DEVELOPMENT OF A CHEMICAL KINETIC MODEL FOR THE COMBUSTION OF A SYNTHESIS GAS FROM A FLUIDIZED-BED SEWAGE SLUDGE GASIFIER IN A THERMAL OXIDIZER

by

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ABSTRACT

The need for sustainability has been on the rise. Municipalities are finding ways of reducing waste, but also finding ways to reduce energy costs. Waste-to-energy is a sustainable method that may reduce bio-solids volume while also producing energy. In this research study bio-solids enters a bubbling bed gasifier and within the gasifier a synthesis gas is produced. This synthesis gas exits through the top of the gasifier and enters a thermal oxidizer for combustion. The thermal oxidizer has an innovative method of oxidizing the synthesis gas. The thermal oxidizer has two air injection sites and the possibility for aqueous ammonia injection for further NO_x reduction. Most thermal oxidizers already include an oxidizer such as air in the fuel before it enters the thermal oxidizer; thus making this research and operation different from many other thermal oxidizers and waste-to-energy plants.

The reduction in waste means less volume loads to a landfill. This process significantly reduces the amount of bio-solids to a landfill. The energy produced from the synthesis is beneficial for any municipality, as it may be used to run the waste-to-energy facility. The purpose of this study is to determine methods in which operators may configure future plants to reduce NO_x emissions. NO_x mixed with volatile organic compounds (VOC) and sunlight, produce ozone (O_3) a deadly gas at high concentrations.

This study developed a model to determine the best methods to reduce NO_x emissions. Results indicate that a fuel-rich then fuel-lean injection scheme results in lower NO_x emissions. This is because at fuel-rich conditions not all of the ammonia in the first air ring is converted to NO_x, but rather a partial of the ammonia is converted to NO_x and N_2 and then the second air

ring operates at fuel-lean which further oxidizes the remaining ammonia which converts to $NO_{x,}$ but also a fraction to N_2. If NO_x standards reach more stringency then aqueous ammonia injection is a recommended method for NO_x reduction; this method is also known as selective non-catalytic reduction (SNCR).

The findings in this study will allow operators to make better judgment in the way that they operate a two air injection scheme thermal oxidizer. The goal of the operator and the organization is to meet air quality standards and this study aims at finding ways to reduce emissions, specifically NO_x.

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“A journey of thousand miles begins with a single step.” – Lao-tzu

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1. INTRODUCTION

This research focuses on combustion of synthesis gas (syngas) in an air injection thermal oxidizer (TO) that follows a sewage sludge fluidized bed gasifier. Syngas is composed of various combustible gases including H_2, CO, CH_4, and tars but also contains N_2, CO_2 and H_2O. The objective of this research is to gain an understanding of how these gases react in the TO as operating conditions change and ultimately to predict the final composition of the exhaust gas. A reaction mechanism was developed to help understand the chemistry and thermodynamics of this phenomenon, especially for NO_x formation. NO_x control is a field of active research at the current moment the detailed mechanisms of NO_x formation in this type of device are not well understood.

1.1 Problem Statement

To better understand the effects of operating conditions and syngas composition on the performance of a thermal oxidizer, the authors developed a computer model for combustion of a syngas from a fluidized-bed sewage sludge gasifier. This work was part of a research project funded by Maxwest Environmental Systems, Inc. Maxwest owns and operates the only commercial-scale sewage sludge gasification facility in the United States of America; gasification provides a better alternative to landfilling waste biosolids. The modeling of the fluidized-bed sewage sludge gasifier predicts the syngas rate and composition going to the thermal oxidizer (TO). The TO modeling is done to provide the information needed for the design of air pollution control devices (APC) required downstream.

1.2 Project Objectives

The objectives of the project were to review the literature concerning combustion of hydrocarbons, ammonia, hydrogen sulfide, hydrogen chloride, carbon monoxide, and hydrogen in order to prepare an up-to-date reaction mechanism (based on elementary reactions). The reaction mechanism would be input into a chemical kinetic software package (CHEMKED) that performs extensive chemical calculations utilizing the reaction mechanism. The main focus of this research, and the focus of this thesis, was on the development of a combustion model that predicts the composition of the gas stream from a thermal oxidizer, as a function of varying operation conditions (Syngas flow, temperatures, compositions, and air and flue gas flow rates). In addition, the effects of NH_3 injection (to control NO_x) will be studied.

1.3 Project Importance

The computer model developed will allow for future designs of a thermal oxidizer and air pollution control (APC) equipment, based on the oxidation of a synthesis gas from a sewage sludge fluidized bed gasifier. The computer model will also aid in APC equipment selection for this type of process. The goal is to have a better understanding of how operating conditions can affect this type of process and how that in turn will affect pollutant formation. The reduction in landfilling sewage sludge and producing a viable source of power will benefit any municipality.

1.4 Thesis organization

This research begins with a literature review of past combustion modeling efforts with respect to syngas. The reader is introduced to fundamental concepts of global mechanism, chemical kinetics, thermodynamics, and equilibrium as well as the process of NO_x reduction.

Next, detail on the development of the theoretical model will be presented. Then finally, pertinent results will be discussed, conclusions will be presented, and recommendations for future research will be made.

2. LITERATURE REVIEW

2.1 Introduction

Synthesis gas from a sewage sludge gasifier (SSG) has been studied in a hard coal-fired boiler as a co-combustion process in order to model emissions with possibilities of NOx reduction (Wei, et al., 2012). Syngas from an SSG has also been used as an additional fuel for the purpose of reducing NOx in an internal combustion engine (Monteiro, Sotton, Bellenoue, Moreira, & Malheiro, 2011). There have been efforts of modeling the combustion of syngas but specifically for this type of air injection thermal oxidizer, no mechanistic models were found in the literature.

The methodology of the modeling effort for this research is modeling a plug flow reactor (PFR) using ChemKed and a java interface that performs essential calculations. CHEMKED models reactions as if in a batch reactor (BR). A series of batch reactors resembles a plug flow reactor. An ideal BR does not have continuous flow into and out of the reactor but rather a set volume is “loaded” with reactants and is allowed to react for a period of time. There is accumulation or depletion of components (non-steady state), because of the degradation or generation reactions occurring in the BR. Figure 1 depicts the thermal oxidizer with two air injection sites and one aqueous ammonia injection sites. The oxidizer is 40 feet long and has an internal diameter of 5 feet 9 inches. The oxidizer was modeled as a series of batch reactors, each 1 foot long.

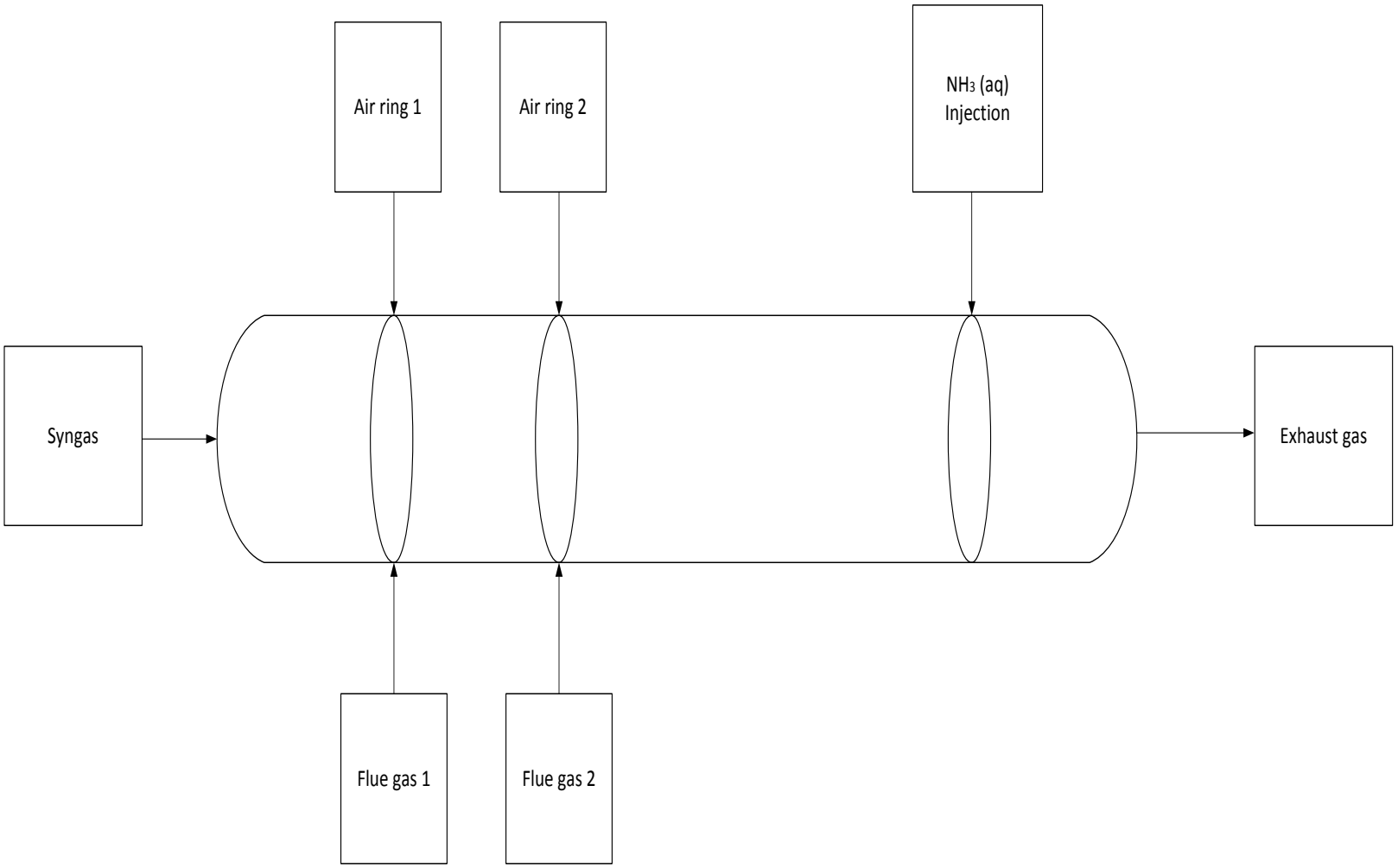

Figure 1 - -Thermal Oxidizer (TO) Scheme

The syngas from the SSG is composed of various gases, such as C_6H_6, CH_4, CO, H_2, HCl, H_2S, NH_3, CO_2, H_2O, and N_2. Ultimately determining the concentrations of all components in the exhaust gas, from the combustion of this syngas, is the modeling effort of this research project.

As shown in Figure 1, the syngas flows from the fluidized bed gasifier into the thermal oxidizer, and almost immediately is injected with air. The air is injected through nozzles placed in such an orientation to promote rapid mixing. There are two injection sites along the length of the TO that introduces air or a combination of air and flue gas. Flue gas is recirculated exhaust gas before it is treated through a wet scrubber. The overall reactor operates at excess oxygen to promote complete combustion. Near the exit of the TO, after all the combustion reactions are done, there is a site for aqueous ammonia injection. Aqueous ammonia is injected for the reduction of NO_x emissions. This process is called selective non-catalytic reduction (SNCR), where ammonia reacts with NO and NO_2 to produce H_2O and N_2. The effectiveness of this reduction reaction depends on temperature, the amount of NO_x, the amount of NH_3 at that point in the reactor, and mixing (Miller & Bowman, 1989). Further discussion of this process will be presented in a later section.

2.1.1 Elementary reactions

The set of all elementary reactions that one thinks are responsible for a chemical transformation is called its *reaction mechanism* (Gardiner, 2000). Combustion mechanisms are all chain reactions. It is important to recognize that each elementary reaction is one step of a mechanism. Initiation occurs when chain centers are produced from stable molecules, (Gardiner, 2000). Chain centers are another way of saying free radicals or active species. For example, heptane can break into two free radicals or two chain centers:

$$\mathbf{C_7H_{16} \rightarrow C_3H_7 + C_4H_9} \quad (2.1)$$

Loss of chain centers occurs when two radicals combine, as in

$$\mathbf{H + CH_3 \rightarrow CH_4} \quad (2.2)$$

and this results in chain termination steps.

Many combustion reactions are initiated by the elementary reaction between H atoms and O_2 molecules (Gardiner, 2000):

$$\mathbf{H + O_2 \rightarrow OH + O} \quad (2.3)$$

Elementary steps in which the number of chain centers increase are called chain branching reactions such as the initiation step just mentioned. Steps in which the number of chain centers remain the same are called chain propagation steps:

$$\mathbf{O + C_2H_5 \rightarrow C_2H_4 + OH} \quad (2.4)$$

A detailed chemical mechanism may have over 1500 reactions and 100 species depending on its complexity. With the right computer software, such as CHEMKIN or CHEMKED, these reactions can be calculated simultaneously producing concentrations, temperatures, etc. All chemical reactions, whether hydrolysis, acid-base, or combustion take place at definite rates and depend on the conditions of the system (Glassman & Yetter, 2008). The most important of these conditions are the concentration of the reactants, the temperature, radiation effects, and the presence of a catalyst or inhibitor. The rate of reaction may be expressed in terms of the concentration of any of the reacting substances or of any reaction product; that is, the rate may be expressed as the rate of decrease of the concentration of a reactant or the rate of increase of reaction product.

A stoichiometric relation describing a one-step chemical reaction of arbitrary complexity can be represented by the equation:

$$\sum_1^{\mathbf{m}} \boldsymbol{\upsilon}_{\mathbf{i}}'(\mathbf{M_i}) \leftrightarrows \sum_1^{\mathbf{n}} \boldsymbol{\upsilon}_{\mathbf{j}}''(\mathbf{N_j}) \tag{2.5}$$

Where:

v_i'	= the stoichiometric coefficient of the reactants
v_j''	= the stoichiometric coefficient of the products
M	= a concentration of all chemical species, reactants
N	= a concentration of all chemical species, products
m, n	= the total number of species involved

The law of mass action, which is confirmed experimentally, states that the rate of disappearance of a chemical species i, defined as RR_i, is proportional to the product of the concentrations of the reacting chemical species (Glassman & Yetter, 2008), where each concentration is raised to a power equal to the corresponding stoichiometric coefficient; that is,

$$\mathbf{RR_i} = \prod_1^{\mathbf{m}} (\mathbf{k_i M_i})^{\boldsymbol{\nu}_{\mathbf{i}}'} \tag{2.6}$$

k_i	= the proportionality constant called the specific reaction rate coefficient for reaction i

$$\mathbf{n} = \sum \boldsymbol{\nu}_{\mathbf{i}}' \tag{2.7}$$

n	= the overall order of the reaction

Equation (2.7) is the overall reaction order where ν_i' is reaction order with respect to the i species. In an actual system the rate of change of the concentration of a species is given by:

$$\frac{\mathbf{d(M_i)}}{\mathbf{dt}} = \left[\boldsymbol{\nu}_{\mathbf{j}}'' - \boldsymbol{\nu}_{\mathbf{i}}'\right] \mathbf{RR} = \left[\boldsymbol{\nu}_{\mathbf{j}}'' - \boldsymbol{\nu}_{\mathbf{i}}'\right] \mathbf{k} \prod_{\mathbf{j=1}}^{\mathbf{m}} \left(\mathbf{M_j}\right)^{\boldsymbol{\nu}_{\mathbf{j}}'} \tag{2.8}$$

More than one set of reaction steps will add complexity to the differential equation for an arbitrary species. For example refer to chemical equations in Figure 2, which depicts a simple 10 step mechanism for the oxidation of methane.

$CH_4 + O_2 \rightarrow CH_3 + HO_2$	chain initiation
$CH_3 + O_2 \rightarrow CH_2 + OH$	chain propagation
$OH + CH_4 \rightarrow H_2O + CH_3$	chain propagation
$OH + CH_2O \rightarrow H_2O + HCO$	chain propagation
$CH_2 + O_2 \rightarrow HO_2 + HCO$	chain branching
$HCO + O_2 \rightarrow CO + HO_2$	chain propagation
$HO_2 + CH_4 \rightarrow H_2O_2 + CH_3$	chain propagation
$HO_2 + CH_2O \rightarrow H_2O_2 + HCO$	chain propagation
$OH \rightarrow$ wall	chain termination
$CH_2O \rightarrow$ wall	chain termination
$CO+O \rightarrow CO_2$	chain termination

Figure 2 - Elementary methane reaction scheme (Cooper & Alley, 2011)

Assume each reaction has a different specific reaction rate coefficient (k_1-k_{10}). The following develops the rate of change of concentration for the intermediate CH_3.

$$\frac{\mathbf{d[CH_3]}}{\mathbf{dt}} = \mathbf{k_1[CH_4][O_2] - k_2[CH_3][O_2] + k_3[CH_4][OH] + k_7[HO_2][CH_4]} \quad (2.9)$$

A similar equation can be developed for each species. As can be seen, the larger the set of species and elementary reactions, the more complex the rate of change for intermediate species. Assumptions can be made to simplify these equations, such as assuming a quasi-steady state for intermediate species. For example for the case of CH_3, $\frac{d[CH_3]}{dt} \approx 0$. The quasi-steady state assumption means that the rate of change is assumed to be zero but in reality it might not be the case (Glassman & Yetter, 2008). This assumption is primarily made for radicals in an elementary set of chemical equations.

2.1.2 The Arrhenius Rate Expression

In most chemical reactions two molecules collide and react to produce products. Thus, most simple reactions are second-order. Other reactions are dominated by a loose bond-breaking step and thus are first-order reactions. The Arrhenius rate expression is based on collision theory (Glassman & Yetter, 2008).

$$\mathbf{k = A \exp\left[-\frac{E_a}{R_u T}\right]} \tag{2.10}$$

A = the pre-exponential factor
E_a = the activation energy required for a reactions to occur, kJ/mol
R_u = the universal, or ideal gas constant, 8.314 Joule/mol-Kelvin
T = temperature, Kelvin

The pre-exponential factor depends on how often molecules collide at 1 mol/L concentration (Glassman & Yetter, 2008).

There is also a modified Arrhenius expression for the rate of reaction:

$$\mathbf{k = A T^b \exp\left[-\frac{E_a}{R_u T}\right]} \tag{2.11}$$

b = experimental constant

The modified Arrhenius equation is more widely used in combustion modeling.

2.2 Chemical kinetics

Oxidation reactions occur in many elementary steps. The actual detailed mechanisms of combustion are very complex; for example the hydrogen mechanism (Li, Zhenwei, Kazakov, & Dryer, 2004) includes 20 steps in the combustion of H_2. The combustion of a simple hydrocarbon, methane, involves a branching chain reaction, the main reactions of which were depicted in Figure 2. Higher order hydrocarbons are further complicated because of the number of possible intermediates, such as benzene, formaldehyde, or heptane.

In order to simplify kinetic models global models were developed. In this research global reaction models were assumed to take place to estimate temperatures and concentrations.

2.3 Overview of CHEMKED Package

Chemked is a program designed for creating and editing thermodynamic and chemical kinetics databases, for formation of reaction mechanisms, and for simulation of problems of complex gas-phase chemistry (Jelezniak & Jelezniak, 2009).

Chemked incorporates a solver for integration of the differential equations of gas phase chemical kinetics at constant pressure or constant volume (density) without mass and heat transfer. The solver is a FORTRAN program based on the RADAU5 subroutines. The necessary information on thermodynamics and reactions is provided for the solver directly from the databases under consideration. The solver output contains numerical and graphical information on mixture-averaged gas parameters and species concentrations (Jelezniak & Jelezniak, 2009).

Using the Chemked tools the user can quickly create desired reaction mechanism and investigate it with numerical solutions. For the reaction mechanism, the program forms a CHEMKIN-II format text file that consists of reaction list and thermodynamics that can be used in other applications (Jelezniak & Jelezniak, 2009).

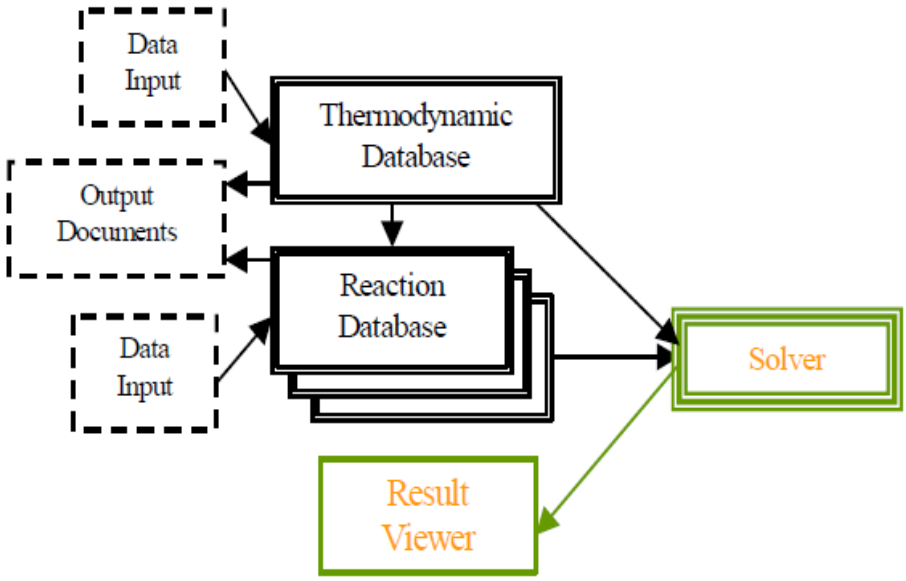

Figure 3 - General structure of CHEMKED – I (Jelezniak & Jelezniak, 2009)

2.4 Types of combustion reactions

Combustion occurs when a fuel and oxidizer react extremely rapidly. Explosion is when the heat is released in an extremely short period of time in a confined space. The primary fuels in syngas are CO, CH_4, H_2, and tars; all ultimately converting to CO_2 and H_2O. The following is a stoichiometric model of combustion of a fuel that contains carbon, hydrogen and oxygen.

$$\mathbf{C_xH_yO_z + a[O_2 + 3.76N_2] \rightarrow xCO_2 + (y/2)H_2O + 3.76aN_2} \quad (2.12)$$

Where:

x = number of carbon atoms, moles
y = number of hydrogen atoms, moles
z = number of oxygen atoms, moles

$$a = [\, x + y/4 - z/2 \,] \quad (2.13)$$

a = the stoichiometric amount of air, moles

There are various species present in a syngas. In this case there are 6 combustible gases (ammonia, hydrogen sulfide, carbon monoxide, methane, benzene, and hydrogen) all burning simultaneously at different rates. It is important to now mention the differences between fuel

lean and fuel rich combustion and the constant phi, ϕ, the fuel-air equivalence ratio, as well as the air-to-fuel ratio.

Stoichiometric air-to-fuel ratio (A/F) = 4.76 a (MW_{Air}/MW_{fuel}) (2.14)

4.76a	= total number of moles of air
MW_{Air}	= molecular weight of air = (32 + 3.76*28)/4.76 = 28.8 lb/lb-mol
MW_{Fuel}	molecular weight of fuel lb/lb-mol

The equivalence ratio (ϕ) is defined as the systems fuel-to-air ratio to the stoichiometric fuel-to-air ratio.

$\phi = (F/A)/(F/A)_{stoic}$ (2.15)

Actual air-to-fuel ratio $(A/F)_{act}$ depends on the equivalence ratio $a = \phi[x + y/4 – z/2]$

Fuel rich ($\phi > 1$) is a condition when there is more fuel then there is oxidizer. An equivalence ratio equal to one ($\phi = 1$) means that the system has exactly the amount of oxidizer necessary for the fuel to theoretically reach complete combustion, complete combustion meaning fully converted to its final products (all hydrocarbons converted to carbon dioxide and water). Finally, fuel lean ($\phi < 1$) is when more oxidizer than is needed for complete combustion to occur is present in the system.

2.4.1 Fuel lean combustion reactions

Fuel lean (excess oxygen) combustion occurs when the equivalence ratio is less than 1. In this state fuels have more than enough oxygen to reach complete combustion, and there is a significant amount of oxygen left in the product gases. Temperatures in this zone are lower, and reaction rates are slower, as the excess air that was introduced acts as a temperature diluent. Thus NOx formation is also limited due to lower reaction rates.

Combustion processes operating under fuel lean conditions have very low emissions and very high efficiency. Pollutant emissions are reduced because flame temperatures are typically low, reducing NO_x formation. In addition, for hydrocarbon combustion, with excess air, complete burnout of fuel occurs (Dunn-Rankin, 2008) reducing hydrocarbon and carbon monoxide (CO) emissions. Achieving these improvements and meeting the demands for the combustion process is complicated by lower reaction rates. The excess air during lean combustion primarily acts as a diluent, reducing temperatures and lowering reaction rates. Exhaust gas and flue gas can be used as diluents as well without quenching the reaction. After excess air combustion, the gases remaining are oxygen, nitrogen, and major products, CO_2, H_2O, NO_x, SO_x.

2.4.2 Fuel rich combustion reactions

Fuel rich combustion occurs when the equivalence ratio , ϕ is greater than 1. This is a physical state in a reactor when the system is oxygen-starved meaning there is a limited amount of oxygen available, and fuel remains after all oxygen has been consumed.

The application of the major products model to fuel rich combustion is only slightly more complicated compared to fuel lean. The major product assumption is an assumption that the only products of combustion are the following: CO_2, CO, NO, N_2, H_2O, H_2 (Gardiner, 2000).

To illustrate fuel-rich combustion propane (C_3H_8) and air are used as an example:

$$\boldsymbol{\phi C_3H_8 + 5(O_2 + 3.76N_2) \rightarrow n_{CO_2}CO_2 + n_{CO}CO + n_{H_2O}H_2O + n_{H_2}H_2 + 18.8N_2} \quad (2.16)$$

In contrast to the fuel-lean solution, the fuel-rich solution for the product species depends on T, through equilibrium constants $K_p(T)$, as well as ϕ.

One can define the equilibrium constant at constant pressure with the following equation, (Gardiner, 2000):

$$\mathbf{aA} + \mathbf{bB} + \cdots \rightarrow \mathbf{rR} + \mathbf{sS} \tag{2.17}$$

$$\mathbf{K_P} = \frac{\mathbf{p_R^r p_S^s}}{\mathbf{p_A^a p_B^b}} \tag{2.18}$$

This equation is usually represented as (Glassman & Yetter, 2008),

$$\mathbf{K_p} = \frac{\mathbf{n_R^r n_S^s}}{\mathbf{n_A^a n_B^b}} * \left(\frac{\mathbf{P}}{\sum \mathbf{n_i}}\right)^{\mathbf{r+s-a-b}} \tag{2.19}$$

Where:

K_p	= equilibrium constant based on partial pressure
n_i	= number of moles of species i
P, p_i	= total pressure, and partial pressure of species i (atm)
r, s, a, b	= stoichiometric coefficient of species i

For fuel rich combustion, the products may contain CO, unburned fuels and other species formed by the degradation of the fuel. Often additional information on the products is needed for complete balance of the chemical reaction.

2.4.3 H_2S oxidation

The reaction mechanisms used to model H_2S oxidation in this study focused on interactions between H_2S and H_2 and O_2 (Mathieu, Deguillaume, & Petersen, 2013); as well as another study (Zhou, Sendt, & Haynes, 2013). In the Zhou (2013) study oxidation of H_2S in an atmospheric flow reactor at temperatures from 950 to 1150 K were studied under fuel-lean conditions ($1.9 < \frac{[O_2]_0}{[H_2S]_0} < 10$). While in the Mathieu (2013) study, ignition delay times were measured behind reflected shock waves for mixtures of 1% H_2 and 1% O_2 diluted in Ar and doped with various H_2S concentrations (100, 400, and 1600 ppm) over large pressure (around 1.6, 13, and 33 atm) and temperature (1045-1860 K). Hydrogen sulfide is a common impurity

that can greatly change the combustion properties of fuels, even when present in small concentrations. However, the combustion chemistry of H_2S is still poorly understood, and this lack of understanding subsequently leads to difficulties in the design of emission-control and energy-production devices (Mathieu, Deguillaume, & Petersen, 2013).

To better understand the high-temperature chemistry of H_2S and to set a base for the comprehension of the interactions between H_2S and the H_2 and O_2 system is of paramount importance (Mathieu, Deguillaume, & Petersen, 2013). The H_2 and O_2 sub-mechanism is critical for the combustion of hydrocarbons as it contains many elementary steps involving radicals (H, O, OH, HO_2) which play a substantial role at every stage of the hydrocarbon oxidation process.

H_2S inhibits the ignition process because it reacts before the H_2 fuel does, taking H atoms away from the main branching reaction $\mathrm{H} + \mathrm{O}_2 \leftrightarrows \mathrm{OH} + \mathrm{O}$ (Mathieu, Deguillaume, & Petersen, 2013).

The Zhou (2013) model shows extraordinary sensitivity to the rates of a significant number of reactions that determine the radical concentrations during the oxidation process. Minor variations (<factor 3) in the rate coefficients of two of the SH self-reaction channels allows accurate description of H_2S consumption profiles: on the one hand, the reaction 2SH = H_2S + S (followed by S + O_2 = SO + O and SO + O_2 = SO_2 + O) is strongly branching whereas on the other, 2SH = HSSH (followed by HSSH + SH = H_2S + HSS and HSS + SH = H_2S + S_2) is a powerful chain termination sequence, especially when the oxygen excess is reduced.

Disulfur interactions are extremely important in the ignition and propagation of H_2S oxidation even under fuel lean conditions (Zhou, Sendt, & Haynes, 2013).

2.4.4 Ammonia injection and NO_x reduction reactions

Selective Noncatalytic Reduction (SNCR) is one method in reducing NO_x ultimately to N_2 gas. The last zone of the thermal oxidizer is the zone where ammonia is injected to act as a reducing agent to reduce NO_x producing nitrogen and water. There is an optimal amount of ammonia injected dependent on operating conditions. NO_x removal rate is a function of temperature and ammonia concentration. Remembering that there is oxygen present and temperatures of 1800 degrees Fahrenheit reaching this zone, there is a possibility for ammonia to be oxidized to more NO_x rather than the NOx being reduced to nitrogen gas and water. Thus this zone must be analyzed thoroughly to ensure that NOx reduction will occur.

At temperatures of 900 – 1000 ℃ (Cooper & Alley, 2011), NH_3 will reduce NO_x to N_2 without a catalyst. At NH_3:NO_x molar ratios of 1:1 to 2:1, about 40-60% NO_x reduction can be achieved (U.S. Environmental Protection Agency, 1983; Farcy, Abou-Taouk, Vervisch, Domingo, & Perret, 2014). Potential problems with SNCR include incomplete mixing of NH_3 with the hot flue gas, and improper temperature control. If the temperature is too low, unreacted ammonia will be emitted; if the temperature is too high, NH_3 will be oxidized to NO.

The following are stoichiometric equations of ammonia reacting with NO_x to form N_2 and H_2O:

$$\mathbf{4NO + 4NH_3 + O_2 \rightarrow 4N_2 + 6H_2O} \quad (2.20)$$

$$\mathbf{2NO_2 + 4NH_3 + O_2 \rightarrow 3N_2 + 6H_2O} \quad (2.21)$$

2.4.4.1 Emergence of selective non-catalytic reduction (SNCR)

Controlling NO_x emissions is becoming a daunting technical challenge as increasingly strict emission limits are being imposed (Javed, Irfan, & Gibbs, 2007). NO_x formed in

combustion processes are usually due either to thermal fixation of atmospheric nitrogen in the combustion air leading to "thermal NO_x" as first postulated by (Zeldovich, 1946), or to the combination of hydrocarbon fragments and atmospheric nitrogen in the flame zone leading to "prompt NO_x" as first noticed by (Fenimore, 1971), or to the conversion of chemically bound nitrogen in the fuel, leading to "fuel NO_x". Fuel NO_x is generally believed to be the major contributor to NO emission in coal-fired combustion systems (Farcy, Abou-Taouk, Vervisch, Domingo, & Perret, 2014). Thermal NO_x formation is a function of oxygen availability, temperature, pressure and residence time in the combustion unit, whereas, formation of fuel NO_x depends on the nitrogen content of the fuel, total excess air rates and relative distribution of primary and secondary combustion air (McInnes & Wormer, 1990).

The advances made in controlling NO_x emissions from stationary combustion sources are evident from the abundant literature that covers several NO_x control technologies, some of which are still in development while others have had successful commercial applications (Khan, Desai, & Gawin, 1990). The NO_x control technologies can broadly be classified into "Pre-combustion", "Combustion Modification" and "Post combustion Techniques" which involve the use of low nitrogen fuels, modifying design and operating features of the combustion unit, and flue gas treatment after the combustion process respectively (Javed, Irfan, & Gibbs, 2007).

The stringency of NO_x emission standards in combination with its concentration in the flue gas after combustion determines the choice of a particular control strategy out of the various options available. These control strategies may vary depending on the combustion technology, fuel properties, whether the plant exists or newly built and the emission standard applicable to it. A wide spectrum of approaches is being used for controlling emissions from

stationary sources spreading from pre-combustion fuel cleaning to post-combustion flue gas treatment (Javed, Irfan, & Gibbs, 2007).

In this research more focus is given to using ammonia injection near the exit of the TO in order to reduce NO_x. NO_x formation is postulated to occur in this device mainly due to oxidation of the NH_3 in the syngas. The initial sludge has nitrogen which forms NH_3 during gasification. The syngas is not pre-mixed with air; rather air is mixed into the syngas in the thermal oxidizer.

'Non-catalytic' reactions were discussed as a method of reducing NO into post-flame gas by (Wendt, Sternling, & Matovich, 1972). Initially very little NO reduction was observed until enough NH_3 was added to completely consume the O_2 present, thus non-selective reduction of NO and O_2 was achieved. They suggested that NH_3 might have been pyrolysed to H_2 and N_2 due to very hot stainless-steel injector, before it entered the combustion effluent; thus, they argued that hydrogen may have been the reducing agent causing selective non-catalytic reduction (SNCR).

The SNCR method removes NO_x it has been formed as a by-product during fuel combustion. The principles of the NO_x removal by the SNCR technique is based on the thermal conversion of nitrogen oxides by injecting a reducing reagent into the flue-gas stream at an appropriate temperature range (Miller & Bowman, 1989). The chemical reagent responsible for NO_x reduction selectively reacts with nitrogen oxides present in the flue gas converting into harmless molecular nitrogen (N_2) and water vapor (H_2O) without employing a catalyst since NO_x reduction reactions occur at relatively high temperatures. Amine-based compounds such as ammonia, urea and cyanuric acid are used as the NO_x reductant. The NH_3 may be injected in

either anhydrous or aqueous form. Under stoichiometric conditions, the overall reactions may be expressed as equations (2.20) and (2.21).

The SNCR is a simple process of NO_x control. At temperatures between 850 °C and 1175 °C, a particular reagent is injected and thoroughly mixed in a flue gas stream containing NO_x. A rapid gas phase homogenous reaction occurs such that in spite of the presence of excess oxygen in the furnace, the reagent selectively reduces NO leaving oxygen largely untouched. The schematic of the SNCR concept is shown in Figure 4.

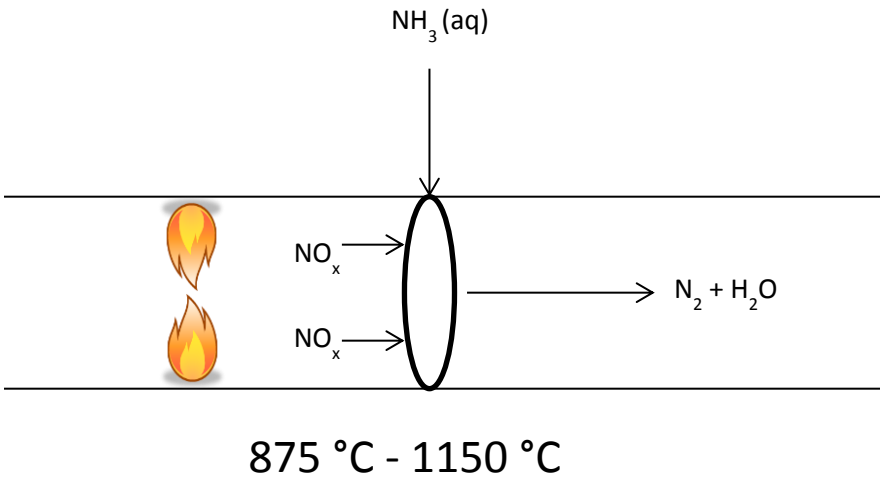

Figure 4 – SNCR concept

The concept is attractive because of its simplicity, catalyst-free system, ease of installation, applicability to all types of stationary-fired equipment, lower capital and operating cost, largely unaffected by fly ash and usability with other NO_x emission control technologies if necessary (Javed, Irfan, & Gibbs, 2007). In most full-scale applications, the reagents of choice are either NH_3 or urea. The focus of this work is on aqueous NH_3 injection and is discussed below.

2.4.4.2 Performance of using ammonia as reagent in SNCR

NH_3 injection for SNCR was introduced by Exxon Research and Engineering in 1975 (Lyon, 1975). The process has been investigated in the laboratory, pilot-scale facilities, and full-scale commercial plants. In spite of the research that has been conducted on the process, there are still significant challenges in its application, described by various features and characteristics of the process.

2.4.4.3 Temperature window

The range of temperatures in which the reaction takes place causing a net reduction of NO is termed the temperature window (Javed, Irfan, & Gibbs, 2007). This is a narrow window because below 800 °C the reaction is too slow to give any reduction and most of the NH_3 will be un-reacted. At higher temperatures, greater than 1000 °C, NH_3 tends to oxidize to form NO.

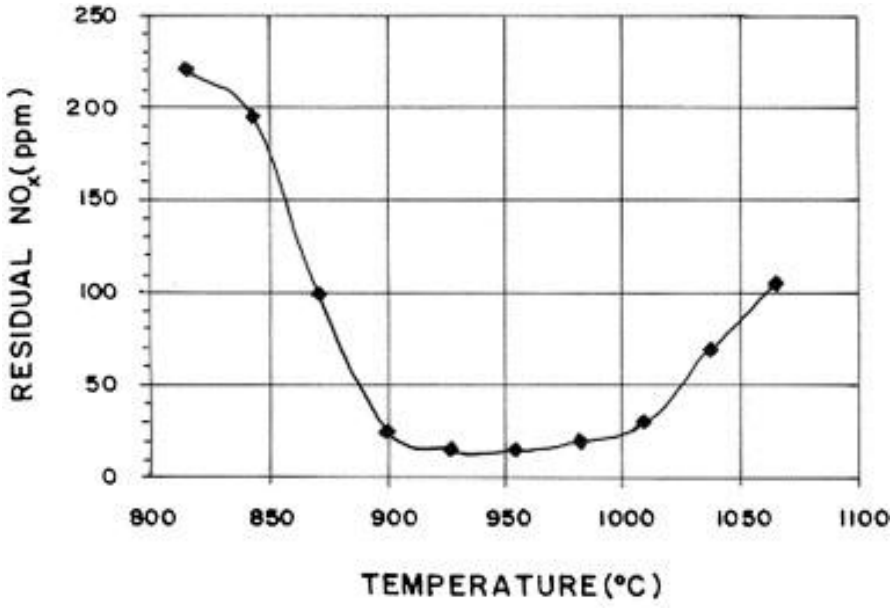

Figure 5 - Temperature window of SNCR process using ammonia at molar ratio (NH3/NOi) = 1.5 (Lyon & Longwell, Selective non-catalytic reduction of NOx by NH3, 1976)

The range over which any significant NO_x removal rates can be achieved varies from one system to the other depending on the system parameters such as flue gas constituents, flue gas velocity, and system geometry which influences the mixing between the reagent and the flue gas.

The NO reduction is initiated by the reaction of NH_3 with hydroxyl radicals giving amidogen ($-NH_2$) via reaction

$$NH_3 + OH \leftrightarrow NH_2 + H_2O \quad (2.22)$$

In the absence of water vapor, amidogen ($-NH_2$) can also be formed by reaction of NH_3 with O_2 atom (O), i.e.

$$NH_3 + O \leftrightarrow NH_2 + OH \quad (2.23)$$

The amidogen radical is highly selective towards NO and causes the overall reduction at optimum temperature even in an oxidizing environment. The mechanism can be explained in terms of OH radicals concentration or the dominance of the chain branching or chain terminating sequence. NO is primarily removed by the reactions (Javed, Irfan, & Gibbs, 2007)

$$NH_2 + NO \leftrightarrow N_2 + H_2O \quad (2.24)$$

$$NH_2 + NO \leftrightarrow NNH + OH \quad (2.25)$$

Reactions (2.24) and (2.25) are dependent on NH_2 formation via reaction (2.22) and (2.23) which in turn depend upon OH and O concentrations. This indicates that the overall reaction would be self-sustaining only if [NH_2 + NO→] reactions, either directly or indirectly, regenerate OH and O radicals to continue the NH_3 to NH_2 conversion. The SNCR process works because [NH_2 + NO→] reactions have a significant chain branching component which regenerates OH and O by the reaction sequence (Javed, Irfan, & Gibbs, 2007)

$$NNH + NO \leftrightarrow N_2 + HNO \quad (2.26)$$

$$HNO + M \leftrightarrow H + NO + M \quad (2.27)$$

The H atom produced in reaction (2.27) reacts with molecular O_2 to produce OH and O via

$$H + O_2 \leftrightarrow OH + O \quad (2.28)$$

The O_2 atom either continues reaction (2.28) or in the presence of water, it reacts via

$$O + H_2O \leftrightarrow OH + OH \quad (2.29)$$

Thus, there is a net gain of chain centers per cycle and as long as the branching sequence occurs at least a quarter of the time, the overall reaction would be self-sustaining (Javed, Irfan, & Gibbs, 2007).

2.4.4.3.1 Below optimum temperature

At a low temperature, less than 730 °C, reactions (2.28) and (2.29), which are strongly temperature dependent, have a low rate, thus OH is not replenished fast enough to convert NH_3 to NH_2, thereby chain termination reactions compete with the branching sequence, resulting in limited NO reduction. The chain terminating reactions are (2.24) and

$$NH_2 + HNO \leftrightarrow NO + NH_3 \quad (2.30)$$

$$OH + HNO \leftrightarrow H_2O + NO \quad (2.31)$$

These are all detrimental to NO reduction because they consume NH_2 and OH radicals, without producing any further radicals; whereas for any substantial reduction to occur, enough [OH] and [O] radicals are required to convert NH_3 to NH_2. Below 730 °C the rates of reactions (2.22) and (2.23) limit the overall process.

2.4.4.3.2 Within the optimum temperature range

The reaction sequences (2.22), (2.23) and (2.24) and (2.22), (2.23) and (2.25) onwards are dominant over the sequence (2.22), (2.24) and (2.32) onwards even up to temperatures below 1000 °C (Javed, Irfan, & Gibbs, 2007). This is so because in the range 730 – 1000 °C, the rate reaction of (2.27) is greater, compared to those of NH_2 oxidation reactions

$$NH_2 + OH \leftrightarrow NH + H_2O \quad (2.32)$$

$$NH_2 + NH_2 \leftrightarrow NH_3 + NH \quad (2.33)$$

Unlike the conditions T<730 °C, where only chain terminating reactions were dominant; in the optimum range 730 – 1000 °C the mix of branching and terminating is just right to cause the growth in chain carrier concentration. With the increase in temperature above 730 °C the reaction path leading to the chain branching reaction (2.41) becomes more important than the one leading to a termination reaction such as (2.45). This can be explained on the basis of the activation energy of the former $\mathrm{E}_{2.41} = 203{,}480 \frac{\mathrm{kJ}}{\mathrm{kmol}}$ which is greater than that of $\mathrm{E}_{2.45} = 0 \frac{\mathrm{kJ}}{\mathrm{kmol}}$ (Miller, Branch, & Kee, 1981; Miller & Bowman, 1989). Now H radicals from the former reactions may react with either molecules of O_2 or water causing more chain branching as follows.

$$H + H_2O \leftrightarrow OH + H_2 \quad (2.34)$$

or

$$H + O_2 \leftrightarrow OH + O \quad (2.35)$$

$$O + H_2O \leftrightarrow OH + OH \quad (2.36)$$

The branching can be observed by viewing the number of OH radicals formed per OH radical consumed in each cycle, e.g. for the sequence (2.22), (2.25), (2.26) and (2.27) involving

(2.34). For each OH consumed in (2.22) of the sequence, two OH radicals are produced (2.25) and (2.27) of the cycle (Javed, Irfan, & Gibbs, 2007).

Similarly in sequence (2.22), (2.25), (2.26) and (2.27) involving (2.28) and (2.29), for each OH consumed in (2.22) four OH radicals are formed in (2.25), (2.28) and (2.29). Due to this branching sequence, enough radicals are produced to drive reactions (2.22) and significant NO reduction is thus achieved within the optimum temperature range.

2.4.4.3.3 Above the optimum temperature

When the temperature is further increased beyond 1000 °C, the OH radical concentrations start building up, due to the branching sequence mentioned above. An excessive increase in OH concentration initiates an NH-forming sequence, and reaction (2.32) may start competing with reaction (2.22). Therefore the NH radical concentration starts building up and NO formation via sequence (2.22), (2.23), (2.27), (2.31), (2.32), (2.35), (2.36), (2.37) starts competing with the NO reduction sequence (Javed, Irfan, & Gibbs, 2007). Once NH is formed, the high-temperature oxidation reaction sequence leads directly to NO formation:

$$NH + O_2 \leftrightarrow HNO + O \quad (2.35)$$

$$NH + OH \leftrightarrow HNO + H \quad (2.36)$$

followed by

$$NH + O_2 \leftrightarrow OH + NO \quad (2.37)$$

$$HNO + OH \leftrightarrow H_2O + NO \quad (2.40)$$

At a temperature around 1230 °C the NO destroyed through the NO reduction sequence would just be balanced by that formed through oxidation sequence. At sufficiently high

temperature the oxidation sequences become significantly dominant resulting in a net increase in NO concentration (Javed, Irfan, & Gibbs, 2007).

2.4.4.4 Effect of O_2

The presence O_2 is a critical criterion for the initiation of the SNCR process. In a laboratory quartz plug flow reactor, (Lyon, 1976) found that without oxygen the NO removal was trivial. (Muzio, Arand, & Teixeira, 1976) reported that by increasing the excess O_2 level from 2% to 4% the magnitude of NO reduction was unaffected; however, at the higher excess oxygen levels, the NH_3 was more effective in removing NO at a temperature around 870 °C. (Robin, Price, & Squires, 1991) tested the effect of O_2 content of the flue gas in a coal ash deposition at two different temperatures. The results obtained are shown in Figure 5.

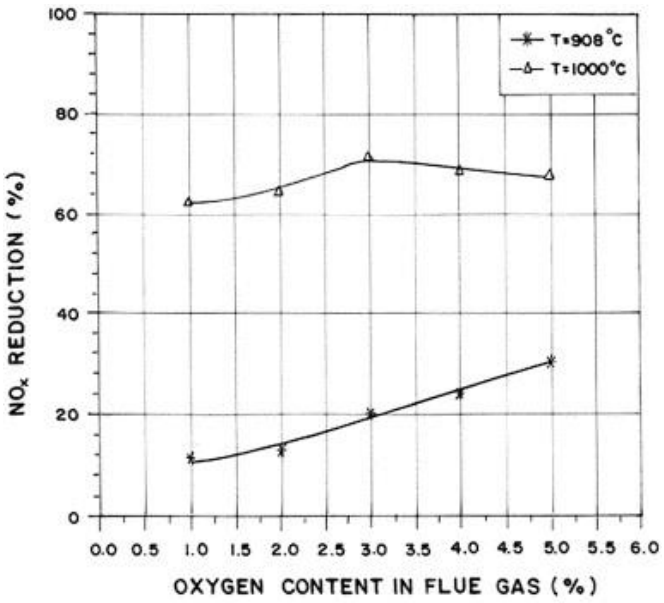

Figure 6 - Effect of oxygen contents at 908 and 1000 °C (Robin, Price, & Squires, 1991)

They inferred that at 1000 °C, the reduction is effectively independent of O_2 concentration, but that at 908 °C, where the effectiveness is lower, NO reduction increases with higher O_2

concentration. The additional O_2 minimizes any NH_3 slip, but emission of nitrous oxide may increase (Caton, Narney II, Cariappa, & W.R., 1995).

Initially it was suggested that NH_2 radicals react with NO by either yielding N_2 and H_2O directly or it may yield N_2, H and OH. Subsequent reactions (2.29), (2.23) and (2.22) regenerate NH_2 radicals. If the fraction of the reaction yielding N_2, H and OH is less than one half, then the overall interaction of NH_2 and NO will be chain terminating, and in the absence of O_2 a self-sustaining chain reaction would not occur (Javed, Irfan, & Gibbs, 2007). When O_2 is added, chain branching may occur by subsequent reactions (2.29), (2.23) and (2.22), and a self-sustaining chain reaction could occur (Lyon, 1976).

Miller, Branch, and Kee (1981) proposed that products of NH_2 + NO reaction were N_2H + OH (and N_2 + H_2O) rather than N_2 + H + OH (and N_2 + H_2O) as had been previously believed. Silver & Kolb (1982) supported this proposition experimentally. According to Miller, Branch, & Kee (1981), the advantage of excess O_2 is firstly, due to its presence, there would be more equilibrium OH present initially in the combustion products in slightly lean conditions. Secondly and more important, is that the reaction sequence (2.29) and (2.30) becomes dominant over (2.35) in lean combustion products, the former resulting in more OH. Even if there is no initial water, such as in the experiments of Lyon and Benn the O_2 atom produced (2.29) reacts directly with NH_3 via (2.23) producing NH_2 and OH (Lyon & Benn, 1978).

In the absence of O_2, reaction (2.29) would not occur and hydrogen atoms would react only with NH_3 at too slow a rate to result in NO removal in the scales of interest (Miller & Bowman, 1989).

2.4.4.5 Effect of initial NH_3/NO molar ratios

Molar ratio, in most of the investigations performed, is defined as the ratio of the number of moles of injected NH_3 with respect to the moles of NO initially present in the flue gas i.e., $R = NH_3/NO_{i.}$ The effect of the quantity of NH_3 injected on the NO reduction performance has been investigated by a number of researchers in the field. The results obtained by (Muzio, Arand, & Teixeira, 1976) on the combustion tunnel experiment, indicated that the largest NO reduction occurred at molar ratios up to 1.6. At optimal temperatures ~1000 °C an R = 2.0 maximized NO reduction.

2.5 Selection of pertinent reaction mechanism

The selection of the elementary steps that ultimately were utilized in the reaction mechanism were those published elementary reactions which closely resembled the conditions of the actual process in the MaxWest thermal oxidizer. The ideal reaction mechanism dealt with atmospheric pressure (1 atm), and temperatures around 1000-1800 Kelvin.

An extensive literature review was performed in order to appropriately decide upon those reactions which seemed to fit for the MaxWest process. The hydrocarbon, carbon monoxide and ammonia reactions were primarily obtained from Klippenstein, Harding, Glarborg, and Miller (2011) and Li, Zhenwei, Kazakov, and Dryer (2004), while the hydrogen sulfide reaction mechanism was obtained from Mathieu, Deguillaume, and Petersen (2013). Hydrogen chloride reactions were obtained from Wei, Wang, Liu, and Sheng (2009). The journal Combustion and Flame is a helpful resource when locating appropriate reactions. In the appendix, the full reaction mechanism is provided.

Experiments reported in the literature varied from internal combustion engines (ICE) to combustion of coal. Data from the combustion of coal, or from ICE's would not be appropriate for this research project. Reactor flow tubes, usually done in a laboratory scale, were the major focus when finding appropriate reactions, because the TO is a larger scale reactor tube. The TO in MaxWest is the first of its kind where air is introduced at specified points along the reactor, versus having the air and the fuel, in this case syngas, mix before flowing through the reactor.

3. DEVELOPMENT OF THE TO MODEL

3.1 Introduction

Provided in Figure 7 is a schematic view of the TO as modeled in this work. Syngas from the gasifier flows into the thermal oxidizer, before it is introduced to the TO the gas goes through a cyclone to remove particulate matter (PM). The first injection site or ring one, as depicted in Figure 7, allows for air and flue gas to be mixed with the combustible syngas. Ring 1 is located 3 feet from the inlet the mixed stream comes in contact with more air and flue gas after ring one and this occurs in ring two, which is located 5 feet from the inlet. The first injection site acts as a combustion region with fuel-rich conditions. The second site is a diluent stage where excess oxygen is present, and any combustible gases that made it through to the second injection site are assumed to completely oxidize in this stage of the reactor. By using staged combustion, peak temperatures (reaction rates) are lowered to minimize NO_x formation. In case NO_x levels are higher than regulatory standards at the exit of the TO, aqueous ammonia can be injected near the end of the reactor.

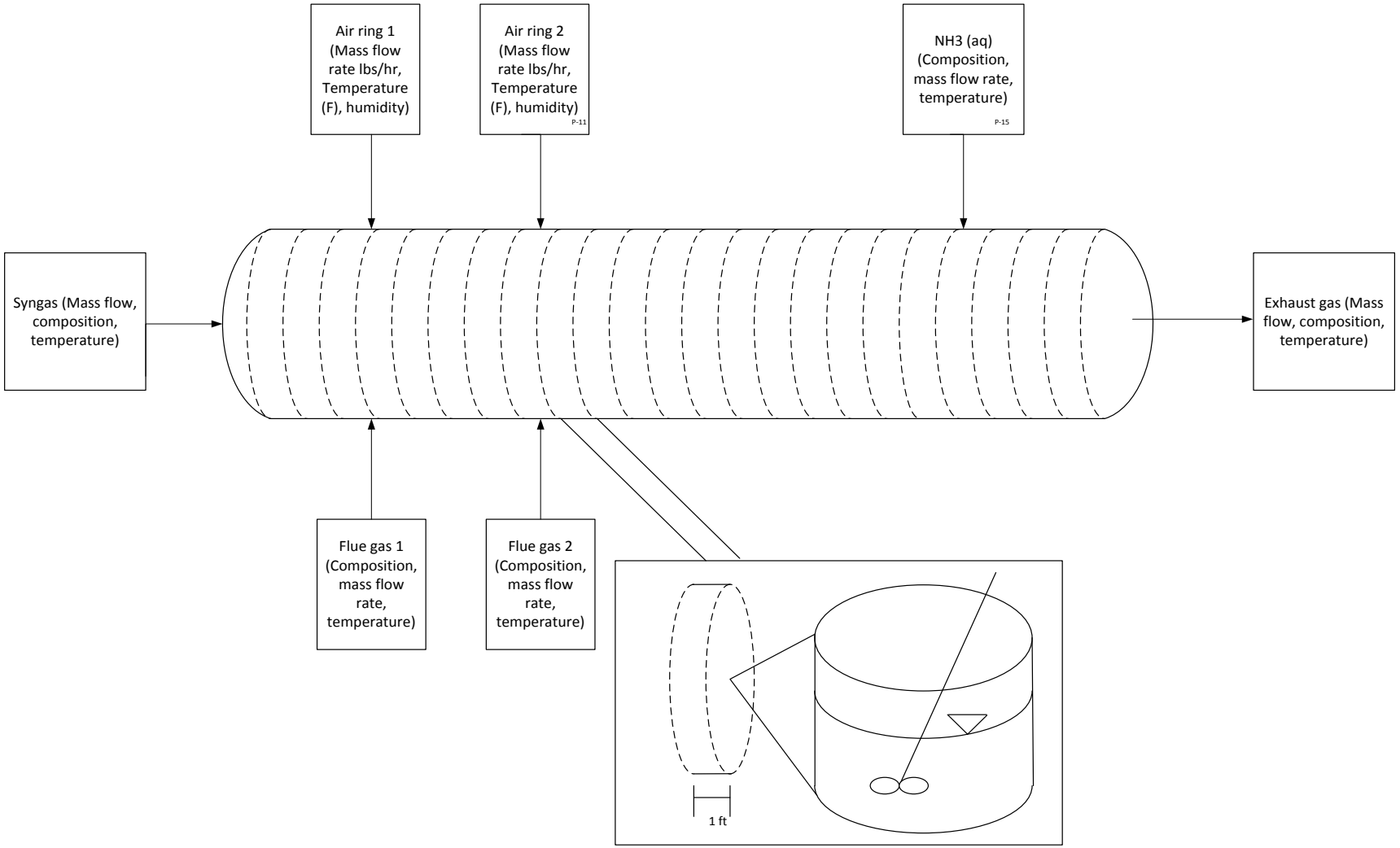

Figure 7 - TO process schematic

The following discussion details how the theoretical energy and material balance calculations were performed in modeling the TO. To help understand these calculations the following concepts are presented. In order to calculate temperature, gas compositions, and temperatures are first assumed. An approximate heat balance is calculated allowing for heat loss effects to take place in order to estimate actual temperatures.

