed from the offgas.

This technology is currently under development, and would need additional testing prior to serious consideration for implementation in the IWVF flowsheet. One potential complication is that because nitrates are not destroyed in this process, they must be managed with the secondary waste stream. In addition, they may necessitate increased scrub blowdown rates, thus increasing the amount of secondary waste generation. However, because of the potential for a PEESP to simultaneously remove NO_x, submicron particulate and mercury from the offgas, this technology warrants further investigation.

2.2 Available Data/Models

One important consideration prior to initiation of model development is to review the models that currently exist, and determine the availability of data for use in model validation. These issues are summarized below for each technology.

2.2.1 Staged Combustion

A kinetic model has been previously developed at the INEEL for NO_x destruction of NWCF offgas using staged combustion.[2] This model incorporates only bulk gas constituents, but includes an extensive kinetic set (500+ reactions) for these components. A review of this model indicates that the following modifications/enhancements should be made to adapt the model for SBW vitrification off-gas use:

- The input off-gas concentration should be updated for SBW vitrification offgas.
- The model was originally developed for natural gas combustion. It should be updated for propane combustion to better align with current IWVF design options.
- The combustion chamber, reducing stage, interstage quench, and reoxidizing stage were modeled as plug-flow reactors. While this approach is suitable for the reducing, quench, and reoxidizing stages, this is not the preferred method for modeling the combustion chamber. It is believed that better agreement with experimental data could be achieved by modeling the combustion chamber as a perfectly stirred reactor.

In addition to the existing kinetic model for staged combustion, some experimental data are also available.[3, 4] Because this data is for staged combustion of simulated NWCF offgas using natural gas, it has only limited utility for SBW vitrification offgas. However, it can be used to quantify the model improvement resulting from modifications to the combustion chamber submodel.

2.2.2 SCR

SCR modeling has not been performed previously at the INEEL. In addition, a brief review of the open literature turned up no articles presenting a detailed approach to SCR modeling. However, it is apparent from the literature that SCR modeling will require catalyst-specific data to achieve acceptable results. Some catalyst data is available in the open literature, although it is anticipated that data for specific catalysts can be obtained from the catalyst manufacturers.

Previous testing with a hydrogen mordenite zeolite catalyst was performed on NWCF offgas at the INEEL during the early 1990s.[5, 6] Kinetic modeling parameters were not regressed from the test data. However, regression of the required parameters could be performed and compared to results from upcoming pilot-scale SCR vitrification off-gas tests.

2.2.3 SNCR

The open literature contains many articles on kinetic and CFD modeling of the SNCR process. Unfortunately, nearly all of these articles address SNCR as method for abating NO_x in existing coal-fired boilers. The NO_x levels anticipated in SBW vitrification offgas differ from that typically observed in coal-fired boilers. In addition, SNCR is applied differently for a coal-fired boiler – ammonia is typically added to the boiler in strategic locations rather than adding a separate reaction vessel specifically for this purpose. Therefore, mixing and temperature control in a coal-fired boiler SNCR application would be significantly different than that anticipated for application of SNCR in the IWVF flowsheet. Hence, although the SNCR process has been previously modeled, existing models are not suitable for use in predicting performance in the IWVF flowsheet.

No data is currently available to validate a model of the SNCR process. Therefore, if modeling indicates that SNCR is a viable option for the IWVF flowsheet, lab and/or pilot-scale testing will be required for both proof-of-principle and model validation.

2.2.4 High-Temperature NO_x Abatement

Due to the pre-developmental state of this NO_x abatement concept, models do not currently exist to predict its performance. In addition, no data are available for model validation.

3. THEORY/APPROACH

3.1 Software Applications

In order to assess the feasibility of these NO_x abatement technologies, key operating variables such as temperature, pressure, gas residence time, and reductant feed rate must be determined. To accurately determine these parameters, both reaction kinetics and fluid dynamics must be considered. Unfortunately, most software packages available today focus on either kinetics or fluid dynamics, while neglecting or over-simplifying effects related to the other phenomena. Hence, some compromises must be made in selecting suitable modeling codes, and limitations must be clearly understood.

For chemical kinetics, the Chemkin Collection[15] was selected as the modeling tool. This package was originally developed at Sandia National Laboratory as a mainframe application, but is now distributed by Reaction Design for use either on a Unix-based workstation or on a MS Windows-based PC. It is suitable for many types of kinetic problems, including those in the fields of combustion, chemical processing, microelectronics, and environmental protection. This package contains extensive thermodynamic and transport property databases, as well as allowing user-supplied input for these properties. Chemkin is recognized throughout the DOE complex and the world as a leading tool for kinetic modeling.

The Chemkin code, although very good at chemical kinetics, is limited in its ability to consider fluid dynamics. User models are available for simple flow geometries such as a plug-flow reactor or a continuous stirred tank reactor. However, in practice, reacting gas flow in NO_x abatement equipment is more complex than in either of these simplified models. Hence, the Chemkin code is likely to produce "best-case" theoretical predictions.

Because chemical kinetics were deemed of primary importance in determining the feasibility of a NO_x abatement technology, only kinetic modeling was performed during FY-01. However, it is anticipated that follow-on fluid dynamic modeling will be required prior to scale-up and implementation at the IWVF. For fluid dynamic modeling, several suitable software packages are commercially available. In previous modeling of staged combustion at the INEEL, CFD Workshop[16] was selected as the modeling tool due to many factors – the ability to accurately model combustion problems, reasonable pricing, flexible licensing, the ability to modify the software to incorporate NO_2 kinetics, and PC platform availability. CFD Workshop is based on the PCGC3 code, which was developed by the Advanced Combustion Engineering Research Center at Brigham Young University and the University of Utah.

3.2 Model Development

An existing kinetic model was used as the starting point for the staged combustion, SNCR and high-temperature NO_x destruction models.[2] For each of these models, a custom interface was built using Microsoft Excel.[17] The following sections document aspects of model development that are common (or similar) to each of the models.

3.2.1 Chemical Reactions

Table 1 summarizes species that were included in all models. The chemistry input file (which contains thermodynamic data, reaction mechanisms, and kinetic data for the model) was supplied to Dr. R. D. Boardman by Sandia National Laboratories' Combustion Research Facility in 1998. This file is based on a previously published reaction set.[18] However, the file has been updated based on recent research, and now includes 546 reactions. One significant addition to the mechanism is the inclusion of reactions involving NO_2. The complete chemistry input file is included in Appendix A, along with specific input files for each model developed.

Table 1. Chemical species included in the Chemkin mechanism.

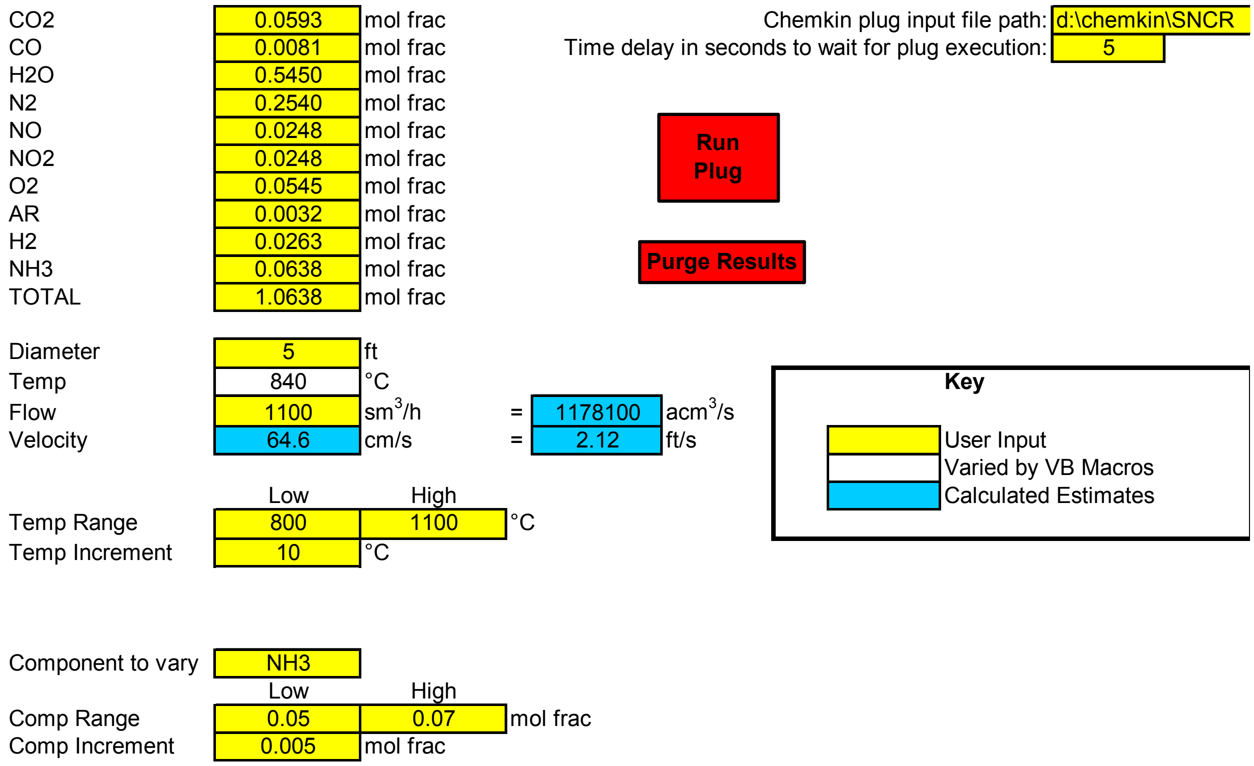
Included Chemkin Species				
H_2	H	CH_4	CH_3	CH_2
CH	CH_2O	HCO	CO_2	CO
O_2	O	OH	HO_2	H_2O_2
H_2O	C_2H	C_2H_2	HCCO	C_2H_3
C_2H_4	C_2H_5	C_2H_6	CH_2OH	CH_3O
HCCOH	H_2CCCH	C_3H_2	$CH_2(S)$	CH_2CO
C	C_4H_2	C_5H_2	$H_2CCCCCH$	HCCCHCCH
C_5H_5	C_6H_2	CH_2CHCCH	HCCHCCH	H_2CCCCH
C_6H_5	C_6H_6	C_3H_4	C_3H_4P	C_6H_5O
$CH_2CHCHCH$	CH_2CHCCH_2	C_2	C_2O	$C_6H_5C_2H$
C_6H_4	OCHCHO	C_4H	CH_3O_2	C_2H_2OH
H_2C_4O	$CH_2CHCHCH_2$	CH_3OH	CH_2HCO	CH_3CO
CH_3HCO	CH_3OOH	Ar	NO	N
NH	NH_2	HNO	HCN	NCO
CN	N_2O	NNH	HNCO	N_2H_2
CH_3CN	CH_2CN	C_2N_2	NO_2	HOCN
HCNO	H_2CN	NH_3	H_2NO	NCN
HONO	NO_3	N_2		

3.2.2 Model Interface

In order to simplify use of the Chemkin code, a user interface was designed in Microsoft Excel for each of the three models. The benefits of the Excel interfaces include:

- The ability to automate running the model repetitively to investigate a range of input conditions
- Convenient storage of model results for multiple cases
- Flexible options for plotting and analyzing model output
- The ability to run the model as a multi-stage process, using output from one stage as input to the subsequent stage.

The Excel interface developed for the SNCR model is shown in Figure 6, and is representative of the interfaces developed for the other NO_x abatement models.



CO2	0.0593	mol frac
CO	0.0081	mol frac
H2O	0.5450	mol frac
N2	0.2540	mol frac
NO	0.0248	mol frac
NO2	0.0248	mol frac
O2	0.0545	mol frac
AR	0.0032	mol frac
H2	0.0263	mol frac
NH3	0.0638	mol frac
TOTAL	1.0638	mol frac

Chemkin plug input file path: d:\chemkin\SNCR
Time delay in seconds to wait for plug execution: 5

Diameter 5 ft
Temp 840 °C
Flow 1100 sm^3/h = 1178100 acm^3/s
Velocity 64.6 cm/s = 2.12 ft/s

	Low	High	
Temp Range	800	1100	°C
Temp Increment	10	°C	

Key

🟨 User Input
⬜ Varied by VB Macros
🟦 Calculated Estimates

Component to vary NH3

	Low	High	
Comp Range	0.05	0.07	mol frac
Comp Increment	0.005	mol frac	

Figure 6. Microsoft Excel interface developed for the SNCR model.

3.3 SCR Modeling Approach

As previously stated, the scope for SCR modeling during fiscal year 2001 was very limited. The primary objective was to review information in the open literature to gain insight into how to approach modeling of the SCR process. The following section documents findings from this review.

3.3.1 Literature Review

The open literature contains numerous articles discussing NO_x abatement using the SCR process. Surprisingly, however, very little SCR catalyst kinetic data are published. Due to this circumstance, kinetic modeling of the SCR process will be hindered unless a suitable source of data is located. This stated, a summary of relevant articles in the literature is given below:

1. Nova, Isabella, et al., “Dynamics of SCR reaction over a TiO2-supported vanadia–tungsta commercial catalyst,” *Catalysis Today*, Vol. 60, 2000, pp. 73–82. This article presents test results for a commercial V_2O_5-WO_3/TiO_2 catalyst (V_2O_5=0.62%w/w, WO_3=9%w/w). Several concentration vs. time plots are presented. Kinetic expressions are given, along with regressed rate parameters. In addition, the effect of water vapor addition is quantified.

2. Tronconi, E., et al., “Experimental and Theoretical Investigation of the Dynamics of the SCR-DeNO$_x$ Reaction,” *Chemical Engineering Science*, Vol. 51, No. 11, 1996, pp. 2965–2970. This article investigates the kinetics of NH_3 adsorption-desorption over V_2O_5-WO_3/TiO_2 catalysts by transient response techniques, and proposes rate expressions that account for heterogeneity of the catalyst surface. Results were successfully validated against laboratory data using a commercial SCR honeycomb catalyst.

3. Radojevic, Miroslav, "Reaction of nitrogen oxides in flue gases," *Environmental Pollution*, Vol. 102, No. S1, 1998, pp. 685–689. This article outlines key reactions for the SCR process. In addition, the operating temperature window for several different commercially available SCR systems, along with the manufacturer and country of origin, is tabulated. Kinetic data are not presented in this article, but the list of catalysts and manufacturers may be a useful reference for obtaining data directly from the manufacturers.

4. Hums, E., "Is advanced SCR technology at a standstill? A provocation for the academic community and catalyst manufacturers," *Catalysis Today*, Vol. 42, 1998, pp. 25-35. This article discusses data gaps that exist in relation to SCR catalysis. Two key points brought out by this article that should be considered when developing and validating a model are:

    a. Deactivation behavior has a significant influence on catalytic performance. Work continues to better understand the mechanisms associated with selective and non-selective catalyst poisoning.

    b. Most discussion and data on the nature of catalytically active sites in the literature address only fresh catalyst performance. Data should be expanded to include the entire operating life of the catalyst.

5. Rogers, Kevin, Mel Albrecht, and Michael Varner, "Numerical Modeling for Design Optimization of SCR Applications," *Presented to ICAC NO$_x$ Forum, Washington D.C., March 23–24, 2000*, Technical Paper BR-1699, Babcock & Wilcox. This article is somewhat generic, but does list key parameters that should be considered when modeling an SCR process. In addition, this article discusses the importance of validation and acceptance criteria.

4. MODELS

4.1 Staged Combustion

Staged combustion was modeled as three plug-flow reactors in series using the Chemkin Plug application. The first Plug model was used to simulate both the combustion chamber and the reduction stage of the combustor. Output temperature and composition were passed as input to the second Plug model. The second Plug model was used to simulate the interstage quench. Output temperature and composition from the second Plug model were passed as input to the third Plug model. The third Plug model was used to simulate the reoxidation stage. Dimensions for each stage were held constant at the following values: 6.5 ft diameter × 23 ft length for the combustion chamber/reduction stage, 6.5 ft diameter × 5 ft length for the quench, and 5.8 ft diameter × 21 ft length for the reoxidation stage. These values were selected to match sizing recommendations provided by a multistage combustion equipment vendor.[19] The off-gas flow rate was fixed at 3100 sm^3/hr, which is representative of the flow expected downstream of the IWVF melter, quench tower, and scrubber during vitrification of SBW.[i] All cases were run at a pressure of 1 atm. The off-gas composition used for this modeling is shown in Table 2.

Table 2. Off-gas composition used for staged combustion modeling.

Component	Mole %
CO_2	2.09
CO	0.29
H_2O	27.40
N_2	54.08
NO	0.88
NO_2	0.88
O_2	13.80
AR	0.11
H_2	0.47
TOTAL	100.00

Natural gas was used as the fuel in this model, primarily due to the availability of a kinetic mechanism for this fuel. The low heat value of 21,518 BTU/lb was assumed, and a fuel input of 15.4 lb/min was used to achieve a heat input of 20 MMBTU/hr. Air was used as the reductant, at an input level of 1898 scfm. A total of 10 gpm of quench water was input (4 gpm for the reduction stage; 6 gpm for the quench). A reoxidation air flow rate of 596 scfm was input. Once again, these inputs were based on equipment vendor specifications.

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[i] This location is downstream of the melter, film cooler, quencher, scrubber, high efficiency mist eliminator (HEME), and high-efficiency particulate air (HEPA) filters. This placement was identified as the optimal location for staged combustion in reference 19.

Some difficulties were experienced in building and running the staged combustion kinetic model. Each of these problems is briefly discussed below:

- The Chemkin Plug module is not flexible enough to allow multiple input streams. Hence, a composite input stream that included all inputs to a particular stage was calculated in Excel prior to generating the input file for Chemkin. To maintain an accurate overall heat balance, Excel was also used to calculate enthalpies of each input stream prior to mixing, thus allowing a reasonable calculation of temperature for the combined feed stream.

- After the model was constructed, it was discovered that grouping the combustion chamber and the reduction stage into a single plug flow reactor model over-simplified the problem. As a result, excessively high temperatures were predicted in the reduction stage. In addition, it was necessary to increase the input stream temperature in order for the model to properly predict initiation of combustion. To compensate for this shortcoming, the following steps were taken:

    1. The enthalpy of the inlet stream was calculated in Excel

    2. The inlet stream temperature was increased so that initiation of combustion would be predicted by the model

    3. The enthalpy of the inlet stream was calculated at the increased temperature

    4. The enthalpy change of the inlet stream was calculated by subtracting the results from steps 3 and 1 above

    5. The first Plug model was run using the increased inlet stream temperature

    6. The enthalpy of the Plug model outlet stream was calculated

    7. The outlet temperature from the Plug model was decreased, and enthalpy of the outlet stream was recalculated

    8. The enthalpy change of the outlet stream was calculated by subtracting the results from steps 6 and 7 above

    9. Steps 7 and 8 above were repeated iteratively until the enthalpy change of the outlet stream equaled the enthalpy change of the inlet stream calculated in step 4 above.

  This fix provides a reasonable estimate of the outlet temperature from the first stage Plug model. However, the inflated temperatures used during kinetic calculations will tend to predict artificially low NO_x concentration exiting the first stage.

- In order to perform an accurate heat balance throughout each stage of the model, the overall heat transfer coefficients must be known. Accurate values for these coefficients will obviously depend on many factors, including refractory type and thickness. Because these parameters have not yet been finalized for the IWVF design, an overall heat transfer coefficient was calculated based on the design of an existing pilot-scale combustion unit (see Appendix B). Based on this calculation, an overall heat transfer coefficient of 2,500 erg/cm^2·s·K was used for each Plug submodel.

4.2 SNCR

For simplicity, the SNCR process was modeled as a single-stage plug-flow reactor using the Chemkin Plug application. Ammonia was included as the reductant in the model. The dimensions of the reactor were fixed at 5 ft diameter × 10 ft length. The off-gas flow rate was fixed at 1100 sm^3/hr, which is representative of the flow expected from the full-scale IWVF melter during vitrification of SBW.[j] All cases were run at a pressure of 1 atm. The off-gas composition used for this modeling is shown in Table 3.

Table 3. Off-gas composition used for SNCR modeling.

Component	**Mole %**
CO_2	5.93
CO	0.81
H_2O	54.50
N_2	25.40
NO	2.48
NO_2	2.48
O_2	5.45
AR	0.32
H_2	2.63
TOTAL	100.00

Because the main interest in modeling the SNCR process was to determine technical feasibility in relation to the IWVF requirements, heat of reaction effects and heat losses to the surroundings were neglected (i.e., the model was run isothermally). By imposing this limitation, identification of the optimal temperature range for NO_x destruction was simplified. A temperature range of 800 – 1100°C was investigated, based on ranges given in the literature for typical SNCR implementations. By using a temperature increment of 10°C, 31 operating temperatures were examined. Input ammonia mole fraction was varied between 0.05 and 0.07, corresponding to NH_3/NO_x ratios of 1.0 – 1.4. The NH_3 mole fraction increment was set at 0.0025, allowing investigation of 9 NH_3/NO_x ratios. In all, 279 cases were run.

