ABSTRACT

The two-stage combustor facility was used to investigate the process of chlorocarbon incineration and formation of products of incomplete combustion. For this purpose methylene chloride was used as a chlorine-containing compound. The propose of this research was to obtain a better understanding of the incineration process of chlorocarbons, such as methylene chloride, especially regarding its destruction efficiency and formation of products of incomplete combustion. For measuring near-real time very low concentrations of benzene and methylene chloride, on-line microtrap gas chromatography system was used.

The experimental system was validated using a known combustion reaction mechanism from literature. Modeling of combustion process has shown different pathways of benzene formation for first (perfectly stirred) and the second (plug flow) zones of the combustor with residence time 0.007 and 0.029 sec respectively. Destruction efficiency of methylene chloride was investigated under different equivalence ratio and inlet concentration. Influence of methylene chloride on formation of products of incomplete combustion such as methane, ethylene, ethane, and acetylene was investigated.

Combustion process was simulated using a reactor model and the reaction mechanism. Rate-of production analysis based on modeling results showed that there are different pathways for destruction of methylene chloride under fuel-lean and fuel-rich conditions. As shown by experimental results, destruction efficiency is lower at its lower concentrations. Simulations of experimental results on destruction of methylene chloride,

methyl chloride, and benzene, has shown that significance of various radicals and destruction channels varies with combustion conditions and concentrations of organics, and that atoms and fragments of destroyed molecules play important role in further destruction of parent species. In order to describe the effect of additional radicals and fragments on the total rate of destruction additional rate function was derived and calculated for methylene chloride combustion cases.

EXPERIMENTAL AND MODELING STUDIES OF FORMATION OF PRODUCTS OF INCOMPLETE COMBUSTION AND CHLOROCARBON INCINERATION

by
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To my beloved family

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CHAPTER 1

INTRODUCTION

1.1 Background

Incineration is widely used for the recovery of energy and the destruction of hazardous industrial, municipal, and medical wastes. The United States Clean Air Act of 1990 regulates the emission of 189 air toxic compounds. These include formaldehyde, butadiene, aromatics and some polyaromatic hydrocarbons (PAH). Since some aromatic and PAH are mutagenic and carcinogenic their emissions are of particular concern.

Typical incineration operations require excess air (fuel-lean conditions). However, poor mixing can result in fuel-rich pockets. Formed during non-optimal combustion conditions, such zones can be responsible for the formation and emission of products of incomplete combustion (PIC), which might include higher molecular weight hydrocarbons, such as benzene. Benzene is a known carcinogen and one of the key intermediates in the formation of polyaromatic hydrocarbons (PAH) and soot. The PAH can then form chlorinated dioxins and furans, if chlorinated species are present.

Incineration is also widely used for disposal of hazardous chlorinated chemical wastes and organic solvents, such as polyvinyl chloride (PVC), pesticides, methylene chloride, carbon tetrachloride, etc. Under the optimal combustion conditions, destruction efficiencies of chlorinated hydrocarbons are high. However, incomplete combustion caused by poor mixing, for example, can lead to low destruction efficiency and high levels of pollutants, such as unburned hydrocarbons, CO, higher molecular weight and aromatic compounds. Chlorine containing compounds are well-recognized inhibitors in

hydrocarbon combustion, which limit CO to CO_2 conversion and promote the formation of PIC.

1.2 Objectives

The goal of this research is to obtain a better understanding of the incineration of chlorocarbons, such as methylene chloride, especially regarding its destruction efficiency and formation of products of incomplete combustion. The specific objectives of this research are to:

1. Validate the reactor and the analytical system using a known combustion reaction mechanism from the literature.

2. Identify pathways of benzene formation under different combustion conditions, based on detailed modeling of near-real time concentration data taken by the microtrap-GC system.

3. Investigate the influence of methylene chloride on the hydrocarbon combustion process and formation of products of incomplete combustion, such as CH_4, C_2H_4, C_2H_6, C_2H_2.