Low temperatures (below 800 K) when used in CHEMKED, the software predicts no occurrence of reactions. Therefore, the simple approach of the iterative process calculating a temperature is based on an assumption of complete combustion of certain species reacting in a certain order until the oxygen is used up. The order of occurrence was verified with CHEMKED. Several runs were performed via CHEMKED in order to determine the order in which these combustible gases oxidize. It was found that benzene is consumed first, then methane, ammonia, hydrogen sulfide, hydrogen and finally carbon monoxide. In the heat balance model it was assumed that each fuel in the sequence burned completely if O_2 was available.

Table 1- Reaction sequence and heats of combustion

Reaction	Heat of combustion(Btu/lb)
$C_6H_6 + 7.5O_2 \rightarrow 6CO_2 + 3H_2O$	17,450
$CH_4 + 1.5O_2 \rightarrow CO + 2H_2O$	17,214
$NH_3 + 1.25O_2 \rightarrow NO + 1.5H_2O$	6,410
$H_2S + 1.5O_2 \rightarrow SO_2 + H_2O$	5,374
$H_2 + 0.5O_2 \rightarrow H_2O$	51,972
$CO + 0.5O_2 \rightarrow CO_2$	4,346

The stoichiometric amount of oxygen needed to combust the base-case syngas (2,040 acfm) is supplied by 2,500 lbs/hr air. Fuel rich (ϕ>1) combustion is known to occur in the first injection site. Air is limited in ring 1 to allow only the more rapidly combustible hydrocarbons (see Table 2) to burn first following the assumed sequence presented earlier. The temperature in ring 1 is calculated using the sum of the heats of reaction and the heat contained in the incoming syngas and air. Knowing that ring one is fuel rich, some of the combustible gases do not oxidize, mainly H_2 and CO.

The second air injection site allows for the remaining fuel to be completely oxidized as this site is fuel lean (ϕ<1). At this site the remaining fuels are oxidized releasing more heat, but the excess air acts as a temperature diluent. This lowers the temperature and reduces reaction rates by orders of magnitude, and works to terminate any more NO_x formation. Overall the device operates with excess air as a preferred method of combustion and air pollution abatement. High temperatures (> 1600 K) may damage air pollution control devices and cause high maintenance costs (Cooper & Alley, 2011). Therefore, a large heat exchanger follows the TO for energy recovery.

The last injection site is to provide NO_x control via SNCR using aqueous ammonia as the reagent. A water solution of ammonia is preferred over having pure ammonia on site. Pure ammonia is a hazardous chemical. Aqueous ammonia can be injected and quickly vaporizes at

the high T in the TO. Aqueous ammonia is injected near the end of the reactor, but with enough length left to allow for an adequate retention time for the SNCR process to occur. As discussed in a previous chapter the SNCR reactions are complex, and processes are different due to characteristics and flow regimes. Syngas can also vary in the amount of ammonia that it contains entering the TO. All the NH_3 entering with the syngas is presumed to be converted to NO and NO_2 in the TO, resulting in more ammonia needed at site 3. All chemical reactions are calculated within Chemked. The mass and energy balance are calculated outside of CHEMKED. A temperature is calculated and used to allow Chemked to run the reactions isothermally.

3.2 Energy and material balance

In this section of the report, the fundamental energy and material balance equations are presented and explained. One of the fundamental principles of this model is a mass balance.

$$\mathbf{M_{in}} = \mathbf{M_{out}} \tag{3.1}$$

$$\dot{\mathbf{m}}_{\mathbf{syngas}} + \dot{\mathbf{m}}_{\mathbf{Air_1}} + \dot{\mathbf{m}}_{\mathbf{Air_2}} + \dot{\mathbf{m}}_{\mathbf{FlueGas_1}} + \dot{\mathbf{m}}_{\mathbf{FlueGas2}} + \dot{\mathbf{m}}_{\mathbf{NH_3Injection}} + \dot{\mathbf{m}}_{\mathbf{H_2O_{NH_3}}} = \dot{\mathbf{m}}_{\mathbf{Effluent}} \tag{3.2}$$

Mole fractions are converted to mass fractions for use in CHEMKED:

$$\mathbf{X_i} = \frac{\mathbf{Y_i MW_i}}{\sum_{\mathbf{i=1}}^{\mathbf{N}} \mathbf{Y_i MW_i}} \tag{3.3}$$

Mass fractions can be converted back to mole fractions:

$$\mathbf{Y_i} = \left(\frac{\mathbf{X_i}}{\mathbf{MW_i}}\right) / \left(\sum_{\mathbf{i=1}}^{\mathbf{N}} \mathbf{X_i / MW_i}\right) \tag{3.4}$$

$$\sum_{\mathbf{i=1}}^{\mathbf{N}} \mathbf{Y_i} = \mathbf{1} \tag{3.5}$$

$$\sum_{\mathbf{i=1}}^{\mathbf{N}} \mathbf{X_i} = \mathbf{1} \tag{3.6}$$

Where,

$\dot{m}_i$ = (lbs/hour or mass/time)=mass flow rate
Y_i = mole fraction

X_i = mass fraction
MW_i = molecular weight of compound i (lb/lbmol or g/gmol)
N = total number of compounds

After a mass balance has been performed the next vital calculation is the energy balance. The thermodynamic equation was based on a three polynomial equation to determine constant specific heat and enthalpy values (Santoleri, Reynold, & Theodore, 2000).

$$\mathbf{c_p = \alpha + \beta T + \gamma T^2 \left(\frac{Btu}{lbmol-R}\ or \frac{cal}{gmol-K}\right)} \quad (3.7)$$

Where,

c_p = specific heat at given temperature ($\frac{Btu}{lbmol-R}$ or $\frac{cal}{gmol-K}$)
α, β, γ = polynomial constants
T = temperature (K)

Integrating the specific heat with respect to temperature the enthalpy is obtained, where:

$$\mathbf{\Delta H_i = n_T \sum Y_i \int_{T_0}^{T_1} c_p\, dT} \quad (3.8)$$

Reference temperature is denoted as $T_0 = 77°F$

$$\mathbf{c_{p_i} = \frac{\Delta H_i}{T_1 - T_0}} \quad (3.9)$$

$$\mathbf{c_{p_i} = \alpha_i + \frac{\beta_i}{2}\left(\frac{T_1^2 - T_0^2}{T_1 - T_0}\right) + \frac{\gamma_i}{3}\left(\frac{T_1^3 - T_0^3}{T_1 - T_0}\right)} \quad (3.10)$$

Where,

c_{p_i} = specific heat of compound i (Btu/lbmol-F)
T = Temperature (K)

The steady state enthalpy balance around any space in the reactor is:

$$\sum \dot{\boldsymbol{n}}_{\boldsymbol{i}} \mathbf{c}_{\mathbf{p}_i} \mathbf{T}_{\mathbf{in}} + \sum \mathbf{n}_i \Delta \mathbf{H}_{\mathbf{rxn}_i} = \sum \dot{\boldsymbol{n}}_{\boldsymbol{i}} \mathbf{c}_{\mathbf{p}_i} \mathbf{T}_{\mathbf{out}} + \mathbf{q} \quad (3.11)$$

Where,

$\sum \dot{\boldsymbol{n}}_{\boldsymbol{i}} c_{p_i} T_{in}$ = heat into a boundary (Btu/hr)

$\sum \dot{\boldsymbol{n}}_{\boldsymbol{i}} c_{p_i} T_{out}$ = heat out of boundary (Btu/hr)

q = heat loss due to walls (Btu/hr)

ΔH_{rxn} = heat released due to combustion reactions (BTU)

The pertinent polynomial constants used for the temperature and heat calculations are displayed in Table 9. Note that when applying equation (3.2) or (3.13), depending on what section of the TO the calculations are being performed certain variables may be neglected. For example if calculations are being performed in ring one there is no need to include the amount of air in ring two or heat in ring two to the mass or energy balance of ring one, respectively. The same is true for the remaining reactor length. More details are shown in the following section.

Table 2 - Polynomial constants for pertinent combustion species (Santoleri, Reynold, & Theodore, 2000)

Species	alpha	beta	gamma
N_2	6.524	1.25E-03	-1.00E-09
O_2	6.148	3.10E-03	-9.23E-07
Ar	6.148	3.10E-03	-9.23E-07
H_2O	7.256	2.30E-03	2.83E-07
CO_2	6.214	1.04E-02	-3.55E-06
CO	6.42	1.67E-03	-1.96E-07
CH_4	3.381	1.80E-02	-4.30E-06
C_6H_6	-0.409	7.76E-02	-2.64E-05
H_2	6.947	-2.00E-04	4.81E-07
HCL	6.732	4.33E-04	3.70E-07
H_2S	6.662	5.13E-03	-8.54E-07
SO_2	7.116	9.51E-03	3.51E-06
NH_3	6.086	8.81E-03	-1.51E-06
NO	7.02	-3.70E-04	2.55E-06

3.2.1 Energy balance equation ring 1

$$\sum_{i=1}^{N}\left(c_{p_i}n_i\right)_{syngas}\Delta T+\sum_{i=1}^{N}\left(c_{p_i}n_i\right)_{Air\ ring\ 1}\Delta T+\sum_{i=1}^{N}\left(c_{p_i}n_i\right)_{FlueGas\ ring\ 1}\Delta T+\sum\Delta H_{reaction}=\sum_{i=1}^{N}\left(c_{p_i}n_i\right)_{Effluent}\Delta T-q_{heatloss} \quad (3.12)$$

3.2.2 Energy balance equation ring 2

$$\sum_{i=1}^{N}\left(c_{p_i}n_i\right)_{ring\ 1\ effluent}\Delta T+\sum_{i=1}^{N}\left(c_{p_i}n_i\right)_{Air\ ring\ 2}\Delta T+\sum_{i=1}^{N}\left(c_{p_i}n_i\right)_{FlueGas\ ring\ 2}\Delta T+\sum\Delta H_{reaction}=\sum_{i=1}^{N}\left(c_{p_i}n_i\right)_{Effluent}\Delta T-q_{heatloss} \quad (3.13)$$

3.2.3 Energy balance equation aqueous ammonia injection

$$\sum_{i=1}^{N}\left(c_{p_i}n_i\right)_{ring\ 2\ effluent}\Delta T+\sum_{i=1}^{N}\left(c_{p_i}n_i\right)_{NH_{3_{injection}}}\Delta T-\Delta H_{vap}=\sum_{i=1}^{N}\left(c_{p_i}n_i\right)_{Effluent}\Delta T-q_{heatloss} \quad (3.14)$$

3.2.4 Energy balance equation of non-injection sites

$$\sum_{i=1}^{N}\left(c_{p_i}n_i\right)_{\text{mixed gas}}\Delta T=\sum_{i=1}^{N}\left(c_{p_i}n_i\right)_{\text{Effluent}}\Delta T-q_{\text{heatloss}} \tag{3.15}$$

To determine the reaction temperature, iteration was done based on the following equations. Constant specific heat is first guessed at an assumed temperature, multiplied by its specific molar flow rate.

$$c_{p_{\text{Guess}}}=\sum_{i=1}^{N}\left(c_{p_i}\dot{n}_i\right)_{\text{Guess}} \tag{3.16}$$

Where:

$\dot{n}$ = molar flow of gas (lbmol/hr)= $\frac{\dot{m}_t}{MW_{gas}}$

MW_{gas} = molecular weight of gas lb/lbmol

With an assumed specific heat enthalpy may also be calculated. In order to converge to an appropriate temperature a numerical method was utilized, the Newton-Rhapson method. The numerical method takes a function and in order to solve for that function it is first set to zero. For example equation 3.15 will be modified for illustration purposes.

$$0=\sum_{i=1}^{N}\left(c_{p_i}n_i\right)_{\text{mixed gas}}\Delta T-\sum_{i=1}^{N}\left(c_{p_i}n_i\right)_{\text{Effluent}}\Delta T+q_{\text{heatloss}} \tag{3.17}$$

Equation 3.17 is now the function and it is a function of temperature or T.

$$f(T)=\sum_{i=1}^{N}\left(c_{p_i}n_i\right)_{\text{mixed gas}}(T_{\text{mix}}-T_{\text{ref}})-\sum_{i=1}^{N}\left(c_{p_i}n_i\right)_{\text{Effluent}}(T-T_{\text{ref}})+q_{\text{heatloss}} \tag{3.18}$$

T is the only variable in equation 3.17 that is to be solved for, so the next step is to find the derivate of the function.

$$f'(T)=-\sum_{i=1}^{N}\left(c_{p_i}n_i\right)_{\text{mixed gas}} \tag{3.19}$$

The specific heat is also a function of temperature. The first assumed temperature is now utilized in equations 3.18 and 3.19 and then the following formula is performed.

$$\boldsymbol{T_{new} = T_{old} - \frac{f(T)}{f'(T)}} \tag{3.20}$$

The new temperature is utilized in equations 3.18 through 3.19 until $T_{new} = T_{old}$. This numerical method is performed for each ring and for the ammonia injection.

3.3 Velocity

Knowing how fast the gas is traveling along the reactor is also import. Knowing the gas flow rate, and velocity allows us to calculate the time it takes for the gas to travel a certain distance. The user enters a distance (the default is 1-foot) of one increment in the reactor. The computer calculates the amount of time it takes to travel one foot from conditions of the run before the reactions take place. The conditions that are needed are the number of moles of species, temperature, mass flow rate and the diameter. CHEMKED gives the user the mass fractions, which are converted back to moles. Once the total amount of moles have been calculated, then the gas law is applied.

$$\mathbf{PQ = \dot{n}RT} \tag{3.21}$$

$$\mathbf{Q = \frac{\dot{n}RT}{P}} \tag{3.22}$$

Where,

P	= Pressure (atm)
$\dot{n}$	= total number of moles (lbmol/s)
Q	= volumetric flow (ft^3/s)
R	= Universal gas constant (0.7302 atm-ft^3/R-lbmol)
T	= gas temperature in degree Rankine

To find the velocity take the volumetric flow and divide by the area:

$$\mathbf{u} = \frac{\mathbf{Q}}{\mathbf{A}} \tag{3.23}$$

$$\mathbf{A} = \left(\frac{\pi \mathbf{D}^2}{4}\right) \tag{3.24}$$

Where:

A	= Area (ft^2)
D	= inside diameter of the thermal oxidizer (feet)
Q	= volumetric flow (ft^3/s)
u	= linear velocity (ft/s)

Once the linear velocity has been determined, the distance increment is divided by the linear velocity, and time has been calculated in seconds.

This time is used in CHEMKED as the reaction time for the increment. The faster the gas velocity the shorter the residence time; the shorter time allowed for reactions to take place along the reactor length and vice versa.

3.4 Heat Loss

A difference in temperature between two bodies in close proximity or between two parts of the same body results in a heat flow from the higher temperature to the lower temperature. There are three different mechanisms by which this heat transfer can occur: conduction, convection, and radiation (Santoleri, Reynold, & Theodore, 2000). When the heat transfer results from macroscopic motion, such as currents in a fluid, the mechanism is that of convection. Conduction through the walls is the mechanism of heat loss for the T.O. The flow of heat from a hot fluid to cooler fluid through a solid wall is a common occurrence in engineering equipment especially a TO.

The rate of heat transfer through a unit of contact area is referred to as the heat flux density and, at any point along the tube length, is given by (Santoleri, Reynold, & Theodore, 2000),

$$dq/dA = U(T-T_a) \quad (3.25)$$

Where,

dq/dA	= local heat flux density (Btu/h-ft^2)
U	= local overall heat transfer coefficient (Btu/h-ft^2-°F)
T	= temperature (°F)
T_a	= ambient temperature (°F)

The contact area is taken as the circumferential area of a reactor tube,

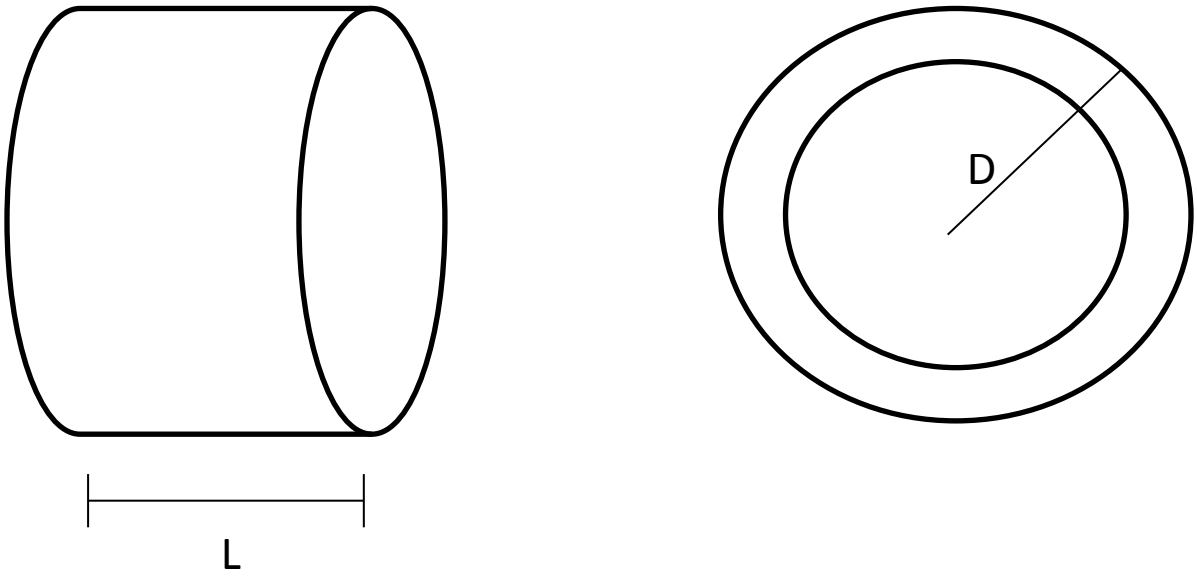

Figure 8 - Section of reactor tube

$$\mathbf{A = \pi DL} \quad (3.26)$$

Where,

A	= contact area (ft^2)
D	= outside diameter of the tube (ft)
L	= horizontal length (ft)
π	= constant, pi (3.1428)

Incorporating the energy balance and heat loss obtains two different equations. As mentioned before each distance increment in the TO is being treated as a batch reactor. The two different equations depend on whether the respective section of reactor has combustion reactions or not. In the rings there will be combustion occurring, and in that case temperature is:

$$\mathbf{T_i = T_o + \Delta t\left[\frac{1}{\sum \dot{n} c_p} * \left(\Delta H_c - UA(T_0 - T_a)\right)\right]} \quad (3.27)$$

Where,

T_o	= old temperature($^\circ F$)
T_i	= new calculated temperature ($^\circ F$)
Δt	= residence time for the specified distance increment
$\sum \dot{n} c_p$	= sum of all species, from i to N, the product of the species individual molar flow rate times the specific heat at the specified temperature $\left(\frac{Btu}{sec-^\circ F}\right)$
ΔH_c	= heat of combustion (Btu/sec)
T_a	= ambient temperature ($^\circ F$)

When no combustion reactions are occurring the following equation is utilized,

$$\mathbf{T_i = T_o - \frac{UA(T_o - T_a)}{\sum \dot{n} c_p}} \quad (3.28)$$

When in the ammonia injection zone the following equation is utilized,

$$\mathbf{T_i = T_o + \Delta t\left[\frac{1}{\sum \dot{n} c_p} * \left(\Delta H_c - \Delta H_{vap} - UA(T_{old} - T_a)\right)\right]} \quad (3.29)$$

Where,

ΔH_{vap}	= heat of vaporization of water (Btu/sec)

4. THE IMPLEMENTATION OF A SYNGAS THERMAL OXIDIZER MODEL AND DISCUSSION OF THE COMPUTER CODE

4.1 Introduction

This section of the report focuses on the implementation of the model using CHEMKED and java. Java was used to develop the graphical user interface (GUI). In order to reduce computing time a program was developed to solve for temperatures in the first two air rings. The program was designed through an integrated development environment (IDE) for development with Java; the IDE is named NetBeans; NetBeans also has the capability for development of a graphical user interface (GUI) design, which was used for ease of data input for this research.

NetBeans is an open source development environment meaning it can be obtained for free online and used for many programming needs (NetBeans, 2013).

The chemical model used in this research, developed from literature, is executed via CHEMKED (Jelezniak & Jelezniak, 2009). Chemked was purchased and used to run various reactions that were found in the literature. Chemked has two programs: one to run the reactions and output the results, and another that is used to reduce large reaction mechanisms to more manageable sizes. Both tools were used for this research project, as described in the following sections.

CHEMKED 1 has a user friendly interface that allows the user to enter a composition of a given gas stream, and CHEMKED performs the simultaneous solutions of all the elementary reactions that the user defines in the CHEMKED program. The program also has an output and

allows the user to graph the concentrations over time and even export data via notepad. With CHEMKED 2 a large reaction mechanism may be reduced. Thus, CHEMKED 2 identifies and eliminates elementary step reactions that are not important to the overall mechanism by performing an automatic sensitivity analysis.

4.2 Flow chart

Figure 9 gives a logic flow chart showing how the program works. The logic flows in the following steps:

1. The necessary data for calculation, such as temperatures, mass flow rates, compositions, and design elements, are input
2. The program checks whether everything has been inputted right, the sum of all gas composition is equal to one; temperatures are not negative values, etc.
3. Preliminary calculations are performed next. These calculations are performed to present the input data in a way that CHEMKED can read it and allow for the solver executable to run the necessary input file. These calculations also allow for mass and energy balances to be calculated at points where new material is input into the TO. For example, the mole fractions for all species are then written into their appropriate line in the input file. Along with the mole fractions, the temperature is inputted. This is all done before the CHEMKED solver is called upon to perform its calculations.
4. This step calculates the volumetric flow of the gas stream based on the ideal gas law and calculates the time it takes for this stream of gas to travel the next incremental distance. CHEMKED will run in batch reactor mode, isothermally, for that specified amount of time.

5. Now the program checks whether the increment is at a location where a new flow (air, flue gas or NH_3 enters). At these locations other calculations are performed:
    a. When the incremental distance has reached an air injection point material and energy balances are performed
    b. All mole fractions are converted to mass fractions. Mass balances (including combustion reactions) are now performed.
    c. The next step is to determine the temperature which these gases attain after the mass balance. When the air is introduced to the syngas complete combustion is assumed to take place until all the O_2 is used up or all the fuels are combusted.
    d. The heats of reaction are calculated and a temperature is determined. Before continuing with the run an external run (this is a mock run) is performed at the new temperature. This is done to verify which components completely oxidized first and this is recorded into variables. The new sequence of reactions is then taken in and a new heat of reaction may be calculated. A new temperature is determined, and no further mock runs are done.
    e. The new temperature will be used in CHEMKED to run this section of reactor (injection site 1 or 2), and this will be run isothermally.
    f. The next distance increment will be followed by the same procedure verifying whether or not the specified distance increment is an air injection site, and until this method is called upon again, thus the process will otherwise continue and proceed to steps 1 through 5 and repeat the procedure.
6. If not an air injection site or the aqueous ammonia site iteration will continue on.

7. When the program has reached the end of the TO, it will output results to excel.
8. All mole fractions have been stored into arrays so that they may be outputted to excel.
9. Only certain specified species were selected to be outputted via excel; the pollutants of concern, along with N_2, H_2O, CO_2 and O_2.

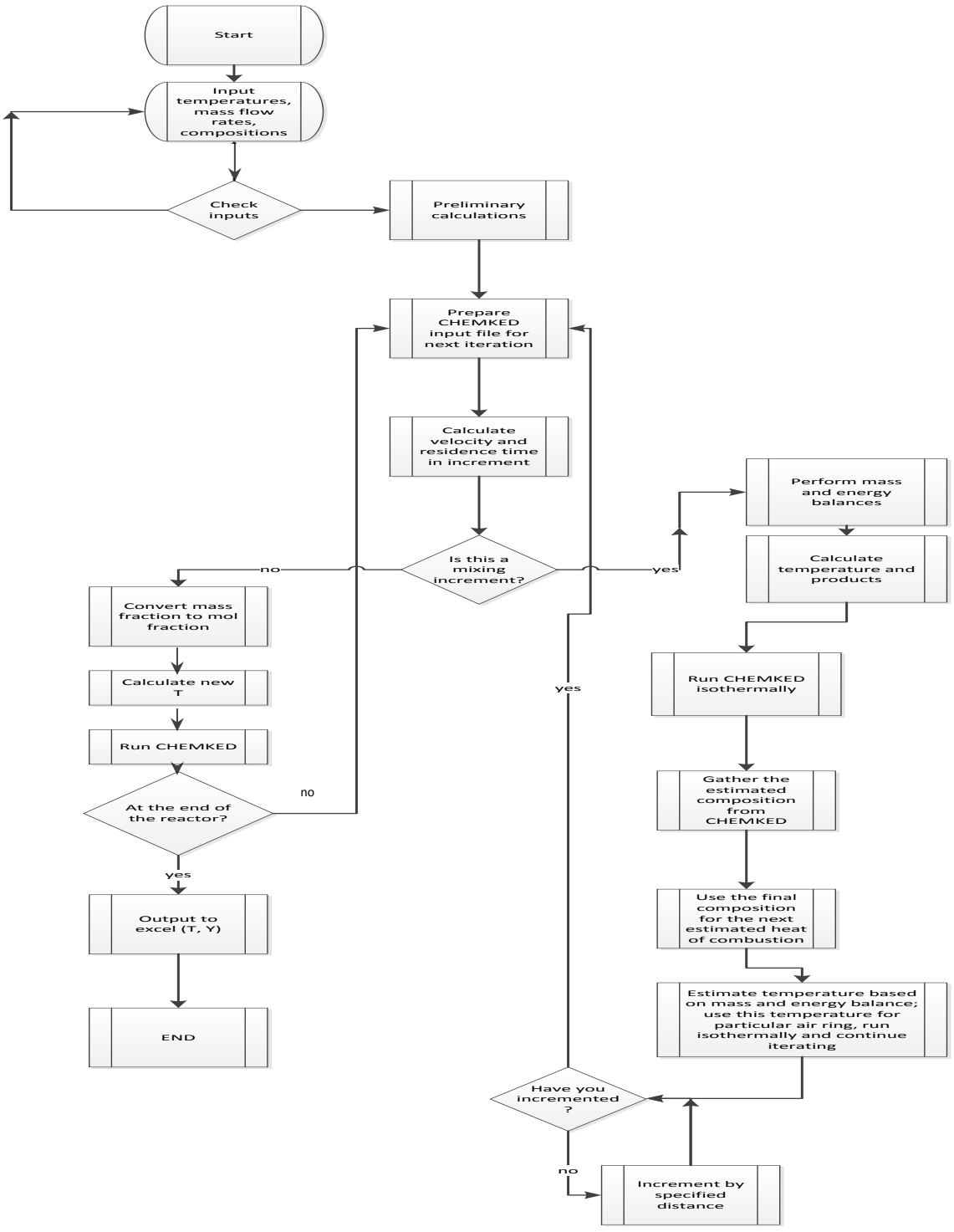

Figure 9 - Logic flow chart

4.3 Graphical User Interface (GUI)

Basic coding in java is similar to C programming. Minor differences exist in the way functions and classes are identified in java. Main function needs to be identified as in C. This main function is what is read by java. Several functions are pre–coded to provide for easier debugging; making appropriate adjustments and just being able to read the code. With this research there were more than 5000 lines of code; commenting and keeping the code organized is vital for the longevity of this project.

A graphical user interface (GUI) was developed as part of this work. Figure 10 shows the screen of the GUI for the input of data:

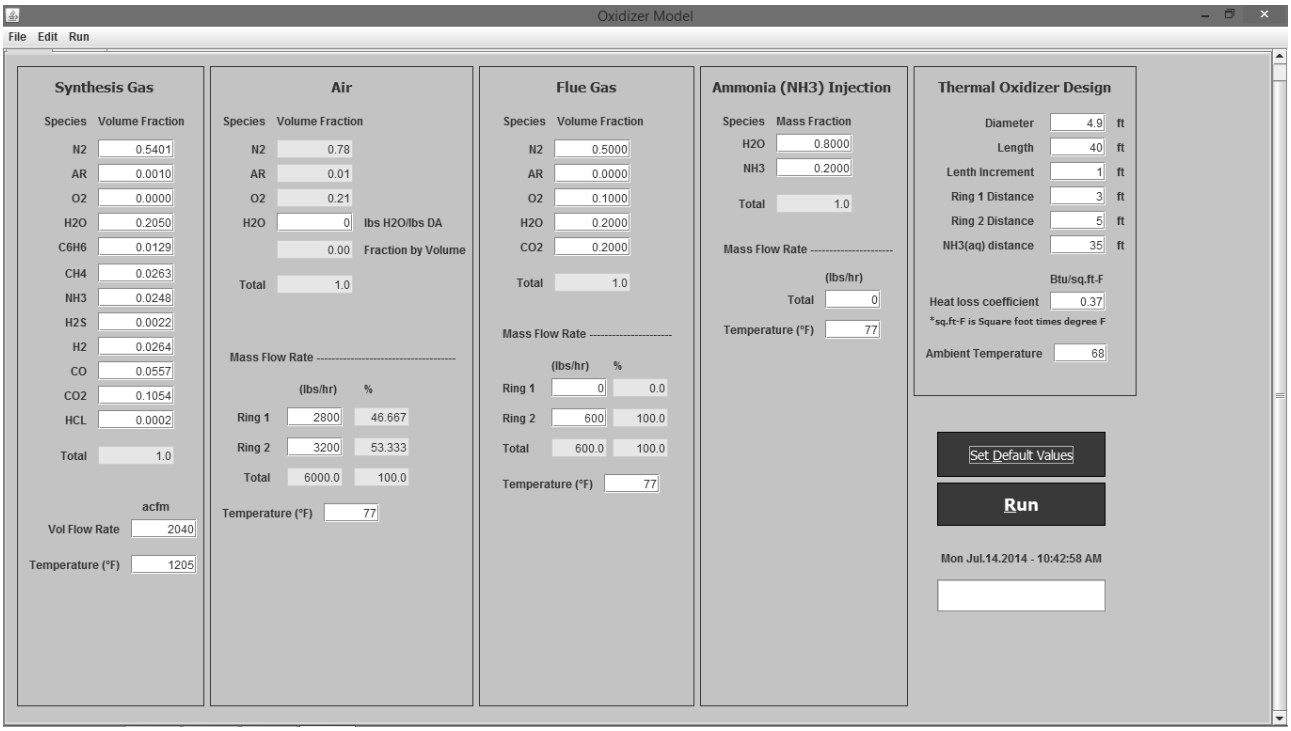

Figure 10 – Screenshot of GUI

Columns break down the GUI. Each column has spaces for different inputs pertinent to the run. Inputs are temperature (F), mass flow rates (lbs/hr), mol fractions (decimal), and

design of the thermal oxidizer all in ft, diameter, length, length increment, distances of ring 1,2 and the liquid ammonia injection site. A default value button was incorporated, but manual input is also allowed.

5. MODELING RESULTS & DISCUSSION

5.1 Reaction Mechanism

There are more than 1500 reactions and over 190 species in the full reaction mechanism. CHEMKED II allows the user to reduce a reaction mechanism. The mechanism was reduced to 496 reactions with 120 species. Reduced mechanisms allow for faster calculating times and similar results. NO_x reduction reactions did not function well in the reduced model, thus the mechanism was switched back to the full mechanism. The full mechanism is provided in the appendix.

5.2 Base case results

Synthesis gas rate and composition were obtained from the gasifier model. The results from the gasifier model are dependent on operating data provided by MaxWest: the air flow, flue gas and biosolids feed rate and composition.

The TO base case uses the synthesis gas rate and composition as predicted by the gasifier model (Champion, 2013). Other inputs for the TO model were obtained from MaxWest operating data.

The following is the base case composition and rates for the TO model followed by results of the base case:

5.2.1 Base case composition and mass or volumetric flow rates

Table 3 - Synthesis gas composition, flow and temperature (base case)

Parameter	Vol%, flow, or temp.
N_2	54.01%
Ar	0.10%
O_2	0.00%
H_2O	20.50%
CO	5.57%
CO_2	10.54%
CH_4	2.63%
C_6H_6	1.29%
H_2	2.64%
NH_3	2.48%
H_2S	0.22%
HCl	0.02%
Volumetric flow rate	2,040 ft^3/min (acfm)
Mass flow rate	2,723 lbs/hr
Temperature (Fahrenheit)	1,205 °F

Table 4 - Air composition, flow and temperature (base case)

Parameter	Vol%, flow, or temp.
N_2	78.00%
Ar	1.00%
O_2	21.00%
H_2O	0.00%
Mass flow rate ring 1	3,900 lbs/hr
Mass flow rate ring 2	4,000 lbs/hr
Total mass flow rate	7,900 lbs/hr
Temperature (Fahrenheit)	77 °F

Table 5 - Flue gas composition, flow and temperature (base case)

Parameter	Vol%, flow, or temp.
N_2	50.00%
Ar	0.00%
O_2	10.00%
H_2O	20.00%
CO_2	20.00%
Mass flow rate ring 1	0 lbs/hr
Mass flow rate ring 2	500 lbs/hr
Total mass flow rate	500 lbs/hr
Temperature (Fahrenheit)	77 °F

Table 6 - Aqueous ammonia composition, flow, and temperature (base case)

Parameter	Vol%, flow, or temp.
NH_3	20.00%
H_2O	80.00%
Mass flow rate	0 lbs/hr
Temperature (Fahrenheit)	77 °F

5.2.2 Base case results

The following are the base case results. The input composition and rates were presented in Tables 3-6. The results indicate that most, but not all of the fuel is burned up in the first air ring, Figure 11. There is a sharp rise in temperature in ring 1 due to combustion of the fuels; then at the second air ring there is an immediate drop in temperature due to dilution with excess air, Figure 12. The base case model NO_x concentrations at base case conditions are 3,300 ppm in the exhaust gas, Figure 13. Base case has an ϕ close to stoichiometric ($\phi = 0.85$) in the first air ring.

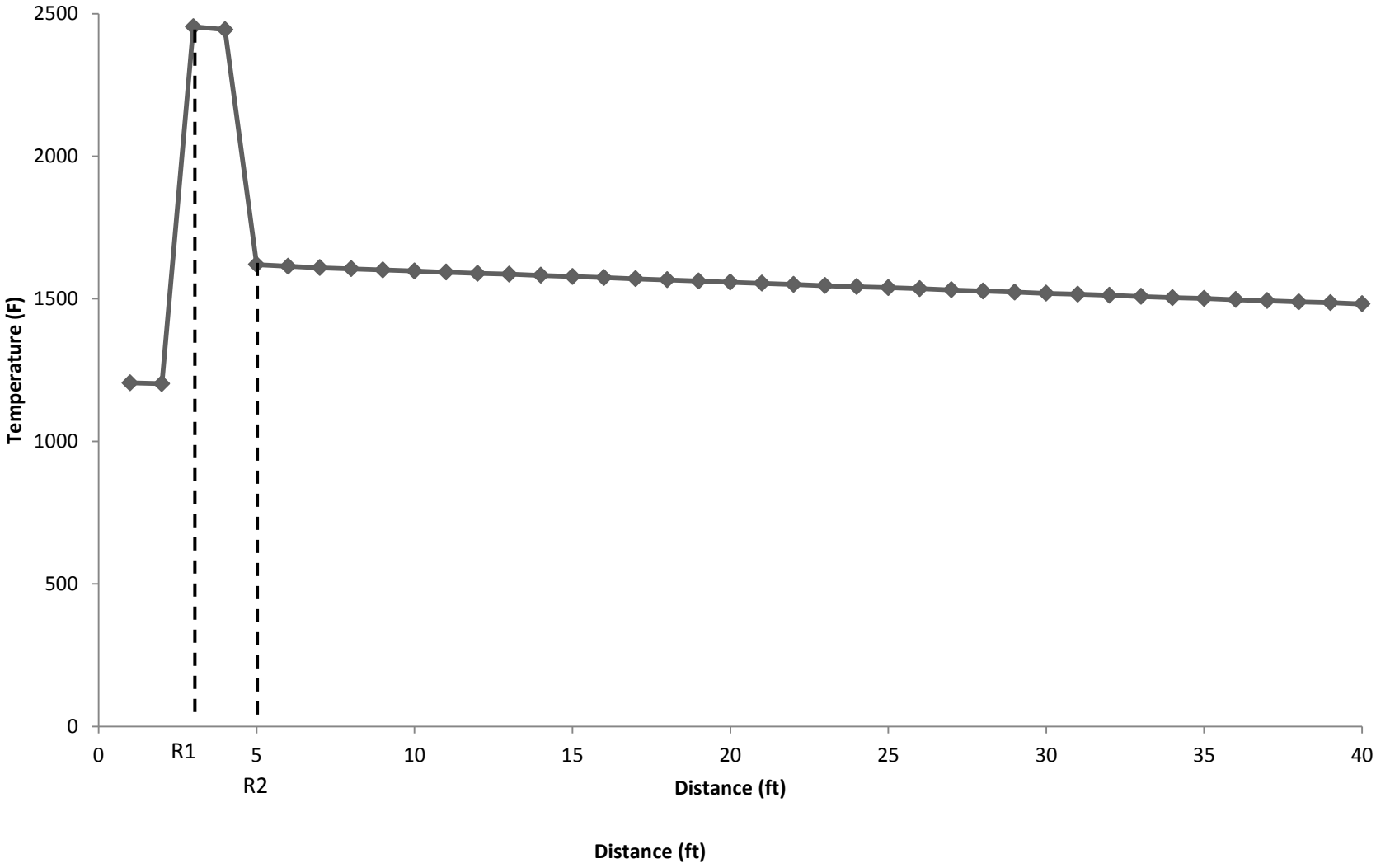

Figure 11 - Base case molar flow rates of combustible gas

Figure 12 - Base case temperature profile (R1 and R2 indicate locations of air rings 1 and 2)

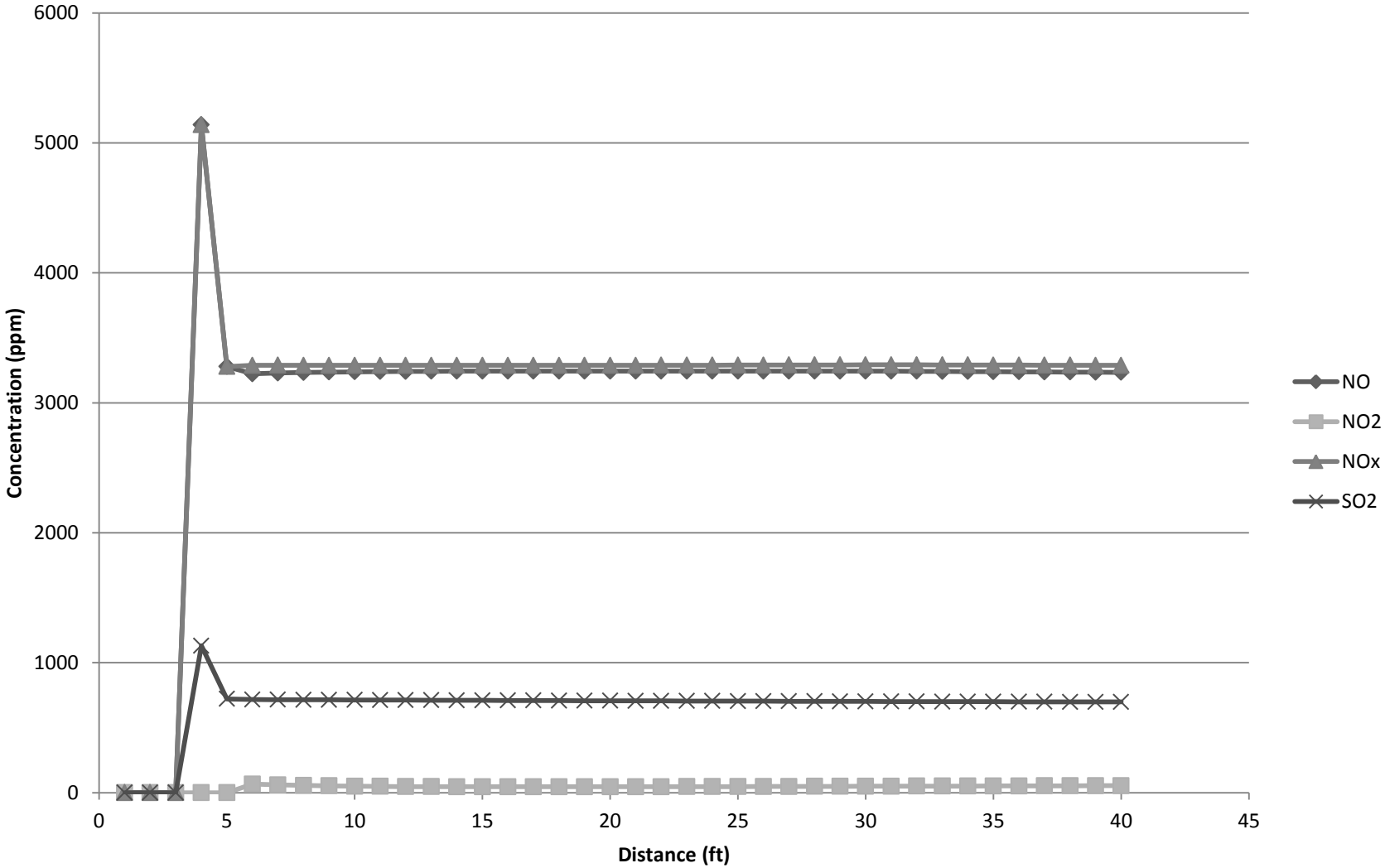

Figure 13 - Base case exhaust gas contaminant concentrations

5.3 Sensitivity Studies

Temperature and NO_x concentrations were analyzed when changes to C_6H_6, CH_4, CO, H_2, NH_3, and H_2S were made. Each fuel species was increased or decreased by 50% from the base case amount; holding air, flue gas and temperature constant.

Figures 14, 16, 18, 20, and 24 are temperature profiles for the combustible gases that were modified. When each fuel was increased by 50%, temperatures were greater than that of the base case, and when decreased by 50%, temperatures were less than that of the base case. This is apparent because more (or less) of a combustible gas will increase (or decrease) the total heat released by combustion, which in turn increases (or decreases) temperature, respectively. Note when changes were made to the combustible gas compositions, all other species were held constant except N_2; i.e. when C_6H_6 was increased by 50%, N_2 was decreased by an equal number of moles.

Figures 15, 17, 19, 21, and 25 are NO_x profiles when the above-mentioned changes were made to the combustible gases. When any of the combustible gases were increased, the production NO_x was greater than the base case and when the fuels were decreased, the NO_x was lower than the base case. This happens because when there is more (or less) of the combustible gas, the temperature increases (or decreases) as stated previously. At higher temperatures, more NO_x is formed due to the kinetics.

Figures 22 and 23 were an exception to what was mentioned in the previous paragraph. Figure 22 did not show a significant increase in temperature compared to Figures 14, 16, 18, 20, and 24, but Figure 23 had a significant increase in NO_x compared to Figures 15, 17, 19, 21, and 25. That is because increasing the NH_3 composition of the syngas while having very little heat

effect, greatly increases the amount of nitrogen in the syngas allowing for higher NO_x concentrations.