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[j] There are two potential placement options for a SNCR in the IWVF flowsheet. First, the SNCR could be located directly downstream of the melter, taking advantage of the elevated process temperature at this point in the off-gas train. Second, the SNCR could be located downstream of the melter and wet-processing equipment, making it less susceptible to plugging. The former location was selected for modeling, as it was deemed that this location would maximize the benefits associated with using SNCR for NO_x abatement in the IWVF flowsheet.

4.3 High-Temperature NO_x Destruction

The high-temperature NO_x destruction process was also modeled as a single-stage plug-flow reactor using the Chemkin Plug application. The dimensions of the reactor were initially fixed at 5 ft diameter × 10 ft length. The off-gas flow rate was fixed at 1100 sm^3/hr, which is representative of the flow expected from the full-scale IWVF melter during vitrification of SBW.[k] All cases were run at a pressure of 1 atm. The off-gas composition used for this modeling is shown in Table 4.

Table 4. Off-gas composition used for high-temperature NO_x destruction modeling.

Component	Mole %
CO_2	5.93
CO	0.81
H_2O	54.50
N_2	25.40
NO	2.48
NO_2	2.48
O_2	5.45
AR	0.32
H_2	2.63
TOTAL	100.00

Because the main interest in modeling the high-temperature NO_x abatement process was to determine technical feasibility in relation to the IWVF requirements, heat of reaction effects and heat losses to the surroundings were neglected (i.e., the model was run isothermally). By imposing this limitation, identification of the optimal temperature range for NO_x destruction was simplified. A temperature range of 800 – 2850°C was investigated. By using a temperature increment of 10°C, 206 operating temperatures were examined.

In addition to kinetic modeling of the high-temperature NO_x abatement process, thermodynamic equilibrium modeling was also performed. The reason for performing thermodynamic modeling was that it represents a "best-case" scenario for high-temperature NO_x destruction, which could then be used for comparison against the kinetic modeling results. To accomplish this modeling, two separate software packages were used. First, a model was built using the Chemkin Equil module. Next, a model was constructed using the Gibbs module of HSC Chemistry for Windows.[20] In each of these models, the temperature window explored was the same as in the kinetic model (800 – 2850°C).

Results of the initial modeling (discussed in the following section) gave rise to two other fundamental questions:

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[k] The location selected for high-temperature NO_x abatement modeling is immediately downstream of the melter. This is the most logical placement to minimize heating requirements.

- Based on kinetic predictions, what gas residence time would be required to achieve equilibrium NO_x outlet concentrations?

- What effect would the addition of a small amount of reductant have on the outlet NO_x concentration?

To address these questions, two follow-on modeling tasks were completed. First, the kinetic model was rerun, but the reactor geometry was changed to 1 ft diameter × 2500 ft length. Although this length is not practical, model results would allow identification of the length (and hence residence time) where reaction kinetic predictions match thermodynamic equilibrium predictions. Second, small amounts of three reductants were added to the model: CH_4 (0.000 – 0.035 mole fraction), H_2 (0.000 – 0.035 mole fraction), and NH_3 (0.000 – 0.010 mole fraction).

5. RESULTS

5.1 Staged Combustion

Model predictions for temperature, key species concentrations, and other important parameters are summarized in Table 5. From these data, it can be seen that outlet stage temperature predictions agree reasonably well with temperatures specified by the equipment vendor. In addition, the predicted outlet NO_x concentrations match results achieved in pilot-scale demonstrations.[1]

Table 5. Results from staged combustion kinetic modeling.

Parameter	Stage		
	Combustion Chamber / Reduction Stage	**Quench**	**Reoxidation Stage**
Gas Residence Time (s)	1.238	0.411	1.211
Gas Exit Velocity (ft/s)	13.0	12.1	17.2
Temperature (°F)			
Inlet	147*	2,314	1,672
Maximum	3,571	2,314	1,777
Outlet	2,314*	1,672	1,749
Vendor spec (for comparison)**	2,400	1,665	1,810
Off-Gas Flow (scfm)			
Inlet	1,813	8,231	9,998
Outlet	8,231	9,998	10,908
Outlet Composition (mol%)			
CO_2	7.084	6.323	6.415
CO	1.375	0.642	23 ppbv
H_2O	38.08	49.17	46.54
N_2	51.11	42.08	45.67
NO	811 ppmv	577 ppmv	528 ppmv
NO_2	67 ppbv	75 ppbv	2 ppmv
O_2	0.108	61 ppmv	0.934
AR	0.407	0.335	0.391
H_2	1.404	1.377	111 ppbv

*Reflects the enthalpy balance correction discussed in Section 4.1.

**From EDF-IWVF-004.

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[1] Pilot-scale demonstrations were conducted at the MSE facility in Butte, Montana (see references 3 and 4). In these demonstrations, the simulated off-gas composition was targeted to match NWCF offgas rather than vitrification offgas. Outlet NO_x concentrations in these tests ranged between 80-1029 ppm total NO_x. The majority of the NO_x was present as NO, as the NO_2 concentration averaged <10 ppmv.

Temperature, CO, and NO_x concentration are shown graphically in Figure 7. From this plot, the effect of modeling the combustion chamber and reduction stage as a single plug flow reactor is evident. The predicted temperature throughout the first stage is representative of the combustion chamber rather than the reduction stage. This condition obviously has an influence on the NO_x concentration exiting the first stage. Even so, the predicted NO_x concentrations looks reasonable as evidenced by agreement with pilot-scale demonstration data.

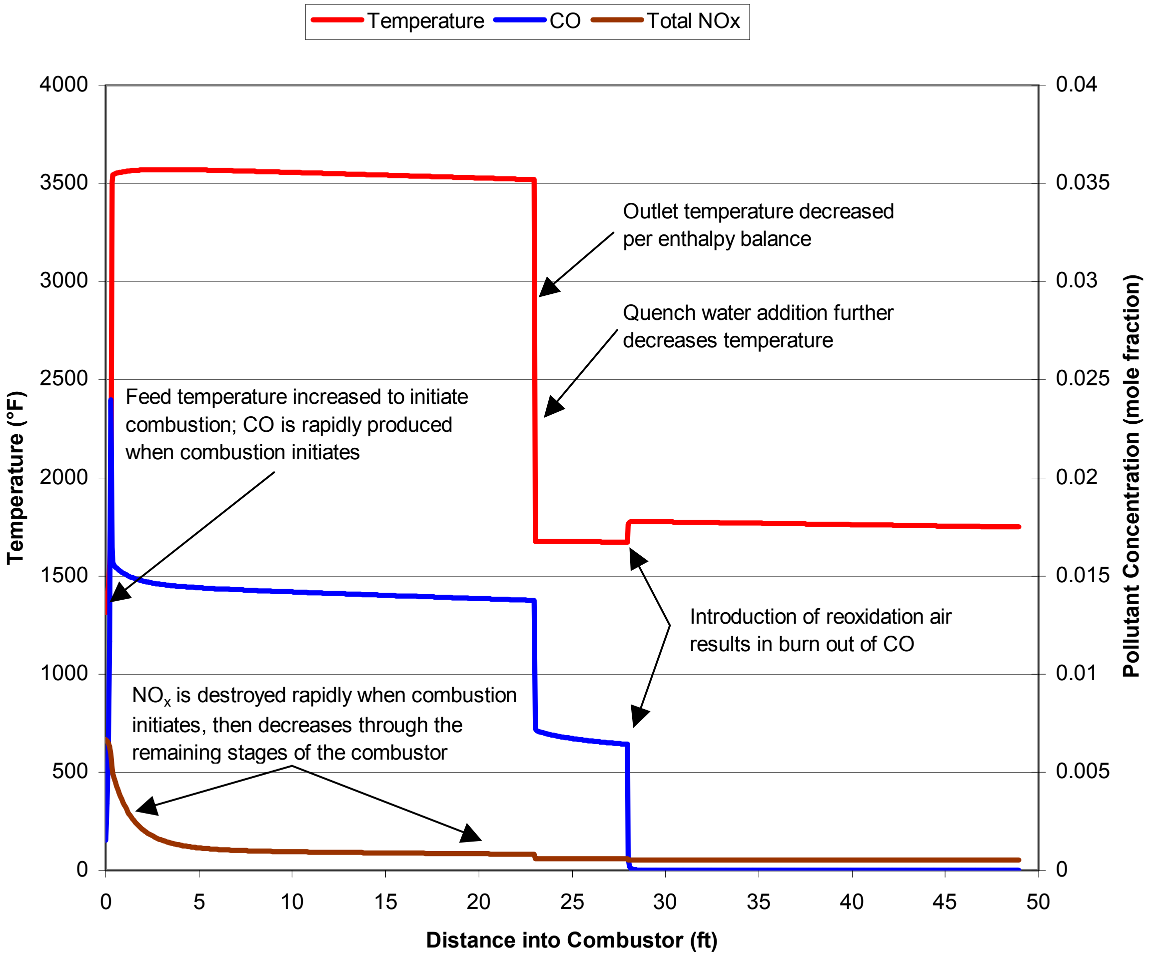

Figure 7. Results from staged combustion kinetic modeling.

5.2 SNCR

Model predictions for key species concentrations, as a function of temperature and amount of NH_3 input, are summarized graphically in Figure 8. From this plot, the following observations can be made:

- The optimal operating temperature range for SNCR would be achieved using an inlet temperature of 850°C, while limiting the outlet temperature to 950°C or less. Below 850°C, NO_x destruction is limited. Above 950°C, NO_x will begin to reform.

- A NH_3/NO_x ratio of 1.2 appears to be optimal (this corresponds to an ammonia input mole fraction of 0.06 in Figure 8). Higher ratios result in excessive NH_3 slip, while lower ratios result in incomplete NO_x destruction.

Figures 9 and 10 display the results as surface plots. Again, it can be seen that an operating temperature range of 850–950°C appears to be optimal, and that the optimal NH_3/NO_x ratio is around 1.2. Figure 11 shows a similar surface plot for CO. From this plot, it can be seen that all CO is essentially destroyed above 880°C in a limited-oxygen environment. Hence, with tight process control, the SNCR can effectively accomplish thermal oxidization of CO, thus eliminating the need for a separate unit operation for this purpose.

From a careful inspection of the modeling results, the optimal operating temperature appears to be around 900°C. At this temperature, the NO_x outlet concentration was minimized to 173 ppmv, with a corresponding NH_3 slip concentration of <5 ppmv. Also at this temperature, CO was effectively reduced to <5 ppmv.

Note the presence of peaks between 840 – 880°C in Figures 9, 10, and 11. It is believed that these peaks are artifacts of using a 10°C step increment in very steep gradient regions. Additional model cases should be performed using a smaller temperature step to further investigate this anomaly.

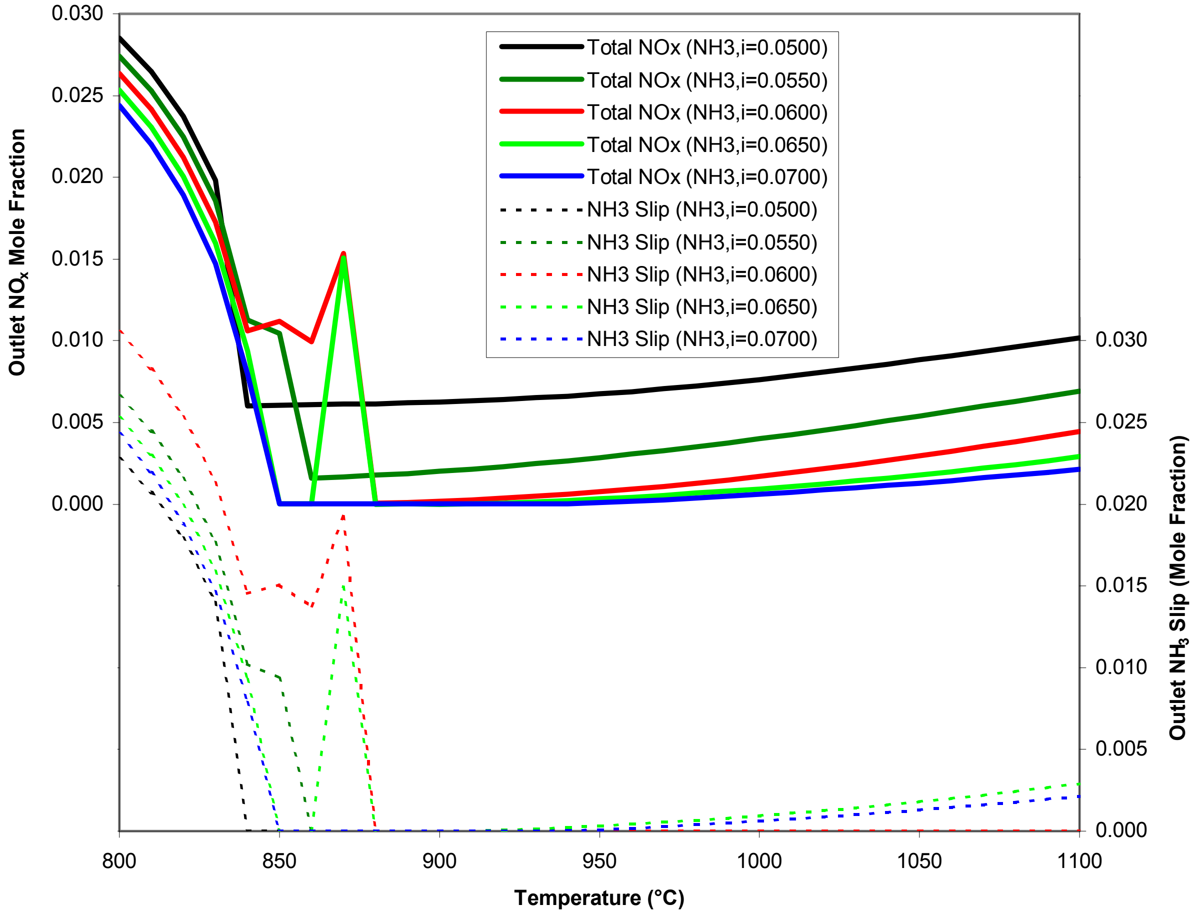

Figure 8. Theoretical NO_x destruction and NH_3 slip achievable with SNCR.

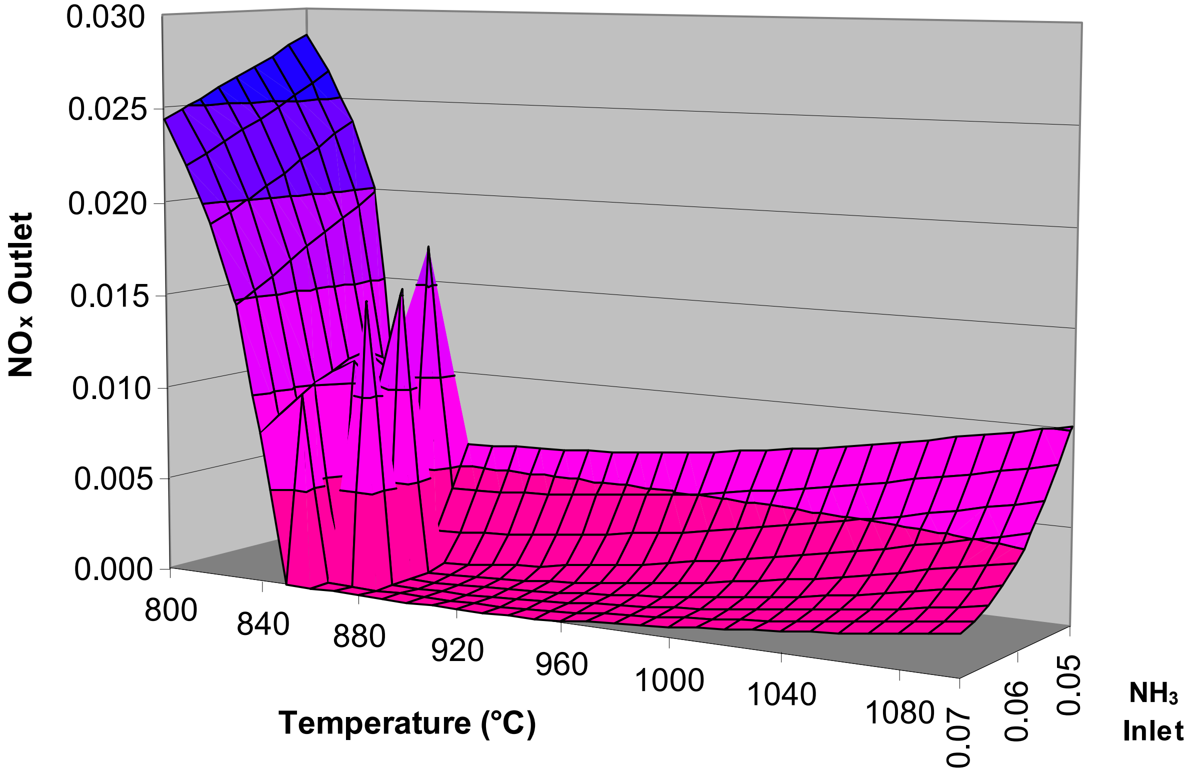

Figure 9. Predicted NO_x response surface for SNCR.

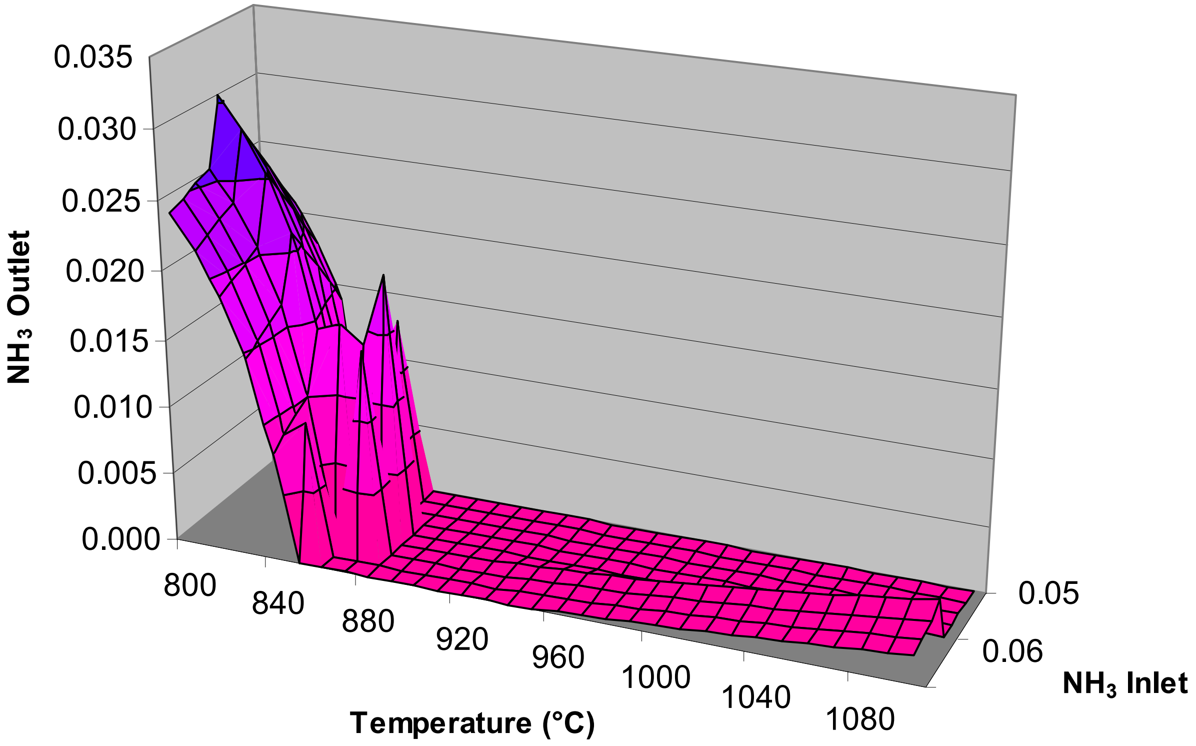

Figure 10. Predicted NH_3 slip response surface for SNCR.