4. Investigate the destruction efficiency of methylene chloride under different fuel/air ratios.

5. Investigate the destruction efficiency of methylene chloride as a function of its inlet concentration.

7. Simulate these combustion runs using a reactor model and the reaction mechanisms. After comparing the calculated results with the experimental data, interpret on the observations.

8. Identify the important reaction pathways responsible for the destruction of methylene chloride via the rate-of-production analysis based on modeling results.

9. Make some explanation on lower destruction efficiency at lower waste concentration (Trenholm data).

1.3 Research Approach

This research used a two-stage turbulent flow reactor as a combustor, which can be considered as a perfectly stirred reactor followed by a plug flow reactor. This type of reactor can simulate many practical combustion systems, such as liquid and gas feed waste incinerators.

Ethylene was used as a fuel for validation of the combustor, and the study of benzene formation and consumption under fuel-rich conditions. Ethylene was also used as a primary fuel for combustion of chlorinated compound. Methylene chloride was used as a model waste chlorocarbon in this study.

The experiments were performed as follows:

a) reactor was validated as a PSR+PFR sequence based on ethylene/air combustion;

b) benzene formation was investigated by measuring its near real-time concentrations using the microtrap-GC system and modeling this process using available reaction mechanism;

c) methylene chloride was burned at different inlet concentrations under fuel-lean and fuel-rich conditions; data taken from these experiments included reactor

temperature, the effects of inlet methylene chloride concentration on efficiency of its destruction, and CO, CO_2, and PICs emission.

Modeling with detailed reaction mechanisms was used to predict the experimental observations. Rate of production analysis based on acceptable model calculations was applied to determine the destruction and formation pathways of the species of interest.

CHAPTER 2

LITERATURE SURVEY

2.1 Formation of Benzene During Combustion

The experimental results performed in isothermal laminar flow reactor has shown that C_2H_2 and molecular hydrogen are controling elements in the reactions for PAH growth in fuel-rich premixed combustion (Roesler, 2000). The kinetic mechanism developed for the formation of benzene and high-molecular-mass aromatic compounds in fuel-rich flames, emphasizes both the role of resonantly stabilized radicals and the standard acetylene addition reactions (D'Anna, et al., 2000).

Combustion studies in engines have investigated the chemistry leading to the formation exhaust hydrocarbons. They showed significant envolvement of postflame reactions. The most important reaction in the formation of benzene was direct demethylation (Gregory, et al., 1999).

Studies of low temperature formation of aromatic hydrocarbons showed that aromatic products such as benzene, toluene, naphthalene are detected between 400 to 600°C. Detectable products formed at temperature above 600°C were methane, benzene, hydrogen (Hajaligol, et al., 2001).

A detailed kinetic model has been used to explore the effect of C/O ratio and temperature on the formation rate and concentration of aromatic hydrocarbons in premixed fuel-rich flames. It has been shown that net formation rate of aromatics increases monotonically with C/O ratio, and at a fixed C/O ratio, it passes through the maximum as temperature is increased (D'Anna, et al., 1998).

In studies of chemical kinetic paths leading to aromatics and PAH in the diffusion, flame benzene was predicted to be formed primarily by the reaction sequence of Allyl+Propagyl↔Fulvene+H+H followed by fulvene isomerization to benzene. This work also demonstrates that there are multipathways to aromatic and PAH formation whose role is dependent on the type of flame (premixed or diffusion) and type of hydrocarbon fuel (Marinov, N. et al., 1998).

Experimental studies on oxidation and pyrolisys of various types of heavy fuels indicated that formation rate of benzene in the different flames is approximately the same, but the mechanism of formation is different. The experiments showed further evidence for a pathway to form benzene through C_3 species, which could occur in parallel to C_4/C_2 pathways (Sidebotham, et al., 1992).

Pope et al. (2000) studied benzene formation reactions in premixed laminar flat flames having an unsaturated C_2 or C_3 hydrocarbon fuel (acetylene, ethylene, and propane). Their results showed that major portion of benzene was formed by reactions of either C_3H_3 + C_3H_3 or C_3H_3 + C_3H_5, with the relative importance being strongly dependent on the fuel. The C_2H_x + C_4H_x reactions did not contribute noticeably to benzene formation. Although the key reactions differed from flame to flame, CH_2 + C_2H_2 and C_3H_3 + H were important for all three flames.