5.3.1 Changes to C_6H_6

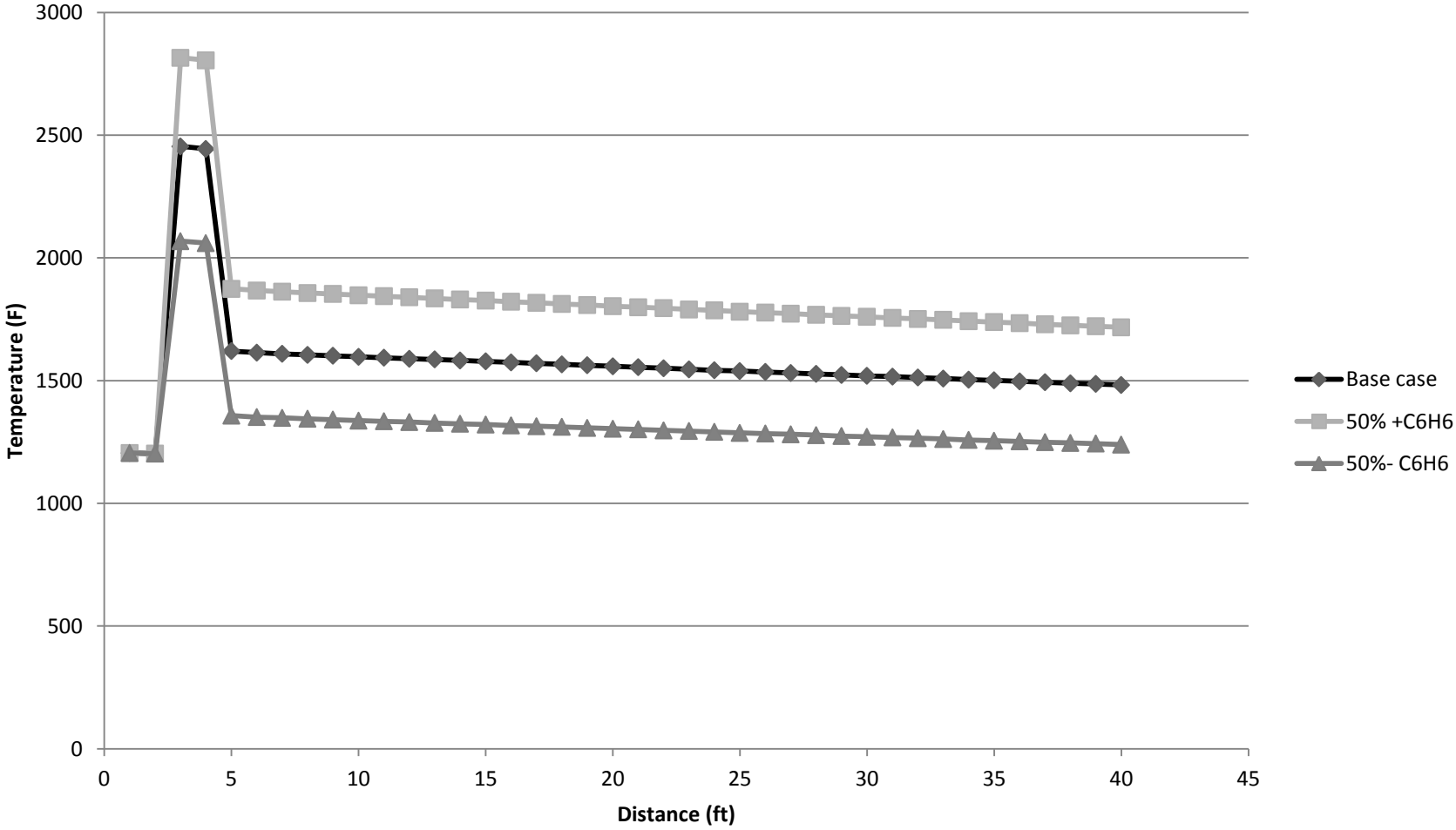

Figure 14 – Temperature profile with change to C6H6

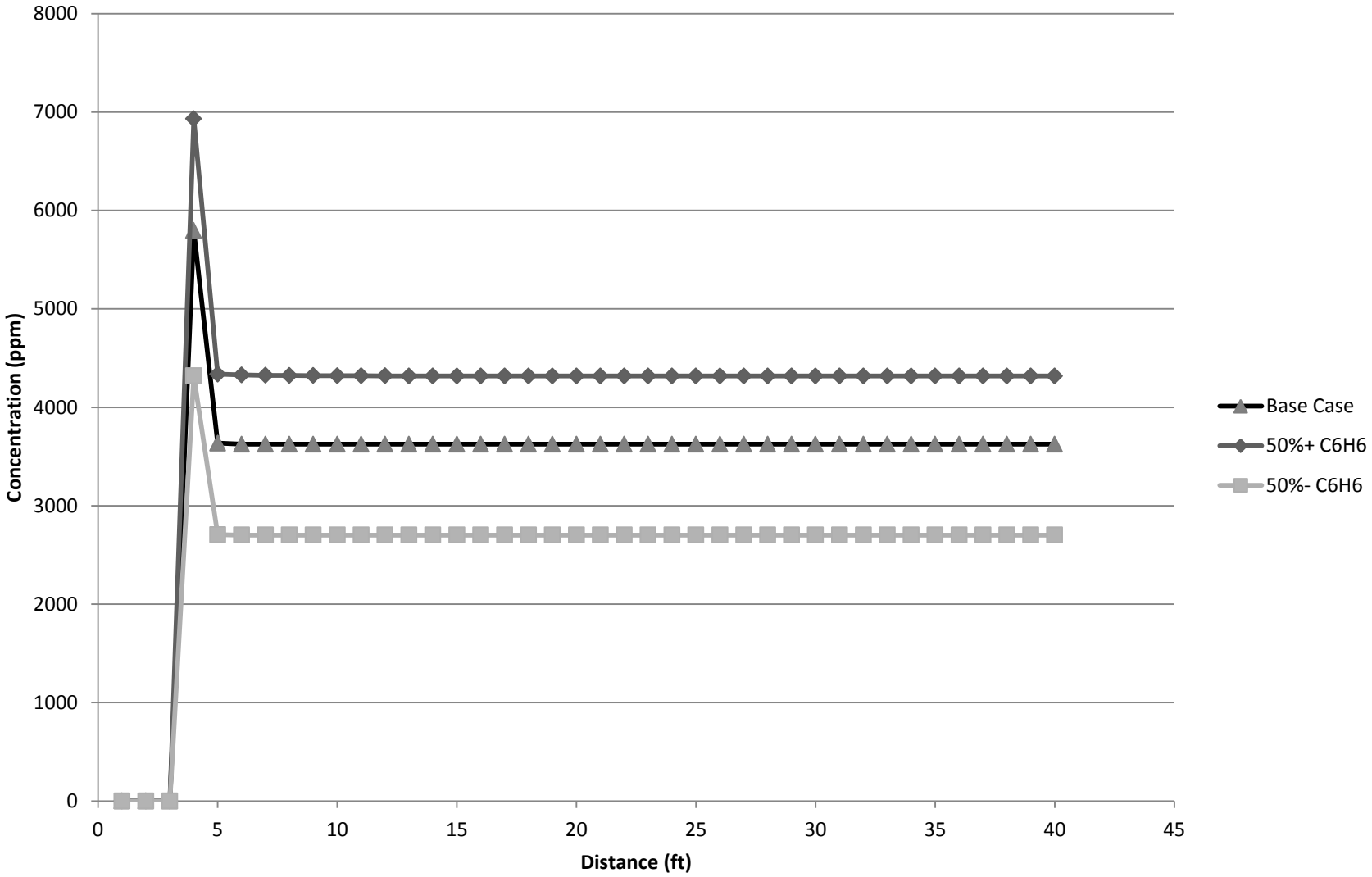

Figure 15 – NOx profile in ppm at actual conditions with changes to C6H6

5.3.2 Changes to CH_4

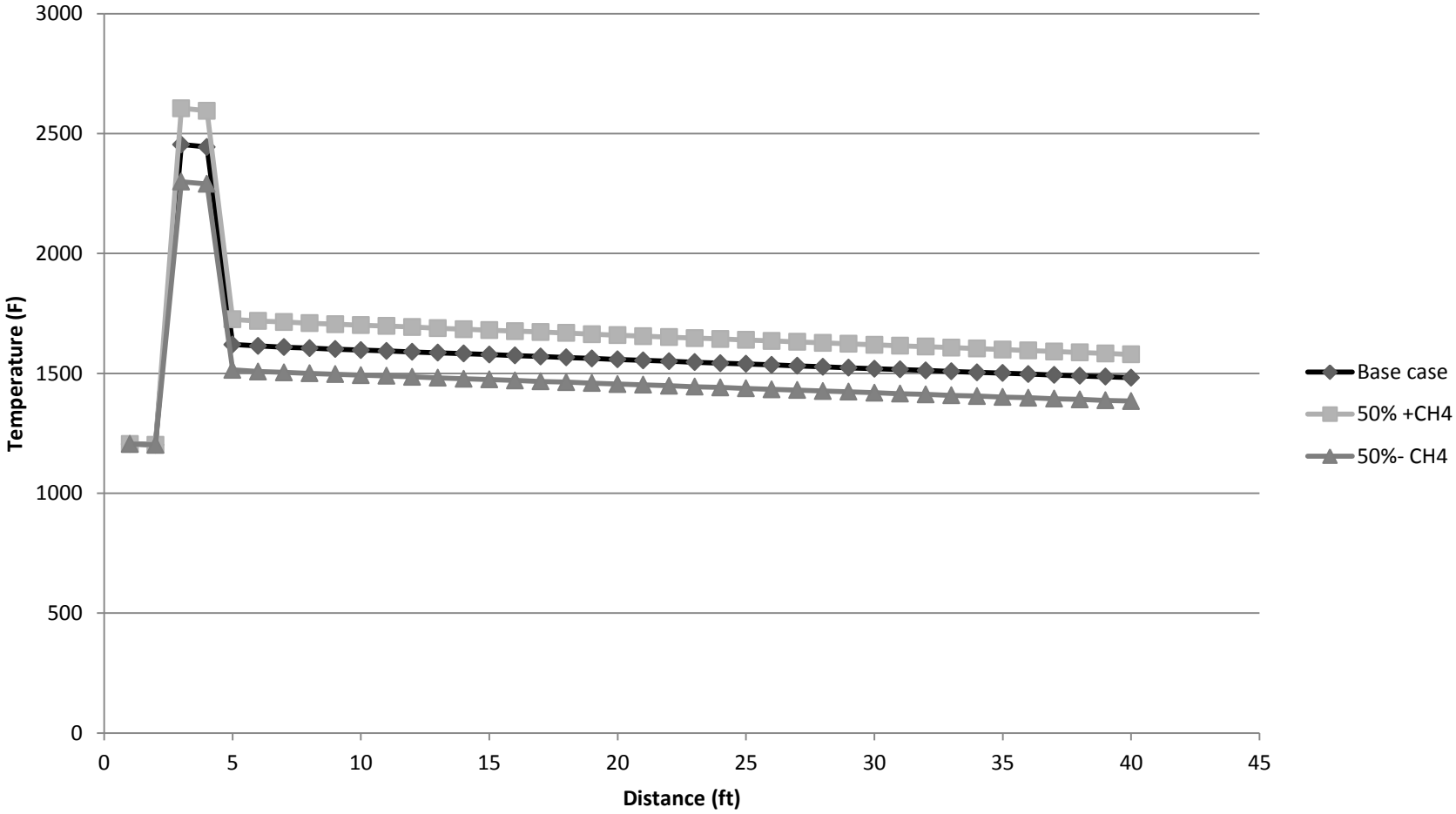

Figure 16 - Temperature profile with change to CH4

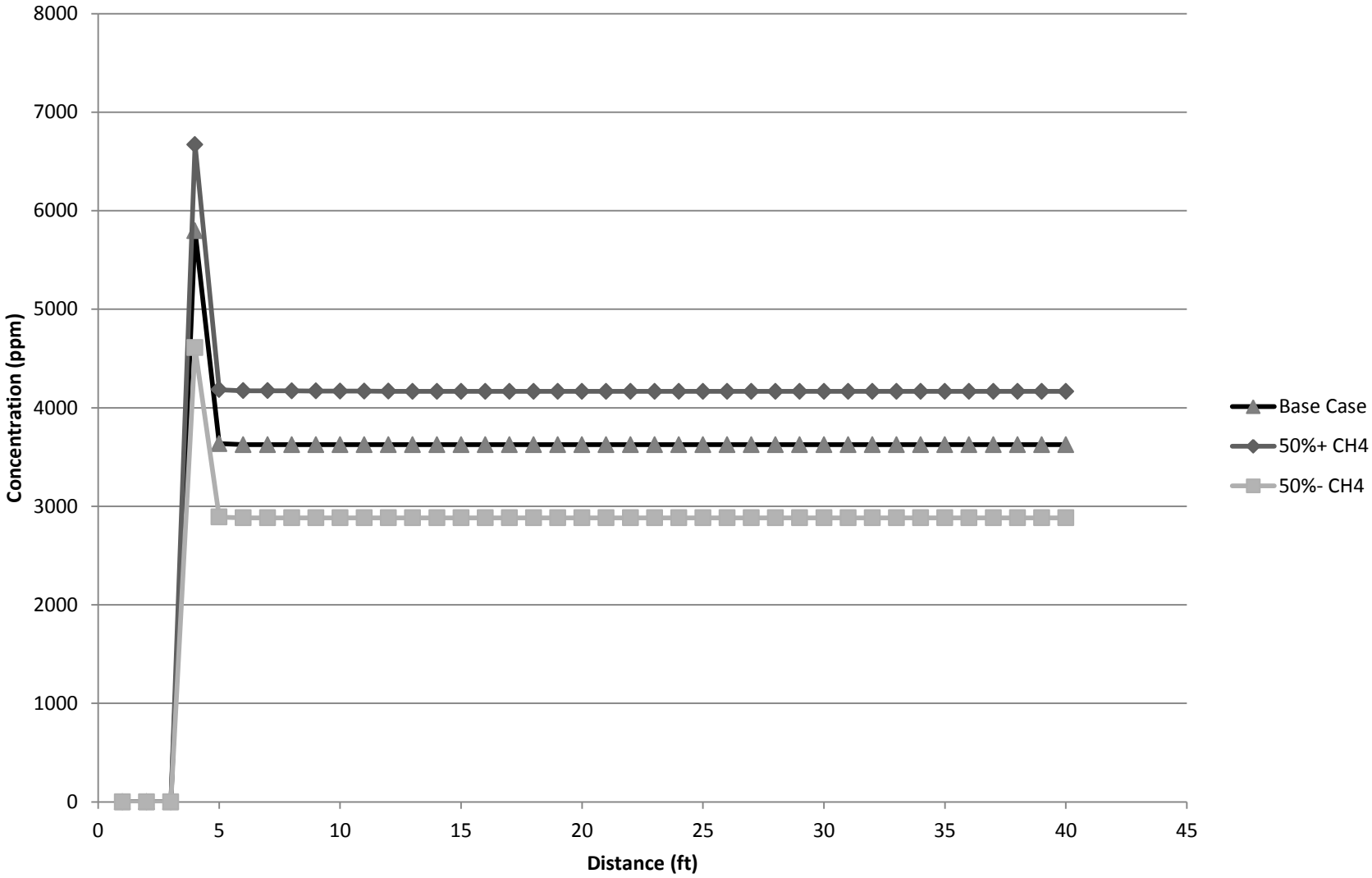

Figure 17 – NOx profile in ppm at actual conditions with changes to CH4

5.3.3 Changes to CO

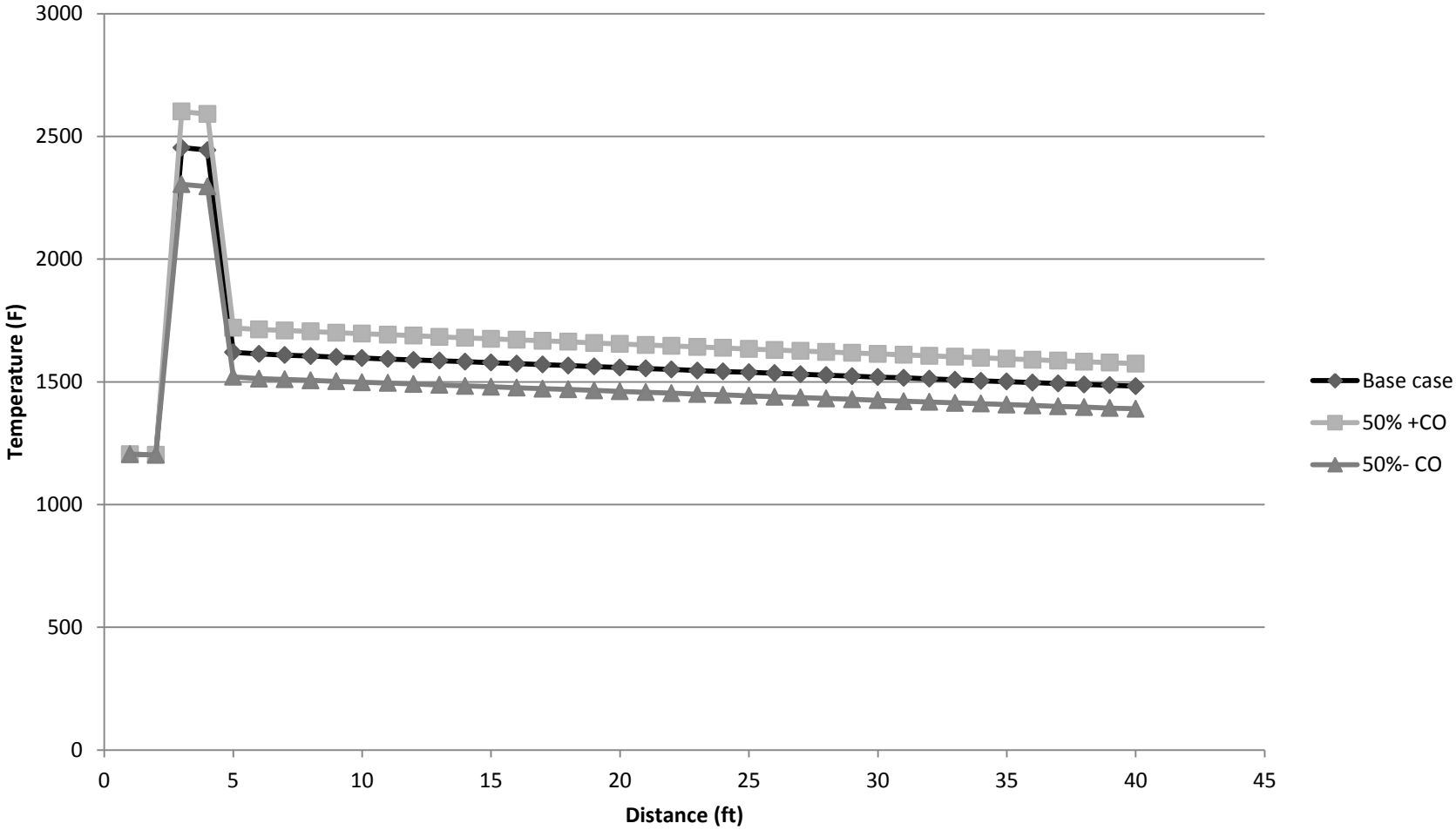

Figure 18 - Temperature profile with change to CO

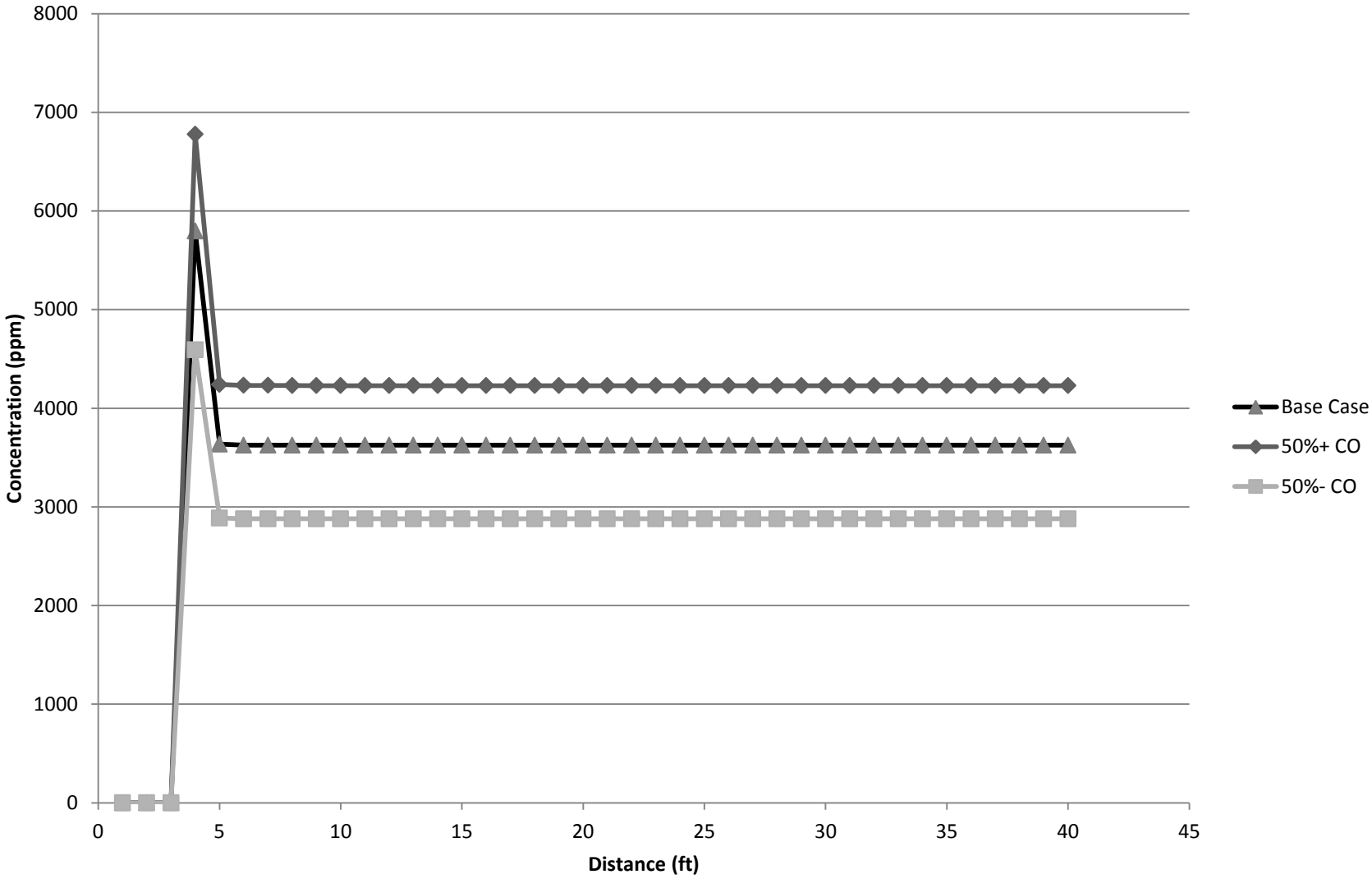

Figure 19 – NOx profile in ppm at actual conditions with changes to CO

5.3.4 Changes to H_2

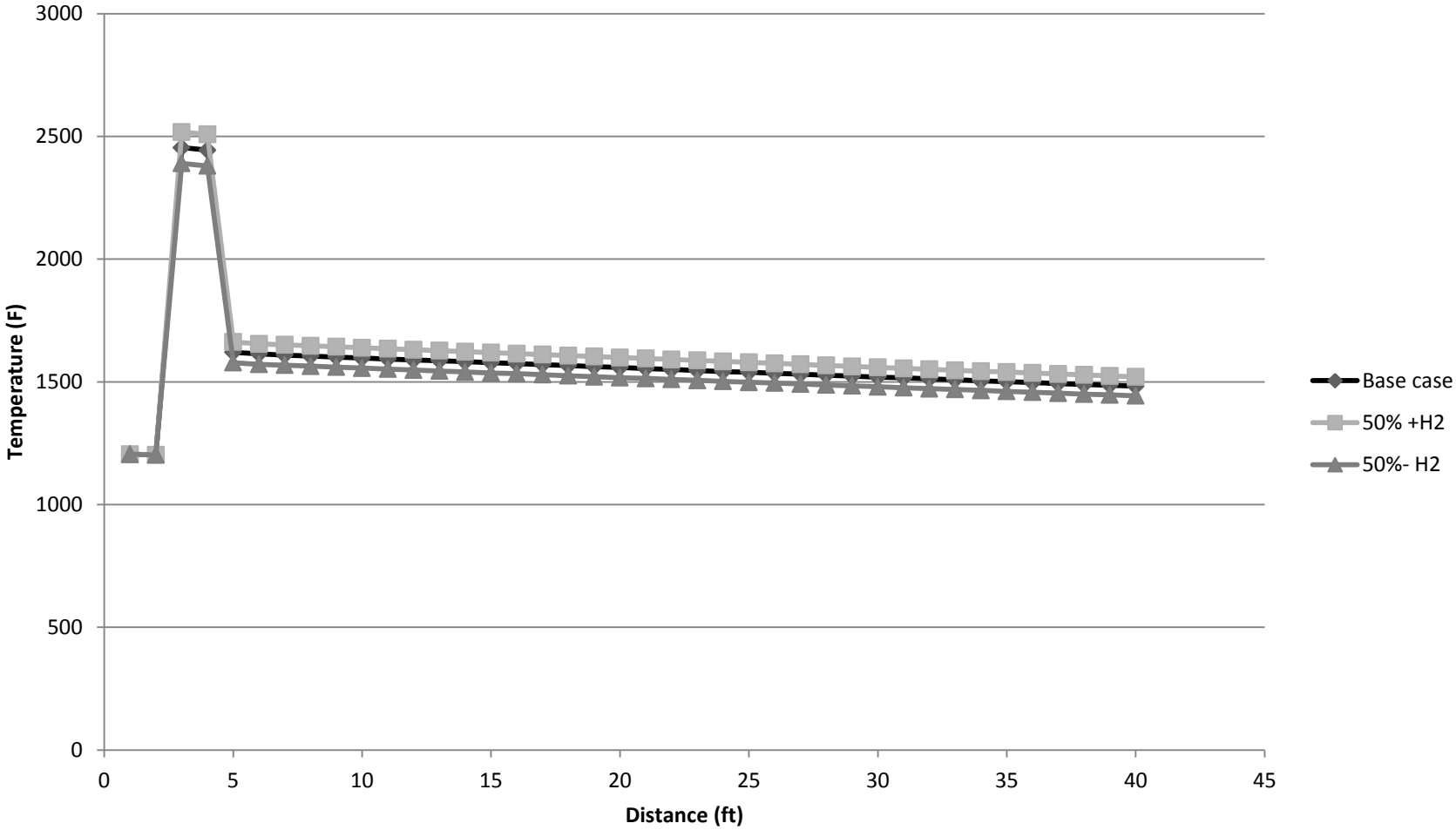

Figure 20 - Temperature profile with change to H2

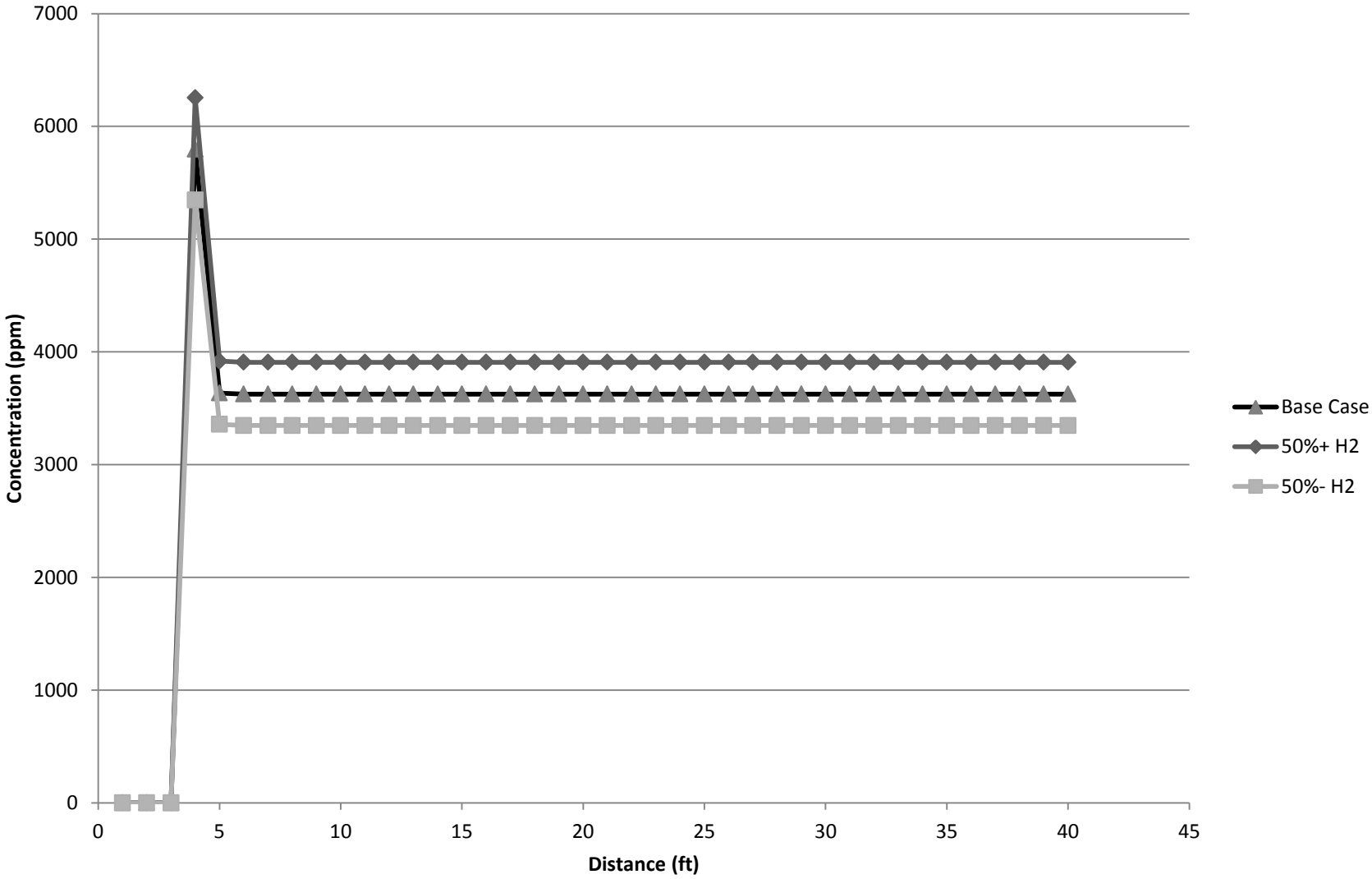

Figure 21 – NOx profile in ppm at actual conditions with changes to H2

5.3.5 Changes to NH_3

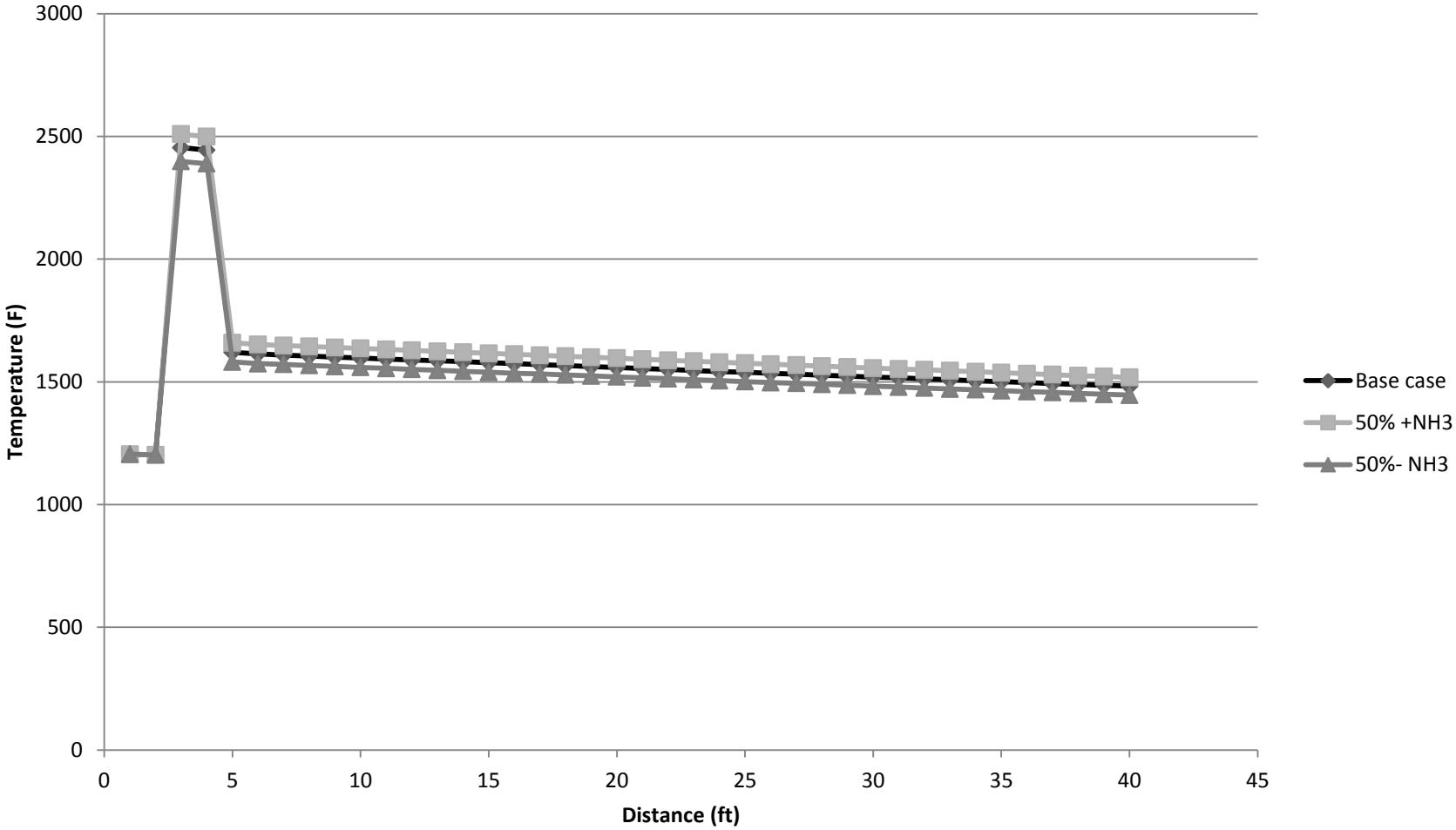

Figure 22 - Temperature profile with change to NH3

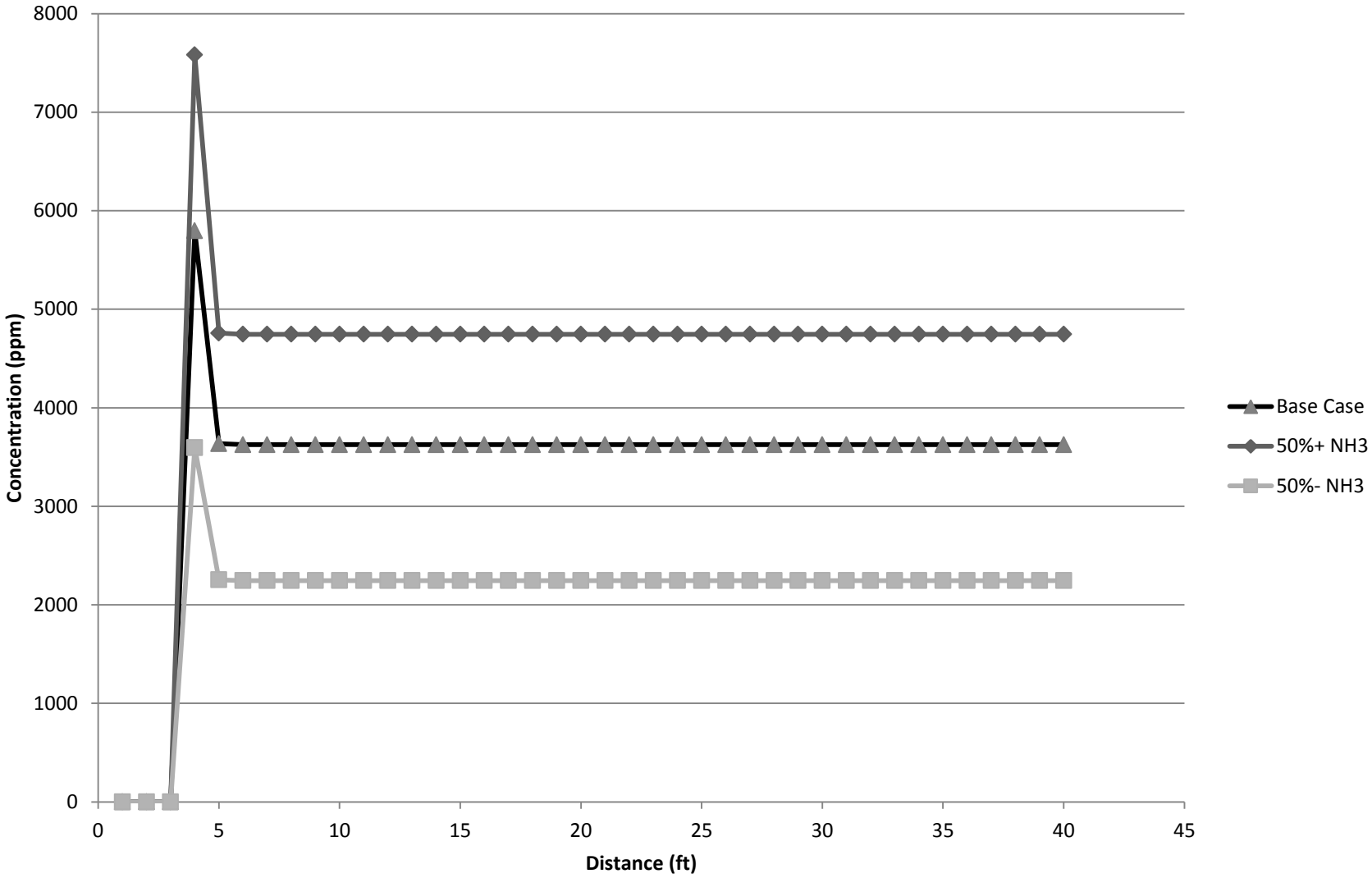

Figure 23 – NOx profile in ppm at actual conditions with changes to NH3

5.3.6 Changes to H_2S

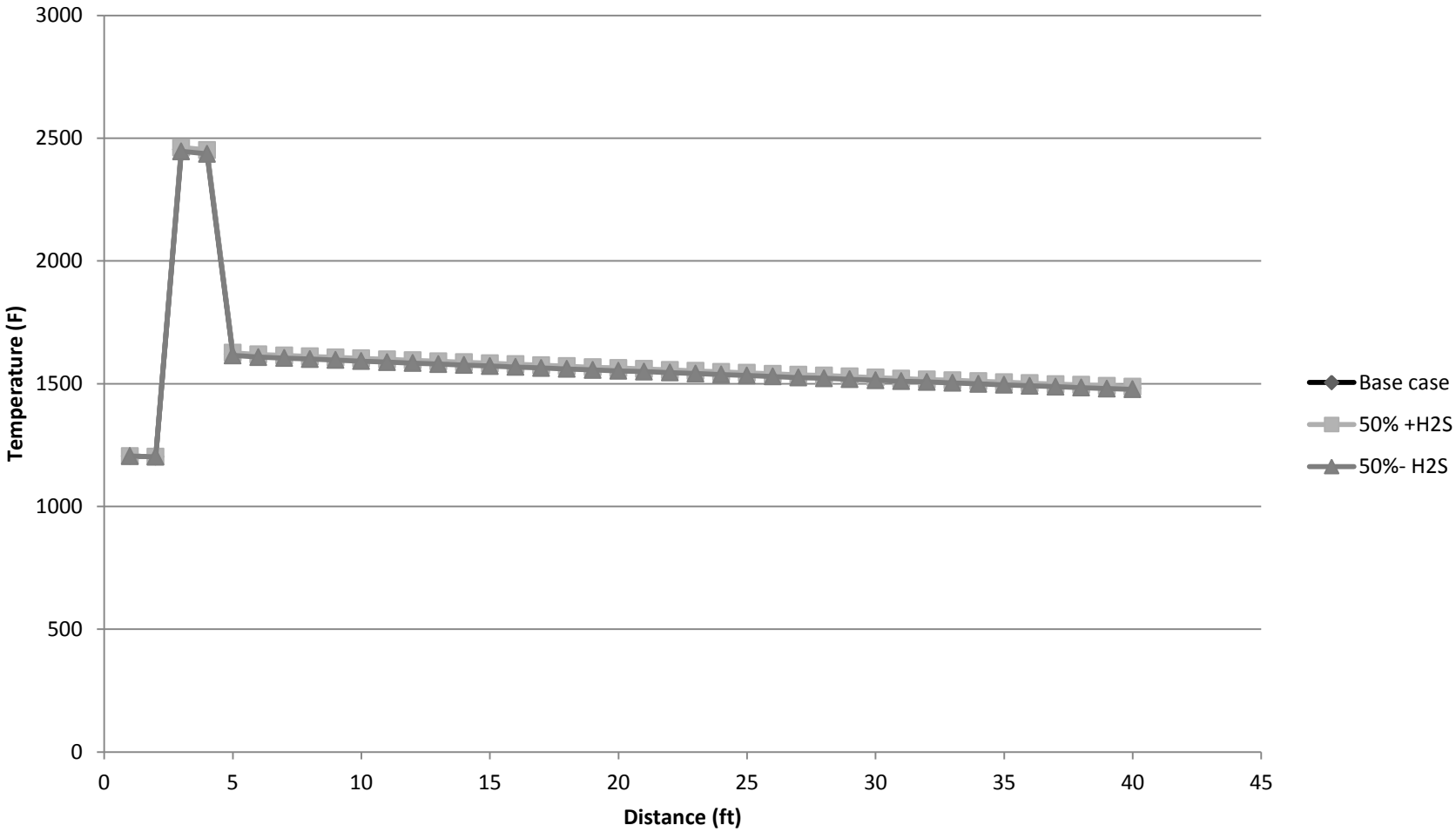

Figure 24 - Temperature profile with change to H2S

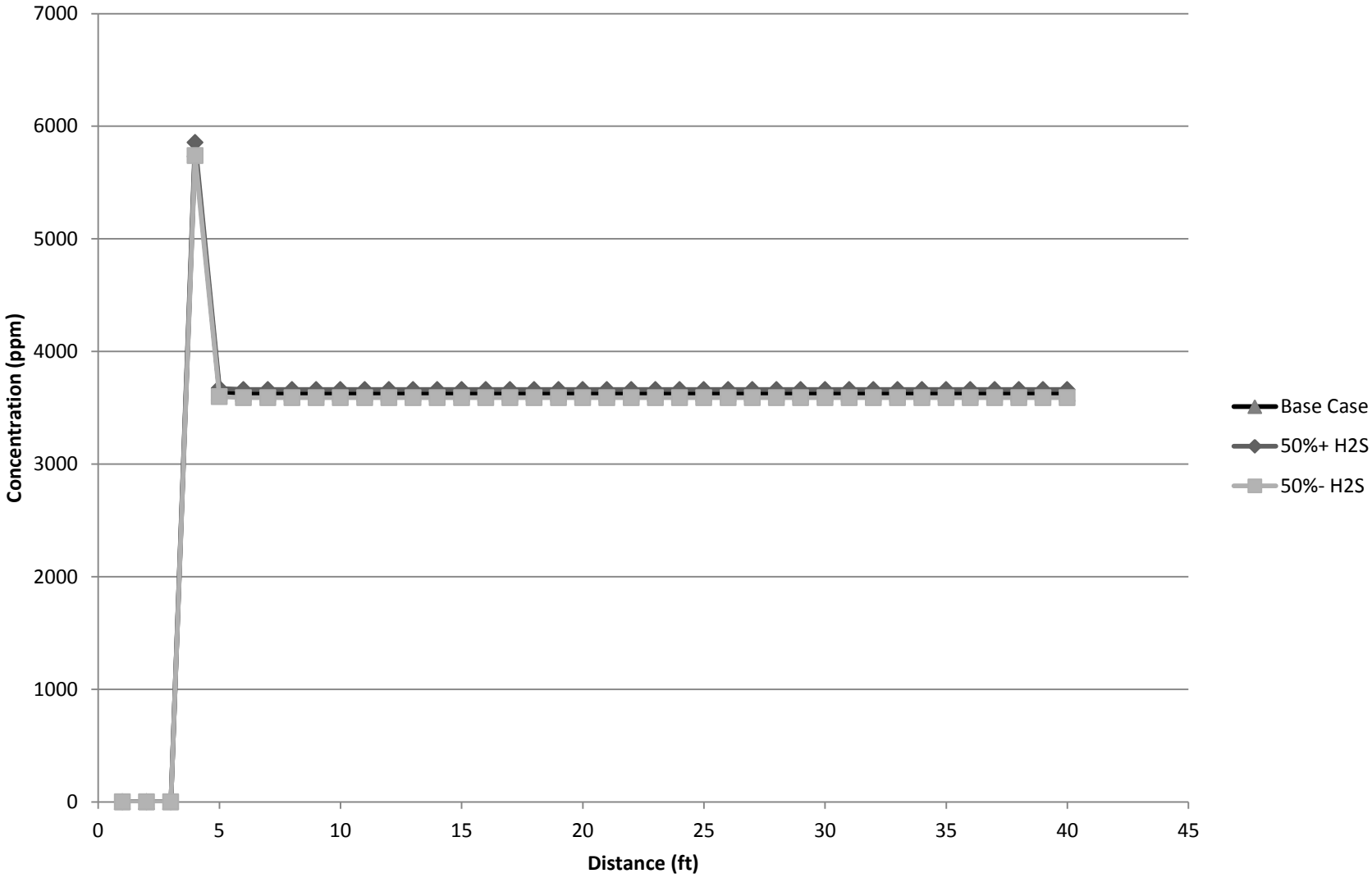

Figure 25 – NOx profile in ppm at actual conditions with changes to H2S

5.4 Discussion of Results

This discussion will focus on parameters that the operator may change during the operation of the TO; such as varying mass air flow rate to rings 1 and 2, total mass air flow rate, and the mass flow rate of aqueous ammonia injection. What will be analyzed is the temperature profile with these changes, NO_x profile, and NO_x removal rates based on the molar ratio of NH_3 to NO_x in the final injection site, as well as other analysis such as NO_x removal rates based on temperature.

5.5 Varying air mass flow rates in rings 1 and 2

The amount of air to rings 1 and 2 were varied in trials 1-3; Table 7 indicating the conditions of the trials. Changing the amount of air to ring 1 changes the equivalence ratio in ring 1. The air into ring 2 was also changed to hold total air constant. Ultimately the temperatures at the end of the reactor are close because the total air flow does not change. The temperatures in the first air ring are different in each trial with respect to the base case. Trial 1 has more ambient air (4800 lbs/hr) in ring 1 and the results indicate a ring 1 temperature about 500 $^{\circ}F$ lower than the base case. Trial 2 has less ambient (1800 lbs/hr) in ring 1 and there was also a drop in temperature with respect to the base case, but ended up with a higher temperature than trial 1. This is because less air is available to dilute the mixed gas stream in ring 1 compared to trial 1, and the heat of combustion is lower because of the lower ϕ (ϕ = 0.55). Trial 3 with 800 lbs/hr air has the lowest of all temperatures in ring 1 but increases in ring 2.

Equivalence ratio is a key factor in the peak temperature in the first air ring. Increasing the equivalence ratio means that more air is available for combustion. Too much air over the stoichiometric amount will dilute the mixed gases in ring 1, lowering the temperature. Lowering the equivalence ratio means there is less oxygen available for combustion, so less fuel is burned and the peak combustion temperature is not reached. To exemplify what is being said the important reactions for the production of NH_3, NO, NO_2, and N_2 were looked at specifically for the case of trial 2 at rings 1 and 2. Trial 2 resulted in the lowest amount of NO_x formation giving it more importance.

The following discussion focuses on results of trial 2. Trial 2 has an ϕ of 0.55, and in this trial not all of the NH_3 is oxidized in the first ring as verified by Figure 26. The combustion of NH_3 forms an important radical NH_2 which is one of the main radicals that reacts with NO to form N_2 and H_2O as can be seen in Figure 27. Figure 27 shows the NO production for trial 2 at ring 1. NO formation is dependent on radicals such as HNO, NO_2, N, NH, OH, and HO_2, but it also reacts with NH_2 and NH to form N_2, H_2O, H, OH, NNH and N_2O. The NO is consumed faster by the reactions that form N_2, H_2O, H, OH, NNH and N_2O than it is formed, thus a negligible amount of NO is present in the first air ring. Figure 28 shows the production of NO_2. NO_2 consumes and produces NO, and in this case NO_2 consumed more NO than it produced. The lack of oxygen in the first air ring limits NO and NO_2 production and allows for radical NH_2 to react with NO to form N_2 and H_2O, as shown in Figure 29.

Table 7 - Trial conditions (compositions held constant)

Trial	Air ring 1 (lbs/hr)	Air ring 2 (lbs/hr)	Total air mass flow rate (lbs/hr)	Humidity (lbs H2O/lbs DA)	Temp. air (Fahrenheit)	Flue gas ring 1 (lbs/hr)	Flue gas ring 2 (lbs/hr)	Total flue gas mass flow rate (lbs/hr)	Temp. flue gas (Fahrenheit)	ϕ (equivalence ratio)
Base case	2800	3200	6000	0	77	0	600	600	77	0.85
1	4800	1200	6000	0	77	0	600	600	77	1.46
2	1800	4200	6000	0	77	0	600	600	77	0.55
3	800	5200	6000	0	77	0	600	600	77	0.24

The rest of the air is introduced by ring 2 where all of the remaining ammonia is oxidized (Figure 30). Figure 31 shows that all the NO is formed in ring 2. The condition of fuel rich in ring 1 allowed for NO to be consumed, and if the operator promotes this condition to occur even further in ring 1, this consumption of N species and to its eventual formation of N_2 will further be realized and even lower NO_x concentrations will result in the exhaust gas.

NO_2 was destroyed and formed into NO, Figure 32. Where NO_2 reacts with radicals H and O to form OH, NO, and O_2; NO_2 was also formed, but the net NO_2 was destroyed rather than formed. The net reaction of NH_3 to N_2 is greater realized especially in these reduced air conditions where there is not enough temperature (T > 2500 °F); thus inhibiting any thermal NO_x formation, so all the nitrogen that converts to N_2 stays as N_2 verified by Figure 33 where N_2 was produced. The important reactions are shown in Table 8, and in Figures 26-33:

Table 8 - Important reactions of production (or destruction) of nitrogen species ultimately forming to NO_x, N_2

No	Reaction
421	CO + N2O <=> N2 + CO2
433	CH3 + NO2 <=> CH3O + NO
434	CH3 + HNO <=> NO + CH4
489	CH4 + NH2 <=> CH3 + NH3
874	N2O + H <=> N2 + OH
903	NO2 + H <=> NO + OH
904	NO + HO2 <=> NO2 + OH
911	HNO + O2 <=> HO2 + NO
912	HNO + OH <=> NO + H2O
914	HNO + H <=> NO + H2
952	H2NN + O2 <=> NH2 + NO2
974	N2H3 + NH2 <=> H2NN + NH3
1002	NNH <=> N2 + H
1003	N + NO <=> N2 + O
1004	N + O2 <=> NO + O
1005	N + OH <=> NO + H
1010	NH + NO <=> N2O + H
1017	NH + O <=> NO + H
1022	NH2 + NO <=> NNH + OH
1023	NH2 + NO <=> N2 + H2O
1024	NH2 + NO <=> N2 + H2O
1026	NH2 + N <=> N2 + H + H
1033	NH2 + OH <=> NH + H2O
1039	NH3 + OH <=> NH2 + H2O
1040	NH3 + O <=> NH2 + OH
1547	H + NO + M <=> HNO + M
1551	HO2 + NO <=> NO2 + OH
1555	NO2 + H <=> NO + OH
1558	HNO + H <=> H2 + NO
1560	HNO + OH <=> NO + H2O

Note - details of all the reactions are in the appendix

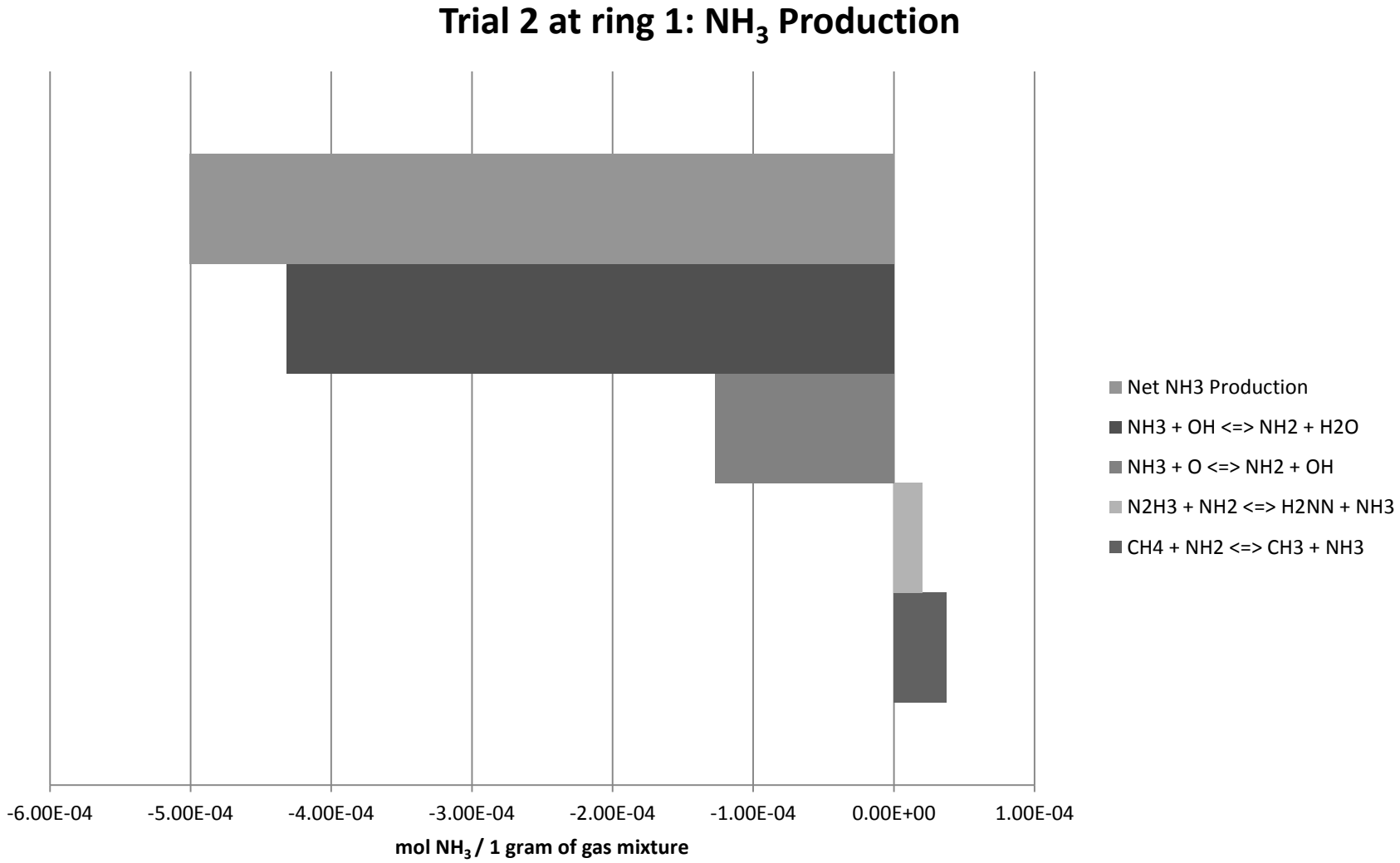

Figure 26 - Important reactions in the production or destruction of NH_3 at ring 1

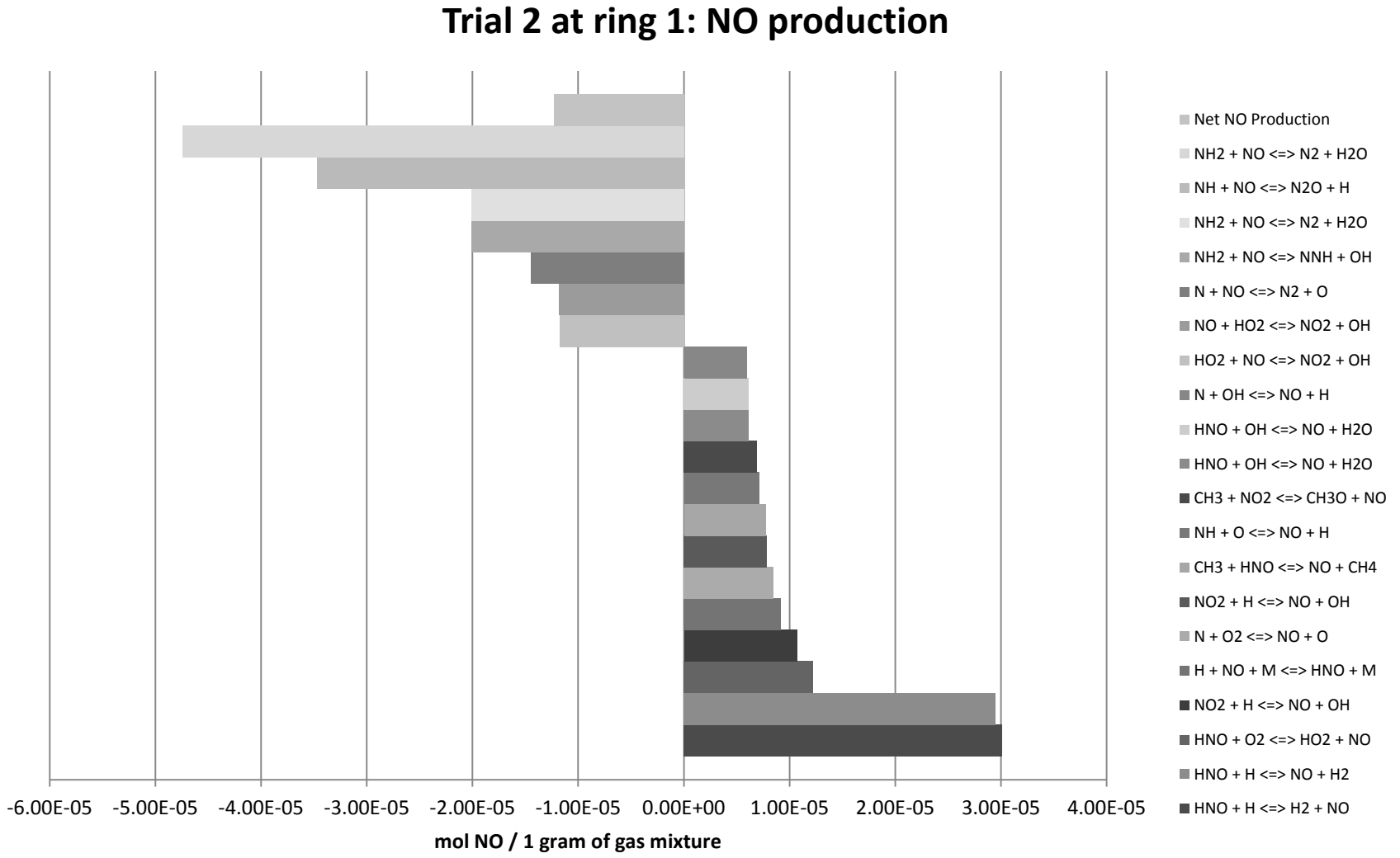

Figure 27 - Important reactions in the production or destruction of NO at ring 1

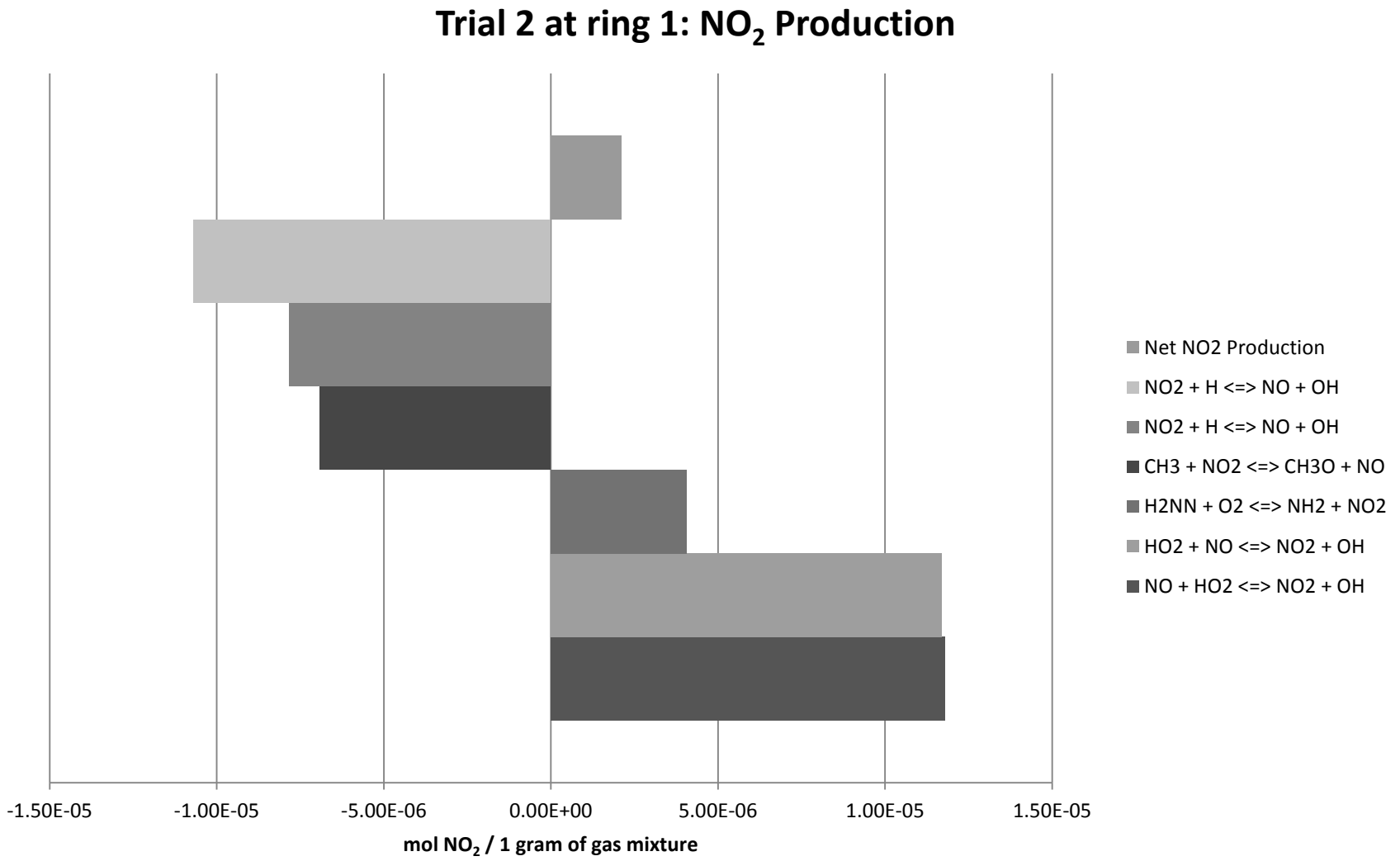

Figure 28 - Important reactions for the production or destruction of NO_2 at ring 1