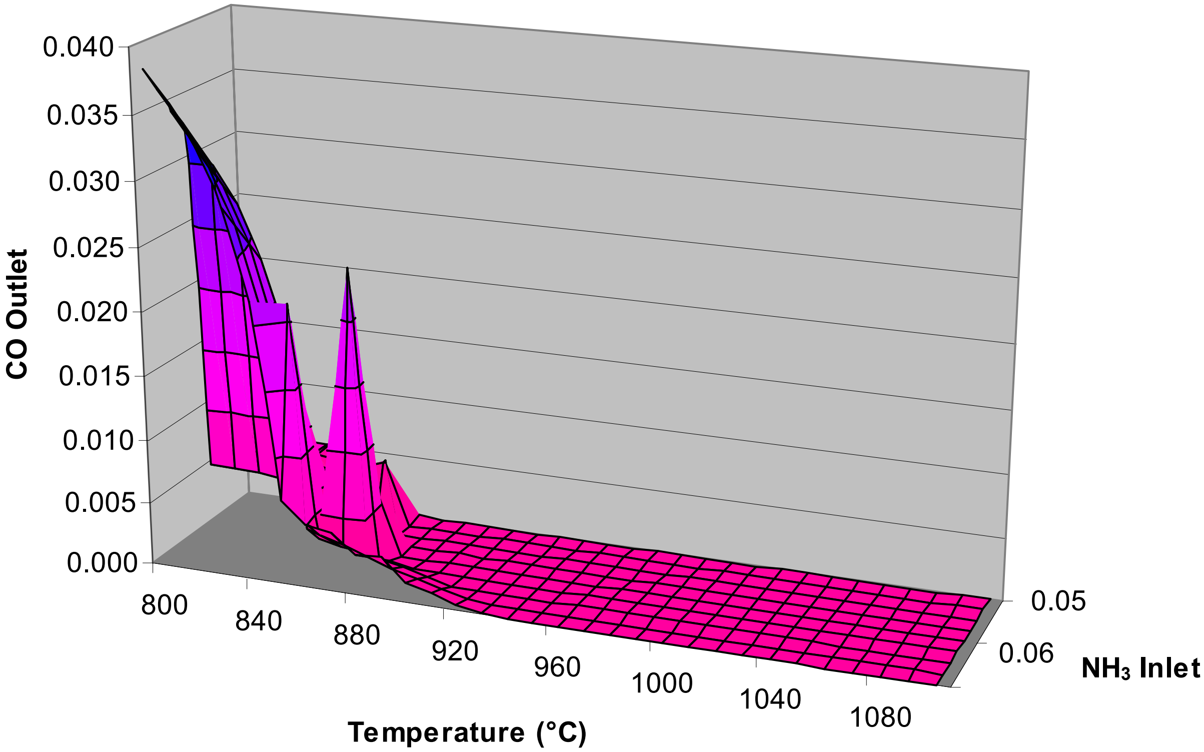

Figure 11. Predicted CO response surface for SNCR.

5.3 High-Temperature NO_x Destruction

Kinetic and thermodynamic model predictions for NO_x outlet concentration as a function of temperature are summarized graphically in Figure 12. From this plot, and from the raw model output, the following observations can be made:

- Kinetic and thermodynamic models predict the same results at 3400°F and above. In addition, reaction kinetics are extremely fast at very high temperatures.
- Kinetic predictions indicate that 3950 ppmv NO_x is the theoretical minimum concentration achievable given the input concentration and reactor size. This minimum is achieved at 3344°F.
- Predictions from the Chemkin Equil and HSC Gibbs codes match very well in the range of 1000 – 4300°F. At higher temperatures, results from these codes differ by 5 – 15%.

If the kinetic curve in Figure 12 could be shifted downward and to the left, it would be possible to match the more favorable thermodynamic curve at cooler temperatures. To investigate this possibility by increasing gas residence time, the following steps were taken:

- The offgas was heated to 1840°C (3344°F) for 1.96 seconds in a 5-ft diameter reactor (i.e., a single point was taken from the modeling results shown in Figure 12). This temperature was selected because it represents a reasonable upper limit for commercially available refractory designed for combustion chamber fabrication. The resulting outlet NO_x concentration was 4172 ppmv.

- The composition resulting from the previous step was input into a Chemkin Plug model using a 1 ft diameter × 2500 ft length reactor at 1200°C. This temperature was selected because it allows flexibility in refractory material selection. The resulting NO_x concentration at the pipe exit (2500 ft length, 36 second residence time) was 4050 ppmv. This is an order of magnitude greater than the equilibrium NO_x concentration at 1200°C of 414 ppmv.

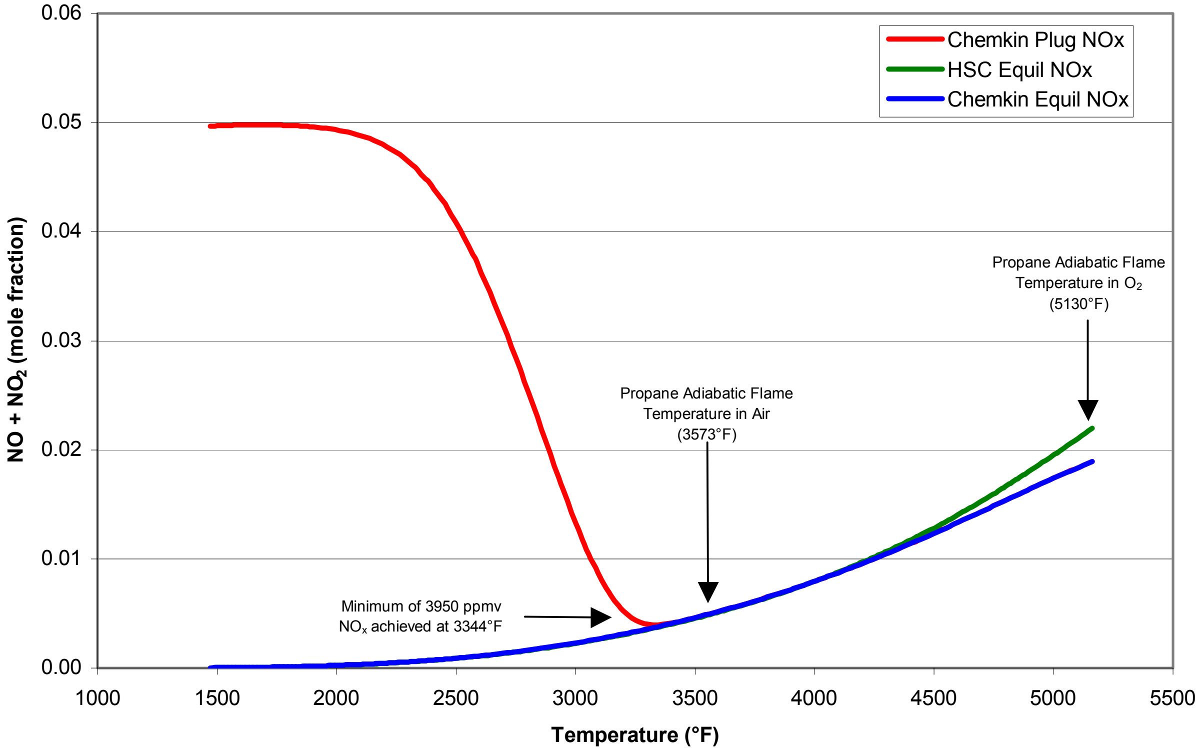

Figure 12. Kinetic and thermodynamic theoretical NO_x destruction at high-temperatures.

Another attempt was made at shifting the kinetic curve from Figure 12 downward and to the left. In this case, however, small amounts of various reductants were added to the offgas. Results of this modeling are shown in Figures 13, 14, and 15. The following observations can be made from these results:

- For CH_4, H_2, and NH_3 addition, a localized minimum NO_x concentration is observed between 3300 – 3400°F. This matches well with predictions for using temperature alone without addition of a reductant.

- H_2 is not effective as a reductant under the conditions modeled. This is evidenced by the fact that increasing the amount of H_2 has little effect on outlet NO_x concentration.

- Both CH_4 and NH_3 enhance NO_x reduction at high temperatures, although the effect is small.

- Both CH_4 and NH_3 enhance NO_x reduction in the 1600 – 1900°F range. However, the effect of NH_3 addition is much more dramatic.

- In order to achieve very low NO_x outlet concentrations (i.e., <100 ppmv) in the 1600 – 1900°F range, NH_3 must be added such that the NH_3/NO_x ratio is slightly above 1. Thus, the high-temperature model and the SNCR model are identical for this condition.

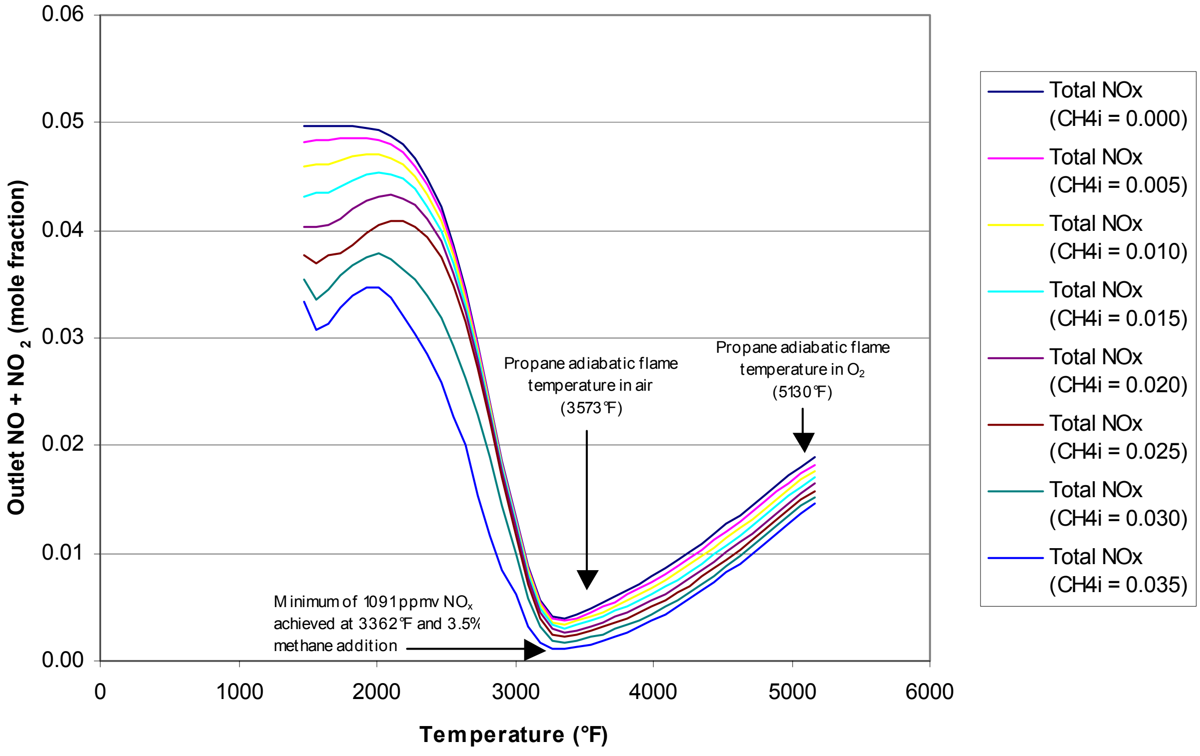

Figure 13. Kinetic predictions for high-temperature NO_x destruction with methane addition.

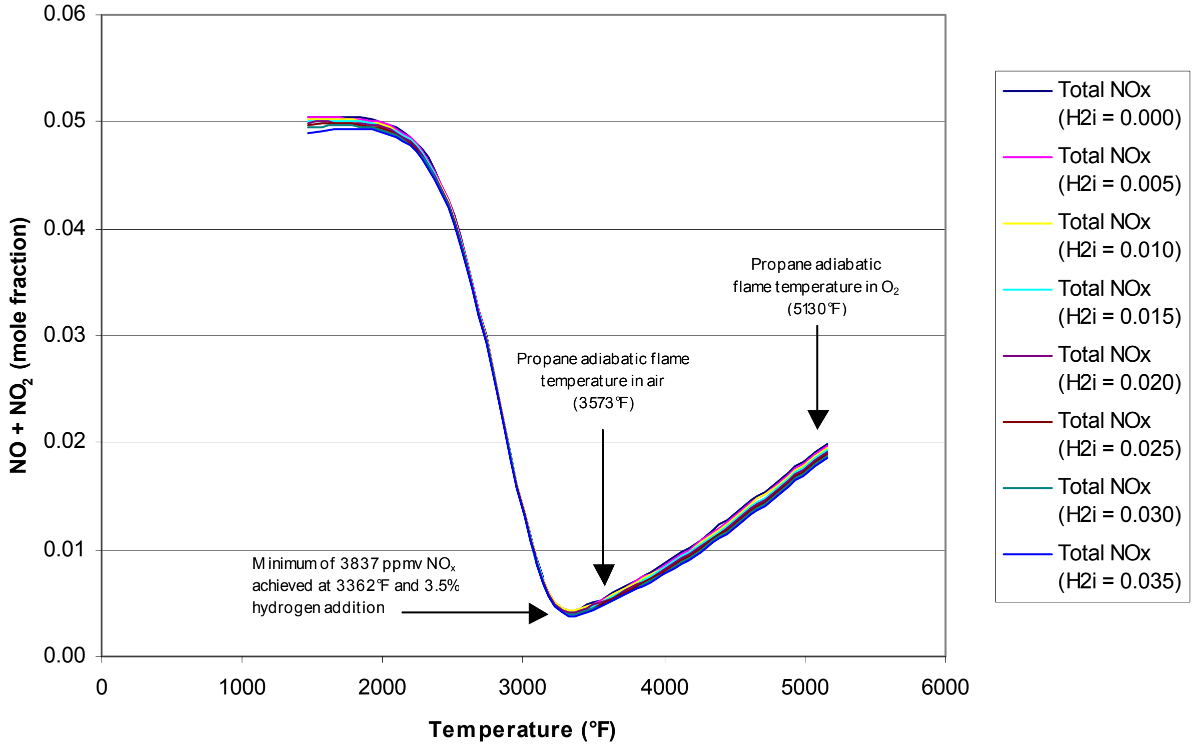

Figure 14. Kinetic predictions for high-temperature NO$_x$ destruction with hydrogen addition.

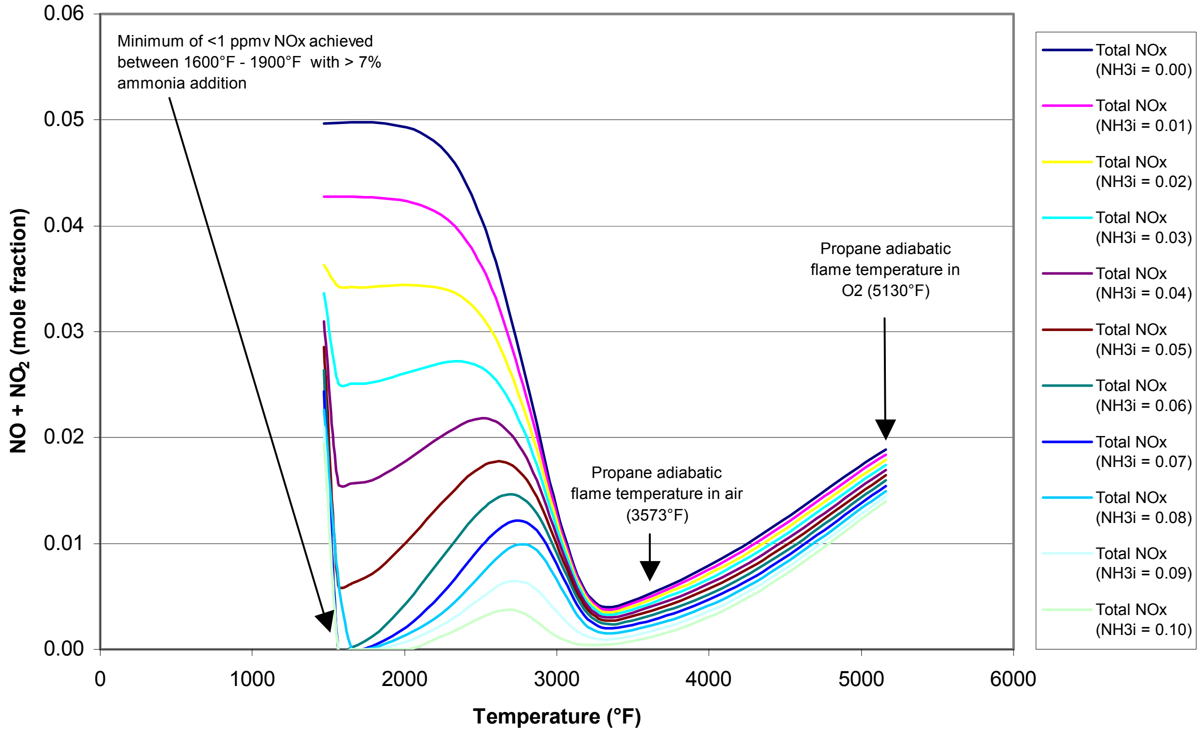

Figure 15. Kinetic predictions for high-temperature NO$_x$ destruction with ammonia addition.

6. CONCLUSIONS & RECOMMENDATIONS

6.1 Conclusions

6.1.1 Feasibility of Technologies

Based on the results of kinetic modeling performed in this study, staged combustion is capable of adequately reducing NO_x in the IWVF off-gas stream. Feasibility of staged combustion for NO_x abatement has previously been demonstrated in pilot-scale testing for an off-gas stream similar to that expected from vitrification of SBW.[3,4] NO_x outlet concentrations from this model and previous models match well with pilot-scale results,[2] signifying that a suitable tool exists for use in design optimization.

Kinetic modeling also indicates that SNCR is a viable option for NO_x abatement in the IWVF flowsheet. Optimal temperature and reductant addition ranges have been identified. In addition, results indicate that SNCR can potentially reduce CO emissions, thus eliminating the need for a separate thermal oxidation step.

Modeling results indicate that NO_x destruction using high temperature alone is inadequate at reducing emissions to target levels (1000 ppm NO, 100 ppm NO_2). The addition of a reductant improves NO_x DRE at high temperature, and additionally lowers the optimal operating temperature. However, to achieve the desired NO_x abatement, significant reductant addition is required; thus, the high-temperature model and the SNCR model are identical for this condition.

As stated previously, results from this study were considered in a broader study to directly compare and down-select IWVF NO_x abatement options. Hence, a more comprehensive comparison of these technologies is documented elsewhere.[1]

6.1.2 Knowledge Gaps (Uncertainty of Models)

Combustion kinetics has been studied for many years. Although work in this area continues to advance, this field is considered mature. Hence, confidence in the reaction chemistry used for this study is high. However, there are some uncertainties associated with the models developed. The following list summarizes the key uncertainties and knowledge gaps:

- Kinetic modeling alone does not adequately consider the effect of mixing and fluid dynamics. This uncertainty is common to all models developed in this study.

- For the staged combustion model, grouping the combustion chamber with the reduction stage into a single plug flow reactor is an over simplification. The error in NO_x outlet concentration and temperature resulting from this assumption should be quantified, or the model should be revised to eliminate this over simplification.

- The SNCR process was modeled isothermally in order to identify optimal temperature ranges for operation. In practice, however, significant heat will be produced from the reaction of NH_3 with NO_x. In addition, the reaction of CO to CO_2 is also exothermic.

6.2 Recommendations

6.2.1 Model Validation Requirements/Needs

6.2.1.1 Staged Combustion. For staged combustion, limited validation of the model has already been performed. Pilot-scale tests have been completed using simulated NWCF offgas, and data from these tests match reasonably well with model predictions.[2] However, additional validation should be considered in two areas. First, the model should be validated against pilot-scale test data utilizing vitrification offgas rather than calcination offgas as the simulant. It is strongly recommended that this validation need be completed. Second, the model predictions could be validated on a larger scale (¼, ½, or full-scale). It is recommended that this validation need be completed if funding is available.

6.2.1.2 SNCR. For SNCR, no model validation has been performed. In addition, SNCR data using an off-gas composition similar to the anticipated IWVF off-gas composition do not exist. Lab or pilot scale proof of principle testing is required using simulated vitrification offgas. In addition to demonstrating NO_x destruction, validation testing should also confirm whether CO can be adequately destroyed using SNCR. In order to adequately validate the model through testing, due consideration must be made to tightly control temperature and the rate of reductant addition. It is strongly recommended that model validation be completed, but only if serious consideration is given to implementation of SNCR in the IWVF flowsheet.

6.2.1.3 High-Temperature NO_x Destruction. For high-temperature NOx abatement, no model validation has been performed. Model validation for this technology is not recommended due to the following reasons:

- Model results do not indicate significant promise for successful implementation of this technology

- Validation testing will be complicated and costly due to anticipated difficulties in identifying suitable materials of construction and heat sources for the high-temperature environment.

6.2.2 Lab/Pilot-Scale Data Needs

In addition to the model validation tasks identified above, other lab and/or pilot-scale data are needed in order to design an optimal NO_x abatement strategy for the IWVF. These needs are briefly summarized below.

6.2.2.1 ***Staged Combustion.*** As shown in Table 5 of this report, the off-gas stream will be diluted by a factor of six due implementation of staged combustion. The result of this dilution is that off-gas equipment downstream of the combustor must be sized significantly larger than if an alternative NO_x abatement technology were selected. Hence, a flow minimization study is needed for staged combustion NO_x abatement. In this study, flow minimization must be balanced with the need to maintain stable combustion, as well as the need to limit combustion chamber temperature to protect the refractory lining. O_2 enrichment and/or flue gas recycle are options that could be considered.

A second data need for staged combustion relates to the fate of chlorinated organics. These trace components were not included in the kinetic model developed for this study. It is anticipated that chlorinated organics will be easily destroyed in the combustion process. However, due to very stringent maximum achievable control technology (MACT) limits that may apply for poly-chlorinated dioxins/furans, DRE for these compounds should be demonstrated. In order to obtain a clear picture of the fate of these compounds, this testing should be performed in a test setup that includes a quench operation immediately downstream of the staged combustor. In this manner, the probability of chlorinated organics to reform upon cooling will be adequately considered.

6.2.2.2 SCR. Significant SCR testing has been performed previously using NWCF offgas. However, due to differences in off-gas composition produced by the calcination and vitrification processes, SCR testing should be performed using a vitrification off-gas simulant.