The formation of benzene in combustion in diesel engines was investigated as a function of the air-fuel ratio, ϕ (Schulz, et al., 1996). A strong dependance of benzene formation with ϕ was observed at minimum ϕ = 1.2-1.4. The extent of fuel-air mixing at the moment of ignition was a dominant factor in pollution formation. This mixing

depends strongly on construction differences of the engines and the efficiency of fuel injection-dispension-evaporation.

2.2 Combustion of Chlorinated Hydrocarbons

Combustion is a major method for destruction of hazardous chlorinated substances, but there are many concerns exist about destruction efficiency and emissions of pollutant byproducts. Incineration of chlorinated substances, even in an oxygen-rich environment, does not always guarantee the removal of the chlorine as the most thermodynamically stable desirable product HCl. For example, phosgene $COCl_2$, hexachlorobenzene C_6Cl_6, molecular chlorine Cl_2, and other hazardous chlorinated byproducts were observed in the flame under the fuel-lean conditions (Chang, et al., 1989).

The early studies on pyrolysis and oxidation of chlorinated hydrocarbons (CHCs) were performed at low temperature ($T < 700°C$) under flameless conditions (Barton et al., 1951; Goodal et al., 1954; Hoare et al. 1959). A large number of breakdown products, including carbon monoxide and chlorinated compounds, were detected in emission gas. These resuls supplied data to the later studies on combustion of CHCs.

Combustion of trichloroethane has been studied by Bose and Senken (1983) using a premixed flat flame. The reaction pathway they proposed is that C2HCl3 undergoes decomposition by oxidative reactions to produce CO, HCl, and Cl2, then HCl and Cl2 inhibited and slow CO burnout reaction. Chlorinated intermediates decomposed relatively fast compared to the slow oxidation of CO. A reaction kinetic model was present in the wotk to explane the flame observations.

Karra and Senkan (1987) performed comparative studies of CH3Cl/CH4 and CH4 flames. The experiments showed that the CH3Cl rapidly decomposes and the concentrations of CO, C2H2, and C2H4 are significantly higher in the CH3Cl/CH4 flame than that in the CH4 flame. Based on the observations and the analysis of reaction mechanism, the authors noted that methyl chloride promotes soot formation in the flame because the increased concentrations of C2H3 and C2H2.

Combustion of dichlorometane in a postflame incinerator region and its effect on byproducts formation was studied by Sgro et al. (2000). Dichloromethane was injectedat concentration 750 ppm, at temperature 900-1200 K. Equivalence ratio varied from 0.6 to 1.1, residence time was 0.28-0.35 sec. This study showed increased destruction efficiency at lower equivalence ratio. However, the experiments reveal increased levels of stable chlorinated organics at lower equivalence ratio, opposite to numerical prediction.

Inhibition and oxidation characteristics of chloromethane were studied by Roesler et al. (1996). In the post flame invironment at temperatures near 1000 K chloromethanes showed stromg inhibition of CO oxidation, with ranking in order of increasing inhibition effectiveness to be CHCl3<CH3Cl<CH2Cl2 on molar basis. Detailed species profiles were obtained and revealed significant formation of products of incomplete conbustion.

A detailed kinetic reaction mechanism based upon fundamental thermochemical and kinetic principles was used for calculations of the stable species concentrations profiles in CH3Cl and CH2Cl2 combustion and pyrolysis environments (Ho, et al., 1992). The model results show that combustion inhibition by chlorocarbons occurs by loss of OH through the fast reaction OH + HCl = H2O + Cl. Therefore CO conversion through reaction with HO2 and ClO become more important.