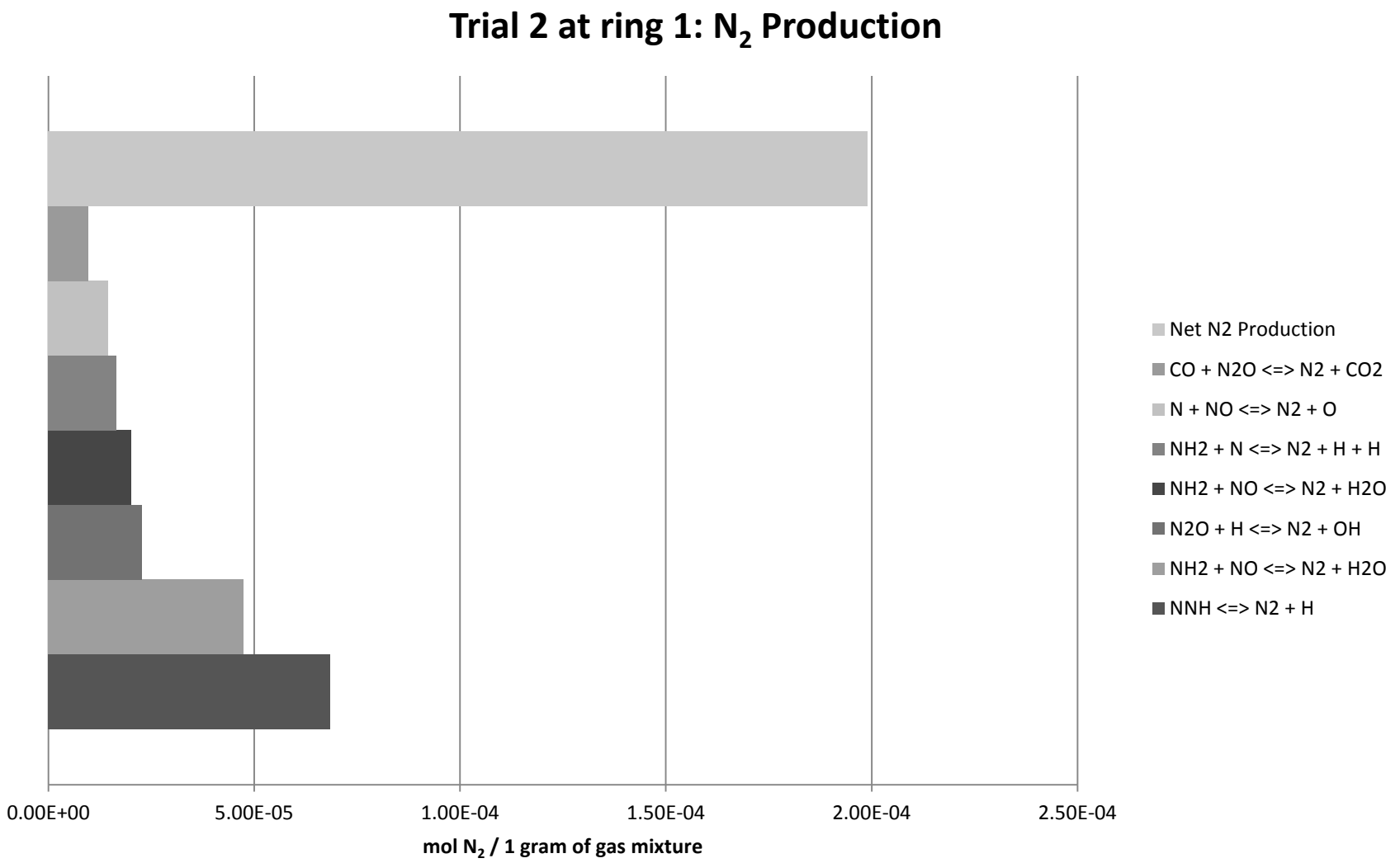

Figure 29 - Important reactions in the production or destruction of N_2 at ring 1

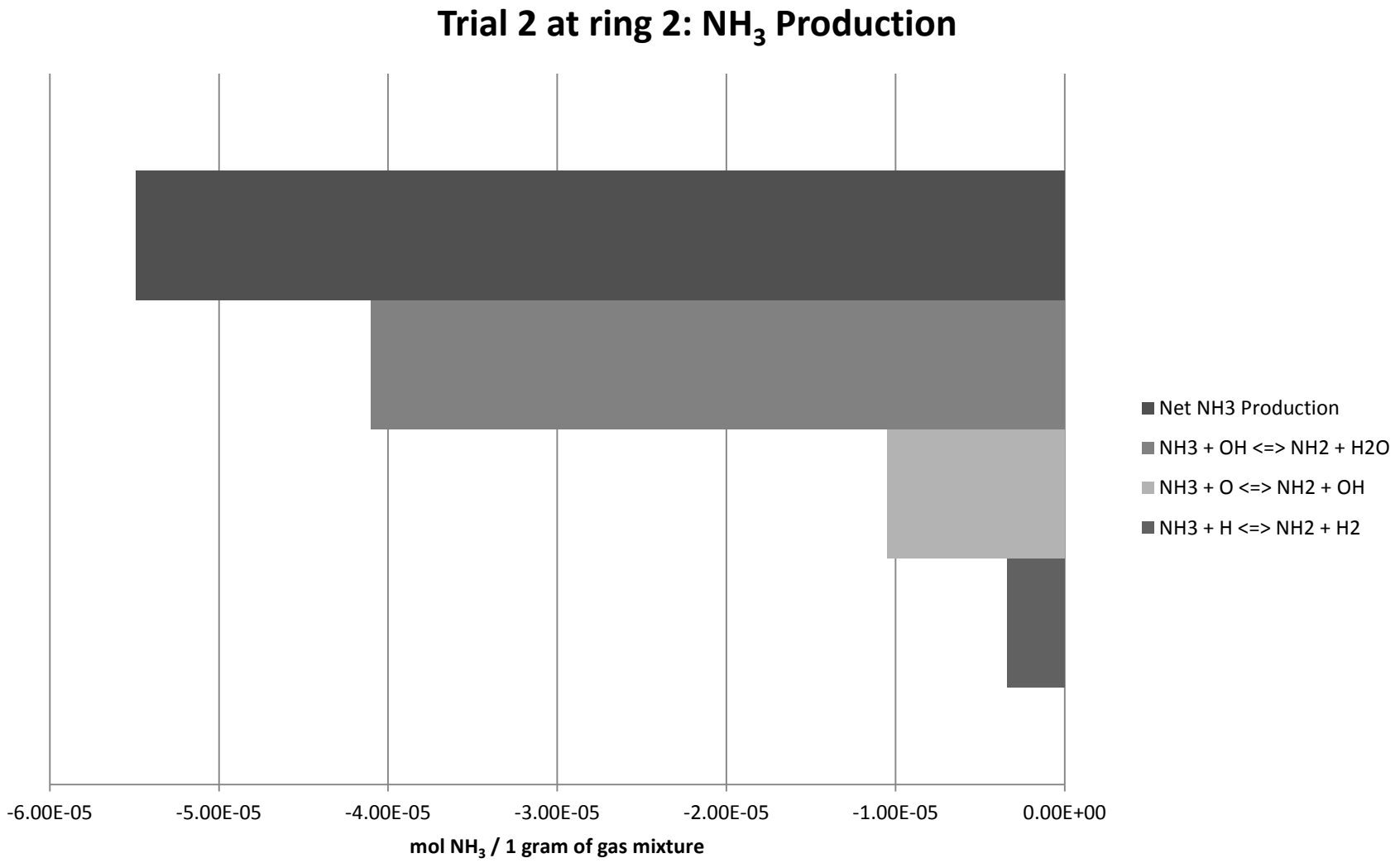

Figure 30 - Important reactions in the production or destruction of NH3 at ring 2

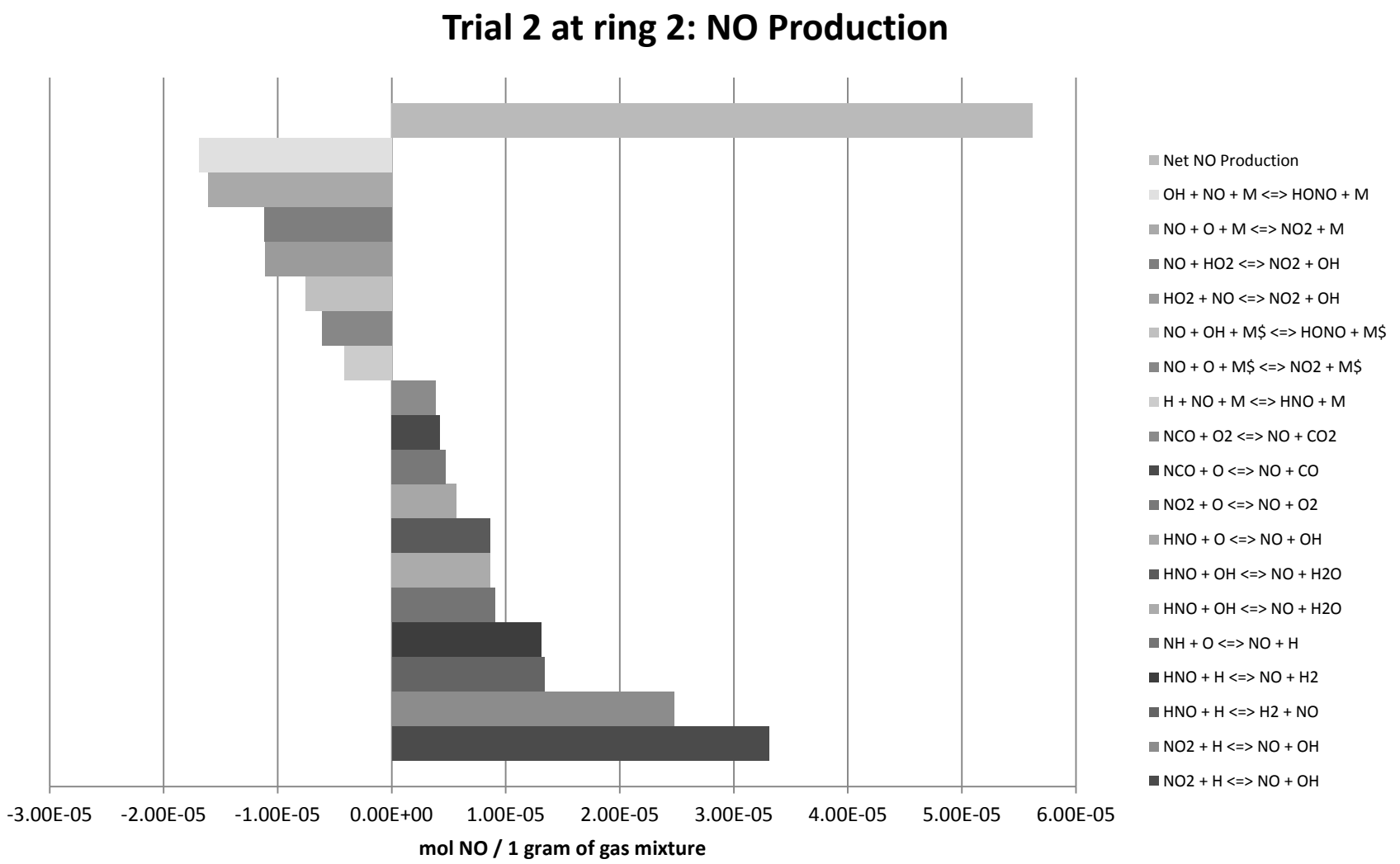

Figure 31 - Important reactions of production or destruction of NO at ring 2

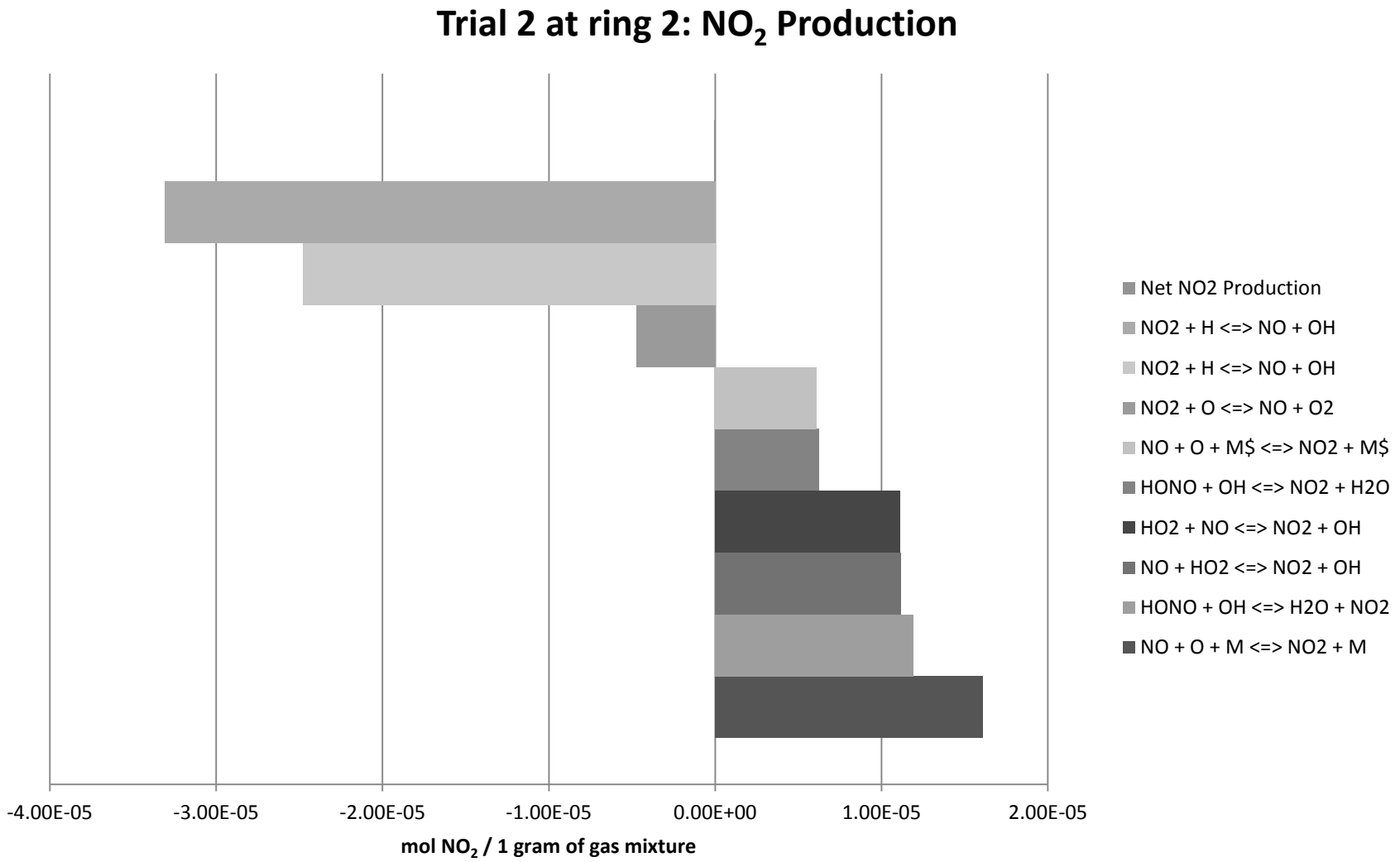

Figure 32 - Important reactions of production or destruction of NO2 at ring 2

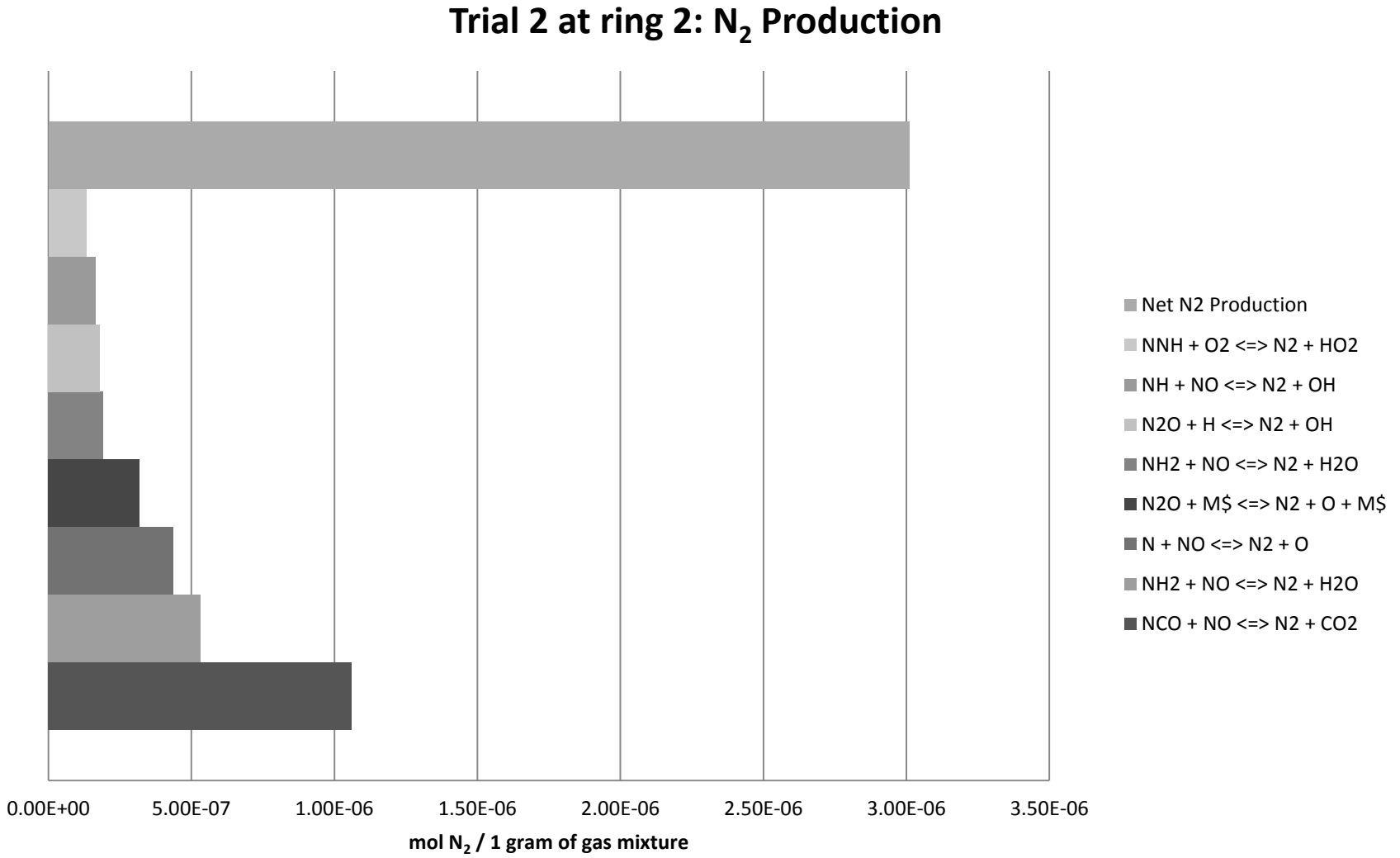

Figure 33 - Important reactions of production or destruction of N2 at ring 2

Still regarding Trial 2 (ϕ = 0.55 in ring 1) NO_x concentrations are dependent on both temperature and equivalence ratio in the first air ring. A lower equivalence ratio in the first air ring allows for the possibility of some of the ammonia forming N_2 rather than NO, resulting in lower NO_x formation. By the time the mixed gas reaches ring 2, and the remaining ammonia reacts the temperatures are lower. The total NO_x that is formed when ring 1 is operated fuel-rich is much less than when a fuel-lean operation occurs in ring 1.

For lower NO_x concentrations with this specific TO configuration, the fuel-rich condition in ring 1 should be the norm of operation. An exhaust NO_x concentration that meets standard may be achieved by just operating in the TO in this fashion, and thus avoiding the use of aqueous ammonia injection for SNCR.

Table 9 and 10 show the fate of NH_3 converting to NO, NO_2, and N_2. Base case shows that approximately 40.2% of the NH_3 is converted to NO and NO_2 (the rest is N_2). Trial 2 shows that approximately 20.5% of the NH_3 is converted to NO and NO_2. Trial 2 unveils that a fuel-rich case in ring 1 allows for lower NO_x emissions.

Figure 34 is a temperature profile of trials 1 – 3 as well as the base case. Trial 1 – 3 all had lower temperatures at ring 1. Trial 1 has an ϕ of 1.46 (Table 7), at this ϕ it is higher than stoichiometric so all the fuel combusts, and there is enough air left for temperature dilution. Trial 2 and 3 had an ϕ of 0.55 and 0.24, respectively; resulting in some of the fuel to combust, but the heat of combustion is much lower than that of the base case, thus the lower temperatures.

Figure 35 is a NO_x concentration profile of trials 1 – 3, as well as the base case. Trial 1 was closer to the base case, than trials 2 and 3. Trials 2 and 3 have lower NO_x concentrations

because more of the nitrogen in NH_3 is converted to N_2 rather than NO_x. Trial 2 was mentioned previously about how it resulted in lower NO_x concentrations. The same may be said about trial 3, but it resulted in a slightly higher NO_x concentration compared to trial 2. This result indicates that some of NH_3 should be allowed to combust in the first air ring too allow for more NH_2 to be present before ring 2, so that the NH_2 may react with the formed NO and produce more N_2. It is also realized that NO_2 should be inhibited in its formation because once it reacts with O radicals it produces more NO.

Figure 36 shows the resulting exhaust gas NO_x concentration with respect to equivalence ratio in the first ring. Figure 36 indicates that there is an optimal ϕ somewhere around 0.55 to achieve lower NO_x concentrations.

Table 9 - Formation of NO and NO_2 and fate of NH_3 at base case

Base case					
Distance (ft)	**Temperature(F)**	**NH_3 (lbmol/hr)**	**NO (lbmol/hr)**	**NO_2 (lbmol/hr)**	**N_2 (lbmol/hr)**
1	1205	2.498	0	0	54.40
2	1202	2.498	1.54E-20	9.73E-33	54.40
3	2389	2.497	2.9E-20	2.26E-32	129.8
4	2378	3.03E-06	1.0057	2.96E-06	130.8
5	1650	3.06E-06	1.0040	2.77E-06	217.0
6	1642	9.45E-10	0.9840	0.01995	217.0

Note – ϕ is 0.55 in ring 1

Table 10 - Formation of NO and NO_2 and fate of NH_3 at trial 2

Trial 2					
Distance (ft)	Temperature(F)	NH_3 (lbmol/hr)	NO (lbmol/hr)	NO_2 (lbmol/hr)	N_2 (lbmol/hr)
1	1205	2.498	0	0	54.40
2	1202	2.498	1.54E-20	9.73E-33	54.40
3	2115	3.051	3.54E-20	2.76E-32	125.6
4	2103	0.5640	0.000295	3.94E-11	127.5
5	1772	0.4660	4.88E-05	6.09E-12	217.6
6	1761	5.22E-07	0.5060	0.005524	217.6

Note – ϕ is 0.55 in ring 1

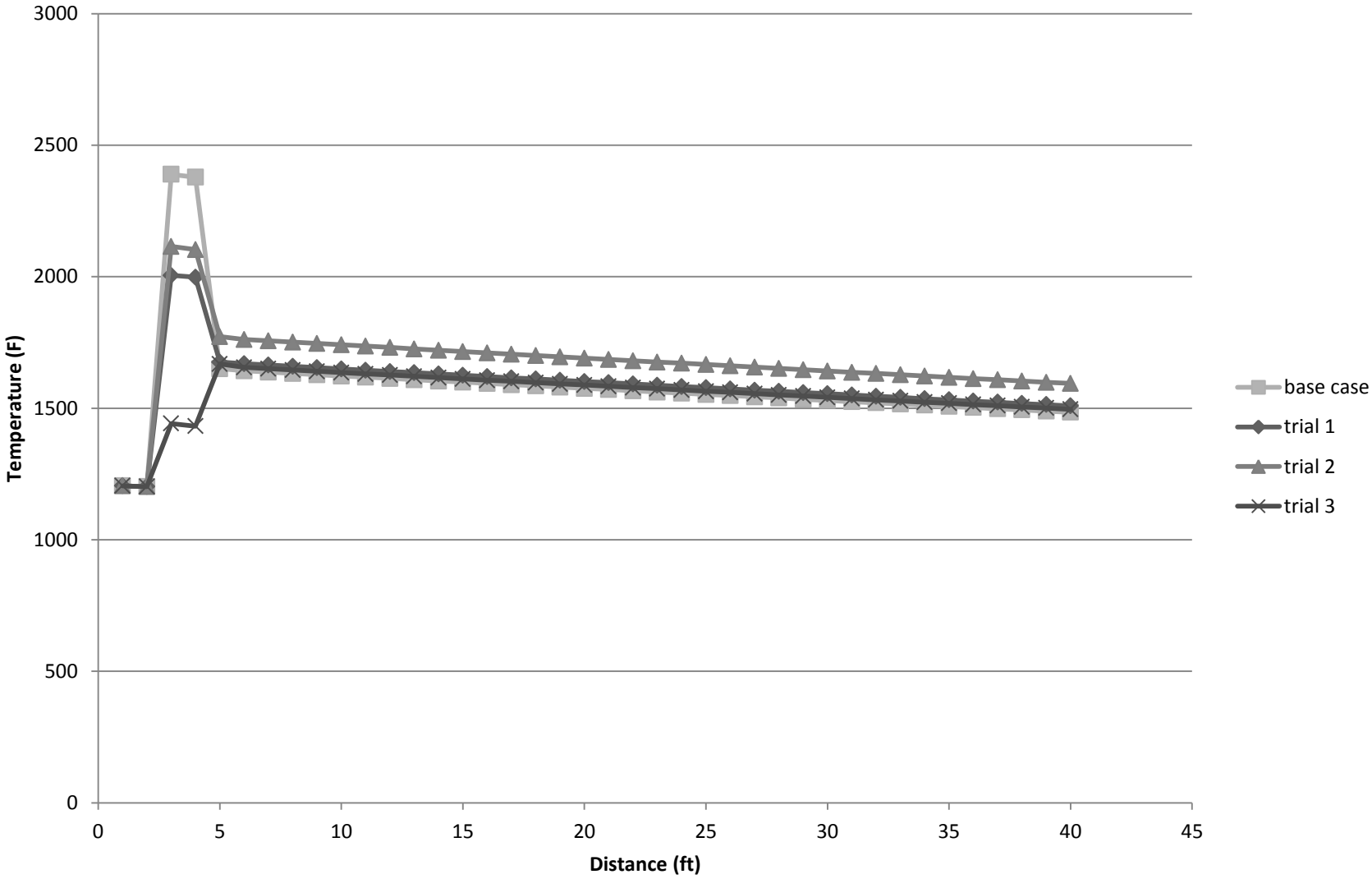

Figure 34 – Temperature profile varying air mass flow rates in ring 1 and 2

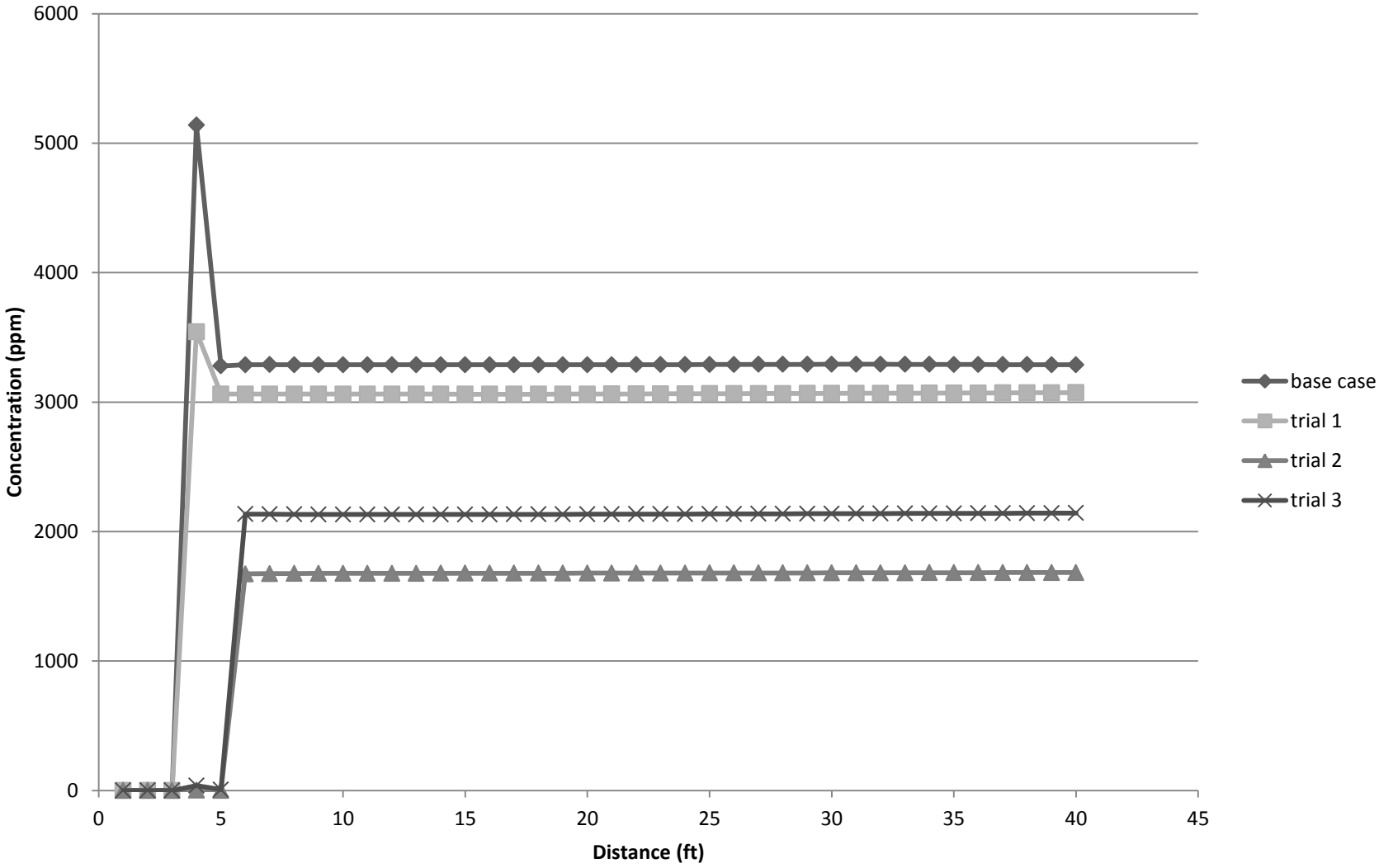

Figure 35 – NO_x concentration profile with varying mass air flow to rings 1 and 2

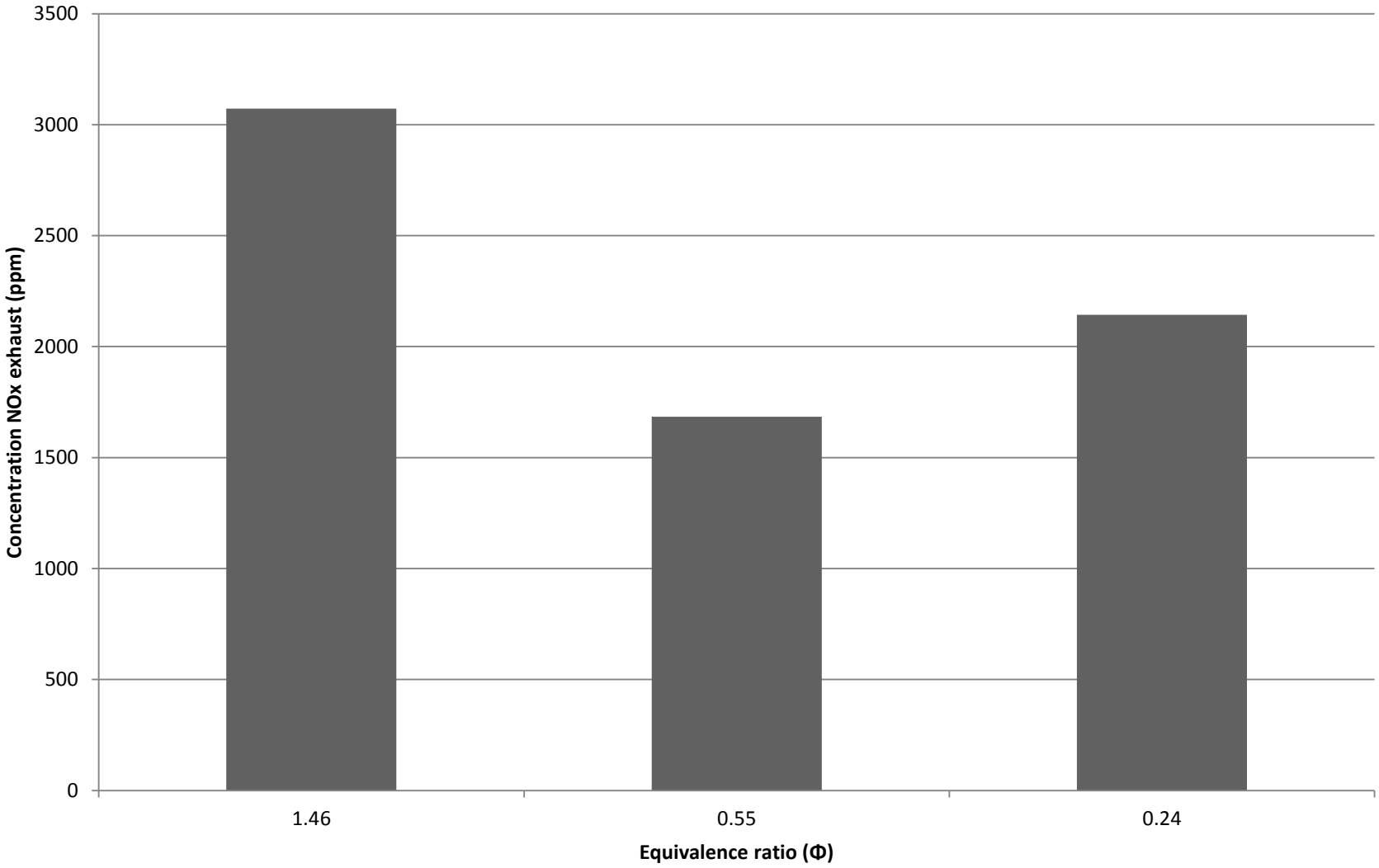

Figure 36 -Final NOx concentration in the exhaust gas as a function of equivalence ratio in the first air ring

5.5.1 Varying total mass air flow rate

The total air mass flow rate was changed, but the ratio of air to rings 1 and 2 with respect to the base case was kept constant. The results indicate that with more total air mass, the final exhaust temperature is lower compared to the base case. Also, with less total air mass flow rate the temperature is higher. Higher temperature was achieved with less total air mass flow rate to rings 1 and 2 as indicated in Figure 37 and this occurs simply because less air is available to dilute the temperature when the mixed stream reaches ring 2. Base case had the highest peak temperature at ring 1 because the ϕ was closest to stoichiometric amount, and at this condition the highest temperatures are realized.

NO_x behavior is indicated by Figure 38. With less total air mass flow rate the NO_x concentration is lower (trial 4), also with more total air the NO_x concentration is lower (trial 5). Trial 4 indicates that less total air will give a lower equivalence ratio in ring 1, and when there is a lower equivalence ratio in the first air ring the nitrogen available in NH_3 is converted to N_2 and some NO; then the nitrogen remaining in the NH_3 is formed to NO_x by the second air ring, but is significantly lower than if all the nitrogen available in NH_3 were to convert directly to NO_x. Trial 5 indicates that increasing the total mass air flow also lowers the concentration of NO_x, but dilution plays more of an effect in this case than it does in the lower total air mass flow rate.

Results indicate that inhibiting the oxidation of ammonia in the first air ring allows for lower final NO_x concentrations in the exhaust gas stream. The operator may increase or decrease the total mass air flow rate, but the main strategy to limit NO_x formation is to only provide enough oxygen for some of the hydrocarbons to react in the first air ring, then allowing

for the remaining fuels to react in the second air ring. For the base case syngas, the best air rate to ring 1 would be 1,800 lbs/hr (ϕ = 0.55).

Table 11 – Increasing total air mass flow rate trials

Trial	Air ring 1 (lbs/hr)	Air ring 2 (lbs/hr)	Total air mass flow rate (lbs/hr)	Humidity (lbs H2O/lbs DA)	Temp. air (Farenheit)	Flue gas ring 1 (lbs/hr)	Flue gas ring 2 (lbs/hr)	Total flue gas mass flow rate (lbs/hr)	Temp. flue gas (Farenheit)	Aqueous ammonia injection (lbs/hr)	Temp. aq. Ammonia (Farenheit)
Base case	2800	3200	6000	0	77	0	600	600	77	0	77
4	3733	4267	8000	0	77	0	600	600	77	0	77
5	1867	2133	4000	0	77	0	600	600	77	0	77

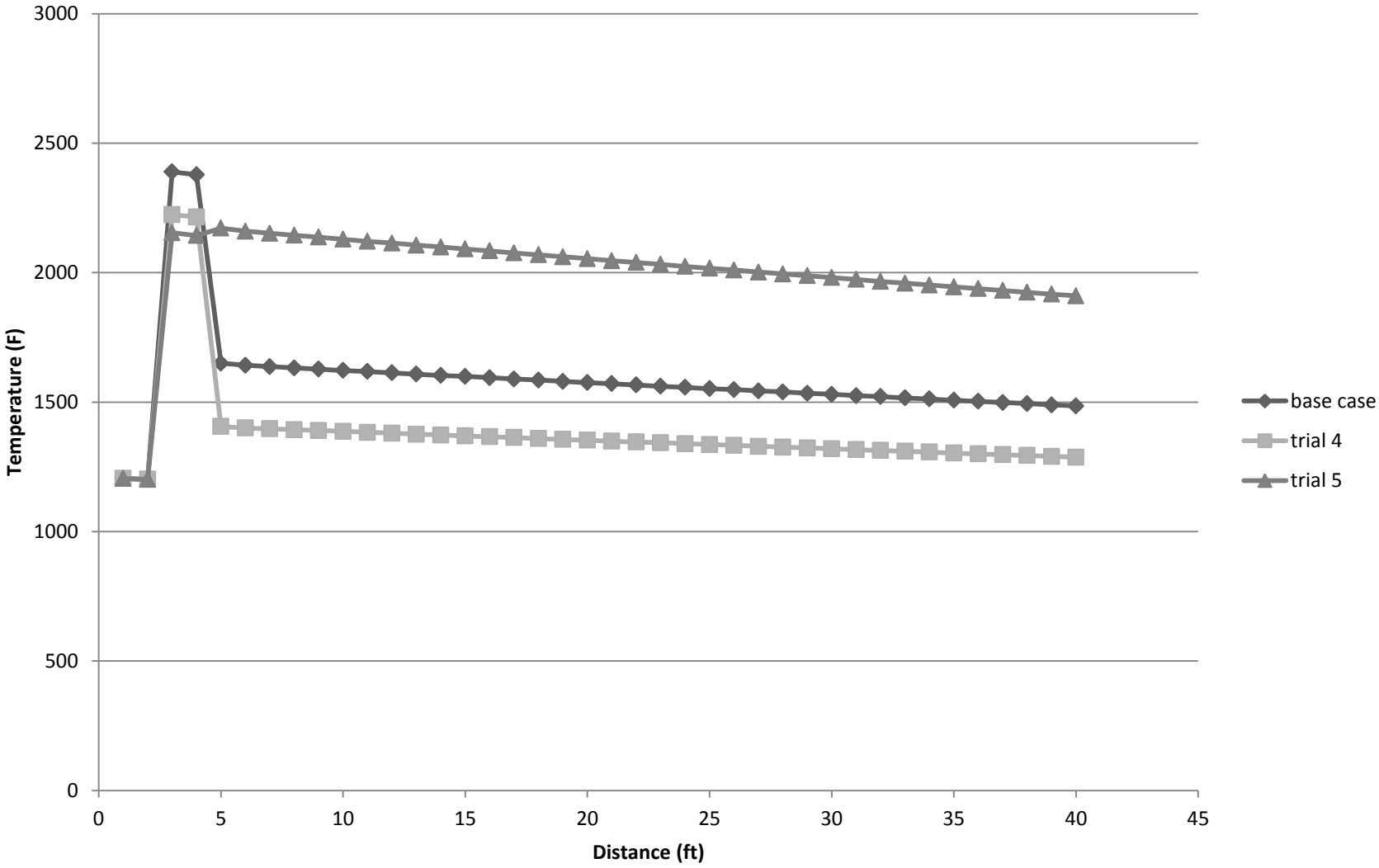

Figure 37 - temperature profile varying total air mass flow rate

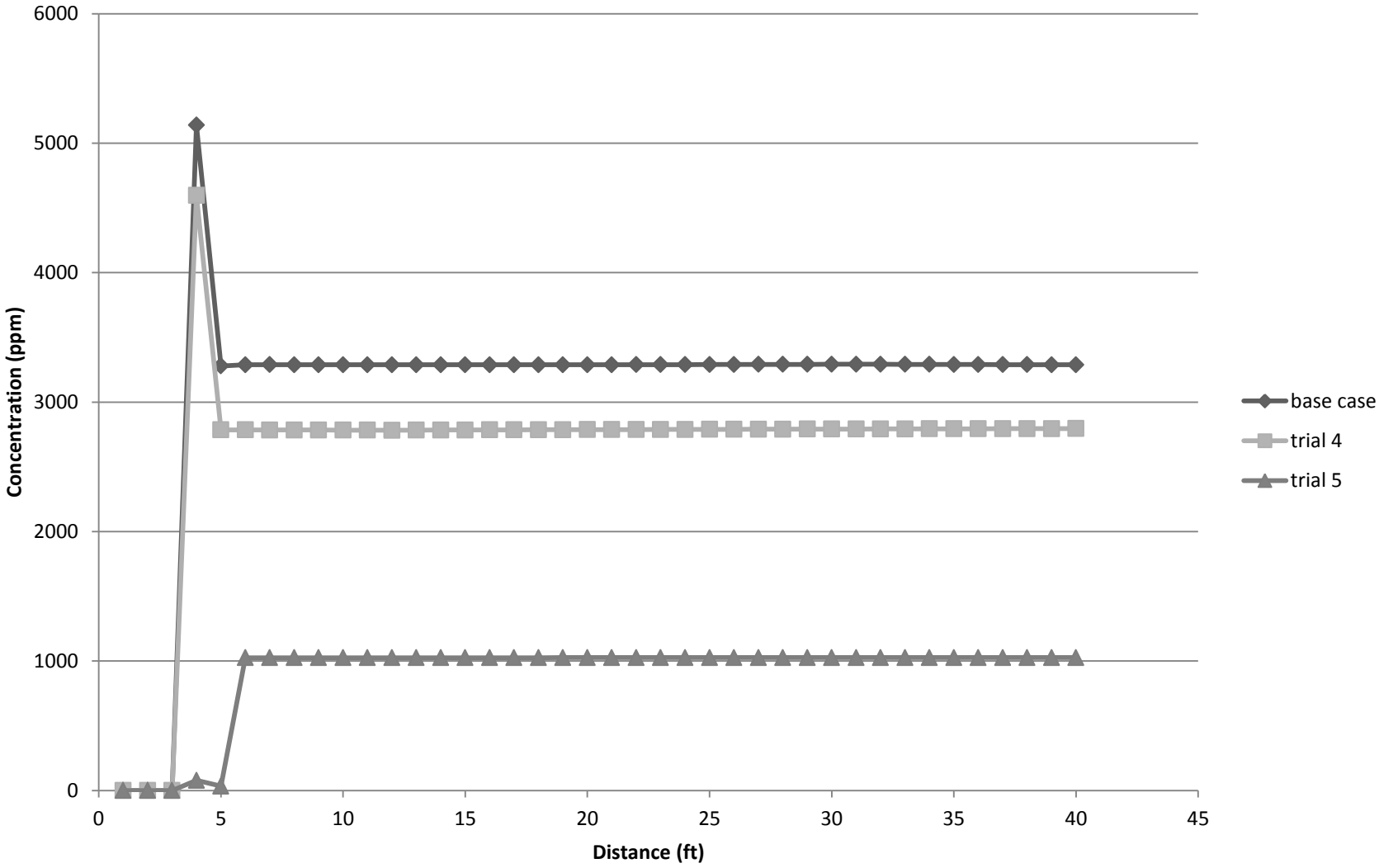

Figure 38 - Concentration profile NOx varying total mass air flow rate

5.5.2 Varying input syngas temperature

The initial syngas temperature from the gasifier to the TO was varied, temperature was plotted in Figure 39 and NO_x concentration was plotted in Figure 40. Results indicate that final exhaust temperatures increase or decrease depending on the initial syngas temperature. NO_x concentrations in the gas stream also change: the higher the initial syngas temperature, the higher the peak NO_x concentration and the lower the initial syngas temperature, the lower the peak NO_x concentration.

Varying initial syngas temperatures is not as effective as varying the mass air flow rates in rings 1 and 2. Having a lower initial syngas temperature allows for a lower temperature at ring 1 as well as a lower peak NO_x concentration, but the overall change in exhaust NO_x concentration is not as significant as inhibiting ammonia from oxidizing in the first air ring by adjusting the air flow rate.

Table 12 – Varying input syngas temperature trials

Trial	Air ring 1 (lbs/hr)	Air ring 2 (lbs/hr)	Total air mass flow rate (lbs/hr)	Temperature syngas (Fahrenheit)	Temp. air (Fahrenheit)	Flue gas ring 1 (lbs/hr)	Flue gas ring 2 (lbs/hr)	Total flue gas mass flow rate (lbs/hr)	Temp. flue gas (Fahrenheit)	Aqueous ammonia injection (lbs/hr)	Temp. aq. Ammonia (Fahrenheit)
Base case	2800	3200	6000	1205	77	0	600	600	77	0	77
6	2800	3200	6000	900	77	0	600	600	77	0	77
7	2800	3200	6000	1400	77	0	600	600	77	0	77

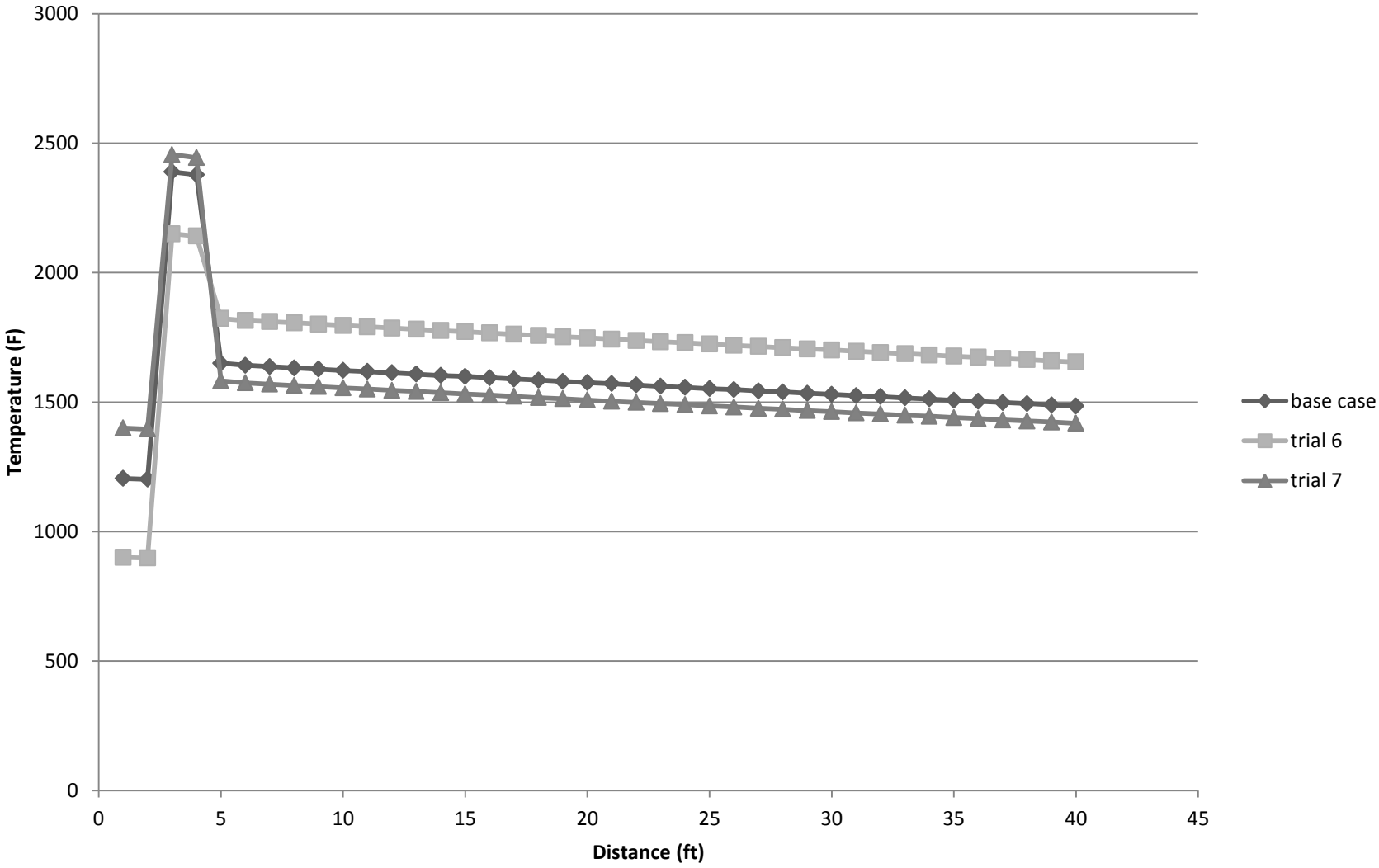

Figure 39 - Temperature profile varying initial syngas temperatures

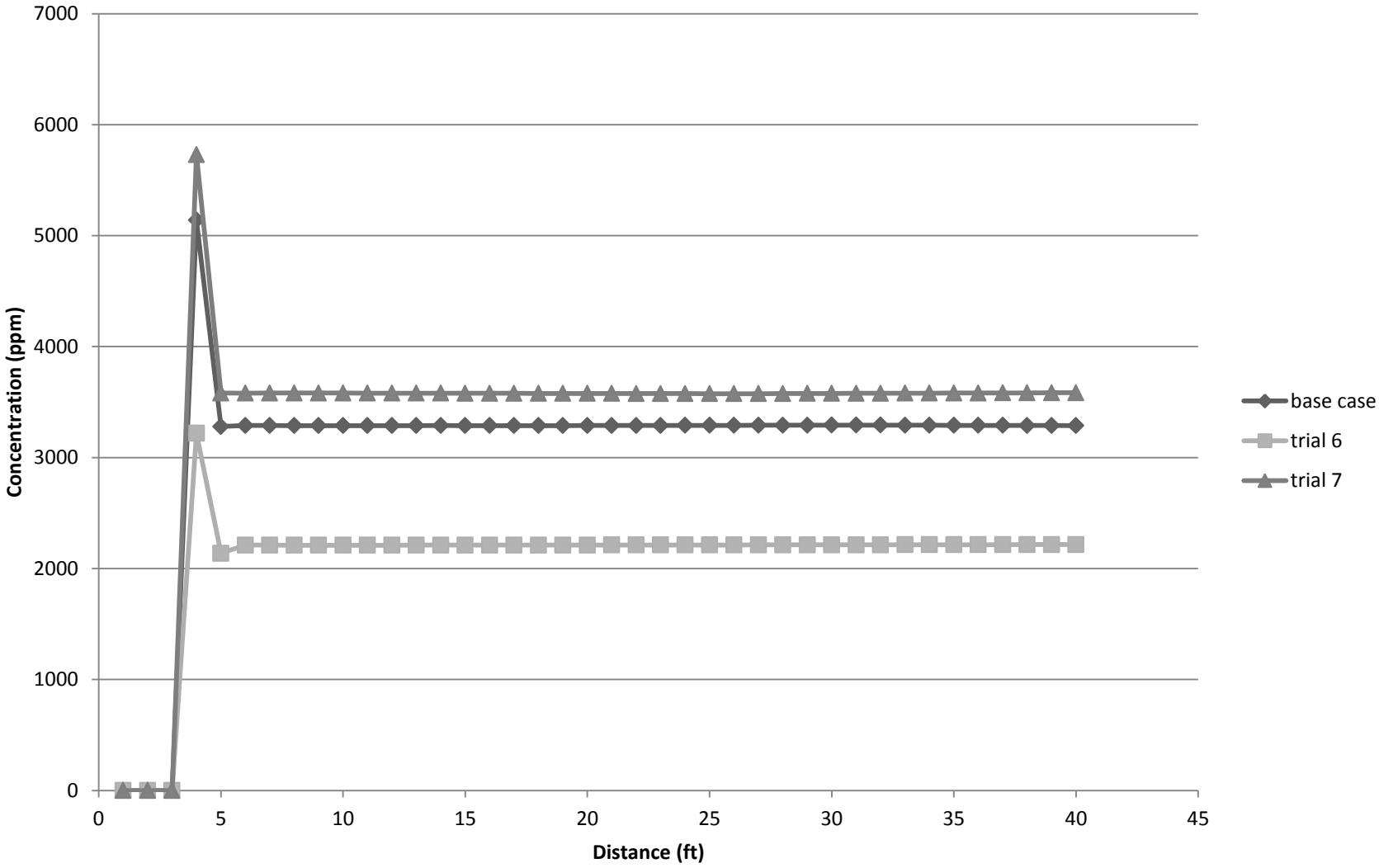

Figure 40 - Concentration profile varying initial syngas temperatures

5.5.3 SNCR results; varying the mole ratio (NH_3:NO_x) and/or exhaust temperature

The final ring in the TO is where aqueous ammonia is injected to further remove NO_x, this allows for the operator to reach even lower levels of NO_x if it is needed. The injection of aqueous ammonia lowers temperatures and quickly reacts to form NH_2 and reacts with the NO and NO_2 to form N_2 and H_2O.

Results indicate that as temperature increases (a range of only 1470 to 1770 °F), NO_x removal increases significantly. Higher temperatures increases the rate at which ammonia reacts with NO_x to form N_2 and H_2O. Higher temperature also prevents ammonia from slipping into the exhaust gas. It is preferential to have temperatures above 1700 °F as indicated in Figure 43.

Varying the molar ratio (lbmol/lbmol) of ammonia to NO_x changes the amount of NO_x removed. Typically, a ratio of NH_3 to NO_x of 1 to 1 gives good removal of NOx (but is a function of temperature). Less aqueous ammonia injected means less of a temperature drop, and the lower temperature drop allows for higher reaction rates and higher NO_x removal is realized due to the higher temperature. There is an optimal range at a certain temperature (T > 1700 °F) and mole ratio (NH_3:NO_x of 1:1) where removal rates will exceed 40%.

Lowering the total air mass flow increases the final temperature. There is also lower NO_x formation in this case and with the higher temperature followed by aqueous ammonia injection, the NO_x removal rates will be higher. Current design limitations in the heat exchanger (after the TO) requires temperatures no greater than 1550 °F, but in the future the heat exchanger should be able to handle higher temperatures (> 1700 °F).