More importantly, a long-term test is required to determine the extent of catalyst deactivation that will occur due to poisoning from trace off-gas species. Other items that should be experimentally verified in a parametric study include:

- Ascertain the effect of PICs, hydrocarbons, and other minor constituents of concern
- Quantify N_2O production
- Quantify the propensity to form ammonium salts such as NH_4NO_3 and $(NH_4)_2SO_4$.

6.2.3 Future Modeling Tasks

6.2.3.1 Staged Combustion. Two enhancements to the current staged combustion kinetic model should be considered. First, the model should be updated to include thermodynamic data and kinetic expressions/rates for combustion of propane. These mechanisms and data are available in the open literature.[21,22] Second, key trace species and pollutants expected in the IWVF offgas should be added to the model.[m]

CFD modeling of a multi-stage combustor should be completed in order to properly consider mixing and fluid dynamics in the design. Using this model in conjunction with the kinetic model, an optimization study could be performed to provide the basis for the best design.

Consideration should be given to integrating the kinetic model developed for this study (or an enhanced kinetic model as outlined above) into the IWVF stead-state process model. This would ensure that impacts to/from the NO_x abatement unit are properly considered when modifications to the flowsheet are evaluated.

6.2.3.2 SCR. Due to the current lack of data, it is recommended that kinetic modeling of the SCR process be delayed until catalyst selection has been finalized. Once this decision has been made, an effort to obtain thermodynamic and kinetic data for the catalyst should be undertaken. This may be as trivial as a vendor request, or as complex as setting up and running laboratory experiments to generate the required data. Once a plan has been arrived at for obtaining the required data, kinetic modeling should be initiated. This modeling ideally should include a rigorous energy balance, which would precede an optimization study on residence time, bed sequencing, and interstage cooling requirements.

Follow-on tasks for SCR modeling that should be considered include CFD modeling and integration with the IWVF steady-state process simulator.

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[m] It is anticipated that sufficient kinetic mechanisms and data may not exist for every pollutant of interest. Therefore, a thorough literature search is required to define the scope for this modeling task.

6.2.3.3 SNCR. The SNCR model developed in this study should be enhanced to include a rigorous energy balance. In addition, an optimization study should be considered to optimize reactor sequencing and interstage cooling.

Because of the narrow operating window for temperature and NH_3 addition, dynamic simulation should also be considered for the SNCR process. This modeling could aid in the development of a suitable control strategy for this process.

Additional follow-on tasks for SNCR modeling should include CFD modeling and integration with the IWVF steady-state process simulator.