2.3 Incineration and Destruction of Organic Compounds

The effect of concentration on destruction or removal efficiency of volatile organic compounds is shown in Figure 2.1 from data based on field testing (EPA, 1984). This same dependence on concentration was duplicated in the laboratory using a spray flame reactor (Kramlich, 1990), as shown in Figure 2.2. These destruction efficiency data correlated inversely with the organic feed concentration indicating that it is much more difficult to get high destruction efficiency at low initial concentrations. The field data indicate that total mass emissions from hazardous waste incinerators vary little over a range of waste feed concentrations approaching six orders of magnitude. This observation suggested that there is some fundamental limit on complete destruction of organics in waste combustion systems. An acceptable explanation of this phenomenon has not

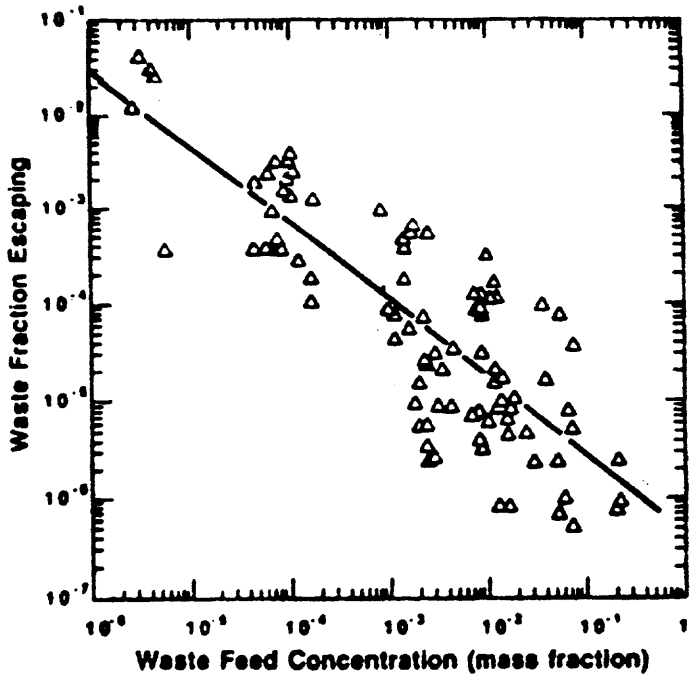


Figure 2.1 Impact of concentration of the organic constituent in the waste stream on the field measurements of destruction efficiency.

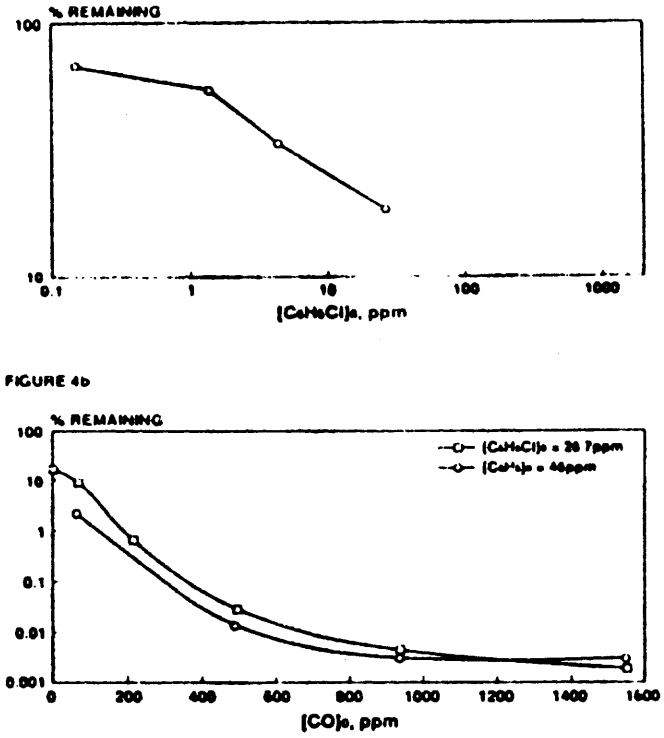


Figure 2.2 Lab scale data on the impact of reactant concentrations on destruction efficiency by benzene and chlorobenzene: (a) impact of reactant concentration, (b) impact of CO (800°C).

yet been found. Equilibrium calculations indicate that if the organics mix with air at moderate temperatures, the thermochemical equilibrium concentration of organics will be insignificant (Kramlich, 1989).