Table 13 – SNCR trials varying flows in air rings and amount of aqueous ammonia injection

Trial	Air ring 1 (lbs/hr)	Air ring 2 (lbs/hr)	Total air mass flow rate (lbs/hr)	Humidity (lbs H2O/lbs DA)	Temp. air (Fahrenheit)	Flue gas ring 1 (lbs/hr)	Flue gas ring 2 (lbs/hr)	Total flue gas mass flow rate (lbs/hr)	Temp. flue gas (Fahrenheit)	Aqueous ammonia injection (lbs/hr)	Temp. aq. Ammonia (Fahrenheit)
Base case	2800	3200	6000	0	77	0	600	600	77	0	77
8	2800	3200	6000	0	77	0	600	600	77	25	77
9	2800	3200	6000	0	77	0	600	600	77	50	77
10	2800	3200	6000	0	77	0	600	600	77	100	77
11	2000	3000	5000	0	77	0	600	600	77	25	77
12	2000	3000	5000	0	77	0	600	600	77	50	77
13	2000	3000	5000	0	77	0	600	600	77	100	77

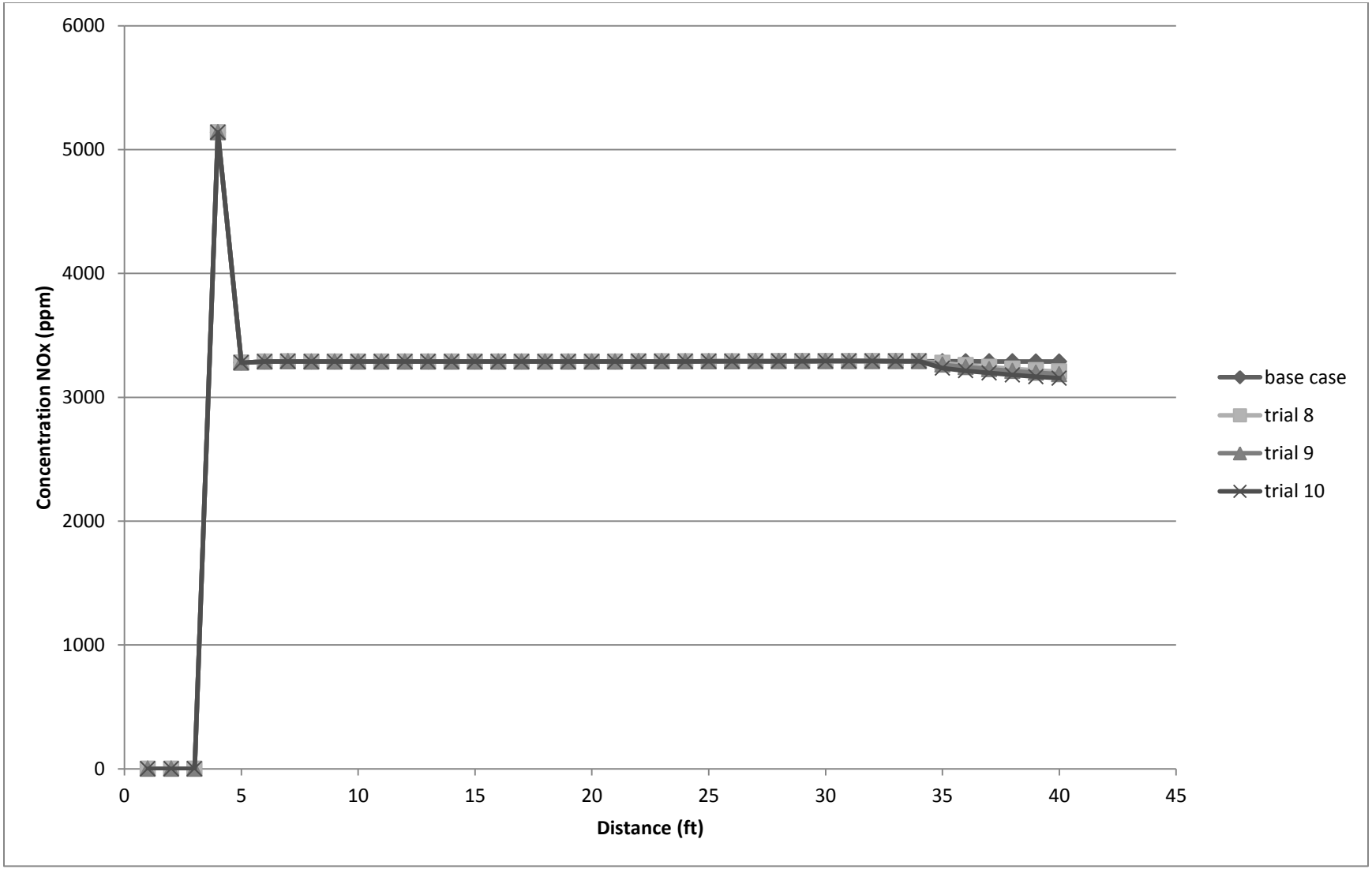

Figure 41 - NO_x concentration profile with SNCR at actual conditions

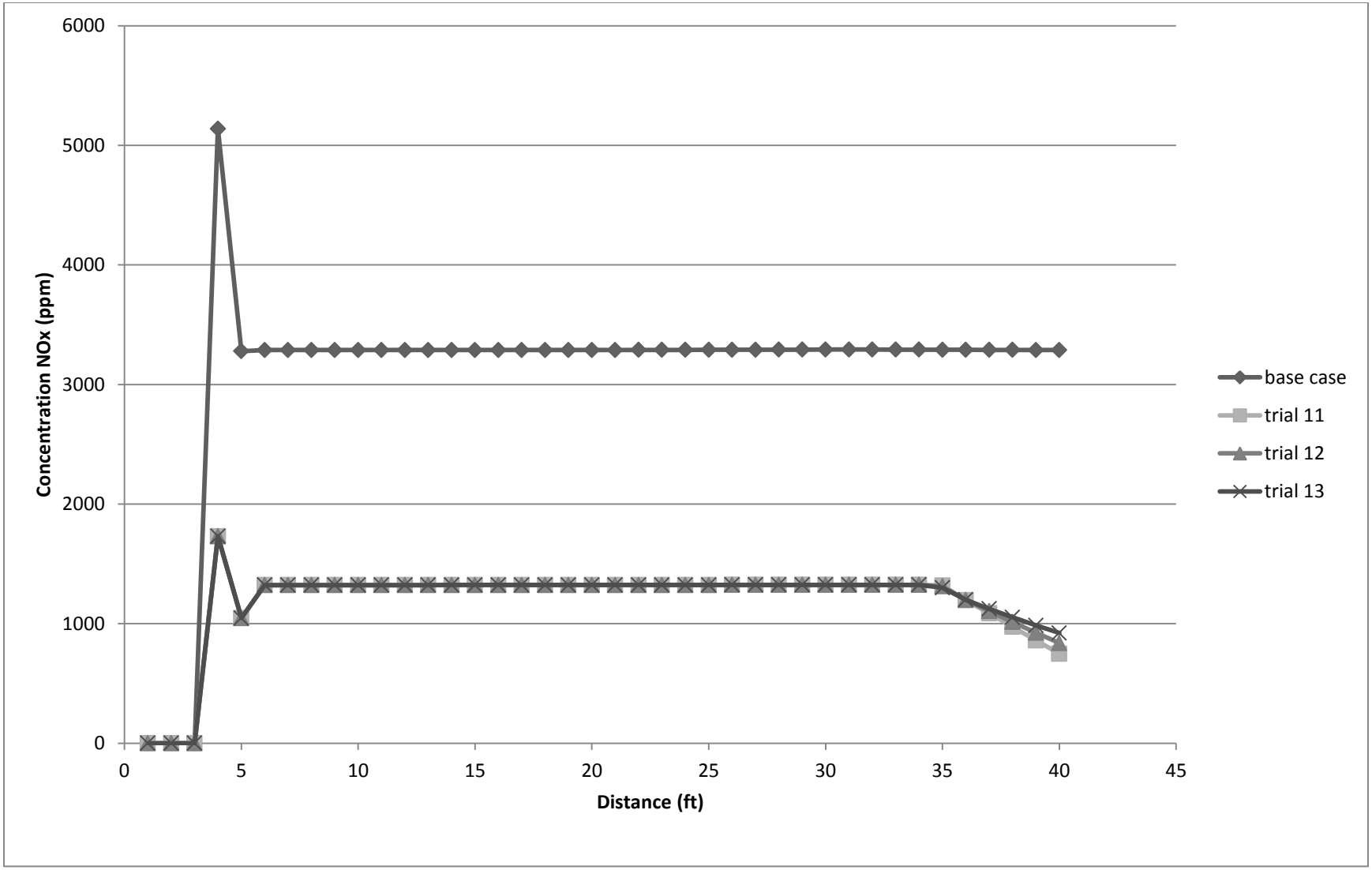

Figure 42 - NO_x concentration profile with SNCR at different air mass flow rates to rings 1 and 2

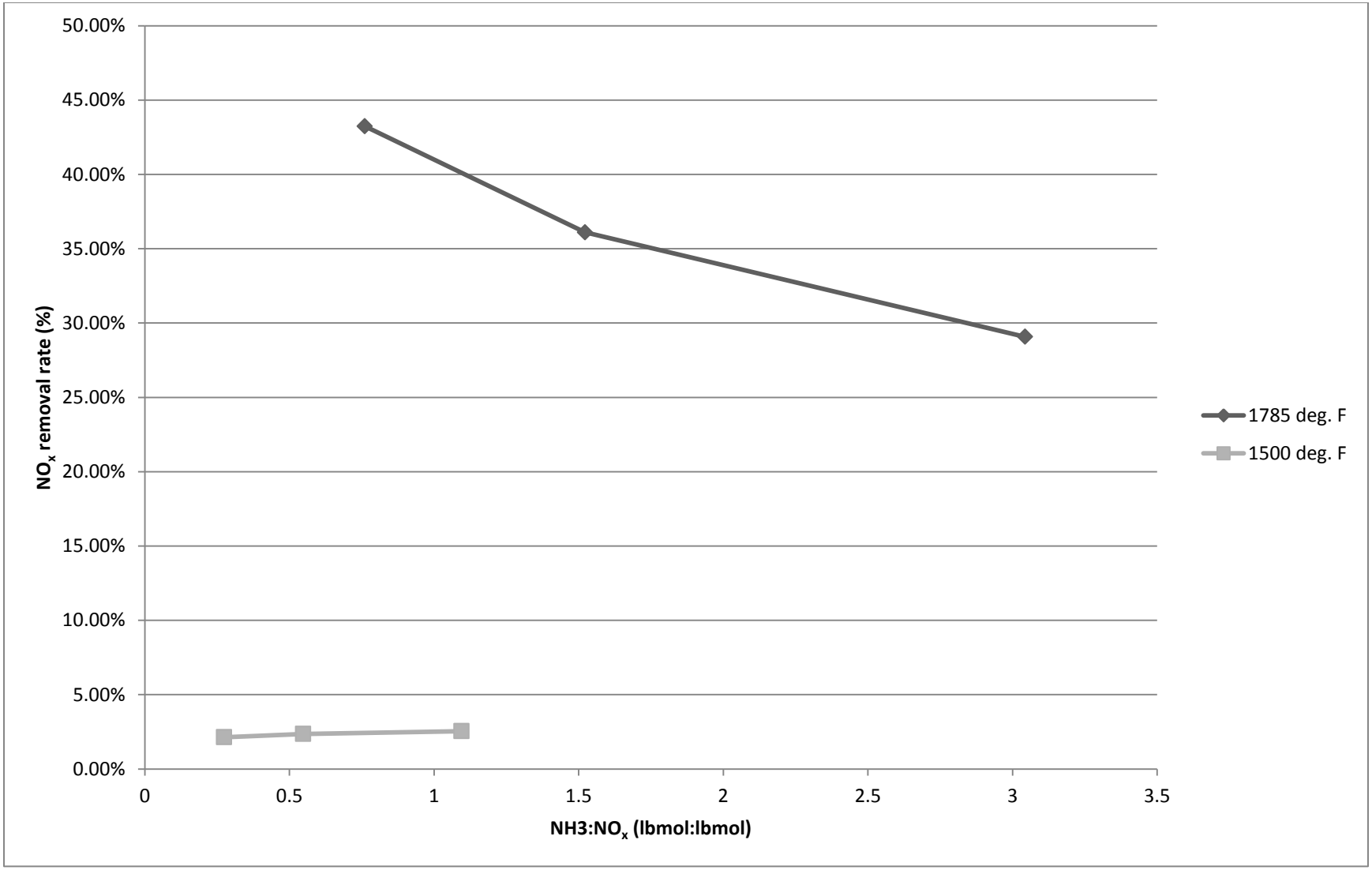

Figure 43 - NO_x removal rates with respect to $NH3:NO_x$ ratio

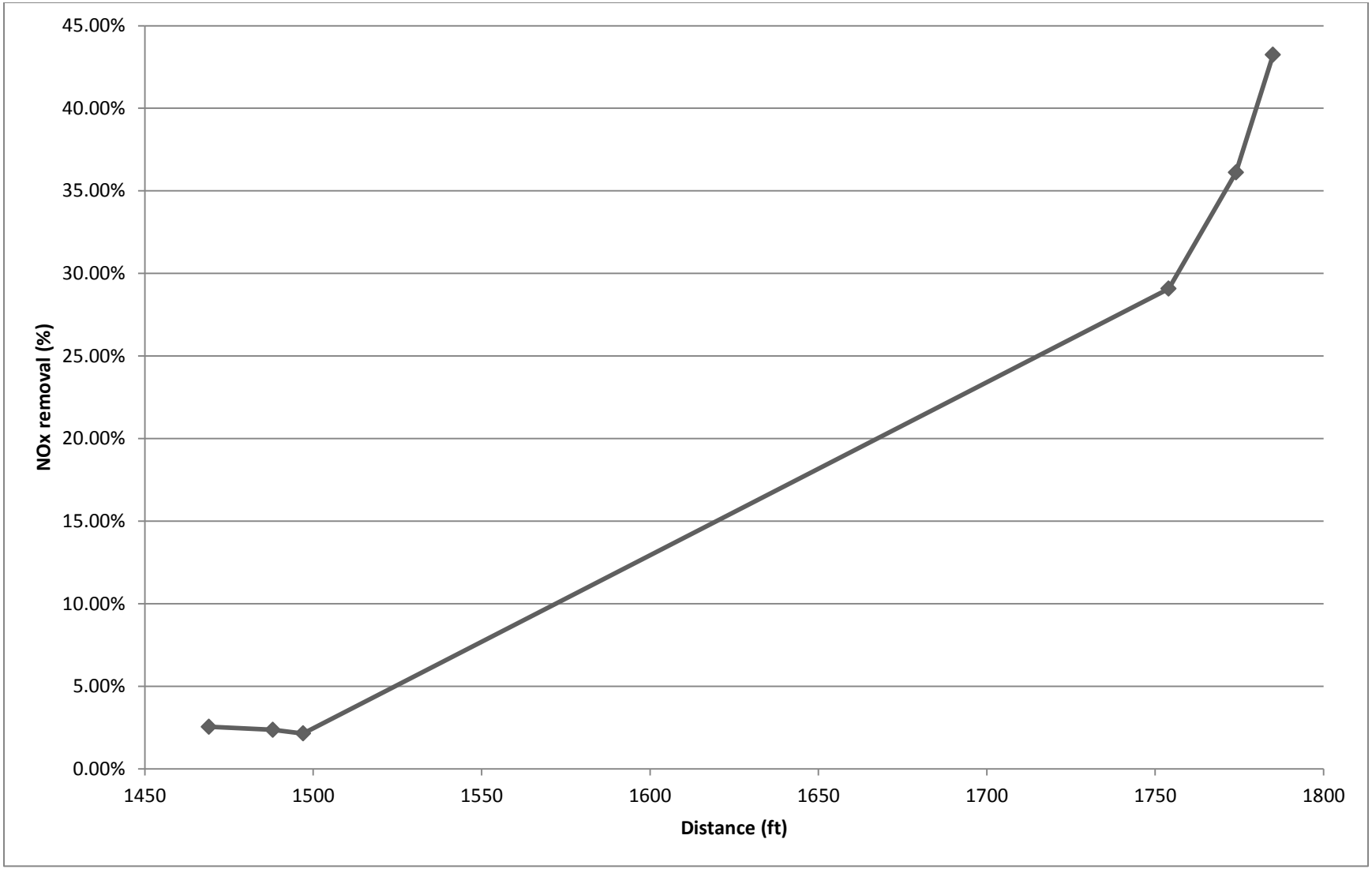

Figure 44 - NO_x removal rates with respect to changes in temperature

6. CONCLUSIONS AND RECOMMENDATIONS

6.1 Conclusions

Varying conditions in a thermal oxidizer with two air rings allows for different strategies to remove NO_x. Increasing and decreasing amounts of air mass flow into rings 1 and 2 may be the best method for NO_x reduction if aqueous ammonia injection is to be avoided. Fuel-rich conditions in ring 1 and fuel-lean in ring 2 results in lower NO_x emissions.

The objective of this modeling was to discover methods in which the gaseous ammonia that is contained in syngas is inhibited from its conversion to NO_x in ring 1. This research indicates that lowering temperatures by adjusting air flow to rings 1 and 2 is one method in the inhibition of NO_x formation. SNCR should always be included in the design for purposes of meeting more stringent standards. Future plants should have the option of aqueous ammonia injection.

NO_x formation is an interesting phenomenon between rings 1 and 2. As NO_x is being formed in ring 1, the remaining NH_3 also reacts with the NO_x to form H_2O and N_2. The nitrogen available in NH_3 to form to NO_x does not completely form into NO_x, but with the right ϕ, can form about 70% N_2 and 30% NO_x, (this split varies with temperature). As temperature increases more of the NH_3 forms NO_x instead of N_2. This is evidence that keeping ring 1 at a certain ϕ (and thus lower temperature) will allow for lower NO_x emissions.

6.2 Recommendations

Reducing the amount of air to ring 1 will allow for lower NO_x emissions and temperatures, and aqueous ammonia might not be necessary to meet standards. Ring 2 should allow for

temperature dilution as this also reduces the formation of NO_x in the remaining length of reactor.

SNCR with aqueous ammonia injection is recommended as needed to meet future possible NO_x emission, but NO_x removal with SNCR is best achieved when temperatures are greater than 1700 °F at the outlet. There is risk in using aqueous ammonia injection due to ammonia slip, but if there is a high enough temperature all the aqueous ammonia that is injected should react and reduce NO_x in the exhaust gas.

Another recommendation for this study is to have more operating data for model validation. Synthesis gas composition was obtained from the gasifier model that was developed by a graduate student at the University of Central Florida. Having the actual operating data for syngas composition, flow, exhaust gas concentrations of NO_x, CO, SO_2, temperature between ring 1 and 2, and exhaust gas mass flow rates will allow for model validation and the further progression of this research. It is realized that this is not affordable at the time of this study. The main limitation of this model is that perfect mixing is assumed throughout the whole length of reactor in each 1-ft increment. CFD modeling may help overcome this limitation.

APPENDIX: REACTION MECHANISM

The reaction mechanism is structured by the CHEMKIN format. The species, thermodynamic data, and reactions are presented in that order respectively.

The text format used in Chemked, and in this research is the format of the CHEMKIN databases. The specific thermodynamic properties of a chemical compound (the heat capacity at constant pressure *Cp*, the enthalpy *H* and the entropy *S*,) are presented as a set of polynomial coefficients.

$$\frac{C_p}{R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\frac{H}{RT} = a_1 + \frac{a_2 T}{2} + \frac{a_3 T^2}{3} + \frac{a_4 T^3}{4} + \frac{a_5 T^4}{5} + \frac{a_6}{T}$$

$$\frac{S}{R} = a_1 \ln(T) + a_2 T + \frac{a_3 T^2}{2} + \frac{a_4 T^3}{3} + \frac{a_5 T^4}{4} + a_7$$

where *R* is the molar gas constant, *T* is temperature in K, *a*1-*a*7 are polynomial coefficients. A set of the seven coefficients is valid for a limited temperature interval. To expand the limits, two coefficient sets for overlapping intervals are used. In the databases, the data are presented in the following order: species name, elemental composition, phase, temperature ranges for which coefficients apply, and the coefficients.

The description of an ordinary reaction has one line that contains a symbol string of reactants and products and 3 numeric values *A, n, E*. Three body reactions contain an M term. The description of the reaction includes additional lines with third-body names and their enhanced efficiencies *Cj*.

```
ELEMENTS
O / 15.999 /
H / 1.00794 /
C / 12.011 /
N / 14.007 /
AR / 39.948 /
HE / 4.0026 /
S / 32.066 /
CL / 35.453 /
END
!Species 197
SPECIES
AR  C  C10H7  C12H10  C12H8O  C2  C2H  C2H2  C2H2OH  C2H3  C2H4  C2H5  C2H5CHO
C2H5CO  C2H6  C2O  C3H2  C3H5  C3H6  C4H  C4H2  C4H3  C5H3  C5H3O  C5H4  C5H4O
C5H4OH  C5H5  C5H5O  C5H5OH  C5H6  C5H7  C6H3O3  C6H4  C6H5  C6H5O  C6H5OH
C6H6  C8H5  C8H6  CC2H3O  CC2H4O  CH  CH2  CH2(S)  CH2CCH3  CH2CCHCO  CH2CH2OH
CH2CHCCH  CH2CHCCH2  CH2CHCH2  CH2CHCH3  CH2CHCHCH  CH2CHCHCH2  CH2CHCHCHCH2
CH2CHCHCHCH2OH  CH2CHCHCHCH3  CH2CHCHCHCHOH  CH2CHCHCHO  CH2CHCHCO
CH2CHCHO
CH2CHCO  CH2CHO  CH2CHOH  CH2CN  CH2CO  CH2HCO  CH2NH  CH2NH2  CH2NO2  CH2O
CH2OH  CH2OOH  CH3  CH3CH2O  CH3CH2ONO  CH3CH2ONO2  CH3CHO  CH3CN  CH3CO
CH3HCO  CH3NH  CH3NH2  CH3NO  CH3NO2  CH3O  CH3OH  CH3ONO  CH3ONO2  CH3OO
CH3OOH  CH4  CHCCCO  CHCCHCHCH2  CHCCHCO  CHCHCH3  CHCHCHCO  CHCHCHO  CHCHOH
CHOCH2CH2CHCHO  CHOCH2CH2CHO  CHOCH2CH2CO  CHOCHCHOH  CL  CL2  CLO  CN  CO
CO2
H  H2  H2C4O  H2CC  H2CCCCH  H2CCCH  H2CCCH2  H2CN  H2NN  H2NO  H2O  H2O2  H2S
H3CCCH  HCCHCCH  HCCO  HCCOH  HCL  HCN  HCNH  HCNO  HCO  HCOO  HE  HNC  HNCO
HNO  HNO2  HNOH  HO2  HOCL  HOCN  HOCO  HON  HONO  HONO2  HOS  HOSO  HOSO2  HSO
HSO2  HSOH  HSOO  HSS  HSSH  HSSO  HSSO2  N  N2  N2H2  N2H3  N2H4  N2O  NCCN
NCN  NCO  NH  NH2  NH2OH  NH3  NNH  NO  NO2  NO3  O  O2  O2CCHOO  O3  OC6H3O
OC6H4O  OCHCHO  OH  OSSO  S  S2  S2O  S3  S4  S5  S6  S7  S8  SH  SO  SO*  SO2
SO3  SSO2
END
THERMO
AR              2 L 6/AR  1    0    0    0G    200.00   6000.00  1000.0      1
 2.50000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
-7.45375000E+02 4.37967490E+00 2.50000000E+00 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00-7.45375000E+02 4.37967490E+00                    4
C               L 7/88C   1    0    0    0G    200.00   6000.00  1000.0      1
 2.60558300E+00-1.95934340E-04 1.06737220E-07-1.64239400E-11 8.18705800E-16    2
 8.54117420E+04 4.19238680E+00 2.55423950E+00-3.21537720E-04 7.33792230E-07    3
-7.32234870E-10 2.66521440E-13 8.54426810E+04 4.53130850E+00                    4
C10H7           T 7/98H   7C  10    0    0G    200.00   6000.00  1000.0      1
 1.83535073E+01 2.77474314E-02-1.00885968E-05 1.64229575E-09-9.89002001E-14    2
```

3.89261241E+04-7.48978150E+01-1.89559772E+00 5.83077290E-02 2.79388931E-05 3
-9.14375172E-08 4.46422302E-11 4.55409775E+04 3.52453263E+01 4
C12H10 g 8/00H 10C 12 0 0G 200.00 6000.00 1000.0 1
2.28963620E+01 3.68453189E-02-1.35016357E-05 2.20802787E-09-1.33358137E-13 2
1.07395923E+04-1.00509573E+02 1.94600056E-01 5.35259888E-02 8.55000841E-05 3
-1.63903525E-07 7.29975666E-11 1.90021492E+04 2.72148992E+01 4
C12H8O T 5/12O 1H 8C 12 0G 200.00 6000.00 1000.0 1
2.38920518E+01 3.42247501E-02-1.25919439E-05 2.06597572E-09-1.25092468E-13 2
-4.81278402E+03-1.07323610E+02-1.94560629E+00 6.63036054E-02 5.55840459E-05 3
-1.35441751E-07 6.29654469E-11 4.01894017E+03 3.50530326E+01 4
C2 T05/09C 2 0 0 0G 200.00 6000.00 1000.0 1
3.43350371E+00 1.07185010E-03-3.97897382E-07 6.67457391E-11-4.10152154E-15 2
1.00178987E+05 4.10588356E+00 3.76163273E+00-2.72143299E-03 8.69879462E-06 3
-8.19304667E-09 2.62415296E-12 1.00254566E+05 3.18038623E+00 4
C2H T 5/10H 1C 2 0 0G 200.00 6000.00 1000.0 1
3.66270248E+00 3.82492252E-03-1.36632500E-06 2.13455040E-10-1.23216848E-14 2
6.71683790E+04 3.92205792E+00 2.89867676E+00 1.32988489E-02-2.80733327E-05 3
2.89484755E-08-1.07502351E-11 6.70616050E+04 6.18547632E+00 4
C2H2 g 1/91H 2C 2 0 0G 200.00 6000.00 1000.0 1
4.65878489E+00 4.88396667E-03-1.60828888E-06 2.46974544E-10-1.38605959E-14 2
2.57517182E+04-3.99838194E+00 8.08679682E-01 2.33615762E-02-3.55172234E-05 3
2.80152958E-08-8.50075165E-12 2.64212948E+04 1.39396761E+01 4
C2H2OH SAND96O 1H 3C 2 0G 300.00 3000.00 1000.0 1
5.72068430E+00 1.07041850E-02-5.03584940E-06 1.13244990E-09-1.00866210E-13 2
1.28494240E+04-4.70817760E+00 8.14982820E-02 3.16406440E-02-3.40853610E-05 3
1.89788380E-08-4.19501650E-12 1.40607830E+04 2.29089770E+01 4
C2H3 ATcT/AH 3C 2 0 0G 200.00 6000.00 1000.0 1
4.15026763E+00 7.54021341E-03-2.62997847E-06 4.15974048E-10-2.45407509E-14 2
3.38566380E+04 1.72812235E+00 3.36377642E+00 2.65765722E-04 2.79620704E-05 3
-3.72986942E-08 1.51590176E-11 3.44749589E+04 7.91510092E+00 4
C2H4 g 1/00H 4C 2 0 0G 200.00 6000.00 1000.0 1
3.99182724E+00 1.04833908E-02-3.71721342E-06 5.94628366E-10-3.53630386E-14 2
4.26865851E+03-2.69081762E-01 3.95920063E+00-7.57051373E-03 5.70989993E-05 3
-6.91588352E-08 2.69884190E-11 5.08977598E+03 4.09730213E+00 4
C2H5 g 7/00H 5C 2 0 0G 200.00 6000.00 1000.0 1
4.28800015E+00 1.24337439E-02-4.41384130E-06 7.06527536E-10-4.20342270E-14 2
1.20564209E+04 8.45299829E-01 4.30642051E+00-4.18635208E-03 4.97137768E-05 3
-5.99121792E-08 2.30507301E-11 1.28416330E+04 4.70738797E+00 4
C2H5CHO T 9/92O 1H 6C 3 0G 273.15 5000.00 1000.0 1
3.31379820E+00 2.66196060E-02-1.04755960E-05 1.88153340E-09-1.27613100E-13 2
-2.54596030E+04 9.66084470E+00 7.60445960E+00-8.64035640E-03 7.39300970E-05 3
-7.96873980E-08 2.80049270E-11-2.54897890E+04-6.76436910E+00 4
C2H5CO T 9/92O 1H 5C 3 0G 298.15 5000.00 1000.0 1
3.04456980E+00 2.32364290E-02-8.63179360E-06 1.47995500E-09-9.68608290E-14 2

-6.17872110E+03 1.31223020E+01 6.73682940E+00-2.69452990E-03 4.99270170E-05 3
-5.00258080E-08 1.50115030E-11-6.57033660E+03-2.33987320E+00 4
C2H6 g 8/88H 6C 2 0 0G 200.00 6000.00 1000.0 1
4.04666411E+00 1.53538802E-02-5.47039485E-06 8.77826544E-10-5.23167531E-14 2
-1.24473499E+04-9.68698313E-01 4.29142572E+00-5.50154901E-03 5.99438458E-05 3
-7.08466469E-08 2.68685836E-11-1.15222056E+04 2.66678994E+00 4
C2O 110203O 1C 2 0 0G 300.00 4000.00 1000.0 1
5.02664790E+00 2.89182270E-03-1.39138410E-06 3.07035460E-10-2.55679050E-14 2
4.48889000E+04-1.78533980E+00 2.96655560E+00 1.05132290E-02-1.35164890E-05 3
9.93339650E-09-3.08813760E-12 4.53859150E+04 8.44327530E+00 4
C3H2 SAND H 2C 3 0 0G 150.00 4000.00 1000.0 1
7.67098100E+00 2.74874900E-03-4.37094200E-07-6.45559900E-11 1.66388740E-14 2
6.32530850E+04-1.23689030E+01 3.16671300E+00 2.48257100E-02-4.59163700E-05 3
4.26801900E-08-1.48215240E-11 6.41600750E+04 8.86944600E+00 4
C3H5 T 9/96H 5C 3 0 0G 200.00 6000.00 1000.0 1
7.00945680E+00 1.31066290E-02-4.65334420E-06 7.45143230E-10-4.43500510E-14 2
1.64129090E+04-1.39461140E+01 1.46980360E+00 1.90343650E-02 1.44804250E-05 3
-3.54686520E-08 1.66475940E-11 1.83258310E+04 1.67241140E+01 4
C3H6 2 L 4/H 6C 3 0 0G 300.00 5000.00 1000.0 1
6.72139740E+00 1.49317570E-02-4.96523530E-06 7.25107530E-10-3.80014760E-14 2
-9.24531490E+02-1.21556170E+01 1.45751570E+00 2.11422630E-02 4.04680120E-06 3
-1.63190030E-08 7.04751530E-12 1.07402080E+03 1.73994600E+01 4
C4H SAND86H 1C 4 0 0G 300.00 5000.00 1000.0 1
6.24288200E+00 6.19368300E-03-2.08593200E-06 3.08220300E-10-1.63648300E-14 2
7.56801900E+04-7.21080600E+00 5.02324700E+00 7.09237500E-03-6.07376200E-09 3
-2.27575200E-09 8.08699400E-13 7.62381300E+04-6.94259400E-02 4
C4H2 SAND86H 2C 4 0 0G 300.00 5000.00 1000.0 1
9.03140700E+00 6.04725300E-03-1.94878900E-06 2.75486300E-10-1.38560800E-14 2
5.29473600E+04-2.38506800E+01 4.00519200E+00 1.98100000E-02-9.86587700E-06 3
-6.63515800E-09 6.07741300E-12 5.42406500E+04 1.84573700E+00 4
C4H3 T06/04H 3C 4 0 0G 200.00 6000.00 1000.0 1
8.44631306E+00 9.07291526E-03-3.18681201E-06 5.06725048E-10-3.00149855E-14 2
6.20007365E+04-1.77938854E+01 5.54263934E-01 3.86185425E-02-4.70818280E-05 3
3.06240321E-08-7.90588421E-12 6.37974910E+04 2.10542043E+01 4
C5H3 BUR94 H 3C 5 0 0G 200.00 6000.00 1000.0 1
1.03975010E+01 1.05482830E-02-3.84625260E-06 6.27384470E-10-3.78364820E-14 2
7.94354810E+04-3.05392130E+01-3.02797430E-01 3.13760320E-02 3.07893830E-06 3
-3.59375350E-08 1.94744410E-11 8.26522820E+04 2.63957220E+01 4
C5H3O OZELLIO 1H 3C 5 0G 300.00 5000.00 1394.0 1
1.37920307E+01 9.94676171E-03-3.53224669E-06 5.62416803E-10-3.32119217E-14 2
2.82749422E+04-5.06039865E+01-2.97900157E+00 5.40428052E-02-4.87013197E-05 3
2.18001279E-08-3.86113970E-12 3.35757242E+04 3.76713392E+01 4
C5H4 BURC94H 4C 5 0 0G 200.00 6000.00 1000.0 1
1.01068090E+01 1.34574660E-02-4.88623830E-06 7.94654240E-10-4.78216910E-14 2

6.17147350E+04-3.01553320E+01 9.83384820E-01 2.14294460E-02 3.33900710E-05 3
-6.69413790E-08 3.05633460E-11 6.49051740E+04 2.06828010E+01 4
C5H4O BURC94O 1H 4C 5 0G 298.15 5000.00 1000.0 1
1.14144290E+01 1.59323960E-02-6.21636120E-06 1.09603370E-09-7.20603790E-14 2
2.58695940E+03-3.88728110E+01-4.02844840E+00 6.10128730E-02-5.56176570E-05 3
2.52217340E-08-4.49574120E-12 5.57756630E+03 4.04869980E+01 4
C5H4OH BURC89O 1H 5C 5 0G 200.00 6000.00 1000.0 1
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3.13805150E+03-4.59200990E+01-1.28208120E+00 4.90400750E-02-1.36874020E-05 3
-2.91344760E-08 1.90068850E-11 6.14207270E+03 3.07978010E+01 4
C5H5 HIPP98H 5C 5 0 0G 300.00 5000.00 1000.0 1
1.53109400E+01 7.47380600E-03-5.83745800E-07-4.38665100E-10 7.69683900E-14 2
2.79935000E+04-5.95159300E+01 1.53109400E+01 7.47380600E-03-5.83745800E-07 3
-4.38665100E-10 7.69683900E-14 2.79935000E+04-5.95159300E+01 4
C5H5O BOZELLO 1H 5C 5 0G 300.00 5000.00 1395.0 1
-4.23394180E+00 6.26896540E-02-5.30483570E-05 2.22659990E-08-3.65777890E-12 2
2.05144080E+04 4.42088160E+01-4.23394180E+00 6.26896540E-02-5.30483570E-05 3
2.22659990E-08-3.65777890E-12 2.05144080E+04 4.42088160E+01 4
C5H5OH BOZELLO 1H 6C 5 0G 300.00 5000.00 1395.0 1
-4.30791350E+00 6.63287430E-02-5.66113450E-05 2.41371720E-08-4.02643430E-12 2
-5.74719240E+03 4.49967210E+01-4.30791350E+00 6.63287430E-02-5.66113450E-05 3
2.41371720E-08-4.02643430E-12-5.74719240E+03 4.49967210E+01 4
C5H6 SAND87H 6C 5 0 0G 300.00 5000.00 1000.0 1
9.68981500E+00 1.83826200E-02-6.26488400E-06 9.39337700E-10-5.08770800E-14 2
1.10212400E+04-3.12290800E+01-3.19673900E+00 4.08136100E-02 6.81650500E-07 3
-3.13745900E-08 1.57722300E-11 1.52906800E+04 3.86993900E+01 4
C5H7 BURC94H 7C 5 0 0G 298.15 5000.00 1000.0 1
1.27856590E+01 1.64578620E-02-4.83996410E-06 7.38140830E-10-4.60003690E-14 2
1.38692960E+04-4.43462430E+01-2.73230950E+00 4.08905690E-02 1.60060140E-05 3
-5.60854660E-08 2.69707360E-11 1.90248060E+04 4.01794070E+01 4
C6H3O3 dummy O 3H 3C 6 0G 300.00 3000.00 1000.0 1
7.29203500E+00 9.25020000E-02-5.16864100E-05 1.36270900E-08-1.38114800E-12 2
1.03167300E+04-1.13273800E+01-1.38895800E+01 1.72098400E-01-1.70066000E-04 3
9.60188800E-08-2.37325300E-11 1.50323400E+04 9.27073600E+01 4
C6H4 A02/05H 4C 6 0 0G 200.00 6000.00 1000.0 1
1.15160949E+01 1.45816929E-02-5.21944977E-06 8.40605048E-10-5.02392470E-14 2
6.35897979E+04-3.41128898E+01 1.72575865E+00 4.58663914E-02-4.46314139E-05 3
2.38247581E-08-5.11679045E-12 6.61423782E+04 1.55428939E+01 4
C6H5 pg9705H 5C 6 0 0G 300.00 4000.00 1000.0 1
1.57758900E+01 9.65110900E-03-9.42941600E-07-5.46911100E-10 1.02652200E-13 2
3.36812300E+04-6.17628000E+01 1.14355700E-01 3.62732500E-02 1.15828600E-06 3
-2.19696500E-08 8.46355600E-12 3.90147900E+04 2.38011700E+01 4
C6H5O SAND89O 1H 5C 6 0G 300.00 4000.00 1000.0 1
1.82263900E+01 1.00398500E-02-9.91566800E-07-5.67280400E-10 1.06837200E-13 2

-2.62084600E+03-7.36139100E+01 1.10749700E+00 3.95694600E-02 8.49729500E-07 3
-2.43631100E-08 9.65066000E-12 3.15967200E+03 1.97349600E+01 4
C6H5OH SAND89O 1H 6C 6 0G 300.00 4000.00 1000.0 1
1.82163300E+01 1.14242700E-02-1.09668400E-06-6.42744200E-10 1.19889300E-13 2
-2.05366400E+04-7.30423400E+01 1.39145600E+00 3.93195800E-02 1.77709600E-06 3
-2.27767300E-08 8.30965900E-12-1.47218100E+04 1.91781300E+01 4
C6H6 SAND87H 6C 6 0 0G 300.00 5000.00 1000.0 1
1.29107400E+01 1.72329700E-02-5.02421100E-06 5.89349700E-10-1.94752100E-14 2
3.66451200E+03-5.00269900E+01-3.13801200E+00 4.72310300E-02-2.96220800E-06 3
-3.26281900E-08 1.71869200E-11 8.89003100E+03 3.65757300E+01 4
C8H5 T12/06H 5C 8 0 0G 200.00 6000.00 1000.0 1
1.45430114E+01 2.02785496E-02-7.36298153E-06 1.19771535E-09-7.20964829E-14 2
7.20671458E+04-5.18466294E+01 1.77837769E+00 3.24193784E-02 3.85015803E-05 3
-8.03841588E-08 3.62690208E-11 7.66004229E+04 1.93639058E+01 4
C8H6 T10/11H 6C 8 0 0G 200.00 6000.00 1000.0 1
1.48427411E+01 2.25477791E-02-8.14867367E-06 1.32148572E-09-7.93819250E-14 2
3.79569346E+04-5.74754012E+01-7.64086880E-01 3.77083180E-02 5.09846183E-05 3
-1.05932407E-07 4.84875074E-11 4.33724909E+04 2.92151372E+01 4
CC2H3O BurcatO 1H 3C 2 0G 200.00 6000.00 1000.0 1
5.60158035E+00 9.17613962E-03-3.28028902E-06 5.27903888E-10-3.15362241E-14 2
1.71446252E+04-5.47228512E+00 3.58349017E+00-6.02275805E-03 6.32426867E-05 3
-8.18540707E-08 3.30444505E-11 1.85681353E+04 9.59725926E+00 4
CC2H4O L 8/88O 1H 4C 2 0G 200.00 6000.00 1000.0 1
5.48876410E+00 1.20461900E-02-4.33369310E-06 7.00283110E-10-4.19490880E-14 2
-9.18042510E+03-7.07996050E+00 3.75905320E+00-9.44121800E-03 8.03097210E-05 3
-1.00807880E-07 4.00399210E-11-7.56081430E+03 7.84974750E+00 4
CH IU3/03H 1C 1 0 0G 200.00 6000.00 1000.0 1
2.52093690E+00 1.76536390E-03-4.61476600E-07 5.92896750E-11-3.34745010E-15 2
7.09948780E+04 7.40518290E+00 3.48975830E+00 3.24321600E-04-1.68997510E-06 3
3.16284200E-09-1.40618030E-12 7.06607550E+04 2.08428410E+00 4
CH2 IU3/03H 2C 1 0 0G 200.00 6000.00 1000.0 1
3.11049513E+00 3.73779517E-03-1.37371977E-06 2.23054839E-10-1.33567178E-14 2
4.59715953E+04 4.62796405E+00 3.84261832E+00-7.36676871E-06 6.16970693E-06 3
-6.96689962E-09 2.64620979E-12 4.58631528E+04 1.27584470E+00 4
CH2(S) IU3/03H 2C 1 0 0G 200.00 6000.00 1000.0 1
3.13501686E+00 2.89593926E-03-8.16668090E-07 1.13572697E-10-6.36262835E-15 2
5.05040504E+04 4.06030621E+00 4.19331325E+00-2.33105184E-03 8.15676451E-06 3
-6.62985981E-09 1.93233199E-12 5.03662246E+04-7.46734310E-01 4
CH2CCH3 ANDIA8H 5C 3 0 0G 300.00 4000.00 1000.0 1
9.10101800E+00 7.96416800E-03-7.88494500E-07-4.56203600E-10 8.52921200E-14 2
2.67068000E+04-2.15055900E+01 3.38581100E+00 1.40453400E-02 3.20412700E-06 3
-3.82412000E-09-9.05374200E-13 2.90906600E+04 1.12664900E+01 4
CH2CCHCO mmy O 1H 3C 4 0G 300.00 5000.00 1401.0 1
-1.86011530E+00 6.58032350E-02-9.32191370E-05 6.32010340E-08-1.59778480E-11 2

2.89970150E+04 3.17474470E+01-1.86011530E+00 6.58032350E-02-9.32191370E-05 3
6.32010340E-08-1.59778480E-11 2.89970150E+04 3.17474470E+01 4
CH2CH2OH T12/01O 1H 5C 2 0G 200.00 6000.00 1000.0 1
7.02824536E+00 1.20037746E-02-4.21306455E-06 6.69471213E-10-3.96371893E-14 2
-5.92493321E+03-9.40355948E+00 4.47893092E+00 7.59782301E-03 2.81794908E-05 3
-4.26953487E-08 1.78878934E-11-4.71446256E+03 6.38921206E+00 4
CH2CHCCH 82489 H 4C 4 0 0G 300.00 4000.00 1000.0 1
1.06977700E+01 6.98201400E-03-6.56774700E-07-3.88451700E-10 7.20094600E-14 2
3.03480300E+04-3.12843000E+01 3.23389300E+00 1.86563400E-02 1.27032000E-06 3
-9.41009600E-09 2.95611100E-12 3.30109700E+04 9.92267600E+00 4
CH2CHCCH2 SANDIAH 5C 4 0 0G 300.00 4000.00 1000.0 1
1.19977600E+01 7.99058000E-03-8.09817300E-07-4.56873300E-10 8.63691000E-14 2
3.22849300E+04-3.52849500E+01 3.87944300E+00 1.99766400E-02 1.87277700E-06 3
-9.30695300E-09 2.38611600E-12 3.52685900E+04 9.84215200E+00 4
CH2CHCH2 2 T 9/H 5C 3 0 0G 200.00 6000.00 1000.0 1
7.00945680E+00 1.31066290E-02-4.65334420E-06 7.45143230E-10-4.43500510E-14 2
1.64129090E+04-1.39461140E+01 1.46980360E+00 1.90343650E-02 1.44804250E-05 3
-3.54686520E-08 1.66475940E-11 1.83258310E+04 1.67241140E+01 4
CH2CHCH3 ANDIA8H 6C 3 0 0G 300.00 5000.00 1000.0 1
6.73225700E+00 1.49083400E-02-4.94989900E-06 7.21202200E-10-3.76620400E-14 2
-9.23570300E+02-1.33133500E+01 1.49330700E+00 2.09251800E-02 4.48679400E-06 3
-1.66891200E-08 7.15814600E-12 1.07482600E+03 1.61453400E+01 4
CH2CHCHCH SANDIAH 5C 4 0 0G 300.00 4000.00 1000.0 1
1.28659700E+01 7.94336900E-03-8.62646600E-07-4.65563500E-10 8.95113100E-14 2
3.78355200E+04-4.18250200E+01 2.99524000E+00 2.28845600E-02 1.97547100E-06 3
-1.14824500E-08 3.19782400E-12 4.14221800E+04 1.28945400E+01 4
CH2CHCHCH2 SANDIAH 6C 4 0 0G 300.00 4000.00 1000.0 1
1.19977600E+01 7.99058000E-03-8.09817300E-07-4.56873300E-10 8.63691000E-14 2
3.22849300E+04-3.52849500E+01 3.87944300E+00 1.99766400E-02 1.87277700E-06 3
-9.30695300E-09 2.38611600E-12 3.52685900E+04 9.84215200E+00 4
CH2CHCHCHCH2 BOZZELH 7C 5 0 0G 298.15 3000.00 1000.0 1
-3.82433560E+00 6.16882580E-02-5.18428620E-05 2.30662500E-08-4.21118690E-12 2
2.36306950E+04 4.37246400E+01-3.82433560E+00 6.16882580E-02-5.18428620E-05 3
2.30662500E-08-4.21118690E-12 2.36306950E+04 4.37246400E+01 4
CH2CHCHCHCH2OH BOZELLO 1H 8C 5 0G 298.15 3000.00 1000.0 1
1.56864064E+01 1.91906779E-02-6.58044838E-06 1.02320738E-09-5.94229022E-14 2
-1.56503172E+04-5.50794572E+01-2.74469890E-01 6.00349537E-02-4.81885682E-05 3
2.08577144E-08-3.72750466E-12-1.03784062E+04 2.95196038E+01 4
CH2CHCHCHCH3 BURC92H 8C 5 0 0G 298.15 3000.00 1000.0 1
1.94031140E+01 9.63254070E-03-1.56831470E-06 0.00000000E+00 0.00000000E+00 2
2.06355710E+02-8.07987130E+01-3.08820870E-01 4.83558980E-02-2.22847580E-05 3
0.00000000E+00 0.00000000E+00 7.29823290E+03 2.68287850E+01 4
CH2CHCHCHCHOH BOZZELO 1H 7C 5 0G 298.15 3000.00 1000.0 1
-4.29455720E+00 7.49453150E-02-7.24872810E-05 3.66141520E-08-7.43473450E-12 2

2.13627670E+03 4.78211050E+01-4.29455720E+00 7.49453150E-02-7.24872810E-05 3
3.66141520E-08-7.43473450E-12 2.13627670E+03 4.78211050E+01 4
CH2CHCHCHO ZELLI O 1H 5C 4 0G 300.00 5000.00 1393.0 1
-1.34293210E-01 4.05564010E-02-2.77279830E-05 9.40211800E-09-1.26944400E-12 2
6.24142910E+03 2.85164780E+01-1.34293210E-01 4.05564010E-02-2.77279830E-05 3
9.40211800E-09-1.26944400E-12 6.24142910E+03 2.85164780E+01 4
CH2CHCHCO ZELLI O 1H 4C 4 0G 300.00 5000.00 1401.0 1
-4.24241180E-01 5.12684600E-02-5.24243190E-05 2.60740100E-08-4.89019190E-12 2
-8.20706910E+02 2.54617220E+01-4.24241180E-01 5.12684600E-02-5.24243190E-05 3
2.60740100E-08-4.89019190E-12-8.20706910E+02 2.54617220E+01 4
CH2CHCHO O 1H 4C 3 0G 300.00 5000.00 1393.0 1
-2.24224150E-01 3.79356310E-02-3.32638600E-05 1.48809720E-08-2.61035640E-12 2
-1.15787540E+04 2.52386110E+01-2.24224150E-01 3.79356310E-02-3.32638600E-05 3
1.48809720E-08-2.61035640E-12-1.15787540E+04 2.52386110E+01 4
CH2CHCO 2 T05/O 1H 3C 3 0G 200.00 6000.00 1000.0 1
6.95842227E+00 1.07193211E-02-3.85218494E-06 6.22009064E-10-3.72401640E-14 2
5.64826498E+03-1.14745786E+01 3.21169467E+00 1.18422105E-02 1.67462582E-05 3
-3.06947176E-08 1.33048816E-11 7.12815750E+03 1.00881663E+01 4
CH2CHO T04/06O 1H 3C 2 0G 200.00 6000.00 1000.0 1
5.91636535E+00 8.84650426E-03-3.14954895E-06 5.05413189E-10-3.01304621E-14 2
-1.04779892E+03-6.10649981E+00 2.66873956E+00 9.62329538E-03 1.60617438E-05 3
-2.87681820E-08 1.25030066E-11 2.19438429E+02 1.25694476E+01 4
CH2CHOH BOZ06 O 1H 4C 2 0G 300.00 1500.00 1500.0 1
-9.61151300E-01 3.94592050E-02-4.51573400E-05 2.68048840E-08-6.20638750E-12 2
-1.62138500E+04 2.65615950E+01-9.61151300E-01 3.94592050E-02-4.51573400E-05 3
2.68048840E-08-6.20638750E-12-1.62138500E+04 2.65615950E+01 4
CH2CN T01/03H 2C 2N 1 0G 200.00 6000.00 1000.0 1
6.14873620E+00 6.06600240E-03-2.17174620E-06 3.49750387E-10-2.09004207E-14 2
2.86491222E+04-6.59235995E+00 2.63064017E+00 1.73644377E-02-1.70284117E-05 3
9.86551140E-09-2.46033517E-12 2.95791691E+04 1.12776223E+01 4
CH2CO T 6/94O 1H 2C 2 0G 200.00 6000.00 1000.0 1
5.75779010E+00 6.34965070E-03-2.25844070E-06 3.62084620E-10-2.15690300E-14 2
-7.97861130E+03-6.10640370E+00 2.14011650E+00 1.80883680E-02-1.73242160E-05 3
9.27674770E-09-1.99150110E-12-7.04305090E+03 1.21986990E+01 4
CH2HCO 110393O 1H 3C 2 0G 300.00 5000.00 1000.0 1
5.97567000E+00 8.13059100E-03-2.74362400E-06 4.07030400E-10-2.17601700E-14 2
4.90321800E+02-5.04525100E+00 3.40906200E+00 1.07385700E-02 1.89149200E-06 3
-7.15858300E-09 2.86738500E-12 1.52147700E+03 9.55829000E+00 4
CH2NH US 88 H 3C 1N 1 0G 300.00 5000.00 1577.0 1
4.54737795E+00 7.17720948E-03-2.47935299E-06 3.87692351E-10-2.26113075E-14 2
8.64056516E+03-1.16687427E+00 2.81849510E+00 5.11983235E-03 6.38887146E-06 3
-6.61374671E-09 1.65531940E-12 9.88442597E+03 1.03390629E+01 4
CH2NH2 M92 H 4C 1N 1 0G 300.00 5000.00 1397.0 1
6.11432288E+00 7.69126269E-03-2.59025729E-06 3.97713575E-10-2.28883272E-14 2

1.55835138E+04-8.93053780E+00 2.56157769E+00 1.60730713E-02-1.05960335E-05 3
4.07638829E-09-6.95570548E-13 1.68563722E+04 1.01987687E+01 4
CH2NO2 T04/98O 2H 2C 1N 1G 200.00 6000.00 1000.0 1
7.67214886E+00 7.04674142E-03-2.55301211E-06 4.14646979E-10-2.49316782E-14 2
1.52307521E+04-1.22510821E+01 2.46754293E+00 1.56130407E-02 4.71686464E-06 3
-2.05123642E-08 1.02705094E-11 1.69015807E+04 1.59016345E+01 4
CH2O L 8/88O 1H 2C 1 0G 200.00 6000.00 1000.0 1
3.16948070E+00 6.19327420E-03-2.25059810E-06 3.65982450E-10-2.20154100E-14 2
-1.44784250E+04 6.04235330E+00 4.79370360E+00-9.90815180E-03 3.73214590E-05 3
-3.79279020E-08 1.31770150E-11-1.43089550E+04 6.02887020E-01 4
CH2OH IU2/03O 1H 3C 1 0G 200.00 6000.00 1000.0 1
5.09312037E+00 5.94758550E-03-2.06496524E-06 3.23006703E-10-1.88125052E-14 2
-4.05813228E+03-1.84690613E+00 4.47832317E+00-1.35069687E-03 2.78483707E-05 3
-3.64867397E-08 1.47906775E-11-3.52476728E+03 3.30911984E+00 4
CH2OOH O 2H 3C 1 0G 200.00 2500.00 1000.0 1
6.98746029E+00 9.00484259E-03-3.24366912E-06 5.24324826E-10-3.13587080E-14 2
5.01257769E+03-1.02619220E+01 5.83126679E+00-3.51771199E-03 4.54550577E-05 3
-5.66903320E-08 2.21633070E-11 6.06187060E+03-5.79143222E-01 4
CH3 IU0702H 3C 1 0 0G 200.00 6000.00 1000.0 1
2.97812060E+00 5.79785200E-03-1.97558000E-06 3.07297900E-10-1.79174160E-14 2
1.64853622E+04 4.72247280E+00 3.65717970E+00 2.12659790E-03 5.45838830E-06 3
-6.61810030E-09 2.46570740E-12 1.63985652E+04 1.67352830E+00 4
CH3CH2O IU3/03O 1H 5C 2 0G 200.00 6000.00 1000.0 1
6.68899820E+00 1.31256760E-02-4.70388400E-06 7.58585520E-10-4.54133060E-14 2
-4.74578320E+03-9.69837550E+00 4.30742680E+00 6.41472050E-03 3.11397140E-05 3
-4.33140830E-08 1.72761840E-11-3.40275240E+03 5.90258370E+00 4
CH3CH2ONO T04/98O 2H 5C 2N 1G 200.00 6000.00 1000.0 1
9.21849299E+00 1.62001532E-02-5.98159944E-06 9.81277173E-10-5.93455530E-14 2
-1.65544389E+04-1.88591687E+01 3.37137598E+00 1.37914267E-02 3.84687528E-05 3
-6.02380553E-08 2.49654782E-11-1.40198744E+04 1.58650733E+01 4
CH3CH2ONO2 T05/98O 3H 5C 2N 1G 200.00 6000.00 1000.0 1
1.21360953E+01 1.70091385E-02-6.43739515E-06 1.07219880E-09-6.54950920E-14 2
-2.41902070E+04-3.71640527E+01 3.75721604E+00 1.93623098E-02 3.87534117E-05 3
-6.64089530E-08 2.82505579E-11-2.08444383E+04 1.11813240E+01 4
CH3CHO L 8/88O 1H 4C 2 0G 200.00 6000.00 1000.0 1
5.40411080E+00 1.17230590E-02-4.22631370E-06 6.83724510E-10-4.09848630E-14 2
-2.26268797E+04-3.48079170E+00 4.72945950E+00-3.19328580E-03 4.75349210E-05 3
-5.74586110E-08 2.19311120E-11-2.16066357E+04 4.10301590E+00 4
CH3CN T01/03H 3C 2N 1 0G 200.00 6000.00 1000.0 1
5.09921882E+00 9.69585649E-03-3.48051966E-06 5.61420173E-10-3.35835856E-14 2
6.60967324E+03-3.36087178E+00 3.82392803E+00 4.08201943E-03 2.16209537E-05 3
-2.89807789E-08 1.12962700E-11 7.44430382E+03 5.52656156E+00 4
CH3CO IU2/03O 1H 3C 2 0G 200.00 6000.00 1000.0 1
5.31371650E+00 9.17377930E-03-3.32203860E-06 5.39474560E-10-3.24523680E-14 2