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Appendix A

Chemkin Input Files

Gas Chemistry Input File for Chemkin Plug and Equil Applications

```
ELEMENTS H   O    C   N  AR END
SPECIES
H2 H
CH4 CH3 CH2 CH CH2O HCO CO2 CO O2 O OH HO2 H2O2 H2O
C2H C2H2 HCCO C2H3 C2H4 C2H5 C2H6 CH2OH CH3O HCCOH H2CCCH
C3H2  CH2(S) CH2CO C C4H2 C5H2 H2CCCCCH HCCCHCCH C5H5 C6H2
CH2CHCCH HCCHCCH H2CCCCH C6H5 C6H6 C3H4 C3H4P C6H5O
CH2CHCHCH CH2CHCCH2 C2 C2O C6H5C2H C6H4 OCHCHO C4H CH3O2 C2H2OH
H2C4O CH2CHCHCH2 CH3OH CH2HCO CH3CO CH3HCO CH3OOH AR
NO N NH NH2 HNO HCN NCO CN N2O NNH HNCO N2H2 CH3CN CH2CN
C2N2 NO2 HOCN HCNO H2CN NH3 H2NO NCN HONO NO3 N2
END
THERMO
C6H5C2H           102494H   6C   8    0    0G   300.000  4000.000 1000.00    0 1
 0.11752088E+02 0.30158901E-01-0.13680864E-04 0.29020322E-08-0.23512366E-12    2
 0.34440183E+05-0.38501116E+02-0.72124976E+01 0.99088942E-01-0.11594625E-03    3
 0.76501033E-07-0.21534190E-10 0.38888275E+05 0.55496023E+02                   4
C2H5               83194H   5C   2    0    0G   300.000  4000.000 1400.00    0 1
 0.87349157E+01 0.54537677E-02-0.37647177E-06-0.31297920E-09 0.52844000E-13    2
 0.10265269E+05-0.23104086E+02 0.24398923E+01 0.13747212E-01-0.85500653E-06    3
-0.31469924E-08 0.93754355E-12 0.13158588E+05 0.13099146E+02                   4
C2H3               83194H   3C   2    0    0G   300.000  4000.000 1400.00    0 1
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 0.32229627E+05-0.15977573E+02 0.24955740E+01 0.10269993E-01-0.10226917E-05    3
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CH2                83194H   2C   1    0    0G   300.000  4000.000 1400.00    0 1
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-0.30893967E-08 0.14288692E-11 0.85533762E+04 0.10920868E+02                   4
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OCHCHO            120596H   2C   2O   2    0G   300.000  3000.000 1000.00    0 1
 0.49087462E+01 0.13182673E-01-0.71416730E-05 0.18461316E-08-0.18525858E-12    2
-0.27116386E+05 0.59148768E+00 0.25068862E+01 0.18899139E-01-0.10302623E-04    3
 0.62607508E-09 0.88114253E-12-0.26427374E+05 0.13187043E+02                   4
CH3O2             BUR95 H   3C   1O   2    0G   200.000  6000.000  1000.000  0 1
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 0.52621851E 03-0.99423847E 01 0.20986490E 01 0.15786357E-01 0.75683261E-07    3
-0.11274587E-07 0.56665133E-11 0.20695879E 04 0.15007068E 02 0.33715510E+04    4
CH3OOH            BUR95 H   4C   1O   2   00G   200.000  6000.000  1000.000    1
 0.61600316E+01 0.10239957E-01-0.36101507E-05 0.57550301E-09-0.34178147E-13    2
-0.17654526E+05-0.61911544E+01 0.49652507E+01 0.92343510E-03 0.34455956E-04    3
-0.44469600E-07 0.17456120E-10-0.16726970E+05 0.29880275E+01-0.14980760E+05    4
C2H2OH HCCO TRAN  121196H   3C   2O   1    0G   300.000  3000.000 1000.00    0 1
 0.57206843E+01 0.10704185E-01-0.50358494E-05 0.11324499E-08-0.10086621E-12    2
 0.12849424E+05-0.47081776E+01 0.81498282E-01 0.31640644E-01-0.34085361E-04    3
 0.18978838E-07-0.41950165E-11 0.14060783E+05 0.22908977E+02                   4
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HNO               121286H   1N   1O   1     G  0300.00   5000.00  1000.00      1
 0.03615144E+02 0.03212485E-01-0.12603370E-05 0.02267297E-08-0.15362358E-13    2
 0.11769108E+05 0.04810263E+02 0.02784402E+02 0.06609646E-01-0.09300223E-04    3
 0.09437980E-07-0.03753146E-10 0.12025976E+05 0.09035629E+02                   4
END
REACTIONS
OH+H2=H2O+H                    2.144E8    1.52    3449.    ! MICHAEL 1992
O+OH=O2+H                      2.02E14     -0.4  0.0      ! MASTEN 1990
O+H2=OH+H                      0.506E+05  2.670   6290.000 ! KLEMM,ET AL 1986
H+O2+M=HO2+M                   2.1E18     -1.0     0.0  ! NH2-NO2 paper
    H2O/10.0/  CO2/4.2/  H2/2.86/  CO/2.11/  N2/0.0/
H+O2+N2=HO2+N2                 6.7E19     -1.42     0.0  ! NH2-NO2 paper
OH+HO2=H2O+O2                  1.9E16     -1.0     0.0 ! Kim et al 25th Symp
H+HO2=2OH                      1.69E14    0.0      874.  ! EURCOM 1992
H+HO2=H2+O2                     4.28E13   0.0     1411.  ! EURCOM 1992
H+HO2=O+H2O                    3.01E13     0.0     1721.  ! EURCOM 1992
O+HO2=O2+OH                    3.25E13     0.0      0.0   ! EURCOM 1992
2OH=O+H2O                      4.331E3    2.7     -2485.7  !MICHAEL 1992
H+H+M=H2+M                     0.100E+19 -1.000      0.000 ! D-L
  H2O/0.0/  H2/0.0/ CO2/0.0/
H+H+H2=H2+H2                   0.920E+17 -0.600      0.000
H+H+H2O=H2+H2O                 0.600E+20 -1.250      0.000
H+H+CO2=H2+CO2                 0.549E+21 -2.000      0.000 ! D-L
H+OH+M=H2O+M                   0.160E+23 -2.000      0.000 ! D-L
    H2O/5/
H+O+M=OH+M                     0.620E+17 -0.600      0.000 ! D-L
    H2O/5/
O+O+M=O2+M                     0.189E+14  0.000  -1788.000 ! NBS
   H2O/5/   CO/2/   CO2/3/  H2/2/
HO2+HO2=H2O2+O2                4.20E14    0.0     11982 ! HIPPLER JCP 1990
 DUP
HO2+HO2=H2O2+O2                1.3E11     0.0     -1629 !
 DUP
H2O2+M=OH+OH+M                 0.130E+18  0.000  45500.000
   H2O/5/ CO/2/ CO2/3/    H2/2/
H2O2+H=HO2+H2                  1.69E12    0.0     3755.  !EURCOM
H2O2+H=OH+H2O                  1.02E13    0.0     3576.  ! 1992
H2O2+O=OH+HO2                  6.63E11    0.0     3974   !
H2O2+OH=H2O+HO2                7.83E12    0.0      1331. !
!CH3+CH3(+M)=C2H6(+M)                9.22E16   -1.174   635.8 ! PILL,WAG 23RD
!   LOW/1.135E36  -5.246 1704.8/
!   TROE/0.405 1120. 69.6/
!    H2/2/ CO/2/ CO2/3/ H2O/5/
CH3+CH3(+M)=C2H6(+M)             2.1E16  -0.97   620. ! GRI2.11
  LOW /1.26E50 -9.67 6220/
  TROE/ 0.5325 151 1038 4970 /
  N2/1.43/ H2O/8.59/ H2/2/ CO/2/ CO2/3/
!CH3+H(+M)=CH4(+M)                  6.0E16   -1.0   0.0
!  LOW/8.0E26  -3.0 0.0/
!   SRI/0.45 797. 979./
!    H2/2/ CO/2/ CO2/3/ H2O/5/
!CH3+H(+M)=CH4(+M)               1.0E17     -0.82   315.   GRI-MECH
!  LOW/7.0E33  -4.88 2225.0/
!  TROE/0.7086  134.0 1784.0 5740.0/
! H2/2.86/ H2O/8.57/ CH4/2.86/  CO/2.14/ CO2/2.86/ C2H6/4.29/
CH3+H(+M)=CH4(+M)               1.3E16     -0.63   383.  ! GRI-MECH2.11
  LOW/1.75E33  -4.76 2440.0/
  TROE/0.783  74.0 2941.0 6964.0/
 H2/2.86/ H2O/8.57/ CH4/2.86/  CO/2.14/ CO2/2.86/ C2H6/4.29/ N2/1.43/
CH4+O2=CH3+HO2                 0.790E+14  0.000  56000.000 ! SKINNER ET AL 1972
!CH4+O2=CH3+HO2                 4.000E+13  0.000  57000.000 !  CEC 1994
CH4+H=CH3+H2                   1.3E4    3.0   8040.  !cec 92
CH4+OH=CH3+H2O                 0.160E+07  2.100   2460.000 ! TULLY
CH4+O=CH3+OH                     1.02E9     1.5     8604. !TSANG
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CH4+HO2=CH3+H2O2               0.180E+12  0.000  18700.000 ! NBS
CH3+HO2=CH3O+OH                8.0E12   0.0  0.0 ! Jam&PG rbn (Troe unpub.)
CH3+O=CH2O+H                      8.0E13   0.0   0.0    !GUTMAN
CH3+O2=CH3O+O                 2.87E13      0.0   30481  !frenk JPC 1995
CH3+O2=CH2O+OH                 1.85E12     0.0   20315 !Frenk jpc 1995
CH3+O2(+M) = CH3O2(+M)      7.8E08  1.20     0 ! CEC94
  LOW  / 5.4E25 -3.30  0 /                     !
  N2/1.1/  H2O/10/
! cec94 (Ar) (300-800) UF=2
!
CH3O2+H = CH3O+OH           1.0E14  0.00     0 ! NBS86
! nbs86 (300-2500) UF=3
!
CH3O2+O = CH3O+O2           3.6E13  0.00     0 ! NBS86
! nbs86 (300-2500) UF=3
!
CH3O2+OH = CH3OH+O2         6.0E13  0.00     0 ! NBS86
! nbs86 (300-2500) UF=5
!
CH3O2+HO2 = CH3OOH+O2       2.5E11  0.00 -1570 ! CEC94
! cec94 (298-700) UF=1.3-2.0
!
CH3O2+H2O2 = CH3OOH+HO2     2.4E12  0.00  9940 ! NBS86
! nbs86 (300-2500) UF=10
!
CH3O2+CH2O = CH3OOH+HCO     2.0E12  0.00 11665 ! NBS86
! nbs86 (300-2500) UF=10
!
CH3O2+CH4 = CH3OOH+CH3      1.8E11  0.00 18500 ! NBS86
! nbs86 (300-2500) UF=10
!
CH3O2+CH3 = CH3O+CH3O       2.4E13  0.00     0 ! NBS86
! nbs86 (300-2500) UF=3
!
CH3O2+CH3O = CH2O+CH3OOH    3.0E11  0.00     0 ! NBS86  10
! nbs86 (300-2500) UF=5
!
CH3O2+CH2OH = CH2O+CH3OOH   1.2E13  0.00     0 ! NBS86/p
! nbs86 (300-2500) UF=5
!
CH3O2+CH3OH = CH3OOH+CH2OH  1.8E12  0.00 13700 ! NBS86
! nbs86 (300-2500) UF=5
!
CH3O2+CH3O2 = CH3O+CH3O+O2  1.0E11  0.00   300 ! CEC94
CH3O2+CH3O2 = CH3OH+CH2O+O2 4.0E09  0.00 -2210 ! CEC94
! cec94 ktot=5.5E10/0/-835 (298-700,UF=1.3-2.0), k1/k2=25/0/1170
!
CH3OOH = CH3O+OH             6.3E14  0.00 42300 ! LIG/LES91 (nist)
! LIG/LES91 (600-700,1atm,N2) UF=*
!
CH3OOH+H = CH3O2+H2          8.8E10  0.00  1860 ! SLE/WAR77 (nist)
! SLE/WAR77 (250-358) UF=*
!
CH3OOH+H = CH3O+H2O          8.2E10  0.00  1860 ! SLE/WAR77 (nist)
! SLE/WAR77 (250-358) UF=*
!
CH3OOH+O = CH3O2+OH          1.0E12  0.00  3000 ! VAG/RAV90/p,est (nist)
! VAG/RAV90 ktot=6.4E9 (297K) UF=*
! Ea est similar to cec rec
! cec92/94 ktot=4.2E11/0.57/2762 (250-2200) UF=2 apparently too fast
!
CH3OOH+OH = CH3O2+H2O        1.8E12  0.00  -378 ! ATK92/p
! ATK92 (220-430) UF=*  CH3O2 channel only 60% (CH2OOH 40%)
CH2OH+H=CH3+OH                 0.100E+15  0.000      0.000 ! NBS 87
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CH3O+H=CH3+OH                  0.100E+15  0.000      0.000 ! EST JAM
CH3+OH=CH2+H2O                 0.750E+07  2.000   5000.000 ! JAM
CH3+HCO=CH4+CO                  1.2E14    0.0     0.0   ! NBS 86
CH3+H=CH2+H2                   0.900E+14  0.000  15100.000 ! PG
CH3+OH(+M)=CH3OH(+M)           6.3E13    0.0     0.0   !GRI2.11
  LOW/1.89E38  -6.3   3100/
  TROE/0.2105 83.5 5398 8370/
  N2/1.43/ H2O/8.58/ CO2/3/ CO/2/ H2/2/
CH3OH+OH=CH2OH+H2O             5.30E4    2.53     960.    ! NBS
CH3OH+OH=CH3O+H2O              1.32E4    2.53     960.    !
CH3OH+O=CH2OH+OH               3.88E5    2.5      3080.    ! NBS
CH3OH+H=CH2OH+H2               1.7E7      2.1     4868     ! NBS
CH3OH+H=CH3O+H2                4.24E6     2.1     4868     ! NBS
CH3OH+HO2=CH2OH+H2O2           9.64E10     0.0   12578.    ! NBS
!CH3O+M=CH2O+H+M                5.45E13     0.0   13497   ! LIN 1990
!     H2/2/ CO/2/ CO2/3/  H2O/5/
CH2O+H(+M)=CH3O(+M)            5.4E11  0.454  2600. ! GRI2.11
  LOW/1.54E30  -4.8  5560 /
  TROE/ 0.758 94 1555 4200/
  N2/1.43/  H2O/8.58/ CO/2/ H2/2/ CO2/3/
!CH2OH+M=CH2O+H+M               0.100E+15  0.000  25000.000 ! PG
!     H2/2/ CO/2/ CO2/3/  H2O/5/
H+CH2O(+M)=CH2OH(+M)           5.4E11   0.454   3600. ! GRI2.11
    LOW/.91E32 -4.82 6530/
    TROE/0.7187 103 1291 4160/
  N2/1.43/ H2O/8.58/ CO/2/ CO2/3/ H2/2/
CH3O+H=CH2O+H2                 0.200E+14  0.000      0.000 ! PG
CH2OH+H=CH2O+H2                0.200E+14  0.000      0.000
CH3O+OH=CH2O+H2O               0.100E+14  0.000      0.000 ! PG
CH2OH+OH=CH2O+H2O              0.100E+14  0.000      0.000
CH3O+O=CH2O+OH                 0.100E+14  0.000      0.000 ! PG
CH2OH+O=CH2O+OH                0.100E+14  0.000      0.000
CH3O+O2=CH2O+HO2               0.630E+11  0.000   2600.000 ! PG
CH2OH+O2=CH2O+HO2              1.57E15    -1.0       0.0   ! EURCOM 1992
 DUP
CH2OH+O2=CH2O+HO2               7.23E13    0.0      3577.  !
 DUP
CH2+H=CH+H2                    0.100E+19 -1.560      0.000 ! THORNE,ET AL
CH2+OH=CH+H2O                  0.113E+08  2.000   3000.000 ! JAM
CH2+OH=CH2O+H                  0.250E+14  0.000      0.000 ! PG
CH+O2=HCO+O                    0.330E+14  0.000      0.000 ! PG
CH+O=CO+H                      0.570E+14  0.000      0.000 ! PG
CH+OH=HCO+H                    0.300E+14  0.000      0.000 ! PG
CH+OH=C+H2O                  4.0E7   2.0    3000.   ! JAM
CH+CO2=HCO+CO                  0.340E+13  0.000    690.000 ! PG
CH+H=C+H2                      0.150E+15  0.000      0.000 ! THORNE
CH+H2O=CH2O+H                  5.72E12    0.0     -751.0    !LIN
CH+CH2O=CH2CO+H                0.946E+14  0.000   -515.000 ! THORNE
CH+C2H2=C3H2+H                 0.100E+15  0.000      0.000 ! THORNE
CH+CH2=C2H2+H                  0.400E+14  0.000      0.000 ! PG
CH+CH3=C2H3+H                  0.300E+14  0.000      0.000 ! PG
CH+CH4=C2H4+H                  0.600E+14  0.000      0.000 ! PG
C+O2=CO+O                      0.200E+14  0.000      0.000 ! THORNE
C+OH=CO+H                      0.500E+14  0.000      0.000 ! THORNE
C+CH3=C2H2+H                   0.500E+14  0.000      0.000 ! PG
C+CH2=C2H+H                    0.500E+14  0.000      0.000 ! PG
CH2+CO2=CH2O+CO                0.110E+12  0.000   1000.000 ! PG
CH2+O=CO+H+H                   0.500E+14  0.000      0.000 ! JAM 2/87
CH2+O=CO+H2                    0.300E+14  0.000      0.000 ! JAM 2/87
!CH2+O2=CO2+H+H                 0.160E+13  0.000   1000.000
!CH2+O2=CH2O+O                  0.500E+14  0.000   9000.000 ! PG
!CH2+O2=CO2+H2                  0.690E+12  0.000    500.000 ! PG
!CH2+O2=CO+H2O                  0.190E+11  0.000  -1000.000 ! PG
!CH2+O2=CO+OH+H                 0.860E+11  0.000   -500.000 ! PG
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!CH2+O2=HCO +OH                  0.430E+11  0.000   -500.000 ! PG
CH2+O2=CO+H2O     2.20E22   -3.3  2867. ! DOMBROWSKY(HGGW) BER.BUN.1992
CH2+O2=CO2+H+H    3.29E21   -3.3  2867.  !
CH2+O2=CH2O+O     3.29E21   -3.3  2867. !
CH2+O2=CO2+H2     2.63E21   -3.3  2867. !
CH2+O2=CO+OH+H    1.64E21   -3.3  2867. !
CH2+CH2=C2H2+H+H                 0.400E+14  0.000      0.000 ! BRAUN,ET AL
CH2+HCCO=C2H3+CO                0.300E+14  0.000      0.000 ! JAM,1/11/82
CH2+C2H2=H2CCCH+H              0.120E+14  0.000   6600.000 ! BOHLAND ET AL,21S
CH2+CH4=CH3+CH3                 4.3E12    0.0     10030. ! PG 86
CH2O+OH=HCO+H2O                 0.343E+10  1.180   -447.000 ! NBS
CH2O+H=HCO+H2                   1.3E8     1.62    2166. ! CEC 94
CH2O+M=HCO+H+M                  0.331E+17  0.000  81000.000 ! DEAN,C 1980
     H2/2/ CO/2/ CO2/3/  H2O/5/
CH2O+O=HCO+OH                   0.180E+14  0.000   3080.000 ! NBS
CH2O+CH3=HCO+CH4                 7.8E-8      6.1     1967. ! CEC 1994
CH2O+HO2=HCO+H2O2                3.0E12    0.0     13000.  !CEC 1994
CH2O+O2=HCO+HO2                 6.0E13    0.0      40660 ! CEC 94
HCO+OH=H2O+CO                   0.100E+15  0.000      0.000 ! TEMPS
HCO+M=H+CO+M                    1.861E17   -1.0    17000.0  ! GUT,AL WAG 1987
    CO/1.87/   H2/1.87/  CH4/2.81/ CO2/3./ H2O/5./
HCO+H=CO+H2                     0.119E+14  0.250    0.000 ! HARD.. 21ST, JAM
HCO+O=CO+OH                     0.300E+14  0.000      0.000 ! PG
HCO+O=CO2+H                     0.300E+14  0.000      0.000 ! PG
HCO+O2=HO2+CO                   7.58E12    0.0    406. !TIMONEN(GUTMAN)JPC 1988
CO+O+M=CO2+M                    0.617E+15  0.000   3000.000 ! NBS
     H2/2/ CO/2/ CO2/3/  H2O/5/
CO+OH=CO2+H                     1.51E7     1.3     -758   ! BAULCH&DRYSDALE
CO+O2=CO2+O                       2.53E12    0.0     47688. !TSANG,BAULCH
HO2+CO=CO2+OH                   0.580E+14  0.000  22934.000 ! ATRI ET AL ,C 197
C2H6+CH3=C2H5+CH4               0.550E+00  4.000   8300.000
C2H6+H=C2H5+H2                  0.540E+03  3.500   5210.000 ! CLARK
C2H6+O=C2H5+OH                  0.300E+08  2.000   5115.000 ! WARNATZ REVIEW
C2H6+OH=C2H5+H2O                7.23E6     2.0      864. ! CEC 1992
C2H6+O2=C2H5+HO2                5.0E13     0.0     55000. ! JAM /SWB 1996
C2H6+HO2=C2H5+H2O2              1.3E13     0.0     20460  ! CEC 94
C2H4+H=C2H3+H2                  5.42E14    0.0     14902    ! EURCOM 1992
C2H4+O=CH3+HCO                  8.1E6      1.88     180. ! CEC 94
C2H4+O=CH2HCO+H                 4.7E6      1.88     180  !
C2H4+O=CH2CO+H2                 6.8E5      1.88     180  !
C2H4+OH=C2H3+H2O                0.202E+14  0.000   5955.000 ! TULLY 1987
C2H4+O2=CH2HCO+OH               2.0E8      1.5     39000 ! JAM /SWB 1996
C2H4+HO2=CH3HCO+OH               2.2E12    0.0     17200 ! CEC 94,PRD JAM
C2H4+CH3=C2H3+CH4               5.0E11     0.0     15000 !JAM&Pg rbn (Zhang 1990)
CH2+CH3=C2H4+H                  0.400E+14  0.000      0.000 ! JAM
C2H4+H(+M)=C2H5(+M)             1.081E12   0.454    1822.  ! MARINOV
   LOW/1.112E34  -5.0   4448.0/
  TROE/0.5 95.0  95.0    200./
    H2/2/ CO/2/ CO2/3/ H2O/5/
C2H5+H=CH3+CH3                  4.89E12   0.35     0.0   ! JAM(Br-UNk,Frank)
H+C2H5(+M)=C2H6(+M)              5.2E17   -0.99    1580  ! GRI-Mech
   LOW/2.0E41  -7.08   6685/
   TROE/0.8422 125 2219 6882/
    H2/2/ CO/2/ CO2/3/ H2O/5/
C2H5+O2=C2H4+HO2                1.0E10   0.0    -2190. !  cec 92
C2H5+O=CH3+CH2O                 4.2E13   0.0   0.0  !JAM&PG rbn (Slagle 1988)
C2H5+O=CH3HCO+H                  5.3E13  0.0   0.0  !
C2H5+O=C2H4+OH                  3.0E13   0.0   0.0  !
C2H5+OH=C2H4+H2O                2.4E13   0.0    0.0 ! NBS 86
C2H5+HCO=C2H6+CO                 1.2E14  0.0   0.0  ! NBS 86
C2H5+CH2O=C2H6+HCO               5.5E3   2.81   5860 ! NBS 86
!C2H5+HCO=C2H5CHO                1.8E13  0.0    0.0 ! PG rbn (NBS 86)
!C2H5CHO+H=C2H5CO+H2               8.0E13  0.0   0.0  ! PG rbn (Baldwin 1969)
!C2H5CHO+O=C2H5CO+OH             7.8E12  0.0  0.0  ! PG rbn (Herron 1988)
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!C2H5CHO+OH=C2H5CO+H2O          1.2E13   0.0   0.0 ! PG rbn (Atkinson 1992)
!C2H5+CO=C2H5CO                 1.5E11   0.0  4800. ! Pg rbn (NBS 86)
C2H5+CH3=C2H4 +CH4             1.1E12   0.0   0.0  ! CEC 92
C2H5+C2H5=C2H6+C2H4             1.5E12  0.0   0.0   ! CEC 92
C2H2+O=CH2+CO                  6.10E6     2.000   1900.000 ! JAM,FONT,PEETERS
C2H2+O=HCCO+H                  1.43E7     2.000   1900.000 ! JAM,FONT,PEETERS
H2+C2H=C2H2+H                  0.409E+06  2.390    864.300 ! HARDING,SHATZ,CHILE
!H+C2H2(+M)=C2H3(+M)            2.345E15   -0.87   3064.! MARINOV 1995
!  LOW/2.254E40  -7.269 6577./
H+C2H2(+M)=C2H3(+M)            3.114E11    0.58    2589 ! Marinov 1996
  LOW/2.254E40  -7.269 6577./
  TROE/0.5 675. 675./
    H2/2/ CO/2/ CO2/3/ H2O/5/
C2H3+H=C2H2+H2                 0.400E+14  0.000      0.000 ! HOYERMANN
C2H3+O=CH2CO+H                 0.300E+14  0.000      0.000 ! HOYERMANN 21ST
!C2H3+O2=CH2O+HCO               3.60E13  -0.3   0.0 !Knyazev&Slagle JPC 1995/JAM
!C2H3+O2=CH2O+HCO                1.1E23  -3.29    3890. ! BOZ/DEAN 93
!C2H3+O2=CH2HCO+O                 2.5E15  -0.78    3135. !
!C2H3+O2=C2H2+HO2                   5.2E15  -1.26   3310. !
C2H3+O2=CH2O+HCO                4.58E16    -1.39   1015 !  Mebel,et al.
C2H3+O2=CH2HCO+O                 3.03E11    -0.29   10.73 !  JACS 1996
C2H3+O2=C2H2+HO2                  1.34E6     1.61    -383.5 !
C2H3+OH=C2H2+H2O                  2.0E13    0.0     0.0   ! JAM
C2H3+CH2=C3H4+H                  3.0E13     0.0     0.0   ! JAM
C2H3+C2H=C2H2+C2H2             0.300E+14  0.000      0.000 ! MMSK
C2H3+C2H=H2CCCCH+H               3.0E13   0.0     0.0 ! JAM 1996
C2H3+CH3=C2H2+CH4                2.1E13   0.0     0.0 ! NBS, Fahr 91(rbn PG)
C2H3+CH2O=C2H4+HCO               5.4E3   2.81   5860 ! NBS 86
C2H3+HCO=C2H4+CO                9.0E13    0.0    0.0  ! NBS 86
!C2H3+C2H3=CH2CHCCH2+H           4.0E13   0.0   0.0 !JAM
C2H3+C2H3=C2H4+C2H2              1.5E13  0.0   0.0 ! Fahr 91(rbn PG)
C2H3+CH=CH2+C2H2               0.500E+14  0.000      0.000 ! JAM
OH+C2H2=C2H+H2O                  3.37E7    2.0   14000. ! MILLER
OH+C2H2=HCCOH+H                  5.04E5    2.3   13500. ! MILLER
OH+C2H2=CH2CO+H                  2.18E-4   4.5   -1000. ! MILLER
OH+C2H2=CH3+CO                   4.83E-4   4.0   -2000. ! MILLER
OH+C2H2(+M)=C2H2OH(+M)           1.52E8  1.7    1000. ! MILLER&MELIUS
   LOW/1.81E23  -2.0   0.0 /                    ! Atkinson(cited in CEC 92)/PG
  H2/2/  CO/2/   CO2/3/   H2O/5/
HO2+C2H2=CH2HCO+O                1.0E12   0.0   10000 ! JAM
HO2+C2H2=CH2O+HCO               1.0E12   0.00   10000 ! JAM
! last 2 k's crudely based on calculations of Mebel,Morokuma,Lin,et al(C2H3+O2)
HCCOH+H=HCCO +H2               3.0E7   2.0     1000. ! JAM
HCCOH+OH=HCCO+H2O              1.0E7   2.0     1000. !JAM
HCCOH+O=HCCO+OH                 2.0E7  3.0     1900. !JAM(O+C2H2)
C2H2+O=C2H+OH                  0.316E+16 -0.600  15000.000 !MMSK
C2H2OH+H=CH2HCO+H                5.0E13  0.0   0.0   ! JAM 1996
C2H2OH+O=OCHCHO+H               5.0E13   0.0     0.0  ! JAM 1996
C2H2OH+O2=OCHCHO+OH             1.0E12   0.0    5000. ! JAM 1996
CH2HCO+H=CH3+HCO                1.0E14   0.0      0.0   ! JAM
CH2HCO+H=CH3CO+H                3.0E13    0.0      0.0   ! JAM
CH2HCO+O=CH2O + HCO             5.0E13    0.0      0.0   !JAM
CH2HCO+OH=CH2CO+H2O             2.0E13     0.0     0.0    ! JAM
CH2HCO+OH=CH2OH+HCO             1.0E13     0.0     0.0   !JAM
CH2HCO+CH3=C2H5+HCO             5.0E13    0.0   0.0    !JAM
!CH2HCO+CH3=C2H5CHO             5.0E13    0.0    0.0  ! PG rbn
CH2HCO+CH2=C2H4+HCO             5.0E13    0.0   0.0     !JAM
CH2HCO+CH =C2H3+HCO             1.0E14    0.0   0.0    !JAM
CH2HCO+O2=OH+OCHCHO             2.22E11  0.0   1500.   !CEC 1992/JAM
!CH2HCO+O2=CH2O +CO+OH          2.2E11   0.0    1500.  ! PG rbn(cec 94)
OCHCHO+M=HCO+HCO+M              1.0E17    0.0  58000. ! JAM
OCHCHO+H=CH2O+HCO               3.0E13    0.0   0.0  !JAM
!H+CH2CO(+M)=CH2HCO(+M)           1.081E12   0.454    1822.  ! MARINOV/JAM(C2H5)
!   LOW/1.112E34  -5.0   4448.0/
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!  TROE/0.5 95.0  95.0    200./
!    H2/2/ CO/2/ CO2/3/ H2O/5/
!assumed to be same as C2H5 dissociation
!CH2HCO+M=CH2CO+H+M              2.0E15    0.0     42000  ! JAM
!    H2/2/ CO/2/ CO2/3/  H2O/5/
CH2HCO+M=CH3+CO+M               2.0E16    0.0     42000  ! JAM
    H2/2/ CO/2/ CO2/3/  H2O/5/
CH3HCO+OH=CH3CO+H2O             2.3E10   0.73     -1110  ! CEC 94
CH3HCO+H=CH3CO+H2               4.10E9   1.16     2400. ! CEC 94
CH3HCO+CH3=CH3CO+CH4            2.0E-6   5.6      2464 ! CEC94
CH3CO(+M)=CH3+CO(+M)            2.8E13   0.0      17100. ! CEC 94
  LOW/2.1E15 0.0 14000./
  TROE/0.5 1.0E-30 1.E30/    ! These parameters force Fcent to be 0.5 always.
     H2/2/ CO/2/ CO2/3/  H2O/5/
CH3CO+H=CH3+HCO                 2.1E13   0.0    0.0  ! PG rbn
CH3CO+H=CH2CO+H2                 1.2E13  0.0    0.0   ! PG rbn
CH3CO+O=CH3+CO2                  1.5E14  0.0    0.0  ! cec 94
CH3CO+O=CH2CO+OH                4.0E13   0.0    0.0  ! CEC 94
CH3CO+OH=CH2CO+H2O               1.2E13  0.0    0.0   ! NBS 86
CH3HCO=CH3+HCO                  7.1E15   0.0    81280 ! CEC 94
CH3HCO+O=CH3CO+OH               5.8E12   0.0     1800. ! CEC 94
CH3HCO+O2=CH3CO+HO2             3.0E13   0.0     39000.! CEC 94
CH3HCO+HO2=CH3CO+H2O2           3.0E12   0.0     12000. ! CEC 94
CH2CO+O=CO2+CH2                0.175E+13  0.000   1350.000 ! SEE WAGNER,TEMPS ET
CH2CO+H=CH3+CO                 5.93E6   2.0    1300. ! CEC 92 / JAM
CH2CO+H=HCCO+H2                3.0E7     2.0  10000.000 ! JAM 1996
CH2CO+O=HCCO+OH                2.0E7  2.0   10000.000 !
CH2CO+OH=HCCO+H2O              1.0E7   2.0   3000.000 !
CH2CO+OH=CH2OH+CO             7.2E12   0.0   0.0 ! Temps,HggW,et al 1992
CH2CO+OH=CH3+CO2               3.0E12  0.0   0.0 ! Grussdorf 94 (PG rbn)
CH2+CO(+M)=CH2CO(+M)          8.1E11    0.5  4510. ! GRI2.11
  LOW/ 1.88E33 -5.11 7095./
  TROE/ 0.5907 275 1226 5185/
     H2/2/ CO/2/ CO2/3/  H2O/8.58/  N2/1.43/
C2H+O2=CO+CO+H           2.52E13    0.0    0.0    ! GLASS&CURL(STEPHENS)JPC1987
C2H+C2H2=C4H2+H                2.47E12   0.5  -391. !LEONE 1993
C2H+CH4=CH3+C2H2              7.23E12   0.0    976 ! Leone JPC 1996
CH+CO(+M)=HCCO(+M)            5.0E13   0.0    0.0  ! GRI2.11
  LOW/ 1.88E28  -3.74 1936 /
  TROE/ 0.5757 237  1652 5069 /
  N2/1.43/ H2O/8.58/ CO/2/ CO2/3/ H2/2/
HCCO+C2H2=H2CCCH+CO           1.0E11   0.0     3000. ! JAM
H+HCCO=CH2(S)+CO               0.100E+15  0.000      0.000 ! PEETERS 1985
O+HCCO=H+CO+CO                 0.100E+15  0.000      0.000 ! PEETERS 1985
HCCO+O2=CO2+CO+H                1.4E7    1.7        1000. ! HGGW.Peeters,JAM
HCCO+O2=CO +CO +OH             2.88E7     1.7       1000. !
CH+HCCO=C2H2+CO                0.500E+14  0.000      0.000 ! JAM EST
HCCO+HCCO=C2H2+CO+CO           0.100E+14  0.000      0.000 ! MMSK
HCCO+OH=C2O+H2O                6.0E13     0.0    0.0    ! JAM
C2O+H=CH+CO                    1.0E13    0.0     0.0    ! JAM
C2O+O=CO+CO                    5.0E13    0.0      0.0   ! JAM
C2O+OH=CO+CO+H                 2.0E13    0.0     0.0    ! JAM
C2O+O2=CO+CO+O                 2.0E13  0.0   0.0  ! JAM
CH2(S)+M=CH2+M                 0.100E+14  0.000      0.000 ! NBS,ADJ
   H/0.0/ H2O/0.0/ C2H2/0.0/ C6H6/0.0/ N2/0.0/ AR/0.0/
CH2(S)+CH4=CH3+CH3             0.400E+14  0.000      0.000 ! NBS
CH2(S)+C2H6=CH3+C2H5           0.120E+15  0.000      0.000 ! NBS
CH2(S)+O2=CO+OH+H             7.0E13    0.0    0.0  ! CBM/ADJ
CH2(S)+H2=CH3+H                0.700E+14  0.000      0.000 ! NBS
!CH2(S)+H2O=CH3+OH                 1.0E14     0.0      0.0  ! WAGNER
CH2(S)+H2O=CH3+OH             3.01E15  -0.6     0.0   !car/wag 95, hack/hggw 88
CH2(S)+H2O=CH2+H2O             3.0E13     0.0      0.0  ! WAGNER
CH2(S)+C2H2=H2CCCH+H           1.8E14   0.0    0.0   ! WAGNER
CH2(S)+C2H2=CH2+C2H2         4.0E13   0.0    00    ! WAGNER
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CH2(S)+H=CH2+H                 0.200E+15  0.000      0.000 ! JAM
CH2(S)+O=CO+H+H               3.0E13  0.0    0.0    !NBS
CH2(S)+OH=CH2O+H              3.0E13  0.0    0.0    ! NBS
CH2(S)+H=CH+H2                3.0E13  0.0    0.0    ! NBS
CH2(S)+CO2=CH2O+CO             3.0E12  0.0    0.0   ! NBS
CH2(S)+CH3=C2H4+H              2.0E13   0.0   0.0   ! NBS
CH2(S)+CH2CO=C2H4+CO            1.6E14  0.0   0.0   ! WAGNER
CH2(S)+C6H6=C6H5+CH3            1.7E14  0.0   0.0   ! WAGNER
CH2(S)+C6H6=CH2+C6H6            7.0E13  0.0  0.0    !WAGNER
CH2(S)+N2=CH2+N2                1.26E13 0.0  430. ! see Hayes,et al  JPC 1996
CH2(S)+AR=CH2+AR                1.45E13 0.0   884. !see Hayes,et al  JPC 1996
C2H+O=CH+CO                    0.500E+14  0.000      0.000 ! BROWNE
C2H+OH=HCCO+H                  0.200E+14  0.000      0.000 ! JAM,12/22
C2H+OH=C2+H2O             4.0E7    2.0     8000.   !  JAM
C2+H2=C2H+H               4.0E5    2.4     1000.   !  JAM
C2+O2=CO+CO                5.0E13    0.0     0.0   ! JAM
C2+OH=C2O+H                5.0E13    0.0     0.0   ! JAM
C4H2+OH=H2C4O+H               0.666E+13  0.000   -410.000 ! PERRY
C3H2+O2=HCCO+CO+H                   2.0E12  0.0    1000.! JAM
C3H2+O=C2H2+CO                       1.0E14    0.0  0.0   !JAM
C3H2+OH=C2H2+HCO                         5.0E13   0.0      0.0  ! JAM
C3H2+CH2=H2CCCCH+H                  3.0E13    0.0   0.0     ! JAM
C3H2+CH3=CH2CHCCH+H                 2.0E13    0.0   0.0   !JAM
C3H2+C2H2=HCCCHCCH+H                5.0E12    0.0  5000. !JAM
C3H2+H2CCCH=C6H4+H                    1.0E13    0.0  0.0  !JAM
C3H2+HCCO=HCCHCCH+CO                3.0E13     0.0  0.0  !JAM
C3H2+CH2(S)=H2CCCCH+H                5.0E13    0.0   0.0  !JAM
!H2C4O+H=C2H2+HCCO                    5.0E13      0.0      3000. ! JAM
!H2C4O+OH=CH2CO+HCCO                  1.0E7       2.0      2000. ! JAM
H2C4O+OH=C2H2 +CO +HCO               1.0E13     0.0  0.0   !JAM , contrived to
! avoid forming HCCO
H2CCCH+O2=CH2CO+HCO              0.300E+11  0.000   2868.000 ! GUTMAN,21ST
H2CCCH+O=CH2O+C2H              1.4E14   0.000      0.000 ! GUTMAN 23RD(PRD JAM)
H2CCCH+H=C3H2+H2                    5.0E13    0.0   1000.  ! JAM
H2CCCH+OH=C3H2+H2O               0.200E+14  0.000      0.000 ! JAM
H2CCCH+CH2=CH2CHCCH+H            4.0E13    0.0   0.0     !JAM
H2CCCH+CH=HCCHCCH+H              7.0E13    0.0   0.0     !JAM
H2CCCH+CH=H2CCCCH+H              7.0E13    0.0   0.0     !JAM
CH2CHCCH+OH=HCCHCCH+H2O          7.5E6     2.0   5000.   !JAM
CH2CHCCH+H=HCCHCCH+H2            2.0E7     2.0   15000.  !JAM
CH2CHCCH+OH=H2CCCCH+H2O          1.0E7     2.0   2000.   !JAM
H+HCCHCCH=H2CCCCH+H              1.0E14    0.0   0.0     !JAM
H2CCCCH+O2=CH2CO+HCCO               1.0E12   0.0    0.0   ! JAM
H2CCCCH+OH=C4H2+H2O                   3.0E13   0.0       0.0  ! JAM
H2CCCCH+O=CH2CO+C2H                   2.0E13   0.0       0.0  ! JAM
H2CCCCH+O=H2C4O+H                2.0E13    0.0     0.0     ! JAM
H2CCCCH+H=C4H2+H2                    5.0E13    0.0      0.0   ! JAM
H2CCCCH+CH2=C3H4+C2H                2.0E13    0.0     0.0   ! JAM
CH2CHCCH+H=H2CCCCH+H2            3.0E7     2.0   5000.   !JAM
CH2CHCHCH+OH=CH2CHCCH+H2O           2.0E7     2.0    1000.  !JAM
CH2CHCHCH+H=CH2CHCCH + H2           3.0E7     2.0    1000.  !JAM
C6H6+H=C6H5+H2                   3.0E7     2.0   8000.   !JAM
C6H6+OH=C6H5+H2O                 7.5E6     2.0   5000.   !JAM
C6H6+O=C6H5+OH                   2.4E13    0.0   4700.  !FONTIJN(JPC 1991)
C2H3+C2H2=CH2CHCCH+H             2.0E12    0.0   5000.  !F&S 22 SYMP
C2H2+CH2CHCHCH=C6H6+H            1.725E6   1.792  2240.!WESTMORELAND(JPC89)
HCCHCCH+C2H2=C6H5                4.12E6    1.646  2500 !WESTMORELAND(JPC89)
C3H4+H=C3H4P+H                    1.0E13    0.0   5000.!JAM
C3H4+H=H2CCCH+H2                   3.0E7    2.0       5000.  !JAM
C3H4+OH=H2CCCH+H2O                 2.0E7    2.0       1000.  !JAM
C3H4P+H=H2CCCH+H2                  3.0E7    2.0       5000.  !JAM
C3H4P+H=CH3+C2H2                    1.0E14    0.0   4000. ! JAM
C3H4P+OH=H2CCCH+H2O                2.0E7    2.0       1000.  !JAM
C6H5+C2H2=C6H5C2H+H                3.6E12   0.0      8000. !HERZLER&FRANK 92
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C6H5+OH=C6H5O+H                  5.0E13      0.0      0.0   !JAM
C6H5+OH=C6H4+H2O                 1.0E7      2.0   1000.
C6H5+O2=C6H5O+O                  2.6E13  0.0    6120. !FRANK 25TH SYMP
DUP
C6H5+O2=C6H5O+O                  3.0E13  0.0  8981 ! FRANK 25TH SYMP
DUP
C6H5O=C5H5+CO                    7.4E11  0.0  43853.!FRANK 25TH SYMP
CH2+C4H2=H2CCCCCH+H            0.130E+14  0.000   4326.000 ! BOH,TEMPS,WAG 21ST
CH+C4H2=C5H2+H                 0.100E+15  0.000      0.000 ! JAM EST
CH2(S)+C4H2=H2CCCCCH+H             0.300E+14  0.000      0.000 ! EST
C4H2+O=C3H2+CO                 0.120E+13  0.000      0.000 ! MMSK
C4H2+OH=C4H+H2O                 1.0E7     2.0        1000. ! JAM 1996
C4H2+H=C4H+H2                   2.0E7     2.0        2000. ! JAM 1996
C4H+O2=CO+CO+C2H                1.0E13     0.0       0.0   ! JAM 1996
C4H2+C2H=C6H2+H                0.400E+14  0.000      0.000 ! GARDINER?
!C2H2+O2=HCCO+OH                0.200E+09  1.500  30100.000 ! MMSK
C2H2+O2=HCO+HCO                0.200E+09  1.500  30100.000 ! MMSK/Benson 1996
C2H2+M=C2H+H+M                 9.08E30    -3.7  127138. !TSANG&HAMP(TAN&GARD)
     H2/2/ CO/2/ CO2/3/  H2O/5/
!C2H4+M=C2H2+H2+M               0.150E+16  0.000  55800.000 ! KIEFER
!     H2/2/ CO/2/ CO2/3/  H2O/5/
C2H4+M=C2H2+H2+M               3.50E+16  0.000  71500. ! CEC 94
     N2/1.5/  H2O/10/
!C2H4+M=C2H3+H+M                0.140E+17  0.000  82360.000 ! KIEFER
!     H2/2/ CO/2/ CO2/3/  H2O/5/
C2H3+H(+M)=C2H4(+M)                6.1E12  0.27  280.000 !   GRI2.11
      LOW /0.98E30 -3.86 3320./
      TROE /0.7820 207.50 2663.00 6095.00/
  H2/2.85/ CO/2.1/ CO2/2.85/  H2O/7.14/ CH4/2.85/ C2H6/4.29/  N2/1.43/
!C2H3+C2H4=CH2CHCHCH2+H           3.0E12   0.0     1000.  ! JAM
C2H3+C2H4=CH2CHCHCH2+H            5.0E11   0.0    7304 !Tsang&Hampson(from SWB)
CH2CHCHCH2+H=CH2CHCHCH+H2              3.0E7     2.0      13000.  ! JAM
CH2CHCHCH2+H=CH2CHCCH2+H2              3.0E7     2.0      6000.  ! JAM
CH2CHCHCH2+OH=CH2CHCHCH+H2O            2.0E7     2.0      5000.  ! JAM
CH2CHCHCH2+OH=CH2CHCCH2+H2O            2.0E7     2.0      2000.  ! JAM
CH2CHCHCH+H=CH2CHCCH2 + H         1.0E14    0.0       0.0   ! JAM
CH2CHCCH2+H=CH3+H2CCCH            1.0E14    0.0      0.0   ! JAM
CH2CHCCH2+OH=CH2CHCCH+H2O         3.0E13    0.0      0.0   ! JAM
H2CCCCH(+M)=C4H2+H(+M)              1.0E14     0.0   55000. ! JAM
     LOW/ 2.0E15  0.0  48000./
     H2/2/ CO/2/ CO2/3/  H2O/5/
HCCHCCH(+M)=C4H2+H(+M)              1.0E14     0.0   36000. !JAM
     LOW/ 1.0E14 0.0   30000./
     H2/2/ CO/2/ CO2/3/  H2O/5/
CH2CHCCH2(+M)=CH2CHCCH+H(+M)            1.0E14   0.0     50000. ! JAM
    LOW/2.0E15  0.0  42000./
     H2/2/ CO/2/ CO2/3/  H2O/5/
CH2CHCHCH(+M)=CH2CHCCH+H(+M)            1.0E14   0.0     37000. ! JAM
    LOW/1.0E14  0.0  30000./
     H2/2/ CO/2/ CO2/3/  H2O/5/
H+C6H5=C6H6                     5.0E13     0.0      0.0     ! JAM
H+C6H5=C6H4+H2                  2.0E7      2.0    1000. ! JAM
H2CCCH+H(+M)=C3H4(+M)           1.0E17     -0.82   315.  ! CH4(k0*0.5)
   LOW/ 3.5E33  -4.88 2225.0/
  TROE/ 0.7086  134.0 1784.0 5740.0 /
 H2/2.86/ H2O/8.57/ CH4/2.86/  CO/2.14/ CO2/2.86/ C2H6/4.29/
H2CCCH+H(+M)=C3H4P(+M)          1.0E17     -0.82   315.  ! CH4(k0*0.5)
   LOW/ 3.5E33  -4.88 2225.0/
  TROE/ 0.7086  134.0 1784.0 5740.0 /
 H2/2.86/ H2O/8.57/ CH4/2.86/  CO/2.14/ CO2/2.86/ C2H6/4.29/
H2CCCH+H2CCCH=C6H5+H                 1.0E13  0.0    0.0     !JAM
CH+N2=HCN+N                    3.68E7     1.42   20723 ! MILLER 1996
C+N2=CN+N                      6.3E13     0.0    46019.!DEAN,HAN&BOW,ROTH 23RD
CH2+N2=HCN+NH                  0.100E+14  0.000  74000.000 ! PG
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H2CN+N=N2+CH2                  0.200E+14  0.000      0.000 ! JAM
H2CN+M=HCN+H+M                 0.300E+15  0.000  22000.000 ! JAM
C+NO=CN+O                     2.0E13     0.0      0.0    !DEAN,HAN&BOW JPC 1991
C+NO=CO+N                      2.8E13     0.0      0.0 ! DEAN,HAN,&BOW JPC 1991
CH+NO=HCN+O                    4.75E13    0.0     0.0 ! DEAN,HAN&BOW 91&REFS
CH+NO=NCO+H                    1.88E13    0.0    0.0 ! Hershberger 1994 for b.f.
CH+NO=NH+CO                    3.37E13    0.0    0.0 !
CH2+NO=HCNO+H                  1.285E12   0.0    -378.!WOLFRUM 24TH
CH2+NO=HCN+OH                  2.189E12    0.0    -378.!WOLFRUM 24TH
CH3+NO=HCN+H2O                 1.5E-1   3.523   3950. ! miller,et al 1996
CH3+NO=H2CN+OH                 1.5E-1   3.523   3950. ! prod assumed
C2H3+NO=C2H2+HNO                1.0E12   0.0     1000. ! JAM
HCCO+NO=HCNO+CO                1.17E11   0.65     0.0 ! Miller 27th Symp.
HCCO+NO=HCN+CO2                1.45E16   -0.968   648 ! Miller 27th Symp.
!HCCO+NO=HCNO+CO                1.00E13     0.0    0.0 !Glass&Curl for k
!HCCO+NO=HCN+CO2                1.35E13    0.0    0.0 ! b.f. like NCO+NO
HCNO+O=HCO+NO                   7.0E13   0.0     0.0   ! Miller 27th Symp.
HCNO+OH=CH2O+NO                 2.0E13   0.0     0.0   ! Miller 27th Symp.
C2H+NO=CN+HCO                  2.1E13   0.0    0.0  !GLASS&CURL(STEPHENS)JPC1987
CH2(S)+NO=HCN+OH               0.200E+14  0.000      0.000 ! JAM
CH2(S)+NO=CH2+NO                1.0E14    0.0      0.0 !CEC 94 & refs
HCNO+H=HCN+OH                  0.100E+15  0.000  12000.000 ! PG
CH2+N=HCN+H                    0.500E+14  0.000      0.000 ! JAM
CH+N=CN+H                      0.130E+14  0.000      0.000 ! JAM
CO2+N=NO+CO                    0.190E+12  0.000   3400.000 ! CRC
HCCO+N=HCN+CO                  0.500E+14  0.000      0.000 ! JAM
CH3+N=H2CN+H                   7.1E13     0.0     0.0     ! DAVIDSON&HANSON 23RD
C2H3+N=HCN+CH2                 0.200E+14  0.000      0.000 ! JAM
H2CCCH+N=HCN+C2H2                0.100E+14  0.000      0.000 ! JAM
HCN+OH=CN+H2O                3.90E6     1.83    10291. ! Wool.,Hanson,Bow IJCK 95
OH+HCN=HOCN+H                  0.585E+05  2.400  12500.000 ! MILLER
OH+HCN=HNCO+H                  0.198E-02  4.000   1000.000 ! MILLER
OH+HCN=NH2+CO                  0.783E-03  4.000   4000.000 ! MILLER
HOCN+OH=NCO+H2O                6.38E5    2.0     2563.  !JAM (HNCO+OH)
HOCN+H=NCO+H2                  2.0E7      2.0    2000.  !JAM
HOCN+O=NCO+OH                  1.5E4      2.64   4000. ! JAM(O+HCN)
HOCN+CH3=CH3CN+OH              5.0E12     0.0    2000. !JAM
H+CH3CN=HCN+CH3                4.0E7      2.0    2000.  ! JAM
O+CH3CN=NCO+CH3                1.5E4      2.64   4980 !JAM(O+HCN)
OH+CH3CN=CH2CN+H2O             2.0E7     2.0   2000. ! JAM
H+CH3CN=CH2CN+H2               3.0E7     2.0    1000. ! JAM
CH2CN+O=CH2O+CN                1.0E14    0.0  0.0    ! JAM
HCN+O=NCO+H                    0.138E+05  2.640   4980.000 ! PERRY
HCN+O=NH+CO                    0.345E+04  2.640   4980.000 ! PERRY
HCN+O=CN+OH                    0.270E+10  1.580  29200.000 ! MILLER,ET AL 1986
HCN+CH2(S)=CH3+CN               5.0E13    0.0      0.0  ! JAM
CN+H2=HCN+H                    0.295E+06  2.450   2237.000 ! WAGNER
CH+HCN=CH2+CN                  3.01E13    0.0     -993.5 !LIN(ZABARNICK)CP1991
CN+O=CO+N                      7.7E13     0.0    0.0 !DAVIDSON,ET AL IJCK91
CN+O2=NCO+O                    7.47E12     0.0   -389. !DURANT&TULLY,DAVIDSON
CN+OH=NCO+H                    4.00E13   0.0    0.0 !Wool(Hanson) 1996
CN+HCN=C2N2+H                  1.51E7    1.71  1530. !
CN+NO2=NCO+NO                  5.324E15  -0.752  344. !WOOLD.(HTGL),PARK&HERSH
CN+NO2=CO+N2O                  4.93E14   -.752  344.! WOOLD.(HTGL),PARK&HERSH.
CN+NO2=N2+CO2                  3.70E14   -.752 344. !WOOLD.(HTGL),PARK&HERSH.
CN+N2O=NCN+NO                  3.85E3    2.6    3696. ! M.C.LIN
CN+CO2=NCO+CO                  3.67E6    2.2    26884. !M.C. LIN 1991
CN+CH4=CH3+HCN                 6.02E4    2.64   -437. !CASTLETON JPC 1991
CN+C2H6=C2H5+HCN               1.20E5    2.77   -1788. !CASTLETON JPC 91
CN+HNCO=HCN+NCO                1.5E13    0.0     0.0  ! TSANG&HERRON
CN+NCO=NCN+CO                  1.8E13    0.0     0.0  ! TSANG&HERRON
CN+CH3=CH2CN+H                  1.0E14   0.0     0.0  ! JAM
CN+CH2OH=CH2CN+OH               5.0E13   0.0   0.0   ! JAM
CN+CH2CO=HCCO+HCN                 2.0E13  0.0   0.0  ! JAM
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C2N2+O=NCO+CN                  0.457E+13  0.000   8880.000 ! STANFORD
C2N2+OH=HOCN+CN                0.186E+12  0.000   2900.000 ! PHILLIPS
NCN+O=CN+NO                    1.0E14      0.0     0.0  !JAM
NCN+OH=HCN+NO                  5.0E13     0.0      0.0  !JAM
NCN+H=HCN+N                    1.0E14     0.0      0.0 !JAM
NCN+O2=NO+NCO                  1.0E13     0.0      0.0 !JAM
HO2+NO=NO2+OH                  0.211E+13  0.000   -479.000 ! HOWARD
HCO+NO=HNO+CO                  7.2E12    0.0       0.0  !TSANG&HERRON
NO2+NO2=NO+NO+O2               1.63E12    0.0       26123. !TSANG&HERRON
NO2+H=NO+OH                    8.4E13    0.0    0.0  !TSANG&HERRON (PG)
NO2+O=NO+O2                    3.9E12     0.0    -238. !TSANG&HERRON (PG)
NO+O+M=NO2+M                   7.5E19     -1.41  0.0   ! PG
  N2/1.7/   O2/1.5/  H2O/10/
NO2+NH=N2O+OH                  1.0E13     0.0       0.0    ! PHILLIPS
NO2+NH2=N2O+H2O                1.62E16   -1.44    268 ! Park&Lin JPC 1997
NH2+NO2=H2NO+NO                6.48E16   -1.44    268 !
NO2+CH2=CH2O+NO                5.9E13    0.0     0.0 !TEMPS,HGGW ET AL JPC89
NO2+CH3=CH3O+NO                1.4E13    0.0    0.0 !gla/troe74, big/car93
NO2+HCO=HONO+CO                1.2E23    -3.29  2355. ! NBS 91
NO2+HCO=H+CO2+NO               8.4E15    -0.75  1930. ! NBS 91
NO2+CH=HCO+NO                  1.0E14    0.0     0.0 !SANDERS&LIN REV
NO2+HCCO=HCNO+CO2              1.6E13   0.0   0.0  !Temps,HGGW,Wolf ZfPC 1992
NO2+HNO=HONO+NO                6.0E11    0.0     2000.! TSANG&HERRON
NO2+CO=CO2+NO                  9.0E13     0.0   33779.!TSANG&HERRON
NO2+CH2O=HCO+HONO              8.0E2     2.80   13730 !
OH+NO+M=HONO+M                 5.08E23  -2.51   -67.6 !TSANG&HERRON
 CO2/0.0/ H2O/5/
OH+NO+CO2=HONO+CO2              1.71E23 -2.3    -246 !TSANG&HERRON
HONO+O=OH+NO2                  1.2E13    0.0    5961.!TSANG&HERRON
HONO+OH=H2O+NO2                4.0E12    0.0    0.0 !RAVI IJCK 1992
!HONO+NH2=NO2+NH3                5.0E12   0.0    0.0    ! JAM
HONO+NH2=NO2+NH3               71.1      3.02   -4941 ! Lin,Morokuma JPC 1996
HONO+H=H2+NO2                  1.2E13     0.0   7352 !TSANG&HERRON
NCO+O2=NO+CO2                  2.0E12     0.0    20000. ! MILLER&BOWMAN IJCK
NCO+H=NH+CO                    0.500E+14  0.000      0.000 ! JAM
NCO+O=NO+CO                    4.7E13     0.0     0.0 !MERTENS 24TH
NCO+N=N2+CO                    0.200E+14  0.000      0.000 ! JAM,LIF
NCO+OH=NO+HCO                     5.0E12    0.0    15000.   !MILLER&BOWMAN IJCK
NCO+M=N+CO+M                   0.310E+17 -0.500  48000.000 ! LOUGE
NCO+NO=N2O+CO                  6.16E17   -1.73  763  !MERTENS,ATAKAN,HERSHBERGER
NCO+NO=N2+CO2                  7.84E17   -1.73  763  !MERTENS,ATAKAN,HERSHBERGER
NCO+H2=HNCO+H                  7.589E2    3.0     4000.    ! JAM&CFM IJCK 1992
NCO+NCO=N2+CO+CO               1.8E13     0.0     0.0   !TSANG&HERRON
NCO+HNO=HNCO+NO                 1.8E13    0.0    0.0    ! TSANG&HERRON
NCO+HONO=HNCO+NO2                3.6E12   0.0    0.0     ! TSANG&HERRON
NCO+NO2=CO+NO+NO                  2.5E11  0.0    -707.  !WOOLD.,HERSH.(JAM)
NCO+NO2=CO2+N2O                  3.0E12   0.0    -707. !WOOLD.,HERSH.(JAM)
NCO+HCO=HNCO+CO                  3.6E13     0.0  0.0    ! TSANG&HERRON
NCO+CH2O=HNCO+HCO                6.0E12     0.0   0.0   ! TSANG&HERRON
NCO+CH4=CH3+HNCO                 9.8E12    0.0   8120. ! SCH 94
NCO+C2H6=C2H5+HNCO               1.5E-9     6.90  -2910. ! SCH 94
NCO+C2H2=HCCO+HCN                 1.4E12   0.0    1815. ! BEC 95
HNCO+H=NH2+CO                    2.247E7  1.7     3800.    !JAM&CFM IJCK 1992
HNCO+M=NH+CO                      1.14E16    0.0     86000.  !M&B WSS
HNCO+NH=NH2+NCO                    3.0E13     0.0     23700.  !M&B WSS
HNCO+NH2=NH3+NCO                  5.0E12     0.0     6200.   !M&B WSS
OH+HNCO=NCO+H2O                6.38E5     2.0     2563. !TSANG&HERRON(TULLY)
HNCO+O=HNO+CO                  1.49E8     1.57    44012   !LIN,CFM 24TH
HNCO+O=NH+CO2                  9.8E7      1.41    8524    !LIN,CFM 24TH
HNCO+O=NCO+OH                  2.2E6      2.11    11425   !LIN,CFM 24TH
HNCO+HO2=NCO+H2O2              3.0E11      0.0    22000. ! MILLER&BOWMAN IJCK
NH+O2=HNO+O                    4.61E5     2.0     6500.    !MILL&MEL 24TH
NH+O2=NO+OH                    1.28E6     1.5      100.    !MILL&MEL 24TH
NH+NO=N2O+H                    2.94E14    -0.4     0.0     !MILL&MEL 24TH
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 DUP
NH+NO=N2O+H                    -2.16E13   -0.23    0.0     !MILL&MEL 24TH
 DUP
NH+NO=N2+OH                    2.16E13    -0.23    0.0     !MILL&MEL 24TH
NH+OH=HNO+H                    0.200E+14  0.000      0.000 ! NH3 CST
NH+OH=N+H2O                    0.500E+12  0.500   2000.000 ! NH3 CST
NH+N=N2+H                      0.300E+14  0.000      0.000 ! JAM
NH+H=N+H2                      3.0E13     0.0    0.0   !DAVIDSON&HANSON 1990
NH+O=NO+H                      9.2E13     0.0       0.0 ! MERTENS
N2O+OH=N2+HO2                  1.29E-2   4.72    36561 ! Mebel,Lin IJCK 1996
N2O+OH=HNO+NO                  1.18E-4   4.33    25081 !
N2O+NO=NO2+N2                  5.26E5    2.23    46281 !
N2O+H=N2+OH                    3.31E10    0.0     4729.    ! FONTIJN 1987
 DUP
N2O+H=N2+OH                    4.40E14     0.0   19254    !  FONTIJN 1987
 DUP
N2O+M=N2+O+M                   4.0E14      0.0   56100.  !PG,ET AL 24TH
 N2/1.7/   O2/1.4/ H2O/12/ CO/1.5/  CO2/3/   !PG,et al 25th except CO
N2O+O=N2+O2                    1.0E14   0.0  28000. ! NBS 91 (PG rbn)
N2O+O=NO+NO                    6.6E13   0.0  16630. ! NBS 91 (PG rbn)
N2O+CH=HCN+NO                  4.7E13       0.0    0.0  !SANDERS&LIN REV
N2O+C=CN+NO                    5.1E12      0.0     0.0 ! DORTHE ET AL JPC 91
N2O+CO=N2+CO2                  3.19E11     0.0    20237. ! TSANG&HERRON
NH2+O=HNO+H                    0.663E+15 -0.500      0.000
NH2+O=NH+OH                    0.675E+13  0.000      0.000
NH2+OH=NH+H2O                  0.400E+07  2.000   1000.000 ! JAM,9/87
NH2+H=NH+H2                    4.0E13    0.0    3650.  ! NH2-NO2 paper
NH2+HO2=NH3+O2                 1.0E13     0.0    0.0    ! PG
NH2+HO2=H2NO+OH                5.0E13     0.0     0.0   !PG
NH2+NH2=N2H2+H2                8.5E11   0.0     0.0   ! NH2-NO2 paper
!NH2+NO=NNH+OH                  8.92E12     -0.35     0.0
!NH2+NO=N2+H2O                  1.3E16     -1.25     0.0   !JAM,PG
! DUP
!NH2+NO=N2+H2O                  -8.92E12    -0.35     0.0
!DUP
NH2+NO=N2+H2O                   2.77E20  -2.654   1258.3 ! JAM 3/98
NH2+NO=NNH+OH                   2.294E10  0.425  -813.56 ! JAM 6/98
NH3+M=NH2+H+M                  2.2E16    0.0     93470. ! NH2-NO2 paper
   CO/2/ H2/2/ CO2/3/  H2O/5/
NH3+OH=NH2+H2O                 0.204E+07  2.040    566.000 ! LOUGE
NH3+H=NH2+H2                   0.636E+06  2.390  10171.000 ! MICHAEL
NH3+O=NH2+OH                   9.4E6      1.90  6460. ! NH2-NO2 paper
NH3+HO2=NH2+H2O2               3.0E11     0.0    22000. !MILLER&BOWMAN IJCK
NNH=N2+H                       6.5E7      0.0     0.0   !JAM 6/98
NNH+O2=N2+HO2                   2.0E14      0.0      0.0 ! JAM
NNH+O2=N2+O2+H                  5.0E13    0.0      0.0 ! JAM
NNH+NO=N2+HNO                  0.500E+14  0.000      0.000
NNH+H=N2+H2                    0.100E+15  0.000      0.000 ! JAM,9/87
NNH+OH=N2+H2O                  0.500E+14  0.000      0.000
NNH+NH2=N2+NH3                 0.500E+14  0.000      0.000
NNH+NH=N2+NH2                  0.500E+14  0.000      0.000
NNH+O=N2+OH                     8.0E13   0.0       0.0
NNH+O=N2O+H                    0.100E+15  0.000      0.000
NNH+O=NH+NO                    5.0E13     0.0        0.0    !JAM&CFM 24TH
H+NO+M=HNO+M                   4.0E20     -1.75   0.0 ! Glarborg,et al 27th
    H2O/10/  O2/1.5/ H2/2/ CO2/3/ N2/0.0/
H+NO+N2=HNO+N2                 4.0E20     -1.75   0.0 ! Glarborg,et al 27th
HNO+OH=NO+H2O                  0.360E+14  0.000      0.000 ! NH3 CST
HNO+H=H2+NO                    4.46E11    0.720     655.  !SOTO&PAGE JCP 1992
HNO+O=OH+NO                     1.0E13    0.0  0.0   ! NH2-NO2 paper
HNO+NH2=NH3+NO                 3.63E6     1.63     -1252 ! Lin,Morokuma JPC 1996
HNO+HNO=N2O+H2O                9.0E8      0.0       3100 ! NH2-NO2 paper
HNO+HCO=CH2O+NO                6.0E11      0.0     2000. ! TSANG&HERRON
HNO+O2=HO2+NO                   2.0E12     0.0    25000. ! JAM 3/98
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H2NO+O2=HNO+HO2                 3.0E12     0.0     25000. ! JAM
H2NO+M=HNO+H+M                 7.5E15     0.0      50000.0 ! JAM 12/96
  H2O/5/  N2/2/
H2NO+NO2=HNO+HONO               6.0E11    0.0       2000. !HNO+NO2
H2NO+H=HNO+H2                  3.0E7      2.0       2000. !JAM,PG EST
H2NO+H=NH2+OH                  5.0E13     0.0       0.0  !
H2NO+O=HNO+OH                  3.0E7      2.0       2000. !
H2NO+OH=HNO+H2O                2.0E7      2.0       1000. !
H2NO+NO=HNO+HNO                 2.0E7     2.0      13000. !
H2NO+NH2=NH3+HNO                3.0E12    0.0       1000. !
N+NO=N2+O                      0.327E+13  0.300      0.000 ! LEEDS,MONAT
N+O2=NO+O                      0.640E+10  1.000   6280.000
N+OH=NO+H                      0.380E+14  0.000      0.000 ! SMITH,FLOWER
NH2+NH=N2H2+H                  0.500E+14  0.000      0.000 ! NH3CST
NH+NH=N2+H+H                   0.254E+14  0.000      0.000 ! NH3 CST
NH2+N=N2+H+H                   0.720E+14  0.000      0.000 ! PG
N2H2+M=NNH+H+M                 0.500E+17  0.000  50000.000 ! NH3 CST
    H2O/15/ O2/2/ N2/2/ H2/2/
N2H2+H=NNH+H2                  0.500E+14  0.000   1000.000 ! NH3 CST
N2H2+O=NH2+NO                  0.100E+14  0.000      0.000 ! NH3 CST
N2H2+O=NNH+OH                  0.200E+14  0.000   1000.000 ! NH3 CST
N2H2+OH=NNH+H2O                0.100E+14  0.000   1000.000 ! NH3 CST
N2H2+NO=N2O+NH2                0.300E+13  0.000      0.000 ! NH3 CST
N2H2+NH=NNH+NH2                0.100E+14  0.000   1000.000 ! NH3 CST
N2H2+NH2=NH3+NNH               0.100E+14  0.000   1000.000 ! NH3 CST
NO2+O(+M)=NO3(+M)              1.3E13     0.0      0.0  !TSANG&HERRON
    LOW/1.0E28  -4.08 2470./
   N2/1.5/ O2/1.5/  H2O/18.6/
NO2+NO2=NO3+NO                 9.6E9   0.73  20900. ! TSANG&HERRON
NO3+H=NO2+OH                    6.0E13  0.0  0.0 !BECKER ET AL 92/N (PG)
NO3+O=NO2+O2                   1.0E13  0.0  0.0  !ATKINSON ET AL 92 (PG)
NO3+OH=NO2+HO2                 1.4E13  0.0  0.0   !ATKINSON ET AL 92 (PG)
NO3+HO2=NO2+O2+OH              1.5E12  0.0  0.0  ! BECKER ET AL 92 (PG)
NO3+NO2=NO+NO2+O2              5.0E10  0.0   2940. ! DEMORE ET AL 90 (PG)
END
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Chemkin Plug Input File for Staged Combustion – Combustion Chamber / Reduction Stage

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XEND    701
DX      2
DIAM    198.12
HEAT
TINF    298
BIGU    2500
TEMP    984.9924728
PRES    1
VEL     248.9536418
MOLE
NNEG
ATOL    1.00E-08
RTOL    1.00E-04
GAS     H2             1.88748E-03
GAS     H              0.00000E+00
GAS     CH4            7.04202E-02
GAS     CH3            0.00000E+00
GAS     CH2            0.00000E+00
GAS     CH             0.00000E+00
GAS     CH2O           0.00000E+00
GAS     HCO            0.00000E+00
GAS     CO2            8.07096E-03
GAS     CO             1.53576E-03
GAS     O2             1.35926E-01
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GAS     O              0.00000E+00
GAS     OH             0.00000E+00
GAS     HO2            0.00000E+00
GAS     H2O2           0.00000E+00
GAS     H2O            2.51612E-01
GAS     C2H            7.39763E-08
GAS     C2H2           7.39763E-08
GAS     HCCO           0.00000E+00
GAS     C2H3           7.39763E-08
GAS     C2H4           1.06526E-04
GAS     C2H5           7.39763E-08
GAS     C2H6           2.88508E-03
GAS     CH2OH          0.00000E+00
GAS     CH3O           0.00000E+00
GAS     HCCOH          0.00000E+00
GAS     H2CCCH         7.39763E-08
GAS     C3H2           7.39763E-08
GAS     CH2(S)         0.00000E+00
GAS     CH2CO          0.00000E+00
GAS     C              0.00000E+00
GAS     C4H2           7.39763E-08
GAS     C5H2           7.39763E-08
GAS     H2CCCCCH       7.39763E-08
GAS     HCCCHCCH       7.39763E-08
GAS     C5H5           0.00000E+00
GAS     C6H2           7.39763E-08
GAS     CH2CHCCH       7.39763E-08
GAS     HCCHCCH        7.39763E-08
GAS     H2CCCCH        7.39763E-08
GAS     C6H5           7.39763E-08
GAS     C6H6           7.39763E-08
GAS     C3H4           7.39763E-08
GAS     C3H4P          7.39763E-08
GAS     C6H5O          7.39763E-08
GAS     CH2CHCHCH      7.39763E-08
GAS     CH2CHCCH2      7.39763E-08
GAS     C2             7.39763E-08
GAS     C2O            7.39763E-08
GAS     C6H5C2H        7.39763E-08
GAS     C6H4           7.39763E-08
GAS     OCHCHO         0.00000E+00
GAS     C4H            7.39763E-08
GAS     CH3O2          0.00000E+00
GAS     C2H2OH         7.39763E-08
GAS     H2C4O          7.39763E-08
GAS     CH2CHCHCH2     7.39763E-08
GAS     CH3OH          0.00000E+00
GAS     CH2HCO         0.00000E+00
GAS     CH3CO          0.00000E+00
GAS     CH3HCO         0.00000E+00
GAS     CH3OOH         0.00000E+00
GAS     AR             4.13699E-03
GAS     NO             3.33278E-03
GAS     N              0.00000E+00
GAS     NH             0.00000E+00
GAS     NH2            0.00000E+00
GAS     HNO            0.00000E+00
GAS     HCN            0.00000E+00
GAS     NCO            0.00000E+00
GAS     CN             0.00000E+00
GAS     N2O            0.00000E+00
GAS     NNH            0.00000E+00
GAS     HNCO           0.00000E+00
GAS     N2H2           0.00000E+00
```

```
GAS     CH3CN          7.39763E-08
GAS     CH2CN          7.39763E-08
GAS     C2N2           0.00000E+00
GAS     NO2            3.33278E-03
GAS     HOCN           0.00000E+00
GAS     HCNO           0.00000E+00
GAS     H2CN           0.00000E+00
GAS     NH3            0.00000E+00
GAS     H2NO           0.00000E+00
GAS     NCN            0.00000E+00
GAS     HONO           0.00000E+00
GAS     NO3            0.00000E+00
GAS     N2             5.16751E-01
END
```