-3.64504140E+03-1.67575580E+00 4.03587050E+00 8.77294870E-04 3.07100100E-05 3
-3.92475650E-08 1.52968690E-11-2.68207380E+03 7.86176820E+00 4
CH3HCO 120186O 1H 4C 2 0G 300.00 5000.00 1000.0 1
5.86865000E+00 1.07942400E-02-3.64553000E-06 5.41291200E-10-2.89684400E-14 2
-2.26456900E+04-6.01294600E+00 2.50569500E+00 1.33699100E-02 4.67195300E-06 3
-1.12814000E-08 4.26356600E-12-2.12458900E+04 1.33508900E+01 4
CH3NH M92 H 4C 1N 1 0G 300.00 5000.00 1404.0 1
4.90528413E+00 8.50385569E-03-2.82356461E-06 4.29267836E-10-2.45297886E-14 2
1.94541503E+04-1.35290137E+00 1.53882571E+00 1.62436539E-02-9.89573425E-06 3
3.49954504E-09-5.53823621E-13 2.06715086E+04 1.68295527E+01 4
CH3NH2 H 5C 1N 1 0G 300.00 5000.00 1387.0 1
5.23365618E+00 1.08525479E-02-3.65205276E-06 5.60552543E-10-3.22553444E-14 2
-5.52829576E+03-5.21507359E+00 1.69170293E+00 1.60389160E-02-4.99028441E-06 3
-3.83481304E-10 3.57345746E-13-3.94057426E+03 1.49835076E+01 4
CH3NO T12/92O 1H 3C 1N 1G 200.00 6000.00 1000.0 1
5.06773970E+00 9.38710790E-03-3.39583170E-06 5.50767290E-10-3.30953010E-14 2
7.18524640E+03-1.07097790E+00 5.24634940E+00-6.81756910E-03 4.67139590E-05 3
-5.34827430E-08 1.99166920E-11 7.92413190E+03 1.86873550E+00 4
CH3NO2 pg/melO 2H 3C 1N 1G 300.00 4000.00 1500.0 1
1.09015800E+01 4.32638100E-03-4.20354800E-07-1.89307100E-10 3.41744400E-14 2
-1.36884891E+04-3.34142701E+01 3.22471700E-01 2.66514700E-02-1.93057400E-05 3
7.76262000E-09-1.39874600E-12-9.57739615E+03 2.45791199E+01 4
CH3O D IU1/O 1H 3C 1 0G 200.00 6000.00 1000.0 1
4.75779238E+00 7.44142474E-03-2.69705176E-06 4.38090504E-10-2.63537098E-14 2
2.87372692E+02-1.96679344E+00 3.71180502E+00-2.80463306E-03 3.76550971E-05 3
-4.73072089E-08 1.86588420E-11 1.20495837E+03 6.57241548E+00 4
CH3OH 2 T06/O 1H 4C 1 0G 200.00 6000.00 1000.0 1
3.52726795E+00 1.03178783E-02-3.62892944E-06 5.77448016E-10-3.42182632E-14 2
-2.60028834E+04 5.16758693E+00 5.65851051E+00-1.62983419E-02 6.91938156E-05 3
-7.58372926E-08 2.80427550E-11-2.56119736E+04-8.97330508E-01 4
CH3ONO A 5/05O 2H 3C 1N 1G 200.00 6000.00 1000.0 1
6.93605239E+00 9.97319424E-03-3.60642537E-06 5.83462161E-10-3.50058729E-14 2
-1.08381899E+04-6.98144573E+00 6.15261387E+00-2.91937431E-03 4.14526828E-05 3
-4.93954776E-08 1.85608328E-11-9.85260262E+03 8.04057190E-01 4
CH3ONO2 T05/98O 3H 3C 1N 1G 200.00 6000.00 1000.0 1
9.77845489E+00 1.10069541E-02-4.25928645E-06 7.18198185E-10-4.42041793E-14 2
-1.88804487E+04-2.39163197E+01 3.91363583E+00 1.52137945E-02 1.73479131E-05 3
-3.37074473E-08 1.44322204E-11-1.66103232E+04 9.44208392E+00 4
CH3OO T04/02O 2H 3C 1 0G 200.00 6000.00 1000.0 1
5.92505819E+00 9.00194542E-03-3.24254309E-06 5.24362718E-10-3.14263003E-14 2
-1.10522082E+03-4.93743168E+00 4.76597792E+00-3.51077148E-03 4.54394152E-05 3
-5.66763729E-08 2.21591482E-11-5.50325261E+01 4.76021720E+00 4
CH3OOH A 7/05O 2H 4C 1 0G 200.00 6000.00 1000.0 1
7.76538058E+00 8.61499712E-03-2.98006935E-06 4.68638071E-10-2.75339255E-14 2

-1.82040949E+04-1.43970452E+01 2.90540897E+00 1.74994735E-02 5.28243630E-06 3
-2.52827275E-08 1.34368212E-11-1.67955597E+04 1.13764198E+01 4
CH4 g 8/99H 4C 1 0 0G 200.00 6000.00 1000.0 1
1.91178600E+00 9.60267960E-03-3.38387841E-06 5.38797240E-10-3.19306807E-14 2
-1.00992136E+04 8.48241861E+00 5.14825732E+00-1.37002410E-02 4.93749414E-05 3
-4.91952339E-08 1.70097299E-11-1.02453222E+04-4.63322726E+00 4
CHCCCO mmy O 1H 1C 4 0G 300.00 5000.00 1401.0 1
-1.86011530E+00 6.58032350E-02-9.32191370E-05 6.32010340E-08-1.59778480E-11 2
2.89970150E+04 3.17474470E+01-1.86011530E+00 6.58032350E-02-9.32191370E-05 3
6.32010340E-08-1.59778480E-11 2.89970150E+04 3.17474470E+01 4
CHCCHCHCH2 BUR94ZH 5C 5 0 0G 298.15 3000.00 1000.0 1
1.48896750E+01 8.21610040E-03-1.51780620E-06 1.62681840E-10-8.80527080E-15 2
4.27192490E+04-5.33828830E+01-2.60852990E+00 6.52369090E-02-8.21913790E-05 3
6.03642700E-08-1.90716070E-11 4.73604050E+04 3.55049200E+01 4
CHCCHCO mmy O 1H 2C 4 0G 300.00 5000.00 1401.0 1
-1.86011530E+00 6.58032350E-02-9.32191370E-05 6.32010340E-08-1.59778480E-11 2
2.89970150E+04 3.17474470E+01-1.86011530E+00 6.58032350E-02-9.32191370E-05 3
6.32010340E-08-1.59778480E-11 2.89970150E+04 3.17474470E+01 4
CHCHCH3 ANDIA8H 5C 3 0 0G 300.00 4000.00 1000.0 1
9.20976400E+00 7.87141300E-03-7.72452300E-07-4.49735700E-10 8.37727200E-14 2
2.85396700E+04-2.23237000E+01 3.16186300E+00 1.51810000E-02 2.72265900E-06 3
-5.17711200E-09 5.43528600E-14 3.09554800E+04 1.19797300E+01 4
CHCHCHCO ZELLI O 1H 3C 4 0G 300.00 5000.00 1401.0 1
-1.86011530E+00 6.58032350E-02-9.32191370E-05 6.32010340E-08-1.59778480E-11 2
2.89970150E+04 3.17474470E+01-1.86011530E+00 6.58032350E-02-9.32191370E-05 3
6.32010340E-08-1.59778480E-11 2.89970150E+04 3.17474470E+01 4
CHCHCHO O 1H 3C 3 0G 300.00 5000.00 1394.0 1
1.54047610E+00 3.19247870E-02-2.96313060E-05 1.34992520E-08-2.35830240E-12 2
1.78761510E+04 1.77579380E+01 1.54047610E+00 3.19247870E-02-2.96313060E-05 3
1.34992520E-08-2.35830240E-12 1.78761510E+04 1.77579380E+01 4
CHCHOH 97/SANO 1H 3C 2 0G 300.00 3000.00 1000.0 1
5.72068430E+00 1.07041850E-02-5.03584940E-06 1.13244990E-09-1.00866210E-13 2
1.13647740E+04-4.70817760E+00 8.14982820E-02 3.16406440E-02-3.40853610E-05 3
1.89788380E-08-4.19501650E-12 1.25761330E+04 2.29089770E+01 4
CHOCH2CH2CHCHO BOZELLO 2H 7C 5 0G 298.15 3000.00 1000.0 1
1.67495698E+01 1.76002589E-02-5.98916805E-06 9.27650094E-10-5.37629506E-14 2
-2.14460869E+04-5.28247697E+01 5.70045881E+00 3.60712265E-02-1.38686845E-05 3
-7.62072050E-11 8.31375090E-13-1.68594701E+04 9.14837948E+00 4
CHOCH2CH2CHO BOZELLO 2H 6C 4 0G 298.15 3000.00 1000.0 1
1.44406255E+01 1.50487556E-02-5.13967301E-06 7.97895590E-10-4.63122524E-14 2
-4.11449658E+04-4.58917536E+01 4.48171350E+00 3.44515192E-02-1.84600554E-05 3
4.48418420E-09-3.58800501E-13-3.72374921E+04 9.07149396E+00 4
CHOCH2CH2CO ZELLI O 2H 5C 4 0G 298.15 3000.00 1000.0 1
1.39398821E+01 1.30768500E-02-4.49050064E-06 6.99619378E-10-4.07081554E-14 2

-2.21572650E+04-4.08348854E+01 5.26873651E+00 2.96232020E-02-1.54390995E-05 3
3.50877521E-09-2.31149542E-13-1.87116524E+04 7.15918873E+00 4
CHOCHCHOH 8 O 2H 4C 3 0G 300.00 5000.00 1389.0 1
1.16730792E+01 1.03596746E-02-3.55282198E-06 5.52699832E-10-3.21154668E-14 2
-3.65802237E+04-3.33350633E+01 2.70595891E+00 3.10758205E-02-2.18671143E-05 3
7.95008194E-09-1.18656764E-12-3.34392510E+04 1.49128069E+01 4
CL 42189 CL 1 0 0 0G 300.00 5000.00 1000.0 1
2.92023700E+00-3.59798500E-04 1.29429400E-07-2.16277600E-11 1.37651700E-15 2
1.37133800E+04 3.26269000E+00 2.38157700E+00 8.89107900E-04 4.07047600E-07 3
-2.16894300E-09 1.16082700E-12 1.38399900E+04 6.02181800E+00 4
CL2 42189 CL 2 0 0 0G 300.00 5000.00 1000.0 1
4.27458700E+00 3.71733700E-04-1.89349000E-07 5.33746500E-11-5.05760200E-15 2
-1.33114900E+03 2.25694700E+00 3.43958700E+00 2.87077400E-03-2.38587100E-06 3
2.89291800E-10 2.91505700E-13-1.13178700E+03 6.47135900E+00 4
CLO 40992 O 1CL 1 0 0G 300.00 4000.00 1500.0 1
4.32062700E+00 1.73097000E-04-7.15787500E-08 1.42463900E-11-1.11554300E-15 2
1.32860100E+04 1.76436200E+00 2.91869600E+00 4.66485700E-03-5.65482600E-06 3
3.13110800E-09-6.51547800E-13 1.36598900E+04 8.87723800E+00 4
CN C 1N 1 0 0G 200.00 6000.00 1000.0 1
3.39912871E+00 7.46548271E-04-1.41493637E-07 1.86747261E-11-1.26032174E-15 2
5.14665281E+04 4.67150296E+00 3.61256066E+00-9.53015376E-04 2.13757148E-06 3
-3.05000108E-10-4.70518899E-13 5.15179601E+04 3.98240466E+00 4
CO RUS 79O 1C 1 0 0G 200.00 6000.00 1000.0 1
3.04848590E+00 1.35172810E-03-4.85794050E-07 7.88536440E-11-4.69807460E-15 2
-1.42661170E+04 6.01709770E+00 3.57953350E+00-6.10353690E-04 1.01681430E-06 3
9.07005860E-10-9.04424490E-13-1.43440860E+04 3.50840930E+00 4
CO2 L 7/88O 2C 1 0 0G 200.00 6000.00 1000.0 1
4.63651110E+00 2.74145690E-03-9.95897590E-07 1.60386660E-10-9.16198570E-15 2
-4.90249040E+04-1.93489550E+00 2.35681300E+00 8.98412990E-03-7.12206320E-06 3
2.45730080E-09-1.42885480E-13-4.83719710E+04 9.90090350E+00 4
H L 6/94H 1 0 0 0G 200.00 6000.00 1000.0 1
2.50000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 2
2.54736600E+04-4.46682850E-01 2.50000000E+00 0.00000000E+00 0.00000000E+00 3
0.00000000E+00 0.00000000E+00 2.54736600E+04-4.46682850E-01 4
H2 RUS 78H 2 0 0 0G 200.00 6000.00 1000.0 1
2.93283050E+00 8.26598020E-04-1.46400570E-07 1.54098510E-11-6.88796150E-16 2
-8.13055820E+02-1.02431640E+00 2.34430290E+00 7.98042480E-03-1.94779170E-05 3
2.01569670E-08-7.37602890E-12-9.17924130E+02 6.83002180E-01 4
H2C4O SAND89O 1H 2C 4 0G 300.00 4000.00 1000.0 1
1.02688800E+01 4.89616400E-03-4.88508100E-07-2.70856600E-10 5.10701300E-14 2
2.34690300E+04-2.81598500E+01 4.81097100E+00 1.31399900E-02 9.86507300E-07 3
-6.12072000E-09 1.64000300E-12 2.54580300E+04 2.11342400E+00 4
H2CC LaskinH 2C 2 0 0G 200.00 6000.00 1000.0 1
4.27803400E+00 4.75628040E-03-1.63010090E-06 2.54628060E-10-1.48863790E-14 2

4.83166880E+04 6.40237010E-01 3.28154830E+00 6.97647910E-03-2.38552440E-06 3
-1.21044320E-09 9.81895450E-13 4.86217940E+04 5.92039100E+00 4
H2CCCCH 82489 H 3C 4 0 0G 300.00 4000.00 1000.0 1
1.13140900E+01 5.01441400E-03-5.35044500E-07-2.82530900E-10 5.40327900E-14 2
5.18121100E+04-3.06243400E+01 6.54579900E+00 1.24247700E-02 5.60322600E-07 3
-5.63114100E-09 1.66521800E-12 5.35250300E+04-4.26408200E+00 4
H2CCCH 032599H 3C 3 0 0G 300.00 4000.00 1000.0 1
8.83104700E+00 4.35719400E-03-4.10906600E-07-2.36872300E-10 4.37652000E-14 2
3.91098120E+04-2.25591940E+01 4.75419900E+00 1.10802770E-02 2.79332300E-07 3
-5.47921200E-09 1.94962900E-12 4.05244520E+04-1.94548824E-01 4
H2CCCH2 SAND93H 4C 3 0 0G 300.00 4000.00 1400.0 1
9.77625600E+00 5.30213800E-03-3.70111800E-07-3.02638600E-10 5.08958100E-14 2
1.95497200E+04-3.07706100E+01 2.53983100E+00 1.63343700E-02-1.76495000E-06 3
-4.64736500E-09 1.72913100E-12 2.25124300E+04 9.93570200E+00 4
H2CN 41687 H 2C 1N 1 0G 300.00 4000.00 1000.0 1
5.20970300E+00 2.96929100E-03-2.85558900E-07-1.63555000E-10 3.04325900E-14 2
2.76771100E+04-4.44447800E+00 2.85166100E+00 5.69523300E-03 1.07114000E-06 3
-1.62261200E-09-2.35110800E-13 2.86378200E+04 8.99275100E+00 4
H2NN BPM3 9H 2N 2 0 0G 300.00 5000.00 1695.0 1
3.13531032E+00 5.68632569E-03-1.93983467E-06 3.01290501E-10-1.74978144E-14 2
3.33678346E+04 7.04815840E+00 2.88544262E+00 4.69495999E-03 7.01983230E-07 3
-1.53359038E-09 3.79345858E-13 3.36030690E+04 8.95096779E+00 4
H2NO 102290O 1H 2N 1 0G 300.00 4000.00 1500.0 1
5.67334600E+00 2.29883700E-03-1.77444600E-07-1.10348200E-10 1.85976200E-14 2
5.56932500E+03-6.15354000E+00 2.53059000E+00 8.59603500E-03-5.47103000E-06 3
2.27624900E-09-4.64807300E-13 6.86803000E+03 1.12665100E+01 4
H2O L 5/89O 1H 2 0 0G 200.00 6000.00 1000.0 1
2.67703890E+00 2.97318160E-03-7.73768890E-07 9.44335140E-11-4.26899910E-15 2
-2.98858940E+04 6.88255000E+00 4.19863520E+00-2.03640170E-03 6.52034160E-06 3
-5.48792690E-09 1.77196800E-12-3.02937260E+04-8.49009010E-01 4
H2O2 T 8/03O 2H 2 0 0G 200.00 6000.00 1000.0 1
4.57977305E+00 4.05326003E-03-1.29844730E-06 1.98211400E-10-1.13968792E-14 2
-1.79847939E+04 6.64969660E-01 4.31515149E+00-8.47390622E-04 1.76404323E-05 3
-2.26762944E-08 9.08950158E-12-1.76843601E+04 3.27373216E+00 4
H2S H 2S 1 0 0G 300.00 5000.00 1000.0 1
2.88314700E+00 3.82783500E-03-1.42339800E-06 2.49799900E-10-1.66027300E-14 2
-3.48074300E+03 7.25816200E+00 3.07102900E+00 5.57826100E-03-1.03096700E-05 3
1.20195300E-08-4.83837000E-12-3.55982600E+03 5.93522600E+00 4
H3CCCH H 4C 3 0 0G 300.00 4000.00 1400.0 1
9.76810200E+00 5.21915100E-03-3.75314000E-07-2.99219100E-10 5.10787800E-14 2
1.83176330E+04-3.02067800E+01 3.02973000E+00 1.49896130E-02-1.39850000E-06 3
-3.96961900E-09 1.38821650E-12 2.11989430E+04 8.00459400E+00 4
HCCHCCH 82489 H 3C 4 0 0G 300.00 4000.00 1000.0 1
1.07527400E+01 5.38115300E-03-5.54963800E-07-3.05226600E-10 5.76174000E-14 2

6.12141900E+04-2.97302500E+01 4.15388200E+00 1.72628700E-02-2.38937400E-07 3
-1.01870000E-08 4.34050500E-12 6.33807100E+04 6.03650700E+00 4
HCCO T 6/94O 1H 1C 2 0G 200.00 6000.00 1000.0 1
5.84690060E+00 3.64059600E-03-1.29590070E-06 2.07969190E-10-1.24000220E-14 2
1.93444192E+04-5.29165330E+00 2.33501180E+00 1.70100830E-02-2.20188670E-05 3
1.54064470E-08-4.34550970E-12 2.01462222E+04 1.19767290E+01 4
HCCOH T 4/93O 1H 2C 2 0G 200.00 6000.00 1000.0 1
6.36602550E+00 5.50387290E-03-1.88519010E-06 2.94464140E-10-1.72185980E-14 2
8.91849650E+03-8.25047050E+00 1.96541730E+00 2.55852050E-02-3.87733340E-05 3
3.15663350E-08-1.00816700E-11 9.76940900E+03 1.26027490E+01 4
HCL 42189 H 1CL 1 0 0G 300.00 5000.00 1000.0 1
2.75533500E+00 1.47358100E-03-4.97125400E-07 8.10865800E-11-5.07206300E-15 2
-1.19180600E+04 6.51511600E+00 3.33853400E+00 1.26820700E-03-3.66691700E-06 3
4.70399200E-09-1.83601100E-12-1.21315100E+04 3.19355500E+00 4
HCN 110193H 1C 1N 1 0G 300.00 4000.00 1000.0 1
3.42645700E+00 3.92419000E-03-1.60113800E-06 3.16196600E-10-2.43285000E-14 2
1.48555200E+04 3.60779500E+00 2.41778700E+00 9.03185600E-03-1.10772700E-05 3
7.98014100E-09-2.31114100E-12 1.50104400E+04 8.22289100E+00 4
HCNH 41687 H 2C 1N 1 0G 300.00 4000.00 1000.0 1
4.92329300E+00 3.33289700E-03-3.37089700E-07-1.90161900E-10 3.53182500E-14 2
3.13266900E+04-1.63250900E+00 2.75945600E+00 6.10338700E-03 7.71314900E-07 3
-2.06309400E-09 1.93192000E-13 3.21724700E+04 1.05748900E+01 4
HCNO O 1H 1C 1N 1G 300.00 5000.00 1000.0 1
6.03562000E+00 4.05933300E-03-1.58877700E-06 2.92048100E-10-2.02305700E-14 2
1.83398800E+04-9.10240500E+00 2.48256400E+00 1.48135600E-02-1.36879800E-05 3
6.04690500E-09-8.77059100E-13 1.92815400E+04 9.03253300E+00 4
HCO T 5/03O 1H 1C 1 0G 200.00 6000.00 1000.0 1
3.92001542E+00 2.52279324E-03-6.71004164E-07 1.05615948E-10-7.43798261E-15 2
3.65008461E+03 3.58077496E+00 4.23754610E+00-3.32075257E-03 1.40030264E-05 3
-1.34239995E-08 4.37416208E-12 3.86906718E+03 3.30835309E+00 4
HCOO BOZELLO 2H 1C 1 0G 300.00 5000.00 1453.0 1
6.40920688E+00 3.28189026E-03-1.18710674E-06 1.91323635E-10-1.13932748E-14 2
-2.20542060E+04-1.04575060E+01 1.52482282E+00 1.26249843E-02-6.61406757E-06 3
7.72750880E-10 2.09088864E-13-2.02040511E+04 1.64205770E+01 4
HE 120186HE 1 0 0 0G 300.00 5000.00 1000.0 1
2.50000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 2
-7.45375000E+02 9.15348900E-01 2.50000000E+00 0.00000000E+00 0.00000000E+00 3
0.00000000E+00 0.00000000E+00-7.45375000E+02 9.15348800E-01 4
HNC H 1C 1N 1 0G 300.00 5000.00 1500.0 1
5.28346400E+00 1.09247600E-03-1.17086500E-07-2.30867200E-11 3.95067300E-15 2
2.16142302E+04-6.38821800E+00 3.59237700E+00 5.56134000E-03-5.93682300E-06 3
3.78232900E-09-9.36509200E-13 2.22826802E+04 2.73216000E+00 4
HNCO O 1H 1C 1N 1G 300.00 5000.00 1000.0 1
5.32884400E+00 4.21433700E-03-1.64739300E-06 3.01842200E-10-2.08448000E-14 2

-1.58921500E+04-3.45005000E+00 3.49918800E+00 6.26365800E-03 3.12576800E-06 3
-8.62520000E-09 3.91337200E-12-1.52332800E+04 6.74499300E+00 4
HNO ATcT/AO 1H 1N 1 0G 200.00 6000.00 1000.0 1
3.16598124E+00 2.99958892E-03-3.94376786E-07-3.85344089E-11 7.07602668E-15 2
1.17654289E+04 7.64513642E+00 4.53525574E+00-5.68543377E-03 1.85198540E-05 3
-1.71881225E-08 5.55818157E-12 1.16110981E+04 1.74318356E+00 4
HNO2 103190O 2H 1N 1 0G 300.00 4000.00 1500.0 1
6.47963000E+00 1.99527400E-03-1.74038700E-07-9.69587200E-11 1.70148000E-14 2
-7.80950291E+03-1.06771518E+01 1.93483800E+00 1.01003600E-02-4.96461600E-06 3
8.70112000E-10-2.32413500E-15-5.91571591E+03 1.47282082E+01 4
HNOH T11/11O 1H 2N 1 0G 200.00 6000.00 1000.0 1
3.98321933E+00 4.88846374E-03-1.65086637E-06 2.55371446E-10-1.48308561E-14 2
1.05780106E+04 3.62582838E+00 3.95608248E+00-3.02611020E-03 2.56874396E-05 3
-3.15645120E-08 1.24084574E-11 1.09199790E+04 5.55950983E+00 4
HO2 L 5/89O 2H 1 0 0G 200.00 6000.00 1000.0 1
4.17226590E+00 1.88120980E-03-3.46292970E-07 1.94685160E-11 1.76091530E-16 2
3.02010736E+01 2.95697380E+00 4.30178800E+00-4.74902010E-03 2.11579530E-05 3
-2.42759610E-08 9.29206700E-12 2.63190983E+02 3.71587740E+00 4
HOCL 40992 O 1H 1CL 1 0G 300.00 4000.00 1500.0 1
4.95315000E+00 1.10005300E-03-1.25629600E-07-3.34995100E-11 6.46450600E-15 2
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NO3 ATcT/AO 3N 1 0 0G 200.00 6000.00 1000.0 1
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S8              tpis89S  8    0    0    0G    200.00   6000.00  1000.0      1
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 5.11843364E+03-6.74373075E+01 4.13158109E+00 9.43298552E-02-2.05775943E-04    3
 2.05747851E-07-7.51844045E-11 8.20318834E+03 7.83537207E+00                    4
SH              H   1S   1    0    0G    300.00   5000.00  1000.0      1
 3.05381000E+00 1.25888400E-03-4.24916900E-07 6.92959100E-11-4.28169100E-15    2
 1.63513273E+04 5.97355100E+00 4.13332700E+00-3.78789300E-04-2.77785400E-06    3
 5.37011200E-09-2.39400600E-12 1.60276973E+04 1.61153500E-01                    4
SO              O   1S   1    0    0G    300.00   5000.00  1000.0      1
 4.02107800E+00 2.58485600E-04 8.94814200E-08-3.58014500E-11 3.22843000E-15    2
-7.11962000E+02 3.45252300E+00 3.08040100E+00 1.80310600E-03 6.70502200E-07    3
-2.06900500E-09 8.51465700E-13-3.98616300E+02 8.58102800E+00                    4
SO*             O   1S   1    0    0G    300.00   5000.00  1000.0      1
 4.02107800E+00 2.58485600E-04 8.94814200E-08-3.58014500E-11 3.22843000E-15    2
 9.51175703E+03 3.45252300E+00 3.08040100E+00 1.80310600E-03 6.70502200E-07    3
-2.06900500E-09 8.51465700E-13 9.82510273E+03 8.58102800E+00                    4
SO2             O   2S   1    0    0G    300.00   5000.00  1000.0      1
 5.25449800E+00 1.97854500E-03-8.20422600E-07 1.57638300E-10-1.12045100E-14    2
-3.75688600E+04-1.14605600E+00 2.91143900E+00 8.10302200E-03-6.90671000E-06    3
 3.32901600E-09-8.77712100E-13-3.68788200E+04 1.11174000E+01                    4
SO3             O   3S   1    0    0G    300.00   5000.00  1000.0      1
 7.05066800E+00 3.24656000E-03-1.40889700E-06 2.72153500E-10-1.94236500E-14    2
-5.02066800E+04-1.10644300E+01 2.57528300E+00 1.51509200E-02-1.22987200E-05    3
 4.24025700E-09-5.26681200E-13-4.89441100E+04 1.21951200E+01                    4
SSO2            O   2S   2    0    0G    300.00   2000.00  1000.0      1
 6.34280650E+00 6.05027505E-03-4.24571996E-06 1.40852829E-09-1.81318004E-13    2
-2.27684952E+04-3.78737520E+00 2.80168627E+00 1.99919280E-02-2.56401242E-05    3
 1.65559742E-08-4.33620009E-12-2.20225598E+04 1.34189370E+01                    4
END
!Reactions 1568
!A-units (mol-cm-sec)  E-units (cal/mol)
REACTIONS     MOLES        CAL/MOLE
H + O2 <=> O + OH                          3.60E+15     -0.41     16600
H + H + M <=> H2 + M                        7.00E+17       -1         0
   N2/0./ H2O/0./ H2/0./
H + H + N2 <=> H2 + N2                      5.40E+18     -1.3         0
H + H + H2 <=> H2 + H2                      1.00E+17     -0.6         0
H + H + H2O <=> H2 + H2O                      1.00E+19       -1         0
H + O + M <=> OH + M                        6.20E+16     -0.6         0
   H2O/5./
H + O2 (+M) <=> HO2 (+M)                      1.50E+12      0.6         0
   LOW /  6.37E+20    -1.72      520 /
```

```
   TROE / 0.8    1.E-30    1.E+30 /
   N2/1./ H2O/11./ H2/2./ O2/0.78/
H + O2 (+AR) <=> HO2 (+AR)                  1.50E+12      0.6        0
   LOW /  9.04E+19     -1.5      490 /
   TROE / 0.5    1.E-30    1.E+30 /
H + O2 (+N2) <=> HO2 (+N2)                  1.50E+12      0.6        0
   LOW /  6.37E+20     -1.72     520 /
   TROE / 0.8    1.E-30    1.E+30 /
O + O + M <=> O2 + M                        1.90E+13        0     -1788
   N2/1.5/ O2/1.5/ H2O/10./
O + H2 <=> OH + H                          3.80E+12        0      7948
   DUPLICATE
O + H2 <=> OH + H                          8.80E+14        0     19175
   DUPLICATE
OH + OH <=> O + H2O                         4.30E+03      2.7     -1822
OH + H + M <=> H2O + M                      4.50E+22       -2        0
   AR/0.38/ H2/0.73/ H2O/12./
OH + H2 <=> H + H2O                         2.10E+08     1.52      3449
H2 + O2 <=> HO2 + H                        7.40E+05     2.433     53502
HO2 + H <=> OH + OH                         8.40E+13        0      400
HO2 + H <=> H2O + O                         1.40E+12        0        0
HO2 + O <=> OH + O2                         1.60E+13        0     -445
HO2 + OH <=> H2O + O2                        3.60E+21     -2.1      9000
   DUPLICATE
HO2 + OH <=> H2O + O2                        2.00E+15     -0.6        0
   DUPLICATE
HO2 + OH => H2O + O2                        2.20E+96      -24     49000
   DUPLICATE
HO2 + HO2 <=> H2O2 + O2                      1.90E+11        0     -1408
   DUPLICATE
HO2 + HO2 <=> H2O2 + O2                      1.00E+14        0     11034
   DUPLICATE
H2O2 (+M) <=> OH + OH (+M)                   4.00E+11        0     37137
   LOW /  2.29E+16        0    43638 /
   TROE / 0.5    1.E-30    1.E+30    1.E+30 /
   H2O/12./ H2/2.5/ AR/0.64/
H2O2 + H <=> H2O + OH                       1.00E+13        0      3580
H2O2 + H <=> HO2 + H2                       1.70E+12        0      3760
H2O2 + O <=> HO2 + OH                       9.60E+06        2      3970
H2O2 + OH <=> H2O + HO2                      1.90E+12        0       427
   DUPLICATE
H2O2 + OH <=> H2O + HO2                      1.60E+18        0     29410
   DUPLICATE
CO + O (+M) <=> CO2 (+M)                    1.80E+10        0      2384
```

```
   LOW /  1.35E+24    -2.79    4191 /
   TROE / 1    1.E-30    1.E+30    1.E+30 /
   H2/2.5/ H2O/12./ CO/1.9/ CO2/3.8/
CO + O2 <=> CO2 + O                        4.70E+12        0    60500
CO + HO2 <=> CO2 + OH                       1.60E+05     2.18    17943
CO + OH <=> CO2 + H                        8.00E+10        0        0
   DUPLICATE
CO + OH <=> CO2 + H                        8.80E+05     1.77      954
   DUPLICATE
CH2O (+M) <=> HCO + H (+M)                  8.00E+15        0    87726
   LOW /  3.73E+15        0    73479 /
CO + OH <=> HOCO                           6.00E+26     -5.6     2881
CH2O (+M) <=> CO + H2 (+M)                  3.70E+13        0    71969
   LOW /  5.66E+15        0    65849 /
CH2O + H <=> HCO + H2                       4.10E+08     1.47     2444
CH2O + O <=> HCO + OH                       4.20E+11     0.57     2760
CH2O + O2 <=> HCO + HO2                     2.40E+05      2.5    36461
CH2O + OH <=> HCO + H2O                     7.80E+07     1.63    -1055
CH2O + HO2 <=> HCO + H2O2                   4.10E+04      2.5    10206
CH2O + CH3 <=> HCO + CH4                    3.20E+01     3.36     4310
HCO <=> H + CO                             9.90E+11    -0.865    16755
HCO + H <=> CO + H2                        1.10E+14        0        0
HCO + O <=> CO + OH                        3.00E+13        0        0
HCO + O <=> CO2 + H                        3.00E+13        0        0
HCO + OH <=> CO + H2O                      1.10E+14        0        0
HCO + O2 <=> CO + HO2                      3.40E+12        0        0
HCO + HO2 <=> CO2 + OH + H                  3.00E+13        0        0
HCO + HCO <=> CO + CH2O                     2.70E+13        0        0
CH3 + H (+M) <=> CH4 (+M)                   2.10E+14        0        0
   LOW /  6.47E+23     -1.8       0 /
   TROE / 0.6376    1.E-30     3230    1.E+30 /
   CH4/1.9/ C2H6/4.8/
CH4 + H <=> CH3 + H2                       4.10E+03     3.156     8755
CH4 + O <=> CH3 + OH                        4.40E+05      2.5     6577
CH4 + OH <=> CH3 + H2O                      1.00E+06     2.182     2506
CH4 + HO2 <=> CH3 + H2O2                    4.70E+04      2.5    21000
CH4 + CH2 <=> CH3 + CH3                     4.30E+12        0    10030
CH4 + CH2(S) <=> CH3 + CH3                  4.30E+13        0        0
CH2 + H (+M) <=> CH3 (+M)                   3.80E+16     -0.8        0
   LOW /  4.80E+27     -3.14     1230 /
   TROE / 0.68       78      1995      5590 /
   N2/1./ H2O/6./ AR/0.7/
CH3 + H <=> CH2 + H2                       9.00E+13        0    15100
CH2(S) + H2 <=> CH3 + H                     7.20E+13        0        0
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CH3 + O <=> CH2O + H                    6.90E+13        0        0
CH3 + O <=> H2 + CO + H                 1.50E+13        0        0
CH3 + OH <=> CH2 + H2O                  1.10E+03        3     2780
CH3 + OH <=> CH2(S) + H2O               6.90E+14   -0.4884        0
CH3 + HO2 <=> CH4 + O2                  1.80E+03     2.83    -3730
CH3 + HO2 <=> CH3O + OH                 2.00E+13        0     1075
CH3 + O2 <=> CH3O + O                   7.50E+12        0    28297
CH3 + O2 <=> CH2O + OH                  1.90E+11        0     9842
CH3 + O2 <=> CH3OO                      5.00E+22    -3.85     2000
CH3 + HCO <=> CH4 + CO                  2.80E+13        0        0
CH3 + CH3 <=> C2H5 + H                  5.40E+13        0    16055
CH3 + CH3 (+M) <=> C2H6 (+M)               3.60E+13        0        0
   LOW /  1.27E+41       -7     2762 /
   TROE / 0.62       73     1180    1.E+30 /
CH2 + M <=> CH + H + M                  5.60E+15        0    89000
CH2 + M <=> C + H2 + M                  5.80E+12      0.5    68500
CH2 + H <=> CH + H2                    1.20E+14        0        0
CH2 + O <=> CO + H + H                  1.20E+14        0      536
CH2 + O <=> CO + H2                     8.00E+13        0      536
CH2 + OH <=> CH2O + H                   2.80E+13   0.1228     -161
CH2 + OH <=> CH + H2O                   8.60E+05    2.019     6776
CH2 + O2 <=> CO + H2O                   1.80E+11        0        0
CH2 + O2 <=> CO2 + H + H                3.80E+11        0        0
CH2 + O2 <=> CH2O + O                   2.90E+11        0        0
CH2 + O2 <=> CO2 + H2                   3.40E+11        0        0
CH2 + O2 <=> CO + OH + H                6.10E+11        0        0
CH2 + CO2 <=> CO + CH2O                 1.00E+11        0     1000
CH2(S) + M <=> CH2 + M                  1.00E+13        0        0
   N2/0./ H2O/0./ AR/0./ H/0./
CH2(S) + N2 <=> CH2 + N2                1.30E+13        0      430
CH2(S) + AR <=> CH2 + AR                1.50E+13        0      884
CH2(S) + H <=> CH2 + H                  2.00E+14        0        0
CH2(S) + H <=> CH + H2                  3.00E+13        0        0
CH2(S) + O <=> CO + H + H               3.00E+13        0        0
CH2(S) + OH <=> CH2O + H                3.00E+13        0        0
CH2(S) + O2 <=> CH2 + O2                3.10E+13        0        0
CH2(S) + H2O <=> CH2 + H2O                 3.00E+13        0        0
CH2(S) + CO2 <=> CH2O + CO                 1.10E+13        0        0
CH + H <=> C + H2                      1.50E+14        0        0
CH + O <=> CO + H                      5.70E+13        0        0
CH + OH <=> HCO + H                     3.00E+13        0        0
CH + OH <=> C + H2O                     4.00E+07        2     3000
CH + O2 <=> HCO + O                     3.30E+13        0        0
CH + H2O <=> CH2O + H                   5.70E+12        0     -755
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CH + CO2 <=> HCO + CO                       8.80E+06     1.75     -1040
C + OH <=> CO + H                          5.00E+13        0        0
C + O2 <=> CO + O                          2.00E+13        0        0
CH3OH (+M) <=> CH3 + OH (+M)                  2.10E+18   -0.6148     92540
   LOW /  2.60E+49     -8.8   101500 /
   TROE / 0.7656     1910     59.51     9374 /
CH3OH (+M) <=> CH2(S) + H2O (+M)               3.10E+18    -1.017     91712
   LOW /  5.40E+23   -8.3446    99596 /
   TROE / 0.9922      943     47310     47110 /
CH3OH + H <=> CH2OH + H2                    2.90E+09     1.24     4491
CH3OH + H <=> CH3O + H2                    5.10E+08     1.24     4491
CH3OH + O <=> CH2OH + OH                    2.10E+13        0     5305
CH3OH + O <=> CH3O + OH                    3.70E+12        0     5305
CH3OH + OH <=> CH2OH + H2O                    1.50E+08    1.4434      113
CH3OH + OH <=> CH3O + H2O                    2.70E+07    1.4434      113
CH3OH + HO2 <=> CH2OH + H2O2                  2.00E+13        0    15000
CH3OH + O2 <=> CH2OH + HO2                    6.00E+13        0    46600
CH3OH + O2 <=> CH3O + HO2                    6.00E+13        0    54800
CH2OH (+M) <=> CH2O + H (+M)                  2.80E+14     -0.73     32820
   LOW /  6.01E+33     -5.39    36200 /
   TROE / 0.96      67.6      1855      7543 /
   H2/2./ H2O/5./ CO/2./ CO2/3./
CH2OH + H <=> CH2O + H2                     4.00E+06     1.86      147
CH2OH + H <=> CH3 + OH                     1.80E+14     0.16      111
CH2OH + H (+M) <=> CH3OH (+M)                 4.30E+15     -0.79        0
   LOW /  3.84E+37     -6.21     1333 /
   TROE / 0.25      210      1434    1.E+30 /
CH2OH + O <=> CH2O + OH                     6.60E+13        0     -693
CH2OH + OH <=> CH2O + H2O                    2.40E+13        0        0
CH2OH + HO2 <=> CH2O + H2O2                   1.20E+13        0        0
CH2OH + O2 <=> CH2O + HO2                    7.20E+13        0     3736
   DUPLICATE
CH2OH + O2 <=> CH2O + HO2                    2.90E+16     -1.5        0
   DUPLICATE
CH2OH + HCO <=> CH3OH + CO                    1.00E+13        0        0
CH2OH + HCO <=> CH2O + CH2O                   1.50E+13        0        0
CH2OH + CH2O <=> CH3OH + HCO                   5.50E+03     2.81     5862
CH2OH + CH2OH <=> CH3OH + CH2O                 4.80E+12        0        0
CH2OH + CH3O <=> CH3OH + CH2O                  2.40E+12        0        0
CH2OH + CH4 <=> CH3OH + CH3                   2.20E+01      3.1    16227
CH3O (+M) <=> CH2O + H (+M)                   6.80E+13        0    26154
   LOW /  1.87E+25       -3    24291 /
   TROE / 0.5     1000     2000 /
CH3O + H <=> CH2O + H2                     7.60E+08      1.5     -519
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CH3O + H <=> CH3 + OH                    4.60E+13    0.283       28
CH3O + H (+M) <=> CH3OH (+M)             2.40E+12    0.515       50
   LOW /  4.66E+41    -7.44    14080 /
   TROE / 0.7      100     90000     10000 /
   N2/1./ H2/2./ H2O/6./ CH4/2./ CO/1.5/ CO2/2./ C2H6/3./
CH3O + O <=> CH2O + OH                   3.80E+12        0        0
CH3O + OH <=> CH2O + H2O                 1.80E+13        0        0
CH3O + HO2 <=> CH2O + H2O2               3.00E+11        0        0
CH3O + O2 <=> CH2O + HO2                 2.20E+10        0     1749
CH3O + CO <=> CH3 + CO2                  9.50E+25    -4.93     9080
CH3O + CH3 <=> CH2O + CH4                2.40E+13        0        0
CH3O + CH4 <=> CH3OH + CH3               1.30E+14        0    15073
CH3O + CH2O <=> CH3OH + HCO              1.00E+11        0     2981
CH3O + CH3O <=> CH3OH + CH2O             6.00E+13        0        0
CH3OOH <=> CH3O + OH                     2.00E+35     -6.7    47450
CH3OOH + H <=> CH2OOH + H2               5.40E+10        0     1860
CH3OOH + H <=> CH3OO + H2                5.40E+10        0     1860
CH3OOH + H <=> CH3O + H2O                1.20E+10        0     1860
CH3OOH + O <=> CH2OOH + OH               1.60E+13        0     4750
CH3OOH + O <=> CH3OO + OH                8.70E+12        0     4750
CH3OOH + OH <=> CH3OO + H2O              1.10E+12        0     -437
CH3OOH + OH <=> CH2OOH + H2O             7.20E+11        0     -258
CH3OOH + HO2 <=> CH3OO + H2O2            4.10E+04      2.5    10206
CH3OO + H <=> CH3O + OH                  1.00E+14        0        0
CH3OO + O <=> CH3O + O2                  1.60E+13        0     -445
CH3OO + OH <=> CH3OH + O2                2.00E+15     -0.6        0
CH3OO + OH <=> CH3O + HO2                4.00E+11      0.6        0
CH3OO + HO2 <=> CH3OOH + O2              2.50E+11        0    -1490
CH3OO + CH3 <=> CH3O + CH3O              5.10E+12        0    -1411
CH3OO + CH4 <=> CH3OOH + CH3             4.70E+04      2.5    21000
CH3OO + HCO <=> CH3O + H + CO2           3.00E+13        0        0
CH3OO + CO <=> CH3O + CO2                1.60E+05     2.18    17940
CH3OO + CH2O <=> CH3OOH + HCO            4.10E+04      2.5    10206
CH3OO + CH3O <=> CH2O + CH3OOH           3.00E+11        0        0
CH3OO + CH3OH <=> CH3OOH + CH2OH         4.00E+13        0    19400
CH3OO + CH3OO <=> CH3O + CH3O + O2       1.10E+18     -2.4     1800
   DUPLICATE
CH3OO + CH3OO <=> CH3O + CH3O + O2       7.00E+10        0      800
   DUPLICATE
CH3OO + CH3OO <=> CH3OH + CH2O + O2      2.00E+11    -0.55    -1600
CH3OO + C2H5 <=> CH3O + CH3CH2O          5.10E+12        0    -1410
CH3OO + C2H6 <=> CH3OOH + C2H5           1.90E+01     3.64    17100
CH2OOH <=> CH2O + OH                     2.40E+12   -0.925     1567
C2H6 + H <=> C2H5 + H2                   9.80E+13        0     9220
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C2H6 + O <=> C2H5 + OH                    1.10E-07      6.5      274
C2H6 + OH <=> C2H5 + H2O                   9.20E+06        2      990
C2H6 + HO2 <=> C2H5 + H2O2                  1.10E+05      2.5    16850
C2H6 + O2 <=> C2H5 + HO2                   7.30E+05      2.5    49160
C2H6 + CH3 <=> C2H5 + CH4                  5.60E+10        0     9418
  DUPLICATE
C2H6 + CH3 <=> C2H5 + CH4                  8.40E+14        0    22250
  DUPLICATE
C2H6 + CH2(S) <=> C2H5 + CH3                1.20E+14        0        0
C2H4 + H (+M) <=> C2H5 (+M)                1.40E+09    1.463     1355
  LOW /  2.00E+39   -6.642    5769 /
  TROE / -0.569      299     9147     152.4 /
C2H5 + H (+M) <=> C2H6 (+M)                5.20E+17    -0.99     1580
  LOW /  1.99E+41    -7.08    6685 /
  TROE / 0.8422      125     2219     6882 /
  N2/1./ H2/2./ H2O/6./ CH4/2./ CO/1.5/ CO2/2./ C2H6/3./ AR/0.7/
C2H5 + O <=> CH3 + CH2O                   4.20E+13        0        0
C2H5 + O <=> CH3CHO + H                   5.30E+13        0        0
C2H5 + O <=> C2H4 + OH                    3.10E+13        0        0
C2H5 + OH <=> C2H4 + H2O                   2.40E+13        0        0
C2H5 + HO2 <=> CH3CH2O + OH                 3.10E+13        0        0
C2H5 + O2 <=> C2H4 + HO2                   1.40E+07     1.09    -1975
C2H5 + CH2O <=> C2H6 + HCO                  5.50E+03     2.81     5860
C2H5 + HCO <=> C2H6 + CO                   4.30E+13        0        0
C2H5 + CH3 <=> C2H4 + CH4                  9.00E+11        0        0
C2H5 + C2H5 <=> C2H6 + C2H4                 1.50E+12        0        0
C2H3 + H (+M) <=> C2H4 (+M)                3.90E+13      0.2        0
  LOW /  2.10E+24     -1.3       0 /
  TROE / 0.5    1.E-30    1.E+30    1.E+30 /
C2H4 (+M) <=> H2CC + H2 (+M)                8.00E+12     0.44    88800
  LOW /  7.00E+50    -9.31    99900 /
  TROE / 0.735      180     1035     5417 /
  H2O/6./ AR/0.7/
C2H4 + H <=> C2H3 + H2                    2.40E+02     3.62    11266
CH4 + CH <=> C2H4 + H                     3.00E+13        0     -400
CH3 + CH2 <=> C2H4 + H                    1.20E+15   -0.3432      153
CH3 + CH2(S) <=> C2H4 + H                  2.00E+13        0        0
C2H4 + O <=> CH3 + HCO                    3.90E+12        0     1494
  DUPLICATE
C2H4 + O <=> CH3 + HCO                    6.20E+13        0     6855
  DUPLICATE
C2H4 + O <=> CH2CHO + H                    1.70E+12        0     1494
  DUPLICATE
C2H4 + O <=> CH2CHO + H                    2.80E+13        0     6855
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   DUPLICATE
C2H4 + OH <=> C2H3 + H2O                 1.30E-01      4.2     -860
C2H4 + OH <=> CH3 + CH2O                 1.80E+06     1.68     2061
C2H4 + OH <=> CH3CHO + H                 2.40E-02     3.91     1723
C2H4 + OH <=> CH2CHOH + H                3.20E+05     2.19     5256
C2H4 + HO2 => CC2H4O + OH                2.20E+12        0    17200
C2H4 + O2 <=> C2H3 + HO2                 7.10E+13        0    60010
C2H4 + CH3 <=> C2H3 + CH4                6.00E+07     1.56    16630
C2H2 + H (+M) <=> C2H3 (+M)              1.70E+10    1.266     2709
   LOW /  6.30E+31    -4.664     3780 /
   TROE / 0.7878    -10212    1.E+30 /
   H2/2./ CO/2./ CO2/3./ H2O/5./
C2H3 + H <=> C2H2 + H2                   4.50E+13        0        0
CH3 + CH <=> C2H3 + H                    3.00E+13        0        0
C2H3 + O <=> CH2CO + H                   3.00E+13        0        0
C2H3 + OH <=> C2H2 + H2O                 2.00E+13        0        0
C2H3 + HO2 <=> CH2CHO + OH               3.00E+13        0        0
C2H3 + O2 <=> CH2O + HCO                 4.00E+15    -0.959      580
C2H3 + O2 <=> CH2CHO + O                 2.00E+09    0.923      226
C2H3 + O2 <=> C2H2 + HO2                 4.40E+01     2.95      186
C2H3 + O2 <=> CH3O + CO                  1.90E+14    -0.959      580
C2H3 + O2 <=> CH3 + CO2                  2.10E+13    -0.959      580
C2H3 + CH2O <=> C2H4 + HCO               5.40E+03     2.81     5860
C2H3 + HCO <=> C2H4 + CO                 9.00E+13        0        0
C2H3 + CH3 <=> C2H2 + CH4                9.00E+12        0     -765
C2H3 + CH <=> CH2 + C2H2                 5.00E+13        0        0
C2H3 + C2H3 <=> C2H4 + C2H2              1.50E+13        0        0
C2H3 + C2H <=> C2H2 + C2H2               3.00E+13        0        0
C2H2 + M <=> C2H + H + M                 9.10E+30     -3.7   127138
   H2/2./ CO/2./ CO2/3./ H2O/5./
CH3 + C <=> C2H2 + H                     5.00E+13        0        0
CH2 + CH <=> C2H2 + H                    4.00E+13        0        0
CH2 + CH2 <=> C2H2 + H + H               7.00E+13   0.0022        8
CH2 + CH2 <=> C2H2 + H2                  1.80E+13   0.0022        8
C2H2 + O <=> HCCO + H                    1.40E+07        2     1900
C2H2 + O <=> CH2 + CO                    6.10E+06        2     1900
C2H2 + O <=> C2H + OH                    3.20E+15     -0.6    15000
C2H2 + OH <=> CH3 + CO                   1.30E+09     0.73     2579
C2H2 + OH <=> HCCOH + H                  2.40E+06        2    12713
C2H2 + OH <=> CHCHOH                     1.90E+44   -11.38     6299
   DUPLICATE
C2H2 + OH <=> CHCHOH                     3.50E+31     -6.2     6635
   DUPLICATE
C2H2 + OH <=> CH2CO + H                  7.50E+06     1.55     2106
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```
C2H2 + HO2 <=> CH2O + HCO                  3.00E+12        0     10000
C2H2 + HO2 <=> CH2CHO + O                  3.00E+12        0     10000
C2H2 + O2 <=> HCO + HCO                    2.20E+07      1.46    33100
C2H2 + CH2(S) <=> C2H2 + CH2               4.00E+13        0        0
H2CC <=> C2H2                              1.00E+07        0        0
H2CC + H <=> C2H2 + H                      1.00E+14        0        0
H2CC + OH <=> CH2CO + H                    2.00E+13        0        0
H2CC + O2 <=> CH2 + CO2                    1.00E+13        0        0
C2 + H2 <=> C2H + H                        4.00E+05      2.4      1000
CH2 + C <=> C2H + H                        5.00E+13        0        0
C2H + O <=> CH + CO                        5.00E+13        0        0
C2H + OH <=> HCCO + H                      2.00E+13        0        0
C2H + OH <=> C2 + H2O                      4.00E+07        2     8000
C2H + H2 <=> C2H2 + H                      4.10E+05      2.39      864
C2H + O2 <=> CO + CO + H                   4.70E+13     -0.16        0
C2H + CH4 <=> CH3 + C2H2                   7.20E+12        0      976
C2H + C6H6 <=> H + C8H6                    1.00E+12        0        0
C2 + M <=> C + C + M                       1.50E+16        0   142300
C2 + O <=> C + CO                          1.00E+14        0        0
C2 + OH <=> C2O + H                        5.00E+13        0        0
C2 + O2 <=> CO + CO                        9.00E+12        0      980
CH3CHO (+M) <=> CH3 + HCO (+M)                4.30E+22     -1.88    85480
   LOW /  2.22E+76    -11.81    95040 /
   TROE / 0.23       80      7000    1.E+30 /
CH3CHO + H <=> CH3CO + H2                  4.70E+13     -0.35     3000
CH3CHO + H <=> CH2CHO + H2                 1.90E+12      0.4      5359
CH3CHO + O <=> CH3CO + OH                  1.80E+18     -1.9      2975
CH3CHO + O <=> CH2CHO + OH                 3.70E+13     -0.2      3556
CH3CHO + OH <=> CH3CO + H2O                2.40E+11      0.3     -1000
CH3CHO + OH <=> CH2CHO + H2O               3.00E+13     -0.6       800
CH3CHO + HO2 <=> CH3CO + H2O2              2.40E+19     -2.2     14030
CH3CHO + HO2 <=> CH2CHO + H2O2             2.30E+11      0.4     14864
CH3CHO + O2 <=> CH3CO + HO2                1.20E+05      2.5     37554
CH3CHO + CH3 <=> CH3CO + CH4               3.90E-07      5.8      2200
CH3CHO + CH3 <=> CH2CHO + CH4              2.50E+01     3.15      5727
CH2CHOH + H <=> CHCHOH + H2                2.40E+02     3.63     11266
CH2CHOH + H <=> CH2CHO + H2                1.50E+07      1.7      3000
CH2CHOH + O <=> CH2OH + HCO                3.90E+12        0     1494
   DUPLICATE
CH2CHOH + O <=> CH2OH + HCO                6.20E+13        0     6855
   DUPLICATE
CH2CHOH + O <=> CH2CHO + OH                1.60E+07        2     4400
CH2CHOH + OH <=> CHCHOH + H2O              1.30E-01      4.2     -860
CH2CHOH + OH <=> CH2CHO + H2O              7.50E+11      0.3     1600
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CH2CHOH + O2 <=> CH2O + HCO + OH                3.50E+07      1.8     39000
CHCHOH <=> HCCOH + H                          1.10E+31    -6.153     51383
CHCHOH + H <=> CH2CHO + H                       5.00E+13         0         0
CHCHOH + O <=> OCHCHO + H                       5.00E+13         0         0
CHCHOH + O2 <=> HCCOH + HO2                      1.40E+02       3.4      3700
CC2H3O => CH2CHO                              8.70E+31      -6.9     14994
CC2H3O => CH2CO + H                           5.00E+13         0     14863
CC2H3O => CH3 + CO                            7.10E+12         0     14280
CH2CHO <=> CH2CO + H                            1.30E+34     -6.57     49454
CH2CHO <=> CH3 + CO                           6.50E+34     -6.87     47191
CH2CHO + H <=> CH3 + HCO                        1.00E+14         0         0
CH2CHO + H <=> CH3CO + H                        3.00E+13         0         0
CH2CHO + H <=> CH2CO + H2                       2.00E+13         0         0
CH2CHO + O <=> CH2CO + OH                       5.00E+13         0         0
CH2CHO + OH <=> CH2CO + H2O                       2.00E+13         0         0
CH2CHO + OH <=> CH2OH + HCO                       1.00E+13         0         0
CH2CHO + O2 <=> CH2O + CO + OH                    5.70E+17    -1.757     11067
CH2CHO + CH3 <=> C2H5 + CO + H                    4.90E+14      -0.5         0
CH2CHO + HO2 <=> CH2O + HCO + OH                    7.00E+12      -0.5         0
CH2CHO + HO2 <=> CH3CHO + O2                      3.00E+12      -0.5         0
CH2CHO + CH2 <=> C2H4 + HCO                       5.00E+13         0         0
CH2CHO + CH <=> C2H3 + HCO                        1.00E+14         0         0
CH3CO <=> CH3 + CO                            6.50E+18     -2.52     16436
CH2CO + H <=> CH3CO                           2.30E+08      1.61      2627
CH3CO + H <=> CH3 + HCO                         2.10E+13         0         0
CH3CO + H <=> CH2CO + H2                        1.20E+13         0         0
CH3CO + O <=> CH3 + CO2                         1.60E+14         0         0
CH3CO + O <=> CH2CO + OH                        5.30E+13         0         0
CH3CO + OH <=> CH2CO + H2O                        1.20E+13         0         0
CH3CO + CH3OO <=> CH3 + CO2 + CH3O                  2.40E+13         0         0
CH3CO + CH3 <=> C2H6 + CO                       3.30E+13         0         0
CH3CO + CH3 <=> CH2CO + CH4                       5.30E+13         0         0
CH3CO + O2 <=> CH2O + CO + OH                     1.90E+12         0         0
CH2 + CO (+M) <=> CH2CO (+M)                      8.10E+11       0.5      4510
   LOW /  2.69E+33     -5.11     7095 /
   TROE / 0.5907       275      1226      5185 /
   N2/1./ H2O/6./ AR/0.7/
CH2CO + H <=> CH3 + CO                        3.30E+10     0.851      2840
CH2CO + H <=> HCCO + H2                         3.00E+07         2     10000
CH + CH2O <=> CH2CO + H                         9.50E+13         0      -517
CH2CO + O <=> CO2 + CH2                         1.80E+12         0      1350
CH2CO + O <=> HCCO + OH                         2.00E+07         2     10000
CH2CO + OH <=> CH2OH + CO                         1.00E+12         0     -1013
CH2CO + OH <=> CH3 + CO2                        6.70E+11         0     -1013
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CH2CO + OH <=> HCCO + H2O                  1.00E+07       2     3000
CH2CO + CH2(S) <=> C2H4 + CO               1.60E+14       0       0
HCCOH + H <=> HCCO + H2                   3.00E+07       2     1000
HCCOH + O <=> HCCO + OH                   2.00E+07       2     1900
HCCOH + OH <=> HCCO + H2O                  1.00E+07       2     1000
CH + CO (+M) <=> HCCO (+M)                 5.00E+13       0       0
   LOW /  2.70E+28    -3.74    1936 /
   TROE / 0.5757      237     1652     5069 /
   N2/1./ H2O/6./ AR/0.7/ H2/2./ CH4/2./ CO/1.5/ CO2/2./ C2H6/3./
HCCO + H <=> CH2(S) + CO                  1.50E+14       0       0
HCCO + O <=> CO + CO + H                  1.00E+14       0       0
HCCO + OH <=> HCO + HCO                    1.00E+13       0       0
HCCO + OH <=> C2O + H2O                    6.00E+13       0       0
HCCO + O2 <=> CO2 + CO + H                 4.90E+12   -0.142     1150
HCCO + O2 <=> CO + CO + OH                 1.60E+11    -0.02     1020
HCCO + O2 <=> HCO + CO + O                 2.20E+02     2.69     3540
HCCO + CH2 <=> C2H3 + CO                  3.00E+13       0       0
HCCO + CH <=> C2H2 + CO                   5.00E+13       0       0
HCCO + HCCO <=> C2H2 + CO + CO                1.00E+13       0       0
C2O + M <=> C + CO + M                    2.00E+15       0    44200
C2O + H <=> CH + CO                       1.30E+13       0       0
C2O + O <=> CO + CO                       5.20E+13       0       0
C2O + OH <=> CO + CO + H                   2.00E+13       0       0
C2O + O2 <=> CO + CO + O                   1.00E+13       0     2600
C2O + O2 <=> CO + CO2                     1.00E+13       0     2600
C2O + C <=> CO + C2                       1.00E+14       0       0
OCHCHO (+M) <=> CO + CO + H2 (+M)             1.10E+14       0    55000
   LOW /  2.60E+16       0    38400 /
OCHCHO + H <=> CH2O + HCO                  3.00E+13       0       0
OCHCHO + OH <=> HCO + CO + H2O                4.00E+06       2    -1630
HCN + M <=> H + CN + M                    3.40E+35    -5.13    133000
   N2/0./ O2/1.5/ H2O/10./
HCN + N2 <=> H + CN + N2                   3.60E+26     -2.6    124890
HCN + M <=> HNC + M                       1.60E+26    -3.23     54600
   AR/0.7/ H2O/7./ CO2/2./
CN + H2 <=> HCN + H                       1.10E+05      2.6     1908
HCN + O <=> NCO + H                       1.40E+04     2.64     4980
HCN + O <=> CN + OH                       4.20E+10      0.4    20665
HCN + O <=> NH + CO                       3.50E+03     2.64     4980
HCN + OH <=> CN + H2O                      3.90E+06     1.83    10300
HCN + OH <=> HOCN + H                      5.90E+04      2.4    12500
HCN + OH <=> HNCO + H                      2.00E-03        4     1000
HCN + OH <=> NH2 + CO                      7.80E-04        4     4000
HCN + O2 <=> CN + HO2                      3.00E+13       0    75100
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HCN + CN <=> NCCN + H                    1.50E+07     1.71     1530
HNC + H <=> HCN + H                     7.80E+13        0     3600
HNC + O <=> NH + CO                     4.60E+12        0     2200
HNC + OH <=> HNCO + H                    2.80E+13        0     3700
HNC + CN <=> NCCN + H                    1.00E+13        0        0
CN + O <=> CO + N                       1.90E+12     0.46      723
CN + OH <=> NCO + H                      1.00E+15   -0.437        0
CN + O2 <=> NCO + O                      7.20E+12        0     -417
  DUPLICATE
CN + O2 => NCO + O                      2.80E+17       -2        0
  DUPLICATE
CN + O2 <=> NO + CO                     2.80E+17       -2        0
CN + NO <=> NCO + N                      9.60E+13        0    42100
CN + NO2 <=> NCO + NO                     5.30E+15   -0.752      344
CN + NO2 <=> CO + N2O                     4.90E+14   -0.752      344
CN + NO2 <=> N2 + CO2                    3.70E+14   -0.752      344
CN + HNO <=> HCN + NO                     1.80E+13        0        0
CN + HONO <=> HCN + NO2                    1.20E+13        0        0
CN + N2O <=> NCN + NO                     3.80E+03      2.6     3700
CN + HNCO <=> HCN + NCO                    1.00E+13        0        0
CN + NCO <=> NCN + CO                     1.80E+13        0        0
HNCO + M <=> CO + NH + M                   1.10E+16        0    86000
  N2/1.5/
HNCO + H <=> NH2 + CO                     3.60E+04     2.49     2345
HNCO + H <=> NCO + H2                     9.00E+07     1.66    13900
HNCO + O <=> NCO + OH                     2.20E+06     2.11    11430
HNCO + O <=> NH + CO2                     9.60E+07     1.41     8520
HNCO + O <=> HNO + CO                     1.50E+08     1.57    44012
HNCO + OH <=> NCO + H2O                    3.60E+07      1.5     3600
HNCO + HO2 <=> NCO + H2O2                   3.00E+11        0    22000
HNCO + O2 <=> HNO + CO2                    1.00E+12        0    35000
HNCO + NH <=> NH2 + NCO                    3.00E+13        0    23700
HOCN + H <=> HNCO + H                     3.10E+08     0.84     1917
HOCN + H <=> NH2 + CO                     1.20E+08     0.61     2076
HOCN + H <=> H2 + NCO                     2.40E+08      1.5     6617
HOCN + O <=> OH + NCO                     1.70E+08      1.5     4133
HOCN + OH <=> H2O + NCO                    1.20E+06        2     -248
HOCN + NH2 <=> NCO + NH3                    9.20E+05     1.94     3646
HCNO <=> HCN + O                        4.20E+31    -6.12    61210
HCNO + H <=> HCN + OH                     7.20E+10    0.841     8612
HCNO + O <=> HCO + NO                     6.30E+13        0        0
HCNO + OH <=> CH2O + NO                    1.00E+12        0        0
HCNO + O <=> NCO + OH                     7.00E+12        0        0
HCNO + OH <=> NO + CO + H2                 6.50E+12        0        0
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HCNO + OH <=> NCO + H + OH                 4.50E+12        0        0
HCNO + OH <=> NCO + H2O                    3.50E+12        0        0
HCNO + OH <=> HCO + HNO                    4.50E+12        0        0
HCNO + CN <=> HCN + NCO                    6.00E+13        0        0
NCO + M <=> N + CO + M                     2.20E+14        0    54050
   N2/1.5/
NCO + H <=> CO + NH                       7.20E+13        0     1000
NCO + O <=> NO + CO                       2.00E+15     -0.5        0
NCO + OH <=> HON + CO                      5.30E+12    -0.07     5126
NCO + OH <=> H + CO + NO                   8.30E+12    -0.05    18042
NCO + HO2 <=> HNCO + O2                    2.00E+13        0        0
NCO + O2 <=> NO + CO2                     1.00E+13        0    10000
NCO + NO <=> N2O + CO                      4.00E+19    -2.19     1743
NCO + NO <=> N2 + CO2                      1.50E+21    -2.74     1824
NCO + NO2 <=> CO + NO + NO                 2.50E+11        0     -707
NCO + NO2 <=> CO2 + N2O                    3.00E+12        0     -707
NCO + HNO <=> HNCO + NO                    1.80E+13        0        0
NCO + HONO <=> HNCO + NO2                  3.60E+12        0        0
NCO + NH3 <=> HNCO + NH2                   2.80E+04     2.48      980
NCO + N <=> N2 + CO                       2.00E+13        0        0
NCO + NCO <=> CO + CO + N2                 1.80E+13        0        0
CO + NO2 <=> NO + CO2                     9.00E+13        0    33800
CO + N2O <=> N2 + CO2                     2.70E+11        0    20237
HOCO + NO <=> CO + HONO                    1.50E+12        0        0
CH2O + NO2 <=> HONO + HCO                  1.40E-07     5.64     9220
CH2O + NO2 <=> HNO2 + HCO                  1.10E-01     4.22    19850
HCO + NO <=> HNO + CO                     6.90E+12        0        0
HCO + NO2 <=> NO + CO2 + H                 2.30E+13        0        0
HCO + NO2 <=> HONO + CO                    5.00E+12        0        0
HCO + NO2 <=> NO + CO + OH                 5.00E+12        0        0
HCO + HNO <=> NO + CH2O                    5.80E-01     3.84      115
CH4 + NO2 <=> HONO + CH3                   6.50E+14        0    45800
CH4 + NO2 <=> HNO2 + CH3                   6.00E+14        0    37600
CH3 + NO (+M) <=> CH3NO (+M)               9.00E+12        0      192
   LOW /  2.50E+16        0    -2841 /
   TROE / 5    1.E-30      120    1.E+30 /
CH3 + NO2 <=> CH3O + NO                   1.10E+13        0        0
CH3 + HNO <=> NO + CH4                    2.30E+14        0     8400
CH3OH + NO2 <=> HONO + CH2OH                1.50E+02     3.32    20035
CH3OH + NO2 <=> HNO2 + CH2OH                2.40E+03      2.9    27470
CH3O + NO <=> HNO + CH2O                   7.50E+12        0     2017
   DUPLICATE
CH3O + NO <=> HNO + CH2O                   2.50E+18    -2.56        0
   DUPLICATE
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CH3O + NO (+M) <=> CH3ONO (+M)                 6.00E+14      -0.6        0
   LOW /  8.14E+25      -2.8        0 /
   TROE / 1    1.E-30      900    1.E+30 /
CH3O + NO2 <=> HONO + CH2O                     6.00E+12        0      2285
CH3O + NO2 (+M) <=> CH3ONO2 (+M)               2.20E+15     -0.88        0
   LOW /  2.91E+23     -1.74        0 /
   TROE / 0.6    1.E-30    1.E+30    1.E+30 /
CH3O + HNO <=> NO + CH3OH                      3.20E+13        0        0
CH2OH + NO <=> CH2O + HNO                      1.30E+12        0        0
CH2OH + NO2 <=> HONO + CH2O                    5.00E+12        0        0
CH2OH + HNO <=> NO + CH3OH                     3.00E+13        0        0
CH3OO + NO <=> NO2 + CH3O                      1.40E+12        0     -715
C2H6 + NO2 <=> HONO + C2H5                     6.50E+14        0    41400
C2H6 + NO2 <=> HNO2 + C2H5                     6.00E+14        0    33200
C2H5 + NO2 <=> CH3CH2O + NO                    4.00E+13     -0.2        0
C2H4 + NO2 <=> C2H3 + HONO                     6.50E+14        0    41400
C2H4 + NO2 <=> C2H3 + HNO2                     6.00E+14        0    33200
C2H3 + NO <=> C2H2 + HNO                       1.00E+12        0     1000
C2H3 + NO2 <=> CH2CHO + NO                     7.70E+14     -0.6        0
CH3CH2O + NO <=> CH3CHO + HNO                  6.60E+12        0        0
CH3CH2O + NO (+M) <=> CH3CH2ONO (+M)           1.20E+13        0     -143
   LOW /  9.43E+19        0        0 /
   TROE / 0.6    1.E-30    1.E+30    1.E+30 /
CH3CH2O + NO2 <=> CH3CHO + HONO                1.70E+12        0        0
CH3CH2O + NO2 (+M) <=> CH3CH2ONO2 (+M)         5.10E+15       -1        0
   LOW /  5.88E+30       -4        0 /
   TROE / 0.6    1.E-30    1.E+30    1.E+30 /
CH2CHO + NO2 <=> CH2CO + HONO                  8.90E+12        0     -159
CH3CO + NO2 <=> CH3 + CO2 + NO                 1.50E+13        0        0
CH2CH2OH + NO2 <=> CH2O + CH2OH + NO           7.00E+12        0        0
CH3NO2 (+M) <=> CH3 + NO2 (+M)                 1.80E+16        0    58500
   LOW /  1.26E+17        0    42000 /
   TROE / 0.183    1.E-30    1.E+30 /
CH3NO2 + H <=> CH3 + HONO                      3.30E+12        0     3730
CH3NO2 + H <=> CH3NO + OH                      1.40E+12        0     3730
CH3NO2 + H <=> CH2NO2 + H2                     5.40E+02      3.5     5200
CH3NO2 + O <=> CH2NO2 + OH                     1.50E+13        0     5350
CH3NO2 + O2 <=> CH2NO2 + HO2                   2.00E+13        0    57000
CH3NO2 + OH <=> CH3OH + NO2                    2.00E+10        0    -1000
CH3NO2 + OH <=> CH2NO2 + H2O                   5.00E+05        2     1000
CH3NO2 + HO2 <=> CH2NO2 + H2O2                 3.00E+12        0    23000
CH3NO2 + CH3 <=> CH2NO2 + CH4                  5.50E-01        4     8300
CH3NO2 + CH3O <=> CH2NO2 + CH3OH               3.00E+11        0     7000
CH3NO2 + NO2 <=> CH2NO2 + HONO                 3.00E+11        0    32000
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CH2NO2 <=> CH2O + NO 1.00E+13 0 36000
CH2NO2 + H <=> CH3 + NO2 5.00E+13 0 0
CH2NO2 + O <=> CH2O + NO2 5.00E+13 0 0
CH2NO2 + OH <=> CH2OH + NO2 1.00E+13 0 0
CH2NO2 + OH <=> CH2O + HONO 1.00E+13 0 0
CH3ONO + H <=> CH3OH + NO 1.20E+11 0 1900
CH3ONO + H <=> CH2O + H2 + NO 1.40E+11 0 1900
CH3ONO + O <=> CH3O + NO2 1.40E+13 0 5210
CH3ONO + OH <=> CH3OH + NO2 6.00E+13 0 3505
CH3ONO2 + H <=> CH3O + HONO 1.00E+12 0 0
CH3ONO2 + O <=> CH3O + NO3 1.50E+13 0 5260
CH3ONO2 + OH <=> CH3O + HONO2 4.90E+11 0 2027
CO2 + CN <=> NCO + CO 3.70E+06 2.16 26900
CH2O + CN <=> HCO + HCN 1.70E+03 2.72 -1427
CH2O + NCO <=> HNCO + HCO 6.00E+12 0 0
HCO + NCO <=> HNCO + CO 3.60E+13 0 0
CH4 + NH2 <=> CH3 + NH3 1.50E+03 3.01 9940
CH4 + CN <=> CH3 + HCN 8.60E+05 2.3 -32
CH4 + NCO <=> CH3 + HNCO 9.80E+12 0 8120
CH3 + NH2 <=> CH3NH2 5.10E+52 -11.99 16790
CH3 + NH2 <=> CH2NH2 + H 1.40E+14 -0.43 11107
CH3 + NH2 <=> CH3NH + H 4.40E+13 -0.31 16641
CH3 + NH2 <=> CH2NH + H2 4.80E+11 -0.2 19403
CH3 + NH2 <=> CH4 + NH 2.80E+06 1.94 9210
CH3 + NH2 <=> CH2 + NH3 1.60E+06 1.87 7570
CH3 + NH <=> CH2NH + H 4.00E+13 0 0
CH3 + NH <=> N + CH4 8.20E+05 1.87 5852
CH3 + N <=> H2CN + H 7.10E+13 0 0
CH3 + N2H2 <=> NNH + CH4 1.60E+06 1.87 2971
CH3 + H2NN <=> CH4 + NNH 1.60E+06 1.87 129
CH3 + N2H4 <=> N2H3 + CH4 3.30E+06 1.87 5325
CH3 + N2H3 <=> N2H2 + CH4 8.20E+05 1.87 1818
CH3 + N2H3 <=> H2NN + CH4 3.00E+13 0 0
CH3 + NO <=> HCN + H2O 1.50E-01 3.52 3950
CH3 + NO <=> H2CN + OH 1.50E-01 3.52 3950
CH3 + H2NO <=> CH3O + NH2 2.00E+13 0 0
CH3 + H2NO <=> CH4 + HNO 1.60E+06 1.87 2961
CH3 + CN <=> CH2CN + H 1.00E+14 0 0
CH3 + HOCN <=> CH3CN + OH 5.00E+12 0 2000
CH2 + N <=> HCN + H 5.00E+13 0 0
CH2 + NO <=> HCNO + H 3.10E+12 0 -378
CH2 + NO <=> HCN + OH 3.90E+11 0 -378
CH2 + NO2 <=> CH2O + NO 5.90E+13 0 0
CH2 + N2 <=> HCN + NH 1.00E+13 0 74000

CH2(S) + NO <=> HCN + OH 2.00E+13 0 0
CH2(S) + NO <=> CH2 + NO 1.00E+14 0 0
CH2(S) + N2O <=> CH2O + N2 3.80E+13 0 0
CH2(S) + NH3 <=> CH2NH2 + H 3.00E+13 0 0
CH2(S) + HCN <=> CH2CN + H 1.80E+14 0 0
CH + NH3 <=> H2CN + H + H 4.40E+13 0 -630
CH + N <=> CN + H 1.30E+13 0 0
CH + NO <=> CO + NH 9.10E+12 0 0
CH + NO <=> NCO + H 1.80E+13 0 0
CH + NO <=> HCN + O 7.90E+13 0 0
CH + NO <=> CN + OH 1.10E+12 0 0
CH + NO <=> HCO + N 6.80E+12 0 0
CH + NO2 <=> HCO + NO 1.00E+14 0 0
CH + N2O <=> HCN + NO 1.90E+13 0 -511
CH + N2 <=> NCN + H 3.70E+07 1.42 20723
C + NO <=> CN + O 2.00E+13 0 0
C + NO <=> CO + N 2.80E+13 0 0
C + N2O <=> CN + NO 4.80E+12 0 0
CN + N <=> C + N2 5.90E+14 -0.4 0
C2H6 + NH2 <=> C2H5 + NH3 4.50E+01 3.46 5600
C2H6 + CN <=> C2H5 + HCN 1.20E+08 1.8 -994
C2H6 + NCO <=> C2H5 + HNCO 1.50E-09 6.89 -2910
C2H5 + N <=> C2H4 + NH 4.30E+13 0 0
C2H5 + N <=> CH3 + H2CN 2.30E+13 0 0
C2H4 + NH2 <=> C2H3 + NH3 5.30E+12 0 10274
C2H3 + NO <=> HCN + CH2O 7.00E+21 -3.382 1025
C2H2 + NCO <=> HCCO + HCN 1.40E+12 0 1815
C2H + NH3 <=> C2H2 + NH2 7.20E+12 0 -735
C2H + NO <=> HCN + CO 6.00E+13 0 570
C2 + NO <=> C2O + N 2.30E+13 0 8640
C2 + N2 <=> CN + CN 1.50E+13 0 41730
HCCO + N <=> HCN + CO 5.00E+13 0 0
HCCO + NO <=> HCNO + CO 5.90E+12 0.089 -457
HCCO + NO <=> HCN + CO2 3.70E+14 -0.75 -90
HCCO + NO2 <=> HCNO + CO2 1.60E+13 0 0
C2O + NO <=> CO + NCO 1.00E+14 0 670
C2O + NO2 <=> CO2 + NCO 5.10E+13 0 125
NCN + H <=> HCN + N 1.00E+14 0 0
NCN + O <=> CN + NO 1.00E+14 0 0
NCN + OH <=> HCN + NO 5.00E+13 0 0
NCN + O2 <=> NO + NCO 4.40E+09 0.51 24580
CH3NH2 + M <=> CH2NH + H2 + M 2.40E+13 0 107260
CH3NH2 + H <=> CH2NH2 + H2 5.60E+08 1.5 5464
CH3NH2 + H <=> CH3NH + H2 4.80E+08 1.5 9706

CH3NH2 + O <=> CH2NH2 + OH 4.00E+08 1.5 5196
CH3NH2 + O <=> CH3NH + OH 3.30E+08 1.5 6348
CH3NH2 + OH <=> CH2NH2 + H2O 1.00E+13 0 0
CH3NH2 + OH <=> CH3NH + H2O 2.40E+06 2 447
CH3NH2 + CH3 <=> CH2NH2 + CH4 1.50E+06 1.87 9170
CH3NH2 + CH3 <=> CH3NH + CH4 1.60E+06 1.87 8842
CH3NH2 + NH2 <=> CH2NH2 + NH3 2.80E+06 1.94 5494
CH3NH2 + NH2 <=> CH3NH + NH3 1.80E+06 1.94 7143
CH2NH2 <=> CH2NH + H 2.40E+48 -10.82 52040
CH2NH2 + H <=> CH2NH + H2 4.80E+08 1.5 -894
CH2NH2 + O <=> CH2O + NH2 7.00E+13 0 0
CH2NH2 + O <=> CH2NH + OH 3.30E+08 1.5 -894
CH2NH2 + OH <=> CH2OH + NH2 4.00E+13 0 0
CH2NH2 + OH <=> CH2NH + H2O 2.40E+06 2 -1192
CH2NH2 + O2 <=> CH2NH + HO2 1.00E+22 -3.09 6756
CH2NH2 + CH3 <=> C2H5 + NH2 2.00E+13 0 2702
CH2NH2 + CH3 <=> CH2NH + CH4 1.60E+06 1.87 -626
CH3NH <=> CH2NH + H 1.30E+42 -9.24 41340
CH3NH + H <=> CH2NH + H2 7.20E+08 1.5 -894
CH3NH + O <=> CH2NH + OH 5.00E+08 1.5 -894
CH3NH + OH <=> CH2NH + H2O 3.60E+06 2 -1192
CH3NH + CH3 <=> CH2NH + CH4 2.40E+06 1.87 -1113
CH2NH + H <=> H2CN + H2 2.40E+08 1.5 7322
CH2NH + H <=> HCNH + H2 3.00E+08 1.5 6130
CH2NH + O <=> H2CN + OH 1.70E+08 1.5 4630
CH2NH + O <=> HCNH + OH 2.20E+08 1.5 5404
CH2NH + O <=> CH2O + NH 1.70E+06 2.08 0
CH2NH + OH <=> H2CN + H2O 1.20E+06 2 -89
CH2NH + OH <=> HCNH + H2O 2.40E+06 2 457
CH2NH + CH3 <=> H2CN + CH4 8.20E+05 1.87 7123
CH2NH + CH3 <=> HCNH + CH4 5.30E+05 1.87 9687
CH2NH + NH2 <=> H2CN + NH3 9.20E+05 1.94 4441
CH2NH + NH2 <=> HCNH + NH3 1.80E+06 1.94 6090
H2CN <=> HCN + H 6.00E+31 -6.46 32110
H2CN + H <=> HCN + H2 2.40E+08 1.5 -894
H2CN + O <=> HCN + OH 1.70E+08 1.5 -894
H2CN + OH <=> HCN + H2O 1.50E+19 -2.18 2166
DUPLICATE
H2CN + OH <=> HCN + H2O 1.20E+06 2 -1192
DUPLICATE
H2CN + O2 <=> CH2O + NO 3.00E+12 0 5961
H2CN + NH2 <=> HCN + NH3 9.20E+05 1.94 -1152
H2CN + N <=> CH2 + N2 2.00E+13 0 0
HCNH <=> HCN + H 6.10E+28 -5.69 24271

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HCNH + H <=> H2CN + H                  2.00E+13        0        0
HCNH + H <=> HCN + H2                  2.40E+08      1.5     -894
HCNH + O <=> HNCO + H                  7.00E+13        0        0
HCNH + O <=> HCN + OH                  1.70E+08      1.5     -894
HCNH + OH <=> HCN + H2O                 1.20E+06        2    -1192
HCNH + CH3 <=> HCN + CH4                8.20E+05     1.87    -1113
CH3CN + H <=> HCN + CH3                4.00E+07        2     2000
CH3CN + H <=> CH2CN + H2                3.00E+07        2     1000
CH3CN + O <=> NCO + CH3                 1.50E+04     2.64     4980
CH3CN + OH <=> CH2CN + H2O               2.00E+07        2     2000
CH2CN + O <=> CH2O + CN                1.00E+14        0        0
CH2OH + CN <=> CH2CN + OH               5.00E+13        0        0
H + CL + M <=> HCL + M                 7.20E+23       -2        0
HCL + H <=> H2 + CL                   2.30E+14        0     3499
HCL + OH <=> H2O + CL                  2.45E+13        0     1099
HCL + O <=> OH + CL                   5.24E+13        0     6400
CL + HO2 <=> HCL + O2                  1.08E+14        0      100
CL2 + H <=> HCL + CL                  8.59E+14        0     1171
CL + CL + M <=> CL2 + M                2.34E+15        0    -1800
CL2 + O <=> CLO + CL                  2.52E+13        0     2720
CLO + O <=> CL + O2                   5.70E+14        0      363
HO2 + CL <=> OH + CLO                  2.42E+14        0     2299
H2O2 + CL <=> HO2 + HCL                 6.62E+13        0     1950
HOCL + CL <=> CLO + HCL                 7.62E+13        0      179
CLO + H2 <=> HOCL + H                  6.03E+12        0    14099
H + HOCL <=> HCL + OH                  9.55E+14        0     7619
CL + HOCL <=> CL2 + OH                 1.81E+13        0      261
O + HOCL <=> OH + CLO                  6.03E+12        0     4369
OH + HOCL <=> H2O + CLO                 1.81E+13        0      989
HOCL <=> OH + CL                      1.76E+21    -3.01    56720
HOCL <=> H + CLO                      8.13E+15    -2.09    93688
H2S + M <=> H2 + S + M                 1.60E+24   -2.613    89170
H2S + H <=> SH + H2                    3.49E+07     1.94      904
H2S + S <=> SH + SH                    7.39E+06    2.297     9007
   DUPLICATE
H2S + S <=> SH + SH                    1.18E+18   -1.685     5975
   DUPLICATE
S + H2 <=> SH + H                     1.35E+14        0    19290
S + SH <=> S2 + H                     3.32E+12    0.543      -29
H + S2 + M <=> HSS + M                  1.15E+25    -2.84     1665
   H2S/1.1/ AR/0.88/ HE/1.39/
H + HSS <=> SH + SH                    9.72E+07     1.62    -1030
   DUPLICATE
H + HSS <=> SH + SH                    1.63E+18   -0.983      261
```

```
   DUPLICATE
SH + SH (+M) <=> HSSH (+M)                3.46E+12    0.155    -1432
   LOW /  2.33E+31   -4.943    1998 /
   TROE / 1      254     2373 /
SH + HSS <=> H2S + S2                     6.27E+03     3.05    -1105
H + HSS <=> H2 + S2                       1.05E+08     1.75     -877
   DUPLICATE
H + HSS <=> H2 + S2                       2.91E+16    -0.894     -56
   DUPLICATE
H + HSS <=> H2S + S                       1.50E+08    1.551     2259
   DUPLICATE
H + HSS <=> H2S + S                       4.19E+18    -1.563     472
   DUPLICATE
S + HSS <=> S2 + SH                       4.17E+06      2.2     -600
HSS + HSS <=> HSSH + S2                    9.56E+00     3.37    -1672
HSSH + H <=> HSS + H2                      4.99E+07    1.933    -1408
HSSH + H <=> H2S + SH                      3.66E+08    1.724     467
HSSH + SH <=> H2S + HSS                    6.40E+03     2.98    -1480
HSSH + S <=> HSS + SH                      2.85E+06     2.31     1204
H + S + M <=> SH + M                      6.20E+16     -0.6       0
S + S + M <=> S2 + M                      1.89E+13        0    -1788
H2S + S (+M) <=> HSSH (+M)                 6.38E+07     1.28     -478
   LOW /  2.40E+21   -1.612    1673 /
   TROE / 0.5      726      726 /
   N2/1.3/
SH + HO2 <=> H2S + O2                      3.80E+04    2.775    -1530
H2S + O2 <=> HSO + OH                      1.00E+11        0    49100
H2S + OH <=> SH + H2O                      8.70E+13     -0.7        0
   DUPLICATE
H2S + OH <=> SH + H2O                      4.07E+07     1.77        0
   DUPLICATE
H2S + O <=> SH + OH                       1.80E+05    2.649     2532
H2S + O <=> HSO + H                       1.36E+09    1.065     5099
H2O2 + SH <=> H2S + HO2                    5.57E+04    2.823     8668
H2O2 + SH <=> HSOH + OH                    9.49E+03    2.817     9829
H2S + HO2 <=> HSO + H2O                    1.03E+00    3.288     6224
H2S + HSO <=> SH + HSOH                    1.00E+13        0    17300
H2S + HOS <=> SH + HSOH                    1.00E+13        0    12500
H2S + SO <=> HSO + SH                      5.38E+03    3.209     26824
H2S + SO <=> HOS + SH                      1.00E+13        0    36500
SH + O2 <=> HO2 + S                       4.72E+06    2.017     36913
SH + O2 <=> HSO + O                       2.29E+06    1.816     20008
SH + O2 <=> SO + OH                       7.50E+04    2.052     16384
SH + O2 <=> H + SO2                       6.50E+11        0    15000
```

```
SH + O <=> OH + S                    1.80E+12       0       0
   DUPLICATE
SH + O <=> OH + S                    4.32E+06    2.103    3583
   DUPLICATE
SH + O <=> SO + H                    4.25E+11    0.724    -1027
SH + OH <=> S + H2O                   1.67E+05    2.465    -1637
SH + OH <=> HOS + H                   1.00E+13       0    7400
H2O2 + S <=> SH + HO2                  4.14E+06    2.164    12619
SH + HO2 <=> HSO + OH                  2.46E+08    1.477    -2169
SH + HO2 <=> H2O + SO                  3.20E+02    2.579    -2071
SH + HSO <=> S + HSOH                  1.00E+11       0    11000
SH + HSO <=> S2O + H2                  1.00E+14       0    14250
H2 + S2O <=> SH + HOS                  1.00E+13       0    46000
SH + SO <=> HSO + S                   1.00E+13       0    25000
SH + SO <=> HOS + S                   1.00E+13       0    30000
SH + SO <=> S2O + H                   1.00E+12       0    5000
HSSO2 + M <=> SH + SO2 + M                1.00E+17       0    3000
SH + O3 <=> HSO + O2                   5.72E+08       0     280
S + OH <=> SO + H                    1.46E+13    0.191    -1361
S + O2 <=> SO + O                    5.43E+05     2.11    -1451
S + HO2 <=> SO + OH                   5.66E+13       0       0
S + HO2 <=> HOS + O                   1.00E+13       0       0
SSO2 + M <=> S + SO2 + M                1.00E+15       0    30000
S + SSO2 <=> S2 + SO2                 1.00E+13       0       0
S + HSOO <=> SH + SO2                  1.00E+13       0       0
S + HSOO <=> SO + HSO                  1.00E+13       0       0
S + HOSO2 <=> SH + SO3                 1.00E+13       0       0
S + SO3 <=> SO + SO2                  1.00E+13       0       0
S + O3 <=> SO + O2                   7.23E+12       0       0
H2O2 + S <=> HOS + OH                  1.00E+12       0       0
HSO + O2 <=> HO2 + SO                  6.44E+05    2.627    19013
HOS + O2 <=> HO2 + SO                  6.44E+05    2.627    19013
HSO + O2 <=> SO2 + OH                  3.70E+01    2.764     6575
HOS + O2 <=> SO2 + OH                  3.70E+01    2.764     6575
HSO + O2 <=> HSO2 + O                  8.40E-07      5.1    11312
HSO + S2 <=> HSS + SO                 1.00E+12       0    3000
HOS + S2 <=> HSS + SO                 1.00E+12       0    1000
HOS + S2 <=> S3 + OH                  1.00E+13       0    13000
H + SO + M <=> HSO + M                  4.93E+29    -5.253     1815
   N2/0./
H + SO + N2 <=> HSO + N2                 2.08E+27    -4.319      812
H + SO + M <=> HOS + M                  3.62E+20    -1.924      -29
   N2/0./
H + SO + N2 <=> HOS + N2                 2.03E+21    -2.093      -72
```

```
HOS + M <=> HSO + M                    5.77E+11       0    32722
   N2/0./
HOS + N2 <=> HSO + N2                  2.93E+11       0    24601
HSO + H <=> H2 + SO                   6.00E+13       0       0
HSO + H <=> SH + OH                   4.90E+19    -1.86     1560
HSO + H <=> S + H2O                   1.60E+09    1.37     -340
HOS + H <=> H2 + SO                   1.00E+13       0       0
HSO + OH <=> H2O + SO                  1.70E+09    1.03      470
HOS + OH <=> H2O + SO                  1.00E+13       0       0
HSO + OH <=> H2 + SO2                  1.00E+11       0       0
HOS + OH <=> H2 + SO2                  1.00E+11       0       0
HSO + O <=> OH + SO                   1.40E+13     0.15      300
HOS + O <=> OH + SO                   1.00E+14       0       0
HSO + O <=> H + SO2                   4.50E+14    -0.4       0
HOS + O <=> H + SO2                   1.00E+14       0       0
H + HSO <=> H + HOS                   1.00E+14       0    4000
HSS + O2 <=> HSSO + O                  1.00E+13       0    26000
HSSO + O <=> S2O + OH                  1.00E+13       0       0
HSSO + O <=> SH + SO2                  1.00E+13       0       0
HSSO + H <=> S2O + H2                  1.00E+13       0       0
HSSO + H <=> HSS + OH                  1.00E+13       0       0
HSSO + OH <=> S2O + H2O                   1.00E+13       0       0
HSSO + OH <=> HSS + HO2                   1.00E+13       0    27000
HSSO + SH <=> S2O + H2S                  1.00E+13       0       0
HSS + HSO <=> HSSO + SH                  1.00E+13       0    7000
HSSO + S <=> HSS + SO                  1.00E+13       0       0
HSSO + S <=> S2O + SH                  1.00E+13       0       0
HSSO + HSS <=> S2O + HSSH                 1.00E+13       0       0
HSSO + HO2 <=> S2O + H2O2                  1.00E+13       0       0
HSSO + S2 <=> S2O + HSS                  1.00E+13       0       0
S2O + HSO2 <=> HSSO + SO2                 1.00E+13       0    32000
HSS + SO3 <=> HSSO + SO2                  1.00E+13       0    10000
S2O + H + M <=> HSSO + M                  6.42E+22    -2.591      287
SO* + M <=> SO + M                    1.00E+13       0       0
SO* + O2 <=> SO2 + O                  1.00E+13       0       0
SO + O2 <=> SO2 + O                   8.91E+06      1.4     3712
SO + O (+M) <=> SO2 (+M)                  3.20E+13       0       0
   LOW /  1.20E+21     -1.54        0 /
   TROE / 0.55    1.E-30    1.E+30 /
   N2/1.5/ SO2/10./ H2O/10./
SO + HO2 <=> SO2 + OH                  3.70E+03     2.42     7660
SO + SO + M <=> OSSO + M                  3.23E+32    -5.75     3044
OSSO + O <=> SO + SO2                  1.00E+13       0       0
OSSO + O <=> O2 + S2O                  1.00E+13       0       0
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```
OSSO + H <=> OH + S2O                  1.00E+13        0        0
OSSO + H <=> SO + HSO                  1.00E+13        0        0
OSSO + H <=> SO + HOS                  1.00E+13        0        0
OSSO + H <=> HO2 + S2                  1.00E+13        0    12570
OSSO + OH <=> HO2 + S2O                  1.00E+13        0    11350
OSSO + OH <=> HOSO + SO                  1.00E+12        0        0
OSSO + SO <=> SO2 + S2O                 2.00E+10        0        0
OSSO + S <=> S2O + SO                  1.00E+13        0        0
OSSO + S <=> S2 + SO2                  1.00E+13        0        0
OSSO + SH <=> HSO + S2O                  1.00E+13        0        0
OSSO + S2 <=> S2O + S2O                 1.00E+12        0        0
S + SO2 <=> SO + SO                    5.88E+12        0     9034
H + SO2 (+M) <=> HSO2 (+M)                 5.30E+08     1.59     2472
   LOW /  1.41E+31    -5.19    4513 /
   TROE / 0.39      167     2191 /
   N2/1./ SO2/10./ H2O/10./
H + SO2 (+M) <=> HOSO (+M)                 2.37E+08     1.63     7339
   LOW /  1.85E+37    -6.14    11075 /
   TROE / 0.283      272     3995 /
   N2/1./ SO2/10./ H2O/10./
HOSO (+M) <=> HSO2 (+M)                    1.00E+09     1.03     50000
   LOW /  1.70E+35    -5.64    55400 /
   TROE / 0.4    1.E-30    1.E+30 /
   N2/1.5/ SO2/10./ H2O/10./
HOSO (+M) <=> OH + SO (+M)                 9.94E+21    -2.54     75891
   LOW /  1.16E+46    -9.02    52953 /
   TROE / 0.95     2989      1.1 /
H + SO2 <=> OH + SO                    6.74E+21    -2.22     30736
SO2 + O (+M) <=> SO3 (+M)                  3.70E+11        0     1689
   LOW /  2.40E+27     -3.6     5186 /
   TROE / 0.442      316     7442 /
   N2/0./ SO2/10./ H2O/10./
SO2 + O (+N2) <=> SO3 (+N2)                3.70E+11        0     1689
   LOW /  2.90E+27    -3.58     5206 /
   TROE / 0.43      371     7442 /
SO2 + OH (+M) <=> HOSO2 (+M)               5.70E+12    -0.27        0
   LOW /  1.70E+27    -4.09       0 /
   TROE / 0.1    1.E-30    1.E+30 /
   H2O/5./ SO2/5./ N2/1./
HOSO2 + O2 <=> SO3 + HO2                   7.83E+11        0      656
SO3 + SO <=> SO2 + SO2                 7.60E+03     2.37     2980
SO3 + O <=> SO2 + O2                   2.80E+04     2.57    29230
SO3 + H <=> SO2 + OH                   8.40E+09     1.22     3322
SO3 + OH <=> SO2 + HO2                   4.80E+04     2.46    27271
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O3 + SO2 <=> O2 + SO3	1.80E+12	0	14000
HSO2 + O2 <=> SO2 + HO2	1.10E+03	3.2	-235
HSO2 + O <=> SO2 + OH	1.00E+13	0	0
HSO2 + H <=> SO2 + H2	5.00E+12	0.46	-262
HSO2 + OH <=> SO2 + H2O	1.00E+13	0	0
HSO2 + SH <=> SO2 + H2S	1.00E+13	0	0
HSO2 + S <=> SO2 + SH	1.00E+13	0	0
HSO2 + HO2 <=> SO2 + H2O2	1.00E+13	0	0
HSO2 + HSS <=> SO2 + HSSH	1.00E+13	0	0
HSO2 + S2 <=> SO2 + HSS	1.00E+13	0	0
HSO2 + SO <=> SO2 + HSO	1.00E+13	0	0
HSO2 + SO <=> SO2 + HOS	1.00E+13	0	0
HSO2 + HSO <=> SO2 + HSOH	1.00E+13	0	0
HOSO + O2 <=> SO2 + HO2	9.60E+01	2.36	-10130
HOSO + O <=> SO2 + OH	1.00E+13	0	0
HOSO + H <=> SO2 + H2	1.80E+07	1.72	-1286
HOSO + H <=> SO* + H2O	2.40E+14	0	0
HOSO + OH <=> SO2 + H2O	6.00E+12	0	0
HOSO + SH <=> SO2 + H2S	1.00E+13	0	0
HOSO + S <=> SO2 + SH	1.00E+13	0	0
HOSO + HO2 <=> SO2 + H2O2	1.00E+13	0	0
HOSO + HSS <=> SO2 + HSSH	1.00E+13	0	0
HOSO + S2 <=> SO2 + HSS	1.00E+13	0	0
HOSO + SO <=> SO2 + HSO	1.00E+13	0	0
HOSO + SO <=> SO2 + HOS	1.00E+13	0	0
HOSO + HSO <=> SO2 + HSOH	1.00E+13	0	0
HOSO + HOS <=> SO2 + HSOH	1.00E+13	0	0
S2 + O <=> SO + S	1.43E+11	0.699	-231
SO + SH <=> S2 + OH	1.00E+12	0	4320
S2 + O2 <=> S2O + O	1.71E+04	2.539	34376
S2 + O2 <=> SO + SO	2.30E+03	2.453	30440
S2 + O + M <=> S2O + M	1.88E+21	-2.8	0
S2O + O <=> SO + SO	9.27E+11	0	0
S2O + S <=> SO + S2	1.00E+13	0	0
S2O + SH <=> HSO + S2	1.00E+12	0	5000
S2O + SH <=> HSS + SO	1.00E+13	0	8000
S2O + OH <=> HO2 + S2	1.00E+13	0	40000
S2O + H <=> OH + S2	1.00E+13	0	0
S2O + SO2 <=> S2 + SO3	1.00E+13	0	20000
HSS + O2 <=> HO2 + S2	4.10E+03	2.527	10585
HSS + O2 <=> HSO + SO	6.61E+03	1.861	7071
HSS + OH <=> H2O + S2	1.00E+14	0	0
HSS + O <=> OH + S2	1.00E+14	0	0
HSS + O <=> SH + SO	1.00E+14	0	0

HSSH + O <=> HSS + OH	1.00E+14	0	0
HSSH + O <=> HSO + SH	1.00E+14	0	0
HSSH + OH <=> HSS + H2O	1.00E+14	0	0
HSSH + O2 <=> HSS + HO2	1.00E+13	0	26000
HSSH + HO2 <=> HSS + H2O2	1.00E+13	0	0
HSSH + SO <=> HSS + HSO	1.00E+13	0	15000
HSSH + SO <=> HSS + HOS	1.00E+13	0	19000
HSSH + HSO <=> HSS + HSOH	1.00E+13	0	2000
HSSH + HOS <=> HSS + HSOH	1.00E+13	0	2000
HSOH + HO2 <=> HSO + H2O2	1.00E+13	0	0
HSOH + HO2 <=> HOS + H2O2	1.00E+13	0	0
HSS + HO2 <=> S2 + H2O2	1.00E+13	0	0
HSO + HO2 <=> SO + H2O2	1.00E+13	0	0
HOS + HO2 <=> SO + H2O2	1.00E+13	0	0
HSS + HSO <=> S2 + HSOH	1.00E+13	0	0
HSS + HOS <=> S2 + HSOH	1.00E+13	0	0
HSO + HSO <=> SO + HSOH	1.00E+13	0	0
HOS + HOS <=> SO + HSOH	1.00E+13	0	0
HSOH + O2 <=> HSO + HO2	1.00E+13	0	26000
HSOH + O2 <=> HOS + HO2	1.00E+13	0	30000
HSOH + O <=> HSO + OH	1.00E+14	0	0
HSOH + O <=> HOS + OH	1.00E+14	0	0
HSOH + H <=> HSO + H2	1.00E+14	0	0
HSOH + H <=> HOS + H2	1.00E+14	0	0
HSOH + OH <=> HSO + H2O	1.00E+14	0	0
HSOH + OH <=> HOS + H2O	1.00E+14	0	0
S + S2 + M <=> S3 + M	1.89E+15	0	-1788
S2 + S2 + M <=> S4 + M	1.89E+15	0	-1788
S2 + S3 + M <=> S5 + M	1.89E+15	0	-1788
S3 + S3 + M <=> S6 + M	1.89E+15	0	-1788
S3 + S4 + M <=> S7 + M	1.89E+15	0	-1788
S4 + S4 + M <=> S8 + M	1.89E+15	0	-1788
SO2 + SH <=> HSO + SO	1.00E+14	0	32000
SO2 + SH <=> HOS + SO	1.00E+14	0	36000
SO2 + SH <=> OH + S2O	1.00E+14	0	32000
SO2 + HSS <=> S2O + HSO	1.00E+14	0	25000
SO2 + S2 <=> S2O + SO	1.00E+14	0	28000
S2O + S2 <=> S3 + SO	1.00E+14	0	18000
S2O + S3 <=> S4 + SO	1.00E+14	0	16000
S2O + S2O <=> S3 + SO2	1.00E+12	0	2600
SH + SO2 <=> HSSO2	1.00E+13	0	33000
HSSO2 <=> S2O + OH	1.00E+13	0	33700
S2O + SH <=> S3 + OH	1.00E+13	0	21450
SO + HSS <=> S3 + OH	1.00E+13	0	14900