Chemkin Plug Input File for Staged Combustion – Quench Stage

```
XEND    152
DX      2
DIAM    198.12
HEAT
TINF    298
BIGU    2500
TEMP    1152.679738
PRES    1
VEL     360.7490169
MOLE
NNEG
ATOL    1.00E-08
RTOL    1.00E-04
GAS     H2             1.15324E-02
GAS     H              5.78100E-04
GAS     CH4            1.74547E-15
GAS     CH3            2.13153E-15
GAS     CH2            1.83665E-16
GAS     CH             1.98203E-17
GAS     CH2O           9.82392E-11
GAS     HCO            1.80133E-09
GAS     CO2            5.81878E-02
GAS     CO             1.12942E-02
GAS     O2             8.85467E-04
GAS     O              7.71539E-05
GAS     OH             2.26706E-03
GAS     HO2            2.13071E-07
GAS     H2O2           3.67001E-08
GAS     H2O            4.91391E-01
GAS     C2H            2.03542E-17
GAS     C2H2           1.07603E-14
GAS     HCCO           2.82397E-16
GAS     C2H3           1.70522E-18
GAS     C2H4           1.95657E-18
GAS     C2H5           1.68879E-22
GAS     C2H6           1.97957E-24
GAS     CH2OH          6.91370E-16
GAS     CH3O           6.31573E-18
GAS     HCCOH          2.90939E-18
GAS     H2CCCH         3.69958E-16
GAS     C3H2           1.82350E-16
GAS     CH2(S)         9.43786E-18
GAS     CH2CO          2.29745E-16
GAS     C              4.59243E-17
GAS     C4H2           7.47226E-16
```

```
GAS     C5H2           7.01720E-28
GAS     H2CCCCCH       1.22799E-21
GAS     HCCCHCCH       2.71554E-29
GAS     C5H5           4.10124E-07
GAS     C6H2           5.67339E-29
GAS     CH2CHCCH       6.69439E-17
GAS     HCCHCCH        5.96745E-17
GAS     H2CCCCH        7.95113E-17
GAS     C6H5           1.03825E-17
GAS     C6H6           7.84435E-18
GAS     C3H4           2.26213E-18
GAS     C3H4P          4.82818E-18
GAS     C6H5O          7.14287E-15
GAS     CH2CHCHCH      8.75610E-21
GAS     CH2CHCCH2      4.35998E-20
GAS     C2             5.13949E-20
GAS     C2O            4.24827E-16
GAS     C6H5C2H        2.04117E-30
GAS     C6H4           2.58083E-17
GAS     OCHCHO         2.94225E-20
GAS     C4H            5.63807E-16
GAS     CH3O2          1.14914E-22
GAS     C2H2OH         1.42923E-20
GAS     H2C4O          1.66251E-16
GAS     CH2CHCHCH2     5.83603E-21
GAS     CH3OH          8.18112E-17
GAS     CH2HCO         6.55640E-22
GAS     CH3CO          1.29042E-22
GAS     CH3HCO         5.72514E-24
GAS     CH3OOH         1.32081E-23
GAS     AR             3.34227E-03
GAS     NO             6.66318E-04
GAS     N              8.37004E-09
GAS     NH             2.95292E-09
GAS     NH2            2.35495E-09
GAS     HNO            2.01325E-08
GAS     HCN            6.81678E-11
GAS     NCO            7.99138E-12
GAS     CN             1.49741E-13
GAS     N2O            2.62272E-08
GAS     NNH            1.02593E-09
GAS     HNCO           6.23769E-10
GAS     N2H2           6.07013E-14
GAS     CH3CN          1.36106E-24
GAS     CH2CN          1.57708E-23
GAS     C2N2           3.27491E-21
GAS     NO2            5.54361E-08
GAS     HOCN           3.92957E-12
GAS     HCNO           1.14174E-16
GAS     H2CN           4.28030E-17
GAS     NH3            1.51794E-08
GAS     H2NO           2.27445E-11
GAS     NCN            2.81411E-17
GAS     HONO           2.82807E-09
GAS     NO3            7.77042E-15
GAS     N2             4.19816E-01
END
```