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H2S + SO* <=> HSO + SH                    1.00E+13    0    11000
N2O + NO <=> NO2 + N2                     5.30E+05    2.23    46280
N2O + OH <=> HNO + NO                     1.20E-04    4.33    25080
N2O + OH <=> N2 + HO2                     1.30E-02    4.72    36560
N2O + O <=> N2 + O2                       3.70E+12    0    15936
N2O + O <=> NO + NO                       9.20E+13    0    27679
N2O + H <=> N2 + OH                       6.40E+07    1.835    13492
N2O (+M) <=> N2 + O (+M)                  1.30E+12    0    62570
  LOW /  4.00E+14    0    56600 /
  N2/1.7/ O2/1.4/ CO2/3./ H2O/12./
HONO2 + H <=> OH + HONO                   3.80E+05    2.3    6976
HONO2 + OH <=> H2O + NO3                  1.00E+10    0    -1240
HONO2 + H <=> H2O + NO2                   6.10E+01    3.3    6285
HONO2 + H <=> H2 + NO3                    5.60E+08    1.5    16400
NO3 + NO2 <=> NO + NO2 + O2               5.00E+10    0    2940
NO3 + HO2 <=> NO2 + O2 + OH               1.50E+12    0    0
NO3 + OH <=> NO2 + HO2                    1.40E+13    0    0
NO3 + O <=> NO2 + O2                      1.00E+13    0    0
NO3 + H <=> NO2 + OH                      6.00E+13    0    0
HNO2 + OH <=> NO2 + H2O                   4.00E+13    0    0
HNO2 + O <=> NO2 + OH                     1.70E+08    1.5    2000
HNO2 (+M) <=> HONO (+M)                   2.50E+14    0    32300
  LOW /  3.10E+18    0    31500 /
  TROE / 1.149    1.E-30    3125    1.E+30 /
HONO + HONO <=> NO + NO2 + H2O            3.50E-01    3.64    12140
HONO + NO2 <=> HONO2 + NO                 2.00E+11    0    32700
HONO + OH <=> NO2 + H2O                   1.70E+12    0    -520
HONO + O <=> NO2 + OH                     1.20E+13    0    5960
HONO + H <=> NO + H2O                     8.10E+06    1.89    3850
HONO + H <=> HNO + OH                     5.60E+10    0.86    5000
NO2 + NO2 <=> NO3 + NO                    9.60E+09    0.73    20900
NO2 + NO2 <=> NO + NO + O2                4.50E+12    0    27599
NO2 + H2 <=> HNO2 + H                     2.40E+00    3.73    32400
NO2 + H2 <=> HONO + H                     1.30E+04    2.76    29770
NO2 + HO2 <=> HNO2 + O2                   1.90E+01    3.26    4983
NO2 + HO2 <=> HONO + O2                   1.90E+00    3.32    3044
NO2 + OH (+M) <=> HONO2 (+M)              3.00E+13    0    0
  LOW /  2.94E+25    -3    0 /
  TROE / 0.4    1.E-30    1.E+30    1.E+30 /
NO2 + O (+M) <=> NO3 (+M)                 3.50E+12    0.24    0
  LOW /  2.50E+20    -1.5    0 /
  TROE / 0.71    1.E-30    1700    1.E+30 /
NO2 + O <=> NO + O2                       1.10E+14    -0.52    0
NO2 + H <=> NO + OH                       1.30E+14    0    362
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NO + HO2 <=> NO2 + OH                    2.10E+12        0      -497
NO + OH (+M) <=> HONO (+M)                1.10E+14      -0.3        0
   LOW /  3.39E+23      -2.5        0 /
   TROE / 0.75    1.E-30    1.E+30    1.E+30 /
NO + O (+AR) <=> NO2 (+AR)                1.30E+15     -0.75        0
   LOW /  7.56E+19     -1.41        0 /
   TROE / 0.75      1000    100000    1.E+30 /
NO + O (+M) <=> NO2 (+M)                  1.30E+15     -0.75        0
   LOW /  4.72E+24     -2.87     1550 /
   TROE / 0.88      1000     10000    1.E+30 /
   AR/0./
NO + H (+M) <=> HNO (+M)                  1.50E+15     -0.41        0
   LOW /  2.40E+14     0.206    -1550 /
   TROE / 0.82    1.E-30    1.E+30    1.E+30 /
   N2/1.6/
HNO + NO2 <=> HONO + NO                    4.40E+04      2.64      4040
HNO + HNO <=> N2O + H2O                    9.00E+08         0      3100
HNO + O2 <=> HO2 + NO                     2.00E+13         0     16000
HNO + OH <=> NO + H2O                     3.60E+13         0         0
HNO + O <=> NO + OH                      2.30E+13         0         0
HNO + H <=> NO + H2                      4.40E+11      0.72       650
HNOH + NO2 <=> HONO + HNO                  6.00E+11         0      2000
HNOH + NH2 <=> NH3 + HNO                   1.80E+06      1.94     -1152
HNOH + NH2 <=> H2NN + H2O                  8.80E+16     -1.08      1113
HNOH + NH2 <=> N2H3 + OH                   1.00E+01      3.46      -467
HNOH + O2 <=> HNO + HO2                    3.00E+12         0     25000
HNOH + HO2 <=> HNO + H2O2                   2.90E+04      2.69     -1600
HNOH + OH <=> HNO + H2O                    2.40E+06         2     -1192
HNOH + O <=> HNO + OH                     3.30E+08       1.5      -358
   DUPLICATE
HNOH + O <=> HNO + OH                      7.00E+13         0         0
   DUPLICATE
HNOH + H <=> HNO + H2                     4.80E+08       1.5       378
HNOH + H <=> NH2 + OH                     4.00E+13         0         0
HNOH + M <=> HNO + H + M                   2.00E+24     -2.84     58934
   H2O/10./
NH2OH + HO2 <=> H2NO + H2O2                 1.40E+04      2.69      6418
NH2OH + HO2 <=> HNOH + H2O2                 2.90E+04      2.69      9557
NH2OH + NH <=> H2NO + NH2                  1.50E-03       4.6      2424
NH2OH + NH <=> HNOH + NH2                  2.90E-03       4.4      1564
NH2OH + NH2 <=> H2NO + NH3                  9.50E+00      3.42     -1013
NH2OH + NH2 <=> HNOH + NH3                  1.10E-01         4       -97
NH2OH + OH <=> H2NO + H2O                  1.50E+05      2.28     -1296
NH2OH + OH <=> HNOH + H2O                  1.50E+04      2.61     -3537
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NH2OH + O <=> H2NO + OH                    1.70E+08      1.5     3010
NH2OH + O <=> HNOH + OH                    3.30E+08      1.5     3865
NH2OH + H <=> H2NO + H2                    2.40E+08      1.5     5067
NH2OH + H <=> HNOH + H2                    4.80E+08      1.5     6249
NH2OH (+M) <=> NH2 + OH (+M)                1.40E+20     -1.31    64080
  LOW /  5.40E+37    -5.96    66783 /
  TROE / 0.31    1.E-30    1.E+30    1.E+30 /
H2NO + NO2 <=> HONO + HNO                   6.00E+11        0     2000
H2NO + NO <=> HNO + HNO                    2.00E+04        2    13000
H2NO + NH2 <=> HNO + NH3                    3.00E+12        0     1000
H2NO + O2 <=> HNO + HO2                    3.00E+12        0    25000
H2NO + HO2 <=> HNO + H2O2                    2.90E+04     2.69    -1600
H2NO + OH <=> HNO + H2O                    2.00E+07        2     1000
H2NO + O <=> HNO + OH                     3.00E+07        2     2000
H2NO + H <=> NH2 + OH                     5.00E+13        0        0
H2NO + H <=> HNO + H2                     3.00E+07        2     2000
H2NO + M <=> HNOH + M                      1.10E+29       -4    44000
  H2O/10./
H2NO + M <=> HNO + H + M                    2.80E+24    -2.83    64915
  H2O/10./
H2NN + NH2 <=> NNH + NH3                    1.80E+06     1.94    -1152
H2NN + O2 <=> NH2 + NO2                    1.50E+12        0     5961
H2NN + HO2 <=> NNH + H2O2                    2.90E+04     2.69    -1600
H2NN + HO2 <=> NH2 + NO + OH                 9.00E+12        0        0
H2NN + OH <=> NH2 + NO + H                  2.00E+12        0        0
H2NN + OH <=> NNH + H2O                    2.40E+06        2    -1192
H2NN + O <=> NH2 + NO                     7.00E+13        0        0
H2NN + O <=> NNH + OH                     3.30E+08      1.5     -894
H2NN + H <=> N2H2 + H                     7.00E+13        0        0
H2NN + H <=> NNH + H2                     4.80E+08      1.5     -894
H2NN <=> NNH + H                         3.40E+26    -4.83    46228
NH2 + NH2 <=> H2NN + H2                     7.20E+04     1.88     8802
N2H2 + NO <=> N2O + NH2                    4.00E+12        0    11922
N2H2 + NH <=> NNH + NH2                    2.40E+06        2    -1192
N2H2 + NH2 <=> NNH + NH3                    8.80E-02     4.05     1610
N2H2 + OH <=> NNH + H2O                    5.90E+01      3.4     1360
N2H2 + O <=> NH2 + NO                     1.00E+13        0        0
N2H2 + O <=> NNH + OH                     3.30E+08      1.5      497
N2H2 + H <=> NNH + H2                     8.50E+04     2.63      230
N2H2 + M <=> NNH + H + M                    1.90E+27    -3.05    66107
  H2O/7./
NH2 + NH2 <=> N2H2 + H2                     1.70E+08     1.62    11783
NH2 + NH <=> N2H2 + H                     4.30E+14   -0.272      -77
N2H3 + NH <=> N2H2 + NH2                    2.00E+13        0        0
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```
N2H3 + NH2 <=> H2NN + NH3                  3.00E+13        0        0
N2H3 + NH2 <=> N2H2 + NH3                  9.20E+05      1.94     -1152
N2H3 + HO2 <=> N2H4 + O2                   9.20E+05      1.94      2126
N2H3 + HO2 <=> N2H2 + H2O2                 1.40E+04      2.69     -1600
N2H3 + OH <=> NH3 + HNO                    1.00E+12        0     15000
N2H3 + OH <=> H2NN + H2O                   3.00E+13        0        0
N2H3 + OH <=> N2H2 + H2O                   1.20E+06        2     -1192
N2H3 + O <=> NH2 + NO + H                  3.00E+13        0        0
N2H3 + O <=> NH2 + HNO                     3.00E+13        0        0
N2H3 + O <=> N2H2 + OH                     1.70E+08      1.5      -646
N2H3 + H <=> N2H2 + H2                     2.40E+08      1.5       -10
NH2 + NH2 <=> N2H3 + H                     1.20E+12     -0.03     10084
N2H3 <=> N2H2 + H                          3.60E+47    -10.38     69009
N2H4 + NH2 <=> N2H3 + NH3                  3.90E+12        0      1500
N2H4 + OH <=> N2H3 + H2O                   4.00E+13        0        0
N2H4 + O <=> N2H3 + OH                     6.70E+08      1.5      2851
N2H4 + O <=> N2H2 + H2O                    4.40E+11        0     -1270
N2H4 + H <=> N2H3 + H2                     7.00E+12        0      2500
NH2 + NH2 (+M) <=> N2H4 (+M)               5.60E+14    -0.414       66
   LOW /  1.60E+34     -5.49     1987 /
   TROE / 0.31    1.E-30    1.E+30    1.E+30 /
NNH + NO <=> N2 + HNO                      5.00E+13        0        0
NNH + NH2 <=> N2 + NH3                     5.00E+13        0        0
NNH + NH <=> N2 + NH2                      5.00E+13        0        0
NNH + O2 <=> N2 + HO2                      5.60E+14    -0.385      -13
NNH + OH <=> N2 + H2O                      5.00E+13        0        0
NNH + O <=> NH + NO                        5.20E+11     0.381     -409
NNH + O <=> N2 + OH                        1.20E+13     0.145     -217
NNH + O <=> N2O + H                        1.90E+14    -0.274      -22
NNH + H <=> N2 + H2                        1.00E+14        0        0
NNH <=> N2 + H                             1.00E+09        0        0
N + NO <=> N2 + O                          2.10E+13        0        0
N + O2 <=> NO + O                          6.40E+09        1     6280
N + OH <=> NO + H                          3.80E+13        0        0
NH + NO2 <=> HNO + NO                      5.90E+12        0        0
NH + NO2 <=> N2O + OH                      4.10E+12        0        0
NH + HONO <=> NH2 + NO2                    1.00E+13        0        0
NH + NO <=> N2 + OH                        2.70E+12   -0.0721     -512
NH + NO <=> N2O + H                        1.80E+14    -0.351     -244
NH + N <=> N2 + H                          3.00E+13        0        0
NH + NH <=> NH2 + N                        5.70E-01     3.88      342
NH + O2 <=> NO + OH                        1.30E+06      1.5      100
NH + O2 <=> HNO + O                        4.60E+05        2     6500
NH + OH <=> N + H2O                        1.60E+07    1.733     -576
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NH + OH <=> HNO + H 3.20E+14 -0.376 -46
NH + O <=> NO + H 9.20E+13 0 0
NH + H <=> N + H2 3.00E+13 0 0
NH2 + HONO <=> NH3 + NO2 7.10E+01 3.02 -4940
NH2 + NO2 <=> H2NO + NO 1.30E+15 -0.77 242
NH2 + NO2 <=> N2O + H2O 3.00E+14 -0.77 242
NH2 + NO <=> NNH + OH 3.10E+13 -0.48 1180
NH2 + NO <=> N2 + H2O 3.10E+13 -0.48 1180
DUPLICATE
NH2 + NO <=> N2 + H2O 1.30E+16 -1.25 0
DUPLICATE
NH2 + HNO <=> NH3 + NO 3.60E+06 1.63 -1250
NH2 + N <=> N2 + H + H 7.00E+13 0 0
NH2 + NH <=> NH3 + N 9.60E+03 2.46 107
NH2 + NH2 <=> NH3 + NH 5.60E+00 3.53 552
NH2 + O2 <=> HNO + OH 2.90E-02 3.764 18185
NH2 + O2 <=> H2NO + O 2.60E+11 0.4872 29050
NH2 + HO2 <=> NH3 + O2 9.20E+05 1.94 -1152
NH2 + HO2 <=> H2NO + OH 5.00E+13 0 0
NH2 + OH <=> NH + H2O 3.30E+06 1.949 -217
NH2 + O <=> NH + OH 8.60E-01 4.01 1673
DUPLICATE
NH2 + O <=> NH + OH 7.00E+12 0 0
DUPLICATE
NH2 + O <=> HNO + H 6.60E+13 0 0
NH2 + H <=> NH + H2 7.20E+05 2.32 799
NH3 + HO2 <=> NH2 + H2O2 3.00E+11 0 22000
NH3 + OH <=> NH2 + H2O 2.00E+06 2.04 566
NH3 + O <=> NH2 + OH 2.80E+02 3.29 4471
NH3 + H <=> NH2 + H2 6.40E+05 2.39 10171
NH3 + M <=> NH2 + H + M 2.20E+16 0 93470
C6H6 + CH3 <=> CH4 + C6H5 4.60E+12 0 14600
C6H6 + C3H5 <=> C3H6 + C6H5 2.85E+12 0 28300
H + C6H6 <=> H2 + C6H5 1.50E+14 0 10000
H + C8H6 <=> H2 + C8H5 1.80E+14 0 14500
C6H6 + HO2 <=> H2O2 + C6H5 6.40E+12 0 25600
C6H6 + O <=> C6H5O + H 1.50E+13 0 4000
C6H6 + O <=> C6H5 + OH 1.60E+14 0 12750
C6H6 + OH <=> C6H5 + H2O 2.00E+13 0 5000
C6H6 + OH <=> C6H5OH + H 4.50E+12 0 8400
C8H5 + C2H2 <=> C10H7 1.00E+12 0 5000
C6H6 + O2 <=> C6H5 + HO2 6.30E+13 0 60000
C6H5 <=> C6H4 + H 3.00E+16 0 89000
C6H5 <=> C2H2 + C4H3 1.00E+17 0 38000

C6H5 + M <=> C6H5 + M 7.00E+18 0 67000
C6H5 + H <=> C6H6 8.50E+13 0 0
C6H5 + H <=> C6H4 + H2 1.00E+13 0 2000
C6H5 + C2H2 <=> H + C8H6 5.00E+12 0 5000
C6H5 + C6H6 <=> H + C12H10 4.00E+11 0 4000
C6H5 + C6H5 <=> C12H10 5.00E+12 0 0
C6H5 + O <=> C5H5 + CO 1.00E+14 0 0
C6H5 + O <=> OH + C6H4 2.00E+13 0 0
C6H5 + OH <=> C6H5O + H 5.00E+13 0 0
C6H5 + OH <=> C6H4 + H2O 2.00E+13 0 0
C6H5 + HO2 <=> C6H5O + OH 2.00E+13 0 1000
C6H5 + H2 <=> C6H6 + H 5.70E+04 2.43 6280
C6H5 + O2 <=> C6H5O + O 2.60E+13 0 6120
C6H5 + O2 <=> OC6H4O + H 1.00E+13 0 9000
C6H5O <=> C5H5 + CO 2.00E+14 0 43920
C6H5O + C6H5O <=> C12H8O + H2O 4.00E+13 0 11000
C6H5O + H <=> C6H5OH 2.50E+14 0 0
H + C6H5O + M <=> C6H5OH + M 4.00E+15 0 0
H + C6H5O <=> C5H6 + CO 2.00E+14 0 0
C6H5O + O <=> OC6H4O + H 1.00E+14 0 0
C6H5O + O <=> C5H5 + CO2 1.00E+13 0 0
C6H5OH <=> C5H6 + CO 2.50E+16 0 72400
C6H5OH + H <=> C6H5O + H2 8.90E+13 0 10700
C6H5OH + H <=> C6H6 + OH 2.20E+13 0 7930
C6H5OH + O <=> C6H5O + OH 5.00E+13 0 9000
C6H5OH + OH <=> C6H5O + H2O 1.50E+13 0 4800
C6H5OH + O2 <=> C6H5O + HO2 6.30E+13 0 49000
C6H5OH + HO2 <=> C6H5O + H2O2 2.00E+12 0 18000
C6H5OH + C2H3 <=> C6H5O + C2H4 6.00E+12 0 0
CH3 + C6H5OH <=> CH4 + C6H5O 1.45E+12 0 12000
C6H5OH + CH2CHCCH2 <=> C6H5O + CH2CHCHCH2 6.00E+12 0 0
C6H5OH + C6H5 <=> C6H5O + C6H6 4.90E+12 0 4400
C3H5 + C6H5OH <=> C3H6 + C6H5O 9.00E+11 0 22200
OC6H4O <=> C5H4O + CO 1.00E+12 0 40000
OC6H4O <=> C5H4O + CO 3.70E+11 0 59000
OC6H4O <=> C5H4 + CO2 3.50E+12 0 67000
OC6H4O + H <=> C5H5O + CO 2.50E+13 0 4700
OC6H4O + H <=> OC6H3O + H2 2.00E+12 0 8100
OC6H4O + O <=> C6H3O3 + H 1.50E+13 0 4530
OC6H4O + O <=> OC6H3O + OH 1.40E+13 0 14700
OC6H4O + OH <=> OC6H3O + H2O 1.00E+06 2 4000
OC6H3O + H <=> C2H2 + CO + C2H2 + CO 1.00E+14 0 0
OC6H3O + H <=> OC6H4O 1.00E+14 0 0
OC6H3O + O <=> C2H2 + HCCO + CO + CO 1.00E+14 0 0

C6H3O3 <=> C2H2 + HCCO + CO + CO 1.00E+12 0 50000
C6H3O3 + H <=> C2H2 + CH2CO + CO + CO 1.00E+14 0 0
C5H6 + H <=> C5H5 + H2 7.20E+13 0 3500
C5H6 + H <=> C5H7 2.40E+73 -17.85 31500
C5H6 + H <=> CH2CHCHCHCH2 1.10E+14 -0.16 3100
C5H6 + O <=> C5H5O + H 8.90E+12 -0.15 590
DUPLICATE
C5H6 + O <=> C5H5O + H 5.60E+12 -0.06 200
DUPLICATE
C5H6 + O <=> C5H5 + OH 4.80E+04 2.71 1100
C5H6 + OH <=> CH2CHCHCHCHOH 1.10E+13 -0.07 870
C5H6 + OH <=> C5H5 + H2O 3.10E+06 2 0
C5H6 + HO2 <=> C5H7 + O2 1.30E+15 -1.07 9530
C5H6 + HO2 <=> C5H5 + H2O2 1.10E+04 2.6 12900
C5H6 + O2 <=> C5H5 + HO2 4.00E+13 0 37150
C5H6 + CH3 <=> C5H5 + CH4 1.80E-01 4 0
C5H6 + C2H3 <=> C6H6 + CH3 2.10E+67 -16.08 42460
C5H6 + C2H3 <=> C5H5 + C2H4 1.20E-01 4 0
C5H6 + C6H5 <=> C6H6 + C5H5 1.00E-01 4 0
C5H6 + CH2CHCCH2 <=> C5H5 + CH2CHCHCH2 6.00E+12 0 0
C5H6 + C6H5O <=> C5H5 + C6H5OH 3.20E+11 0 8000
C5H7 <=> CH2CHCHCHCH2 3.20E+15 0 39500
C5H7 + H <=> C5H6 + H2 3.60E+12 0 0
C5H7 + O <=> C5H6 + OH 1.00E+13 0 0
C5H7 + OH <=> C5H6 + H2O 2.40E+13 0 0
C5H7 + O2 <=> CHOCH2CH2CHCHO 8.00E+24 -3.8 20000
CHOCH2CH2CHCHO + O2 <=> CHOCH2CH2CHO + HCOO 6.30E+05 1.65 17480
CH2CHCHCHCH2 <=> CH2CHCHCHCH2 5.40E+11 -0.7 60
CH2CHCHCHCH2 + O2 <=> CH2CHCHO + CH2HCO 1.20E+36 -7.25 33600
CH2CHCHCHCH2 + H <=> CH2CHCHCHCH3 2.30E+20 -1.6 3020
CH2CHCHCHCH2 + H <=> CH2CHCHCH + CH3 2.90E+26 -2.18 36770
CH2CHCHCHCH2 + O <=> CH2CHCHO + C2H3 2.00E+14 0 0
CH2CHCHCHCH2 + OH <=> CH2CHCHCHCH2OH 1.50E+13 0 0
CH2CHCHCHCH2 + O2 <=> CH2CHCHCHO + CH2O 8.20E+10 0.18 9140
CH2CHCHCHCH3 + H <=> CH2CHCHCH2 + CH3 5.20E+71 -16.38 51000
CH2CHCHCHCH3 + H <=> CH2CHCHCHCH2 + H2 7.00E+06 2 5000
CH2CHCHCHCH3 + OH <=> CH2CHCHCHCH2 + H2O 7.00E+06 2 0
CH2CHCHCHCH2OH + H <=> CH2CHCHCH2 + CH2OH 2.50E+34 -6.12 16250
CH2CHCHCHCHOH + O2 <=> CHOCHCHOH + CH2HCO 1.20E+36 -7.25 33600
C5H5 <=> CHCCHCHCH2 1.00E+12 1 77000
CHCCHCHCH2 <=> H2CCCH + C2H2 1.00E+12 1 31000
C5H5 + H <=> C5H6 1.50E+14 0 0
C5H5 + O <=> CH2CHCHCH + CO 3.20E+13 -0.17 440
C5H5 + O <=> C5H4O + H 5.80E+13 -0.02 20

C5H5 + OH <=> C5H5OH 6.50E+14 -0.85 -2730
DUPLICATE
C5H5 + OH <=> C5H5OH 1.10E+43 -8.76 18730
DUPLICATE
C5H5 + OH <=> C5H5OH 1.10E+59 -13.08 33450
DUPLICATE
C5H5 + OH <=> C5H4OH + H 3.50E+57 -12.18 48350
C5H5 + HO2 <=> C5H5O + OH 6.30E+29 -4.69 11650
C5H5 + O2 <=> CH2CHCHCO + HCO 1.20E+19 -2.48 10970
C5H5OH + H <=> C5H4OH + H2 3.20E+12 0 0
C5H5OH + H <=> C5H5O + H2 4.00E+13 0 6094
C5H5OH + O <=> C5H4OH + OH 4.70E+11 0 0
C5H5OH + O <=> C5H5O + OH 1.00E+13 0 4683
C5H5OH + OH <=> C5H4OH + H2O 5.50E+12 0 1731
C5H5OH + OH <=> C5H5O + H2O 1.00E+13 0 1697
C5H5OH + HO2 <=> C5H4OH + H2O2 3.60E+03 2.55 10531
C5H5OH + HO2 <=> C5H5O + H2O2 1.00E+13 0 15800
C5H5O <=> C5H4O + H 2.90E+32 -6.5 21220
C5H5O <=> CH2CHCHCH + CO 1.10E+79 -19.62 66250
C5H4OH <=> C5H4O + H 2.10E+13 0 54000
C5H4OH + H <=> C5H5OH 1.00E+14 0 0
C5H4OH + O2 <=> C5H4O + HO2 1.00E+13 0 10000
C5H4O <=> C2H2 + C2H2 + CO 5.70E+32 -6.76 68500
DUPLICATE
C5H4O <=> C2H2 + C2H2 + CO 6.20E+41 -7.87 98700
DUPLICATE
C5H4O + H <=> CH2CHCHCH + CO 2.10E+61 -13.27 40810
C5H4O + H <=> C5H3O + H2 2.00E+12 0 8100
C5H4O + O <=> CH2CHCCH + CO2 1.00E+13 0 2000
C5H4O + O <=> C5H3O + OH 1.40E+13 0 14700
C5H4O + OH <=> C5H3O + H2O 1.10E+08 1.42 1450
C5H3O + H <=> C5H4O 1.00E+14 0 0
C5H3O + O2 <=> CHCHCHCO + CO2 9.70E+58 -13.47 38180
C5H4 + H <=> C5H3 + H2 1.00E+06 2.5 5000
C5H4 + O <=> C5H3 + OH 1.00E+06 2.5 3000
C5H4 + OH <=> C5H3 + H2O 1.00E+06 2 0
C5H3 + H <=> C5H4 1.00E+14 0 0
C5H3 + O2 <=> C2H2 + HCCO + CO 1.00E+12 0 0
CHOCH2CH2CHO + H <=> CHOCH2CH2CO + H2 2.30E+10 1.05 3279
CHOCH2CH2CHO + OH <=> CHOCH2CH2CO + H2O 3.50E+09 1.18 -447
CHOCH2CH2CO + O2 <=> C2H4 + O2CCHOO 1.60E+45 -9.92 20670
CH2CHCHCHO <=> CH2CHCH2 + CO 6.10E+05 0.92 -1120
CH2CHCHCHO + O2 <=> CH2CHCHO + HCOO 1.20E+36 -7.25 33600
CH2CHCHCO + H <=> CH2CHCH2 + CO 6.60E+13 -0.02 2740

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CH2CHCHCO + H <=> CH2CCHCO + H2                1.50E+07        2      6000
CH2CHCHCO + O <=> CH2HCO + HCCO                3.00E+08      1.45      -860
CH2CHCHCO + OH => CHCHCHCO + H2O               1.00E+07        2      5000
CH2CHCHCO + OH <=> CH2CCHCO + H2O              1.00E+07        2      2000
CH2CHCHCO + OH <=> CH2CHCH2 + CO2              3.00E+12        0         0
CH2CCHCO + H <=> H2CCCH + HCO                  1.00E+14        0         0
CH2CCHCO + OH <=> CHCCHCO + H2O                3.00E+13        0         0
CHCHCHCO <=> H2CCCH + CO                      6.10E+05      0.92     -1120
CHCHCHCO + H <=> CH2CCHCO + H                  1.00E+14        0         0
CHCHCHCO + H <=> CHCCHCO + H2                  3.00E+07        2      1000
CHCHCHCO + OH <=> CHCCHCO + H2O                2.00E+07        2      1000
CHCHCHCO + O2 <=> CHCCHCO + HO2                1.00E+07        2     10000
CHCCHCO + H <=> CHCCCO + H2                   3.00E+07        2      5000
CHCCHCO + OH <=> CHCCCO + H2O                  1.00E+07        2      2000
CHCCCO + H <=> C3H2 + CO                     5.00E+13        0         0
CHCCCO + O <=> C2H + CO + CO                  1.00E+13        0         0
CHCCCO + OH <=> C2H2 + CO + CO                 1.00E+13        0         0
CHCCCO + O2 => HCCO + CO + CO                 1.00E+12        0         0
CH2CHCHCH2 + H <=> CH2CHCHCH + H2              3.00E+07        2     13000
CH2CHCHCH2 + H <=> CH2CHCCH2 + H2              3.00E+07        2      6000
CH2CHCHCH2 + O <=> CH2CHCH2 + HCO              6.00E+08      1.45      -858
CH2CHCHCH2 + O <=> CH2HCO + C2H3               1.00E+12        0         0
CH2CHCHCH2 + OH <=> CH2CHCHCH + H2O            2.00E+07        2      5000
CH2CHCHCH2 + OH <=> CH2CHCCH2 + H2O            2.00E+07        2      2000
CH2CHCHCH2 + O2 <=> CH2CHCHCH + HO2            3.00E+13        0     57800
CH2CHCHCH2 + O2 <=> CH2CHCCH2 + HO2            3.00E+13        0     45850
CH2CHCHCH (+M) <=> CH2CHCCH + H (+M)           1.00E+14        0     37000
   LOW /  1.00E+14        0    30000 /
   H2/2./ CO/2./ CO2/3./ H2O/5./
CH2CHCHCH + H <=> CH2CHCCH2 + H                1.00E+14        0         0
CH2CHCHCH + H <=> CH2CHCCH + H2                3.00E+07        2      1000
CH2CHCHCH + OH <=> CH2CHCCH + H2O              2.00E+07        2      1000
CH2CHCHCH + O2 <=> CHCHCHO + CH2O              1.00E+12        0         0
CH2CHCHCH + O2 <=> CH2CHCCH + HO2              1.00E+07        2     10000
CH2CHCCH2 (+M) <=> CH2CHCCH + H (+M)           1.00E+14        0     50000
   LOW /  2.00E+15        0    42000 /
   H2/2./ CO/2./ CO2/3./ H2O/5./
CH2CHCCH2 + H <=> H2CCCH + CH3                 1.00E+14        0         0
CH2CHCCH2 + OH <=> CH2CHCCH + H2O              3.00E+13        0         0
CH2CHCCH + H <=> HCCHCCH + H2                  2.00E+07        2     15000
CH2CHCCH + H <=> H2CCCCH + H2                  3.00E+07        2      5000
CH2CHCCH + O <=> C2H3 + HCCO                  1.40E+07        2      1900
CH2CHCCH + O <=> H2CCCH + HCO                  8.10E+06      1.88       180
CH2CHCCH + OH <=> HCCHCCH + H2O                7.50E+06        2      5000
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CH2CHCCH + OH <=> H2CCCCH + H2O                1.00E+07        2      2000
CH2CHCCH + O2 <=> HCCHCCH + HO2                3.00E+13        0     60750
CH2CHCCH + O2 <=> H2CCCCH + HO2                3.00E+13        0     42200
HCCHCCH (+M) <=> C4H2 + H (+M)                 1.00E+14        0     36000
   LOW /  1.00E+14        0    30000 /
   H2/2./ CO/2./ CO2/3./ H2O/5./
HCCHCCH + H <=> H2CCCCH + H                    1.00E+14        0        0
HCCHCCH + OH <=> C4H2 + H2O                    1.00E+13        0        0
HCCHCCH + O2 <=> C2H2 + CO + HCO               3.00E+12        0        0
HCCHCCH + C2H2 <=> C6H5                        2.80E+03      2.9     1400
H2CCCCH (+M) <=> C4H2 + H (+M)                 1.00E+14        0     55000
   LOW /  2.00E+15        0    48000 /
   H2/2./ CO/2./ CO2/3./ H2O/5./
H2CCCCH + H <=> C4H2 + H2                      5.00E+13        0        0
H2CCCCH + O <=> CH2CO + C2H                    2.00E+13        0        0
H2CCCCH + O <=> H2C4O + H                      2.00E+13        0        0
H2CCCCH + OH <=> C4H2 + H2O                    3.00E+13        0        0
H2CCCCH + O2 <=> CH2CO + HCCO                  1.00E+12        0        0
H2CCCCH + CH2 <=> H3CCCH + C2H                 2.00E+13        0        0
C4H2 + H <=> C4H + H2                          2.00E+07        2     2000
C4H2 + O <=> C3H2 + CO                         1.20E+12        0        0
C4H2 + OH <=> H2C4O + H                        6.70E+12        0     -410
C4H2 + OH <=> C4H + H2O                        1.00E+07        2     1000
H2C4O + H <=> C2H2 + HCCO                      5.00E+13        0     3000
H2C4O + OH <=> CH2CO + HCCO                    1.00E+07        2     2000
C4H + O2 <=> CO + CO + C2H                     1.00E+13        0        0
CH2CHCH3 + H <=> C2H4 + CH3                    7.20E+12        0     1300
CH2CHCH3 + H <=> CH2CHCH2 + H2                 1.70E+05      2.5     2490
CH2CHCH3 + H <=> CH2CCH3 + H2                  4.10E+05      2.5     9800
CH2CHCH3 + H => CHCHCH3 + H2                   8.00E+05      2.5    12300
CH2CHCH3 + O <=> C2H5 + HCO                    1.60E+07     1.76    -1216
CH2CHCH3 + O <=> CH2CHCH2 + OH                 5.20E+11      0.7     5884
CH2CHCH3 + O <=> CHCHCH3 + OH                  1.20E+11      0.7     8960
CH2CHCH3 + O <=> CH2CCH3 + OH                  6.00E+10      0.7     7630
CH2CHCH3 + OH <=> CH2CHCH2 + H2O               3.10E+06        2     -298
CH2CHCH3 + OH <=> CH2CCH3 + H2O                1.10E+06        2     1451
CH2CHCH3 + OH <=> CHCHCH3 + H2O                2.10E+06        2     2778
CH2CHCH3 + HO2 <=> CH2CHCH2 + H2O2             9.60E+03      2.6    13909
CH2CHCH3 + O2 <=> CH2CHCH2 + HO2               2.00E+13        0    47600
CH2CHCH3 + O2 <=> CHCHCH3 + HO2                2.00E+13        0    47600
CH2CHCH3 + O2 <=> CH2CCH3 + HO2                2.00E+13        0    47600
CH2CHCH2 + H <=> H2CCCH2 + H2                  5.00E+13        0        0
CH2CHCH2 + H <=> CH2CHCH3                      1.90E+26     -3.6     5470
CH2CHCH2 + O <=> CH2CHCHO + H                  1.80E+14        0        0
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CH2CHCH2 + OH <=> H2CCCH2 + H2O                1.00E+13        0        0
CH2CHCH2 + HO2 <=> CH2CHCHO + H + OH           1.00E+13        0        0
CH2CHCH2 + O2 <=> CH2CHCHO + OH                1.80E+13     -0.41     22860
CH2CHCH2 + O2 <=> H2CCCH2 + HO2                5.00E+15     -1.4      22430
CH2CHCH2 + O2 <=> CH2HCO + CH2O                1.10E+10     0.34      12840
CH2CHCH2 + O2 <=> C2H2 + CH2O + OH             2.80E+25     -4.8      15470
CHCHCH3 + H <=> CH2CHCH2 + H                   1.00E+14        0        0
CHCHCH3 + H <=> H3CCCH + H2                    2.00E+13        0        0
CHCHCH3 + OH <=> H3CCCH + H2O                  1.00E+13        0        0
CHCHCH3 + O2 <=> CH3HCO + HCO                  1.10E+23     -3.29      3900
CH2CCH3 + H <=> CH2CHCH2 + H                   1.00E+14        0        0
CH2CCH3 + H <=> H3CCCH + H2                    4.00E+13        0        0
CH2CCH3 + O <=> CH2CO + CH3                    1.00E+14        0        0
CH2CCH3 + OH <=> H3CCCH + H2O                  2.00E+13        0        0
CH2CCH3 + O2 <=> CH3CO + CH2O                  1.10E+22     -3.29      3900
H2CCCH2 <=> H3CCCH                             2.20E+14        0     68100
H2CCCH2 + H <=> H3CCCH + H                     1.00E+13        0      5000
H2CCCH2 + H (+M) <=> CH2CHCH2 (+M)             1.20E+11     0.69      3000
   LOW /  5.60E+33       -5     4450 /
   TROE / 0.7086      134      1784      5740 /
H2CCCH2 + H (+M) <=> CH2CCH3 (+M)              8.50E+12        0      2000
   LOW /  1.10E+34       -5     4450 /
   TROE / 0.7086      134      1784      5740 /
H2CCCH2 + O <=> C2H4 + CO                      1.30E+07     1.88       180
H2CCCH2 + H <=> H2CCCH + H2                    3.00E+07        2      5000
H2CCCH2 + OH <=> H2CCCH + H2O                  2.00E+07        2      1000
H3CCCH + H <=> H2CCCH + H2                     3.00E+07        2      5000
H3CCCH + H <=> CH3 + C2H2                      1.00E+14        0      4000
H3CCCH + H (+M) <=> CH2CCH3 (+M)               6.50E+12        0      2000
   LOW /  8.50E+39     -7.27     6580 /
   TROE / 0.7086      134      1784      5740 /
H3CCCH + OH <=> H2CCCH + H2O                   2.00E+07        2      1000
H3CCCH + O <=> C2H4 + CO                       1.50E+13        0      2100
CH2CHCHO + H <=> C2H4 + HCO                    2.00E+13        0      3500
CH2CHCHO + H <=> CH2CHCO + H2                  4.00E+13        0      4200
CH2CHCHO + O <=> CH2CHCO + OH                  7.20E+12        0      1970
CH2CHCHO + O <=> CH2CO + HCO + H               5.00E+07     1.76        76
CH2CHCHO + OH <=> CH2CHCO + H2O                1.00E+13        0        0
CH2CHCHO + O2 <=> CH2CHCO + HO2                3.00E+13        0     36000
H2CCCH + H (+M) <=> H2CCCH2 (+M)               1.00E+17     -0.82       315
   LOW /  3.50E+55     -4.88     2225 /
   TROE / 0.7086      134      1784      5740 /
   H2/2./ CO/2./ CO2/3./ H2O/8.6/
H2CCCH + H (+M) <=> H3CCCH (+M)                1.00E+17     -0.82       315
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   LOW /  3.50E+55    -4.88    2225 /
   TROE / 0.7086      134      1784      5740 /
   H2/2./ CO/2./ CO2/3./ H2O/8.6/
H2CCCH + H <=> C3H2 + H2                    5.00E+13        0      1000
H2CCCH + O <=> CH2O + C2H                   1.40E+14        0         0
H2CCCH + OH <=> C3H2 + H2O                  2.00E+13        0         0
H2CCCH + O2 <=> CH2CO + HCO                 3.00E+10        0      2868
H2CCCH + H2CCCH <=> C6H5 + H                1.00E+13        0         0
CH2CHCO <=> C2H3 + CO                       1.00E+14        0     34000
CH2CHCO + O <=> C2H3 + CO2                  1.00E+14        0         0
CH2CHCO + O2 <=> CH2HCO + CO2               5.40E+20    -2.72      7000
C3H2 + O <=> C2H2 + CO                      1.00E+14        0         0
C3H2 + OH <=> C2H2 + HCO                    5.00E+13        0         0
C3H2 + O2 <=> HCCO + CO + H                 2.00E+12        0      1000
C3H2 + CH3 <=> CH2CHCCH + H                 2.00E+13        0         0
C3H2 + HCCO <=> HCCHCCH + CO                3.00E+13        0         0
C3H2 + H2CCCH <=> C6H4 + H                  1.00E+13        0         0
O2CCHOO <=> HCOO + CO2                      3.00E+13        0      4000
O + OH <=> O2 + H                         2.00E+14      -0.4         0
O + H2 <=> OH + H                         5.00E+04      2.67      6290
OH + H2 <=> H2O + H                         2.10E+08      1.52      3450
OH + OH <=> O + H2O                         4.30E+03       2.7     -2486
H + H + M <=> H2 + M                        1.00E+18        -1         0
   H2O/0./
H + H + H2O <=> H2 + H2O                    6.00E+19     -1.25         0
H + O + M <=> OH + M                        6.20E+16      -0.6         0
   H2O/5./
H + OH + M <=> H2O + M                      1.60E+22        -2         0
   H2O/5./
O + O + M <=> O2 + M                        1.90E+13         0     -1788
   H2O/5./
H + O2 + M <=> HO2 + M                      2.10E+18        -1         0
   H2O/10./ N2/0./
H + O2 + N2 <=> HO2 + N2                    6.70E+19     -1.42         0
H + HO2 <=> H2 + O2                       4.30E+13         0      1411
H + HO2 <=> OH + OH                         1.70E+14         0       874
H + HO2 <=> O + H2O                         3.00E+13         0      1721
O + HO2 <=> O2 + OH                         3.30E+13         0         0
OH + HO2 <=> H2O + O2                       1.90E+16        -1         0
HO2 + HO2 <=> H2O2 + O2                     1.30E+11         0     -1629
   DUPLICATE
HO2 + HO2 <=> H2O2 + O2                     4.20E+14         0     11982
   DUPLICATE
H2O2 + M <=> OH + OH + M                    1.30E+17         0     45500
```

```
   H2O/5./
H2O2 + H <=> HO2 + H2                    1.70E+12        0     3755
H2O2 + H <=> OH + H2O                    1.00E+13        0     3576
H2O2 + O <=> OH + HO2                    6.60E+11        0     3974
H2O2 + OH <=> H2O + HO2                    7.80E+12        0     1330
   DUPLICATE
H2O2 + OH <=> H2O + HO2                    5.80E+14        0     9560
   DUPLICATE
CO + O + M <=> CO2 + M                    6.20E+14        0     3000
   H2O/5./
CO + OH <=> CO2 + H                      1.50E+07      1.3     -758
CO + O2 <=> CO2 + O                      2.50E+12        0    47700
HO2 + CO <=> CO2 + OH                      5.80E+13        0    22934
CH2O + M <=> HCO + H + M                    3.30E+16        0    81000
   H2O/5./
CH2O + H <=> HCO + H2                     1.30E+08     1.62     2166
CH2O + O <=> HCO + OH                     1.80E+13        0     3080
CH2O + OH <=> HCO + H2O                     3.40E+09     1.18     -447
CH2O + HO2 <=> HCO + H2O2                    3.00E+12        0    13000
CH2O + O2 <=> HCO + HO2                     6.00E+13        0    40660
HCO + M <=> H + CO + M                     1.90E+17       -1    17000
   H2O/5./
HCO + H <=> CO + H2                      1.20E+13     0.25        0
HCO + O <=> CO + OH                      3.00E+13        0        0
HCO + O <=> CO2 + H                      3.00E+13        0        0
HCO + OH <=> H2O + CO                      1.00E+14        0        0
HCO + O2 <=> HO2 + CO                      7.60E+12        0      406
CH3 + H (+M) <=> CH4 (+M)                    1.30E+16    -0.63      383
   LOW /  1.75E+33    -4.76     2440 /
   TROE / 0.783       74      2941      6964 /
   H2O/8.57/ N2/1.43/
CH4 + H <=> CH3 + H2                     2.20E+04        3     8750
CH4 + O <=> CH3 + OH                      1.00E+09      1.5     8604
CH4 + OH <=> CH3 + H2O                      1.60E+06      2.1     2460
CH4 + HO2 <=> CH3 + H2O2                    1.80E+11        0    18700
CH4 + O2 <=> CH3 + HO2                     7.90E+13        0    56000
CH3 + H <=> CH2 + H2                     9.00E+13        0    15100
CH2(S) + H2 <=> CH3 + H                     7.20E+13        0        0
CH3 + O <=> CH2O + H                      8.40E+13        0        0
CH3 + OH <=> CH2 + H2O                      7.50E+06        2     5000
CH2(S) + H2O <=> CH3 + OH                    3.00E+15     -0.6        0
CH2OH + H <=> CH3 + OH                     1.00E+14        0        0
CH3O + H <=> CH3 + OH                     1.00E+14        0        0
CH3 + OH (+M) <=> CH3OH (+M)                 6.30E+13        0        0
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LOW / 1.89E+38 -6.3 3100 /
TROE / 0.2105 83.5 5398 8370 /
N2/1.43/ H2O/8.58/
CH3 + HO2 <=> CH3O + OH 8.00E+12 0 0
CH3 + O2 <=> CH3O + O 2.90E+13 0 30481
CH3 + O2 <=> CH2O + OH 1.90E+12 0 20315
CH3 + CH3 (+M) <=> C2H6 (+M) 2.10E+16 -0.97 620
LOW / 1.26E+50 -9.67 6220 /
TROE / 0.5325 151 1038 4970 /
N2/1.43/ H2O/8.59/ H2/2./ CO/2./ CO2/3./
CH3 + CH2O <=> CH4 + HCO 7.80E-08 6.1 1967
CH3 + HCO <=> CH4 + CO 1.20E+14 0 0
CH2 + H <=> CH + H2 1.00E+18 -1.56 0
CH2 + O <=> CO + H + H 5.00E+13 0 0
CH2 + O <=> CO + H2 3.00E+13 0 0
CH2 + OH <=> CH + H2O 1.10E+07 2 3000
CH2 + OH <=> CH2O + H 2.50E+13 0 0
CH2 + O2 <=> CO + H2O 2.20E+22 -3.3 2867
CH2 + O2 <=> CO2 + H + H 3.30E+21 -3.3 2867
CH2 + O2 <=> CH2O + O 3.30E+21 -3.3 2867
CH2 + O2 <=> CO2 + H2 2.60E+21 -3.3 2867
CH2 + O2 <=> CO + OH + H 1.60E+21 -3.3 2867
CH2 + CO2 <=> CH2O + CO 1.10E+12 0 1000
CH2 + CH4 <=> CH3 + CH3 4.30E+12 0 10030
CH2 + CH3 <=> C2H4 + H 4.20E+13 0 0
CH2 + CH2 <=> C2H2 + H + H 4.00E+13 0 0
CH2 + HCCO <=> C2H3 + CO 3.00E+13 0 0
CH2(S) + M <=> CH2 + M 1.00E+13 0 0
H/0./ H2O/0./ N2/0./
CH2(S) + N2 <=> CH2 + N2 1.30E+13 0 430
CH2(S) + H <=> CH2 + H 2.00E+14 0 0
CH2(S) + H2O <=> CH2 + H2O 3.00E+13 0 0
CH2(S) + H <=> CH + H2 3.00E+13 0 0
CH2(S) + O <=> CO + H + H 3.00E+13 0 0
CH2(S) + OH <=> CH2O + H 3.00E+13 0 0
CH2(S) + O2 <=> CO + OH + H 7.00E+13 0 0
CH2(S) + CO2 <=> CH2O + CO 3.00E+12 0 0
CH2(S) + CH4 <=> CH3 + CH3 4.30E+13 0 0
CH2(S) + CH3 <=> C2H4 + H 2.00E+13 0 0
CH2(S) + CH2CO <=> C2H4 + CO 1.60E+14 0 0
CH2(S) + C2H6 <=> CH3 + C2H5 1.20E+14 0 0
CH + H <=> C + H2 1.50E+14 0 0
CH + O <=> CO + H 5.70E+13 0 0
CH + OH <=> HCO + H 3.00E+13 0 0

```
CH + OH <=> C + H2O                    4.00E+07    2    3000
CH + O2 <=> HCO + O                    3.30E+13    0    0
CH + H2O <=> CH2O + H                  5.70E+12    0    -751
CH + CO2 <=> HCO + CO                  3.40E+12    0    690
CH + CH4 <=> C2H4 + H                  6.00E+13    0    0
CH + CH3 <=> C2H3 + H                  3.00E+13    0    0
CH + CH2 <=> C2H2 + H                  4.00E+13    0    0
CH + CH2O <=> CH2CO + H                9.50E+13    0    -515
CH + HCCO <=> C2H2 + CO                5.00E+13    0    0
C + OH <=> CO + H                      5.00E+13    0    0
C + O2 <=> CO + O                      2.00E+13    0    0
C + CH3 <=> C2H2 + H                   5.00E+13    0    0
C + CH2 <=> C2H + H                    5.00E+13    0    0
CH3OH + H <=> CH2OH + H2               1.70E+07    2.1  4868
CH3OH + H <=> CH3O + H2                4.20E+06    2.1  4868
CH3OH + O <=> CH2OH + OH               3.90E+05    2.5  3080
CH3OH + OH <=> CH2OH + H2O             5.30E+04    2.53 960
CH3OH + OH <=> CH3O + H2O              1.32E+04    2.53 960
CH3OH + HO2 <=> CH2OH + H2O2           9.60E+10    0    12578
CH2O + H (+M) <=> CH3O (+M)            5.40E+11    0.454  2600
   LOW /  1.54E+30    -4.8    5560 /
   TROE / 0.758      94    1555    4200 /
   N2/1.43/ H2O/8.58/
CH3O + H <=> CH2O + H2                 2.00E+13    0    0
CH3O + O <=> CH2O + OH                 1.00E+13    0    0
CH3O + OH <=> CH2O + H2O               1.00E+13    0    0
CH3O + O2 <=> CH2O + HO2               6.30E+10    0    2600
H + CH2O (+M) <=> CH2OH (+M)           5.40E+11    0.454  3600
   LOW /  9.10E+31    -4.82    6530 /
   TROE / 0.7187     103    1291    4160 /
   N2/1.43/ H2O/8.58/ CO/2./ CO2/3./ H2/2./
CH2OH + H <=> CH2O + H2                2.00E+13    0    0
CH2OH + O <=> CH2O + OH                1.00E+13    0    0
CH2OH + OH <=> CH2O + H2O              1.00E+13    0    0
CH2OH + O2 <=> CH2O + HO2              1.60E+15    -1   0
   DUPLICATE
CH2OH + O2 <=> CH2O + HO2              7.20E+13    0    3577
   DUPLICATE
C2H6 + H <=> C2H5 + H2                 5.40E+02    3.5  5210
C2H6 + O <=> C2H5 + OH                 3.00E+07    2    5115
C2H6 + OH <=> C2H5 + H2O               7.20E+06    2    864
C2H6 + HO2 <=> C2H5 + H2O2             1.30E+13    0    20460
C2H6 + O2 <=> C2H5 + HO2               5.00E+13    0    55000
C2H6 + CH3 <=> C2H5 + CH4              5.50E-01    4    8300
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C2H4 + H (+M) <=> C2H5 (+M)                 1.10E+12    0.454     1822
   LOW /  1.11E+34       -5     4448 /
   TROE / 0.5       95       95       200 /
   H2O/5./
C2H5 + H (+M) <=> C2H6 (+M)                 5.20E+17    -0.99     1580
   LOW /  2.00E+41     -7.08     6685 /
   TROE / 0.8422      125      2219      6882 /
   N2/1./ H2O/6./
C2H5 + H <=> CH3 + CH3                    4.90E+12     0.35        0
C2H5 + O <=> CH3 + CH2O                    4.20E+13        0        0
C2H5 + O <=> CH3HCO + H                    5.30E+13        0        0
C2H5 + O <=> C2H4 + OH                    3.00E+13        0        0
C2H5 + OH <=> C2H4 + H2O                    2.40E+13        0        0
C2H5 + O2 <=> C2H4 + HO2                    1.00E+10        0    -2190
C2H5 + CH2O <=> C2H6 + HCO                    5.50E+03     2.81     5860
C2H5 + HCO <=> C2H6 + CO                    1.20E+14        0        0
C2H5 + CH3 <=> C2H4 + CH4                    1.10E+12        0        0
C2H5 + C2H5 <=> C2H6 + C2H4                    1.50E+12        0        0
C2H3 + H (+M) <=> C2H4 (+M)                    6.10E+12     0.27      280
   LOW /  9.80E+29     -3.86     3320 /
   TROE / 0.782     207.5      2663      6095 /
   H2/2.85/ CO/2.1/ CO2/2.85/ H2O/7.14/ CH4/2.85/ C2H6/4.29/ N2/1.43/
C2H4 + M <=> C2H2 + H2 + M                    3.50E+16        0     71500
   N2/1.5/ H2O/10./
C2H4 + H <=> C2H3 + H2                    5.40E+14        0     14900
C2H4 + O <=> CH2HCO + H                    4.70E+06     1.88       180
C2H4 + O <=> CH3 + HCO                    8.10E+06     1.88       180
C2H4 + O <=> CH2CO + H2                    6.80E+05     1.88       180
C2H4 + OH <=> C2H3 + H2O                    2.00E+13        0     5940
C2H4 + HO2 <=> CH3HCO + OH                    2.20E+12        0     17200
C2H4 + O2 <=> CH2HCO + OH                    2.00E+08      1.5     39000
C2H4 + CH3 <=> C2H3 + CH4                    5.00E+11        0     15000
H + C2H2 (+M) <=> C2H3 (+M)                    3.10E+11     0.58      2590
   LOW /  2.25E+40    -7.269     6577 /
   TROE / 0.5       675       675 /
   H2/2./ CO/2./ CO2/3./ H2O/5./
C2H3 + H <=> C2H2 + H2                    4.00E+13        0        0
C2H3 + O <=> CH2CO + H                    3.00E+13        0        0
C2H3 + OH <=> C2H2 + H2O                    2.00E+13        0        0
C2H3 + O2 <=> CH2O + HCO                    1.10E+23    -3.29     3890
C2H3 + O2 <=> CH2HCO + O                    2.50E+15    -0.78     3135
C2H3 + O2 <=> C2H2 + HO2                    5.20E+15    -1.26     3310
C2H3 + CH2O <=> C2H4 + HCO                    5.40E+03     2.81     5860
C2H3 + HCO <=> C2H4 + CO                    9.00E+13        0        0
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```
C2H3 + CH3 <=> C2H2 + CH4                 2.10E+13        0        0
C2H3 + C2H3 <=> C2H4 + C2H2                1.50E+13        0        0
C2H2 + M <=> C2H + H + M                  9.10E+30      -3.7    127138
   H2/2./ CO/2./ CO2/3./ H2O/5./
H2 + C2H <=> C2H2 + H                     4.10E+05      2.39      864
C2H2 + O <=> CH2 + CO                     6.10E+06         2     1900
C2H2 + O <=> HCCO + H                     1.40E+07         2     1900
C2H2 + O <=> C2H + OH                     3.20E+15      -0.6     15000
OH + C2H2 <=> C2H + H2O                     3.40E+07         2     14000
OH + C2H2 <=> HCCOH + H                     5.00E+05       2.3     13500
OH + C2H2 <=> CH2CO + H                     2.20E-04       4.5     -1000
OH + C2H2 <=> CH3 + CO                     4.80E-04         4     -2000
OH + C2H2 (+M) <=> C2H2OH (+M)                1.50E+08       1.7      1000
   LOW /  1.81E+23        -2        0 /
   H2/2./ CO/2./ CO2/3./ H2O/5./
HO2 + C2H2 <=> CH2HCO + O                   1.00E+12         0     10000
HO2 + C2H2 <=> CH2O + HCO                   1.00E+12         0     10000
C2H2 + O2 <=> HCO + HCO                    2.00E+08       1.5     30100
C2 + H2 <=> C2H + H                       4.00E+05       2.4      1000
C2H + O <=> CH + CO                       5.00E+13         0         0
C2H + OH <=> HCCO + H                      2.00E+13         0         0
C2H + OH <=> C2 + H2O                      4.00E+07         2      8000
C2H + O2 <=> CO + CO + H                    2.50E+13         0         0
C2H + CH4 <=> CH3 + C2H2                    7.20E+12         0       976
C2 + OH <=> C2O + H                       5.00E+13         0         0
C2 + O2 <=> CO + CO                       5.00E+13         0         0
CH3HCO <=> CH3 + HCO                       7.10E+15         0     81280
CH3HCO + H <=> CH3CO + H2                    4.10E+09      1.16      2400
CH3HCO + O <=> CH3CO + OH                    5.80E+12         0      1800
CH3HCO + OH <=> CH3CO + H2O                    2.30E+10      0.73     -1110
CH3HCO + HO2 <=> CH3CO + H2O2                  3.00E+12         0     12000
CH3HCO + O2 <=> CH3CO + HO2                  3.00E+13         0     39000
CH3HCO + CH3 <=> CH3CO + CH4                  2.00E-06       5.6      2464
CH2HCO <=> CH3 + CO                        1.00E+13         0     42000
CH2HCO + H <=> CH3 + HCO                     1.00E+14         0         0
CH2HCO + H <=> CH3CO + H                     3.00E+13         0         0
CH2HCO + O <=> CH2O + HCO                    5.00E+13         0         0
CH2HCO + OH <=> CH2CO + H2O                    2.00E+13         0         0
CH2HCO + OH <=> CH2OH + HCO                    1.00E+13         0         0
CH2HCO + O2 <=> CH2O + CO + OH                  2.20E+11         0      1500
CH2HCO + CH3 <=> C2H5CHO                     5.00E+13         0         0
CH2HCO + CH2 <=> C2H4 + HCO                    5.00E+13         0         0
CH2HCO + CH <=> C2H3 + HCO                    1.00E+14         0         0
C2H5 + HCO <=> C2H5CHO                     1.80E+13         0         0
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```
C2H5CHO + H <=> C2H5CO + H2                  8.00E+13        0        0
C2H5CHO + O <=> C2H5CO + OH                  7.80E+12        0     1730
C2H5CHO + OH <=> C2H5CO + H2O                1.20E+13        0        0
C2H5 + CO <=> C2H5CO                        1.50E+11        0     4800
C2H2OH + H <=> CH2HCO + H                    5.00E+13        0        0
C2H2OH + O <=> OCHCHO + H                    5.00E+13        0        0
C2H2OH + O2 <=> OCHCHO + OH                  1.00E+12        0     5000
CH3CO (+M) <=> CH3 + CO (+M)                 2.80E+13        0    17100
   LOW /  2.10E+15        0    14000 /
   TROE / 0.5    1.E-30    1.E+30 /
   H2/2./ CO/2./ CO2/3./ H2O/5./
CH3CO + H <=> CH3 + HCO                      2.10E+13        0        0
CH3CO + H <=> CH2CO + H2                     1.20E+13        0        0
CH3CO + O <=> CH3 + CO2                      1.50E+14        0        0
CH3CO + O <=> CH2CO + OH                     4.00E+13        0        0
CH3CO + OH <=> CH2CO + H2O                   1.20E+13        0        0
CH2 + CO (+M) <=> CH2CO (+M)                 8.10E+11      0.5     4510
   LOW /  1.88E+33     -5.11     7095 /
   TROE / 0.5907      275      1226      5185 /
   H2/2./ CO/2./ CO2/3./ H2O/8.58/ N2/1.43/
CH2CO + H <=> CH3 + CO                       5.90E+06        2     1300
CH2CO + H <=> HCCO + H2                      3.00E+07        2    10000
CH2CO + O <=> CO2 + CH2                      1.80E+12        0     1350
CH2CO + O <=> HCCO + OH                      2.00E+07        2    10000
CH2CO + OH <=> HCCO + H2O                    1.00E+07        2     3000
CH2CO + OH <=> CH2OH + CO                    7.20E+12        0        0
CH2CO + OH <=> CH3 + CO2                     3.00E+12        0        0
HCCOH + H <=> HCCO + H2                      3.00E+07        2     1000
HCCOH + OH <=> HCCO + H2O                    1.00E+07        2     1000
HCCOH + O <=> HCCO + OH                      2.00E+07        3     1900
OCHCHO + M <=> HCO + HCO + M                 1.00E+17        0    58000
OCHCHO + H <=> CH2O + HCO                    3.00E+13        0        0
CH + CO (+M) <=> HCCO (+M)                   5.00E+13        0        0
   LOW /  1.88E+28     -3.74     1936 /
   TROE / 0.5757      237      1652      5069 /
   N2/1.43/ H2O/8.58/ CO/2./ CO2/3./ H2/2./
H + HCCO <=> CH2(S) + CO                     1.00E+14        0        0
O + HCCO <=> H + CO + CO                     1.00E+14        0        0
HCCO + OH <=> C2O + H2O                      6.00E+13        0        0
HCCO + O2 <=> CO2 + CO + H                   1.40E+07      1.7     1000
HCCO + O2 <=> CO + CO + OH                   2.90E+07      1.7     1000
HCCO + HCCO <=> C2H2 + CO + CO               1.00E+13        0        0
C2O + H <=> CH + CO                         1.00E+13        0        0
C2O + O <=> CO + CO                         5.00E+13        0        0
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```
C2O + OH <=> CO + CO + H                    2.00E+13        0        0
C2O + O2 <=> CO + CO + O                    2.00E+13        0        0
H + NO + M <=> HNO + M                      2.70E+15        0     -600
   H2O/10./ O2/1.5/ H2/2./ CO2/3./ N2/0./
H + NO + N2 <=> HNO + N2                    2.40E+18       -1        0
NO + O + M <=> NO2 + M                      7.50E+19    -1.41        0
   N2/1.7/ O2/1.5/ H2O/10./
OH + NO + M <=> HONO + M                    5.10E+23    -2.51      -68
   H2O/5./
HO2 + NO <=> NO2 + OH                       2.10E+12        0     -479
HONO + H <=> H2 + NO2                       1.20E+13        0     7352
HONO + O <=> OH + NO2                       1.20E+13        0     5961
HONO + OH <=> H2O + NO2                     4.00E+12        0        0
NO2 + H <=> NO + OH                         8.40E+13        0        0
NO2 + O <=> NO + O2                         3.90E+12        0     -238
NO2 + NO2 <=> NO + NO + O2                  1.60E+12        0    26123
HNO + H <=> H2 + NO                         4.50E+11     0.72      655
HNO + O <=> NO + OH                         1.00E+13        0        0
HNO + OH <=> NO + H2O                       3.60E+13        0        0
HNO + O2 <=> HO2 + NO                       1.00E+13        0    25000
HNO + NO2 <=> HONO + NO                     6.00E+11        0     2000
CO + NO2 <=> CO2 + NO                       9.00E+13        0    33779
CH2O + NO2 <=> HCO + HONO                   8.00E+02     2.77    13730
HCO + NO <=> HNO + CO                       7.20E+12        0        0
HCO + NO2 <=> CO + HONO                     1.20E+23    -3.29     2355
HCO + NO2 <=> H + CO2 + NO                  8.40E+15    -0.75     1930
HCO + HNO <=> CH2O + NO                     6.00E+11        0     2000
END
```

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