Chemkin Plug Input File for Staged Combustion – Reoxidation Stage

```
XEND    640
DX      2
```

```
DIAM    176.784
HEAT
TINF    298
BIGU    2500
TEMP    1121.781779
PRES    1
VEL     484.4496045
MOLE
NNEG
ATOL    1.00E-08
RTOL    1.00E-04
GAS     H2             1.25594E-02
GAS     H              3.63191E-07
GAS     CH4            7.25380E-10
GAS     CH3            4.57957E-13
GAS     CH2            6.00880E-18
GAS     CH             1.22584E-23
GAS     CH2O           8.90102E-11
GAS     HCO            1.67185E-11
GAS     CO2            5.76974E-02
GAS     CO             5.85466E-03
GAS     O2             1.84746E-02
GAS     O              2.38966E-10
GAS     OH             9.60423E-08
GAS     HO2            1.52774E-09
GAS     H2O2           5.74704E-12
GAS     H2O            4.48471E-01
GAS     C2H            2.08685E-22
GAS     C2H2           2.65416E-14
GAS     HCCO           1.27236E-19
GAS     C2H3           5.07848E-19
GAS     C2H4           4.48380E-15
GAS     C2H5           3.90098E-19
GAS     C2H6           1.39731E-17
GAS     CH2OH          1.32799E-16
GAS     CH3O           7.09418E-19
GAS     HCCOH          2.62862E-18
GAS     H2CCCH         1.44839E-17
GAS     C3H2           1.37998E-19
GAS     CH2(S)         5.46429E-20
GAS     CH2CO          2.77273E-15
GAS     C              7.10969E-26
GAS     C4H2           1.76488E-21
GAS     C5H2           9.95083E-27
GAS     H2CCCCCH       1.12095E-21
GAS     HCCCHCCH       1.50585E-29
GAS     C5H5           3.74957E-07
GAS     C6H2           2.18626E-31
GAS     CH2CHCCH       1.14558E-20
GAS     HCCHCCH        3.50422E-24
GAS     H2CCCCH        4.31598E-22
GAS     C6H5           4.95535E-17
GAS     C6H6           2.23460E-13
GAS     C3H4           3.85355E-17
GAS     C3H4P          2.11603E-17
GAS     C6H5O          3.99492E-13
GAS     CH2CHCHCH      6.17663E-24
GAS     CH2CHCCH2      1.59341E-22
GAS     C2             1.65361E-29
GAS     C2O            7.22552E-22
GAS     C6H5C2H        2.89039E-26
GAS     C6H4           8.26256E-14
GAS     OCHCHO         2.38236E-19
GAS     C4H            6.17571E-24
```

```
GAS     CH3O2          2.60673E-19
GAS     C2H2OH         9.01047E-22
GAS     H2C4O          4.93893E-22
GAS     CH2CHCHCH2     9.96907E-21
GAS     CH3OH          1.21125E-13
GAS     CH2HCO         6.30523E-21
GAS     CH3CO          1.82052E-19
GAS     CH3HCO         3.45588E-17
GAS     CH3OOH         1.38910E-24
GAS     AR             3.87311E-03
GAS     NO             5.25816E-04
GAS     N              3.22057E-12
GAS     NH             3.47139E-12
GAS     NH2            6.60257E-10
GAS     HNO            1.40278E-07
GAS     HCN            1.56331E-10
GAS     NCO            5.18793E-14
GAS     CN             5.45426E-18
GAS     N2O            4.36249E-07
GAS     NNH            2.63592E-13
GAS     HNCO           3.08284E-08
GAS     N2H2           8.37110E-14
GAS     CH3CN          4.45005E-19
GAS     CH2CN          2.45624E-20
GAS     C2N2           1.44930E-21
GAS     NO2            6.79684E-08
GAS     HOCN           1.55237E-12
GAS     HCNO           2.72530E-15
GAS     H2CN           3.18408E-17
GAS     NH3            1.57699E-05
GAS     H2NO           1.86977E-08
GAS     NCN            9.91434E-20
GAS     HONO           1.26323E-09
GAS     NO3            2.23096E-16
GAS     N2             4.52459E-01
END
```

Sample Chemkin Plug Input File for SNCR

```
XEND            300
DX               30
DIAM         152.40
ISO
TEMP        1073.15
PRES              1
VEL           62.26
MOLE
NNEG
ATOL       1.00E-08
RTOL       1.00E-04
GAS      CO2           0.056335
GAS      CO            0.007695
GAS      H2O           0.517750
GAS      N2            0.241300
GAS      NO            0.023560
GAS      NO2           0.023560
GAS      O2            0.051775
GAS      AR            0.003040
GAS      H2            0.024985
GAS      NH3           0.050000
END
```

Sample Chemkin Plug Input File for High-Temperature NO_x Destruction

```
XEND            300
DX               10
DIAM         152.40
ISO
TEMP        1073.15
PRES              1
VEL           62.26
MOLE
NNEG
ATOL       1.00E-08
RTOL       1.00E-04
GAS      CO2          0.059300
GAS      CO           0.008100
GAS      H2O          0.545000
GAS      N2           0.254000
GAS      NO           0.024800
GAS      NO2          0.024800
GAS      O2           0.054500
GAS      AR           0.003200
GAS      H2           0.026300
GAS      NH3          0.000000
END
```

Sample Chemkin Equil Input File for High-Temperature NO_x Destruction

```
REAC     CO2        0.059300
REAC     CO         0.008100
REAC     H2O        0.545000
REAC     N2         0.254000
REAC     NO         0.024800
REAC     NO2        0.024800
REAC     O2         0.054500
REAC     AR         0.003200
REAC     H2         0.026300
REAC     NH3        0.000000
REAC     CH4        0.000000
TP
TEMP     3123.15
PRES     1.00
FREE
END
```

Species Included in HSC Gibbs Model for High-Temperature NO_x Destruction

Solid Species:

C
C(A)
C(D)

Gas Species:

H2O(g)
N2(g)
CO2(g)
C4N2(g)
C5N4(TCMg)
CNN(g)
(H3)O2(g)
(H3)2O(Tg)
HOCN(g)

```
O2(g)
H2(g)
NO(g)
NO2(g)
CO(g)
Ar(g)
C(g)
C2(g)
C3(g)
C4(g)
C5(g)
CCN(g)
CH(g)
CH2(g)
CH3(g)
C(H3)(g)
CH4(g)
C2H(g)
C2H2(g)
C2H3(g)
C2H4(g)
C2H5(g)
C2H6(g)
CN(g)
CN2(g)
C2N(g)
C2N2(g)
C3N2O(OPDNg)
C2O(g)
C3O2(g)
COOH(g)
H(g)
H3(Tg)
HCCN(g)
HCN(g)
H2CNN(g)
HCO(g)
HCOOH(g)
HCOOH(Cg)
HCOOH(Tg)
HH3(Tg)
HH3O(Tg)
HH3O2(Tg)
HN3(g)
H4N2(TDHg)
HNO(g)
HNO2(g)
HNO2(Cg)
HNO2(Tg)
HNO3(g)
HO(g)
HO2(g)
H2O2(g)
H3O(Tg)
N(g)
N3(g)
NCN(g)
NCO(g)
NH(g)
NH2(g)
NH3(g)
N2H2(g)
N2H2(Bg)
N2H2(Cg)
N2H2(Tg)
N2H2(tg)
N2H4(g)
N3H(g)
NH(H3)2(g)
N2H4*H2O(g)
NH2NO2(g)
NH2OH(g)
NO3(g)
N2O(g)
N2O2(g)
N2O3(g)
N2O4(g)
N2O5(g)
O(g)
O3(g)
```

Chemkin Plug Input File for High-Temperature NO$_x$ Destruction Using a Long Reactor

```
XEND     76200
DX       100
DIAM     30.48
ISO
TEMP     1473.15
PRES     1
VEL      2133.16
MOLE
NNEG
ATOL     1.00E-08
RTOL     1.00E-04
GAS      NO              0.0041690
GAS      NO2             0.0000033
GAS      CO              0.0007932
GAS      CO2             0.0667300
GAS      H2              0.0013660
GAS      H2O             0.5677000
GAS      N2              0.2772000
GAS      O2              0.0718500
GAS      AR              0.0032060
GAS      NH3             0.0000000
GAS      CH3              1.77E-19
GAS      CH2O             6.86E-13
```

```
GAS      OH             6.41E-03
GAS      HCCO           6.16E-23
GAS      C2H5           5.60E-36
GAS      CH3O           9.77E-21
GAS      C3H2           9.82E-32
GAS      C              4.43E-20
GAS      H2CCCCCH       9.45E-24
GAS      C6H2          -3.58E-50
GAS      H2CCCCH        7.26E-31
GAS      C3H4           5.29E-35
GAS      CH2CHCHCH      1.06E-37
GAS      C2O            1.06E-21
GAS      OCHCHO         1.07E-23
GAS      C2H2OH         2.31E-31
GAS      CH3OH          6.00E-20
GAS      CH3HCO         1.37E-29
GAS      NH2            1.34E-10
GAS      NCO            2.27E-13
GAS      NNH            1.15E-10
GAS      CH3CN          6.24E-31
GAS      H2CN           1.11E-20
GAS      NCN            3.46E-20
GAS      H              1.24E-04
GAS      CH2            2.22E-20
GAS      HCO            2.69E-11
GAS      HO2            5.31E-06
GAS      C2H            1.29E-28
GAS      C2H3           2.45E-31
GAS      C2H6          -5.83E-39
GAS      HCCOH          3.17E-26
GAS      CH2(S)         1.04E-21
GAS      C4H2           9.25E-29
GAS      HCCCHCCH      -3.90E-53
GAS      CH2CHCCH       6.32E-33
GAS      C6H5           2.34E-33
GAS      C3H4P          1.25E-34
GAS      CH2CHCCH2      1.31E-36
GAS      C6H5C2H        2.63E-55
GAS      C4H            2.50E-29
GAS      H2C4O          5.89E-29
GAS      CH2HCO         6.86E-29
GAS      CH3OOH         7.38E-26
GAS      N              2.35E-09
GAS      HNO            3.78E-08
GAS      CN             2.49E-16
GAS      HNCO           1.05E-11
GAS      CH2CN          1.60E-29
GAS      HOCN           5.21E-14
GAS      HONO           6.78E-08
GAS      CH4            7.95E-20
GAS      CH             7.29E-21
GAS      O              4.04E-04
GAS      H2O2           4.10E-07
GAS      C2H2           5.34E-26
GAS      C2H4           2.46E-31
GAS      CH2OH          1.15E-18
GAS      H2CCCH         1.89E-32
GAS      CH2CO          4.03E-23
GAS      C5H2           2.12E-43
GAS      C5H5           1.49E-21
GAS      HCCHCCH        5.65E-33
GAS      C6H6           1.04E-33
GAS      C6H5O          1.91E-30
GAS      C2             5.11E-31
```

```
GAS      C6H4            7.49E-32
GAS      CH3O2           8.27E-25
GAS      CH2CHCHCH2      5.51E-38
GAS      CH3CO           6.88E-28
GAS      NH              3.51E-10
GAS      HCN             7.47E-14
GAS      N2O             1.15E-07
GAS      N2H2            2.30E-15
GAS      C2N2            2.92E-26
GAS      HCNO            4.64E-19
GAS      H2NO            1.49E-11
GAS      NO3             3.31E-12
END
```

Sample Chemkin Plug Input File for High-Temperature NO_x Destruction with CH_4 Addition

```
XEND             300
DX                30
DIAM          152.40
ISO
TEMP         1073.15
PRES               1
VEL            62.26
MOLE
NNEG
ATOL        1.00E-08
RTOL        1.00E-04
GAS      CO2           0.057521
GAS      CO            0.007857
GAS      H2O           0.528650
GAS      N2            0.246380
GAS      NO            0.024056
GAS      NO2           0.024056
GAS      O2            0.052865
GAS      AR            0.003104
GAS      H2            0.025511
GAS      CH4           0.030000
END
```

Sample Chemkin Plug Input File for High-Temperature NO_x Destruction with H_2 Addition

```
XEND             300
DX                30
DIAM          152.40
ISO
TEMP         1073.15
PRES               1
VEL            62.26
MOLE
NNEG
ATOL        1.00E-08
RTOL        1.00E-04
GAS      CO2           0.059684
GAS      CO            0.008152
GAS      H2O           0.548526
GAS      N2            0.255643
GAS      NO            0.024960
GAS      NO2           0.024960
GAS      O2            0.054853
GAS      AR            0.003221
```

```
GAS      H2            0.020000
GAS      NH3           0.000000
END
```

Sample Chemkin Plug Input File for High-Temperature NO_x Destruction with NH_3 Addition

```
XEND            300
DX               30
DIAM         152.40
ISO
TEMP        1073.15
PRES              1
VEL           62.26
MOLE
NNEG
ATOL       1.00E-08
RTOL       1.00E-04
GAS      CO2           0.056335
GAS      CO            0.007695
GAS      H2O           0.517750
GAS      N2            0.241300
GAS      NO            0.023560
GAS      NO2           0.023560
GAS      O2            0.051775
GAS      AR            0.003040
GAS      H2            0.024985
GAS      NH3           0.050000
END
```

Appendix B

Calculation of Overall Heat Transfer Coefficient for Staged Combustion

(ALL CALCULATIONS PERFORMED USING MATHCAD 2000)

Known Temperatures, Flows, Pressures, Dimensions & Constants:

$T_G := 2350K$ $T_{Ambient} := 273K$ $r_1 := 1.958333ft$ $r_2 := 2.958333ft$ $r_3 := 3.458333ft$

$L := 2.25ft$ $T_G := 2350K$ $\sigma := 5.67 \cdot 10^{-8} \cdot \frac{W}{m^2 \cdot K^4}$ $r_4 := 3.5ft$ $m_{dot} := 72.8 \frac{g}{s}$

$P := 1atm$

Initial Guesses & Simplifying Assumptions:

$T_4 := 467K$ Initial Guess (after first try, make this match final answer)

Properties of Air at the mean external temperature (0°C + 150°C) / 2 = 75°C

$\nu := 20.92 \cdot 10^{-6} \frac{m^2}{s}$ $\alpha := 29.9 \cdot 10^{-6} \frac{m^2}{s}$ $Pr := 0.700$ $K_{Air} := 30 \cdot 10^{-3} \frac{W}{m \cdot K}$

$\beta := \frac{1}{T_4 + T_{Ambient}}$ (see Incropera & Dewitt, 2nd Edition, p. 767)

Refractory & Pipe Properties:

$K_A := 2.3 \frac{W}{m \cdot K}$ for A P Green Greencast-94 at 1500°F (see www.hwr.com)

$K_B := 0.37 \frac{W}{m \cdot K}$ for A P Green Greenlite-45L at 800°F (see www.hwr.com)

$K_C := 48 \frac{W}{m \cdot K}$ for carbon steel at 620°F (see Incropera & Dewitt, 2nd Edition, p. 756)

$\varepsilon := 0.8$ emissivity for carbon steel pipe (reasonable guestimate)

$e := 1000 \cdot 10^{-6} m$ guestimate of roughness for refractory

Properties of the Combustion Gas:

Assumed Conditions:

$T_{CombGas} := 2366K$

$X_{CO} := 0.07$

$X_{CO2} := 0.05$

$X_{H2} := 0.05$

$X_{N2} := 0.61$

$X_{H2O} := 0.22$

From Aspen (using RKS-BM Property Set):

$\rho_{CombGas} := 1.302 \cdot 10^{-4} \frac{g}{cm^3}$

$\mu_{CombGas} := 7.95 \cdot 10^{-2} \frac{g}{m \cdot s}$ This unit is equivalent to a cP (Mathcad seems to have problems with viscosity units!)

$cp_{CombGas} := 1630.5 \frac{J}{kg \cdot K}$

$k_{CombGas} := 0.2023 \frac{W}{m \cdot K}$

Heat Transfer Coefficient Calculation for Comb. Gas to Refractory Surface via Convection:

$u_{CombGas} := \frac{m_{dot}}{\rho_{CombGas} \cdot \pi \cdot r_1^2}$ $u_{CombGas} = 1.64 \frac{ft}{s}$

$Re_{CombGas} := \frac{\rho_{CombGas} \cdot u_{CombGas} \cdot 2r_1}{\mu_{CombGas}}$ (see Incropera & Dewitt, 2nd Edition, p. 369)

$Re_{CombGas} = 977$

$\mu_{CombGas} := \mu_{CombGas} \cdot 10^{-2} \cdot \frac{m \cdot s \cdot poise}{g}$ $\mu_{CombGas} = 7.95 \times 10^{-5} \frac{kg}{ms}$

$Pr_{CombGas} := \frac{cp_{CombGas} \cdot \mu_{CombGas}}{k_{CombGas}}$ (see Incropera & Dewitt, 2nd Edition, p. 283)

$Pr_{CombGas} = 0.641$

$Roughness := \frac{e}{2 \cdot r_1}$

$Roughness = 0.000838$

Since we are in the laminar flow regime (i.e, Re < 2300), then:

$f := \frac{64}{Re_{CombGas}}$ $f = 0.06553$ (see Incropera & Dewitt, 2nd Edition, p. 372)

Assuming a constant heat flux boundary condition:

$Nu_{CombGas} := 4.36$ (see Incropera & Dewitt, 2nd Edition, p. 389)

$$h_{CombGas} := \frac{Nu_{CombGas} \cdot k_{CombGas}}{2 \cdot r_1}$$ (see Incropera & Dewitt, 2nd Edition, p. 389)

$$h_{CombGas} = 0.7388 \frac{W}{m^2 K}$$

Heat Transfer Coefficient Calculation for Comb. Gas to Refractory Surface via Radiation:

Since I don't have a chart of emissivity for CO, I'll group CO and CO2 together, thus looking at 12% CO2 and 22% H2O for radiation purposes. N2 and H2 don't readily absorb or emit radiation.

$X_{COCO2} := X_{CO} + X_{CO2}$ $X_{COCO2} = 0.12$

$L_{BeamEquiv} := 1$ (see Schaums Heat Transfer, p. 281 for a long cylinder)

$L_{Equiv} := L_{BeamEquiv} \cdot 2 \cdot r_1$ (see Schaums Heat Transfer, p. 281 for a long cylinder)

$L_{Equiv} = 1.19 m$

$pL_{CO2} := L_{Equiv} \cdot X_{COCO2} \cdot P$ $pL_{CO2} = 0.47 atm \cdot ft$

$pL_{H2O} := L_{Equiv} \cdot X_{H2O} \cdot P$ $pL_{H2O} = 0.862 atm \cdot ft$

From Schaum's, using a temperature of 2200K (see p. 281 & 282):

$\varepsilon_{CO2} := 0.059$

$\varepsilon_{H2O} := 0.090$

$\varepsilon_{CombGas} := \varepsilon_{CO2} + \varepsilon_{H2O}$

$\varepsilon_{CombGas} = 0.149$

Heat Transfer Coefficient Calculation for Air External to NOxidizer:

$$Ra := \frac{g \cdot \beta \cdot (T_4 - T_{Ambient}) \cdot (r_3 \cdot 2)^3}{\nu \cdot \alpha}$$ (see Incropera & Dewitt, 2nd Edition, p. 429 for free convection)

$Ra = 3.851 \times 10^{10}$

$$Nu := \left[0.60 + 0.387 \cdot \frac{Ra^{\frac{1}{6}}}{\left[1 + \left(\frac{0.559}{Pr}\right)^{\frac{9}{16}}\right]^{\frac{8}{27}}}\right]^2$$

(free convection over a long horizontal cylinder – not the best assumption, but it should provide an order of magnitude reasonable estimate even though end effects are neglected)

$Nu = 370.54$

$$h_{Air} := Nu \cdot \frac{K_{Air}}{(2 \cdot r_4)}$$

(see Incropera & Dewitt, 2nd Edition, p. 435 for free convection)

$$h_{Air} = 5.21 \frac{W}{m^2 K}$$

Initial Guesses (Needed to Facilitate Convergence):

$q_{1a} := 1W$ $q_2 := 1W$ $q_4 := 1W$ $q_6 := 1W$ $T_2 := 900K$ $T_4 := 400K$

$q_{1b} := 1W$ $q_3 := 1W$ $q_5 := 1W$ $T_1 := 1200K$ $T_3 := 700K$

Standard Conduction, Convection, and Radiation Equations:

Given

$$q_{1a} = \varepsilon_{CombGas} \cdot 2 \cdot \pi \cdot r_1 \cdot L \cdot \sigma \cdot \left(T_G^{\,4} - T_1^{\,4}\right)$$

(Radiative Heat Transfer to a Surface – See Incropera &DeWitt, 2nd Edition, p. 9)

$$q_{1b} = 2 \cdot \pi \cdot r_1 \cdot L \cdot h_{CombGas}\left(T_G - T_1\right)$$

(Steady-State Convection for a Cylinder – See Incropera &DeWitt, 2nd Edition, p. 8)

$$q_2 = \frac{2 \cdot \pi \cdot K_A \cdot L\left(T_1 - T_2\right)}{\ln\left(\frac{r_2}{r_1}\right)}$$

(One Dimensional Steady-State Conduction for a Cylinder - See Incropera &DeWitt, 2nd Edition, p. 76)

$$q_3 = \frac{2 \cdot \pi \cdot K_B \cdot L\left(T_2 - T_3\right)}{\ln\left(\frac{r_3}{r_2}\right)}$$

(One Dimensional Steady-State Conduction for a Cylinder - See Incropera &DeWitt, 2nd Edition, p. 76)

$$q_4 = \frac{2 \cdot \pi \cdot K_C \cdot L\left(T_3 - T_4\right)}{\ln\left(\frac{r_4}{r_3}\right)}$$

(One Dimensional Steady-State Conduction for a Cylinder – See Incropera & DeWitt, 2nd edition, p. 76)

$q_5 = 2\cdot\pi\cdot r_4\cdot L\cdot h_{Air}\left(T_4 - T_{Ambient}\right)$ (Steady-State Convection for a Cylinder - See Incropera &DeWitt, 2nd Edition, p. 8)

$q_6 = \varepsilon\cdot 2\cdot\pi\cdot r_4\cdot L\cdot\sigma\cdot\left(T_4{}^4 - T_{Ambient}{}^4\right)$ (Radiative Heat Transfer from a Surface – See Incropera &DeWitt, 2nd Edition, p. 9)

Heat Balance Equations (Conservation of Energy):

$q_{1a} + q_{1b} = q_2$ (Conduction through the inner surface must equal convection plus radiation away from the gas)

$q_2 = q_3$ (Conduction from one layer to the next must be equal)

$q_3 = q_4$ (Conduction from one layer to the next must be equal)

$q_4 = q_5 + q_6$ (Conduction to the outer surface must equal convection plus radiation away from the outer surface)

Solve the Equations:

$\text{Answer} := \text{Find}\left(q_{1a}, q_{1b}, q_2, q_3, q_4, q_5, q_6, T_1, T_2, T_3, T_4\right)$

Answer =

	0
0	[1,1]
1	[1,1]
2	[1,1]
3	[1,1]
4	[1,1]
5	[1,1]
6	[1,1]
7	[1,1]
8	[1,1]
9	[1,1]
10	[1,1]

$q_{1a} := \text{Answer}_0$ $q_{1a} = 13378\text{W}$

$q_{1b} := \text{Answer}_1$ $q_{1b} = 23\,\text{W}$

$q_2 := \text{Answer}_2$ $q_2 = 13400\text{W}$ $q_2 = 3201\frac{\text{cal}}{\text{s}}$

$q_3 := \text{Answer}_3$ $q_3 = 13400\text{W}$

$q_4 := \text{Answer}_4$ $q_4 = 13400\text{W}$

$q_5 := \text{Answer}_5$ $q_5 = 4645\text{W}$

$q_6 := \text{Answer}_6$ $q_6 = 8755\text{W}$

$T_1 := \mathrm{Answer}_7$ $\qquad T_1 = 2338\mathrm{K}$

$T_2 := \mathrm{Answer}_8$ $\qquad T_2 = 1780\mathrm{K}$

$T_3 := \mathrm{Answer}_9$ $\qquad T_3 = 468\mathrm{K}$

$T_4 := \mathrm{Answer}_{10}$ $\qquad T_4 = 467\mathrm{K}$

Now solve for the overall heat transfer coefficient:
(Note: This is not rigorous, but may match the way the data will be used in the Chemkin Plug module)

$$U_i := \frac{q_{1a} + q_{1b}}{\left(T_G - T_{Ambient}\right)\cdot\left(2\cdot\pi\cdot r_1\cdot L\right)} \qquad U_i = 2508\frac{\mathrm{erg}}{\mathrm{cm}^2\mathrm{s}\cdot\mathrm{K}}$$

Based on inside area.

Now perform a more rigorous calculation:

$$h_r := \varepsilon_{CombGas}\cdot\sigma\cdot\left(T_G + T_1\right)\cdot\left(T_G^{\ 2} + T_1^{\ 2}\right)$$

(Incropera & DeWitt, 2nd Edition, p. 10, eq. 1.8)

$$h_r = 435230\frac{\mathrm{erg}}{\mathrm{cm}^2\mathrm{s\ K}}$$

$$h_{r2} := \varepsilon\cdot\sigma\cdot\left(T_4 + T_{Ambient}\right)\cdot\left(T_4^{\ 2} + T_{Ambient}^{\ \ 2}\right)$$

(Incropera & DeWitt, 2nd Edition, p. 10, eq. 1.8)

$$h_{r2} = 9820\frac{\mathrm{erg}}{\mathrm{cm}^2\mathrm{s\ K}}$$

$$U_i := \frac{1}{\frac{1}{h_{CombGas}} + \frac{1}{h_r} + \frac{r_1}{K_A}\cdot\ln\left(\frac{r_2}{r_1}\right) + \frac{r_2}{K_B}\cdot\ln\left(\frac{r_3}{r_2}\right) + \frac{r_3}{K_C}\cdot\ln\left(\frac{r_4}{r_3}\right) + \frac{r_1}{r_4}\cdot\frac{1}{h_{Air}} + \frac{1}{h_{r2}}} \qquad U_i = 487\frac{\mathrm{erg}}{\mathrm{cm}^2\mathrm{s\ K}}$$