The measurements of the destruction and removal efficiency (DRE) of designated principal organic constituents was used by the U.S. EPA to assess the ability of hazardous waste combustion units to destroy organics (Moran, et al., 1999). The test was based on the temperature for 99% destruction at two seconds gas phase residence time under

oxygen starved conditions. Statistical evaluation of this data show strong correlations of both DRE and CO concentrations to combustion temperature.

Experimental and modeling studies on destruction of CH_3Cl in postflame combustion gases showed that the concentration influences the extent of destruction (Koshland et al., 1993). Researches reported the optimal concentration level of 100 ppm where CH_3Cl was most effectively destroyed in the postflame region of a reactor. Higher and lower levels were more difficult to destroy. Results indicated that injection of the fuels in postflame region can increase the destruction efficiency or reduce the peak temperature needed for adequate destruction of CH_3Cl by increasing radical concentrations and the rate of subsequent destruction reactions.

Incineration tests performed using CCl_4 as a surrogate for PCBs demonstrated that strong dependence of DRE on combustion temperature. The residual concentration of CCl_4 was 2.0 e-7 at 2000°F with residence time 40 ms (Xiong, et al., 1991).

The existence of a second threshold during incineration of methyl chloride under fuel-lean conditions was proposed by experimental study (Tsang, 1990). When the incinerator was operated below the threshold, efficiency of destruction of the toxic organic compounds was limited. It shown that when methylene chloride molar concentration in the feed was lower than 100 ppm, the fraction of undecomposed methyl chloride remaining in the emission gas reached about 30 percent. However, when the feed concentration was higher, the methyl chloride decomposed to about 97 percent at 1200 K, and 0.52 second residence time.

Mixing and kinetic inadequacies may be the limiting factors for destruction of organics in waste combustion systems. Numerous studies on the kinetics of nonflame

thermal oxidation of pure and mixed organic compounds have been carried out. Several studies have been conducted on detailed chemical kinetics of flame zone processes of simple organic compounds (Chang, et al., 1989). The non-flame studies have been used to define the temperature at which a one second residence time is sufficient to produce 99.99% oxidation of the initial compound even in the absence of flame radical concentrations. These temperatures are typically below 1650° F (900° C) for most investigated organics. Kinetic modeling studies by Tsang (1990) using the available elementary rate data suggested the importance of the reaction mixture and mixing on the destruction of chlorinated organics. Research by Lyon et al. (1985) suggested that the extent to which a compound is destroyed by incineration may be dependent on its concentration due to a kinetic threshold of oxidation that exists at low concentrations. They suggest that the kinetic threshold arises from the fact that generating a high enough equilibrium concentration of free radicals to sustain the oxidation rate requires a minimum amount of fuel. Laboratory studies in a flow reactor (Kee, et al.) have shown a strong dependence of destruction on concentration for benzene, chloroform and chlorobenzene, and it can be accelerated with the addition of a co-oxidizing fuel at higher concentrations in order to generate higher concentrations of radicals. These data suggest that kinetic limitations can be important at low concentrations even at high temperatures typically encountered in waste combustion systems.

CHAPTER 3

EXPERIMENTAL METHODS

3.1 Schematic of Experimental System

The schematic of the experimental system is shown in Figure 3.1. It can be divided into three parts: feed and mixing system, two-stage combustor, and analytical system.

The primary fuel used for this study is ethylene (C_2H_4), which was supplied by Matheson Gas Company. The ethylene purity grade was UHP. The purity specifications are listed in Table 3.1.

Table 3.1 Ethylene Purity Specifications

Typical contaminants	vppm
Acetylene	5
Carbon Dioxide	5
Carbon Monoxide	5
Ethane	5
Hydrogen	2
Methane	20
Nitrogen	20
Oxygen	10
Propane	5
Water	5

Two cylinders with ethylene are connected in parallel to the feed line through a two-stage regulator, which decreases the ethylene pressure to 60 psig at the inlet of the ethylene flowmeter. In order to prevent regulator freeze-up due to Joule-Thomson cooling, the

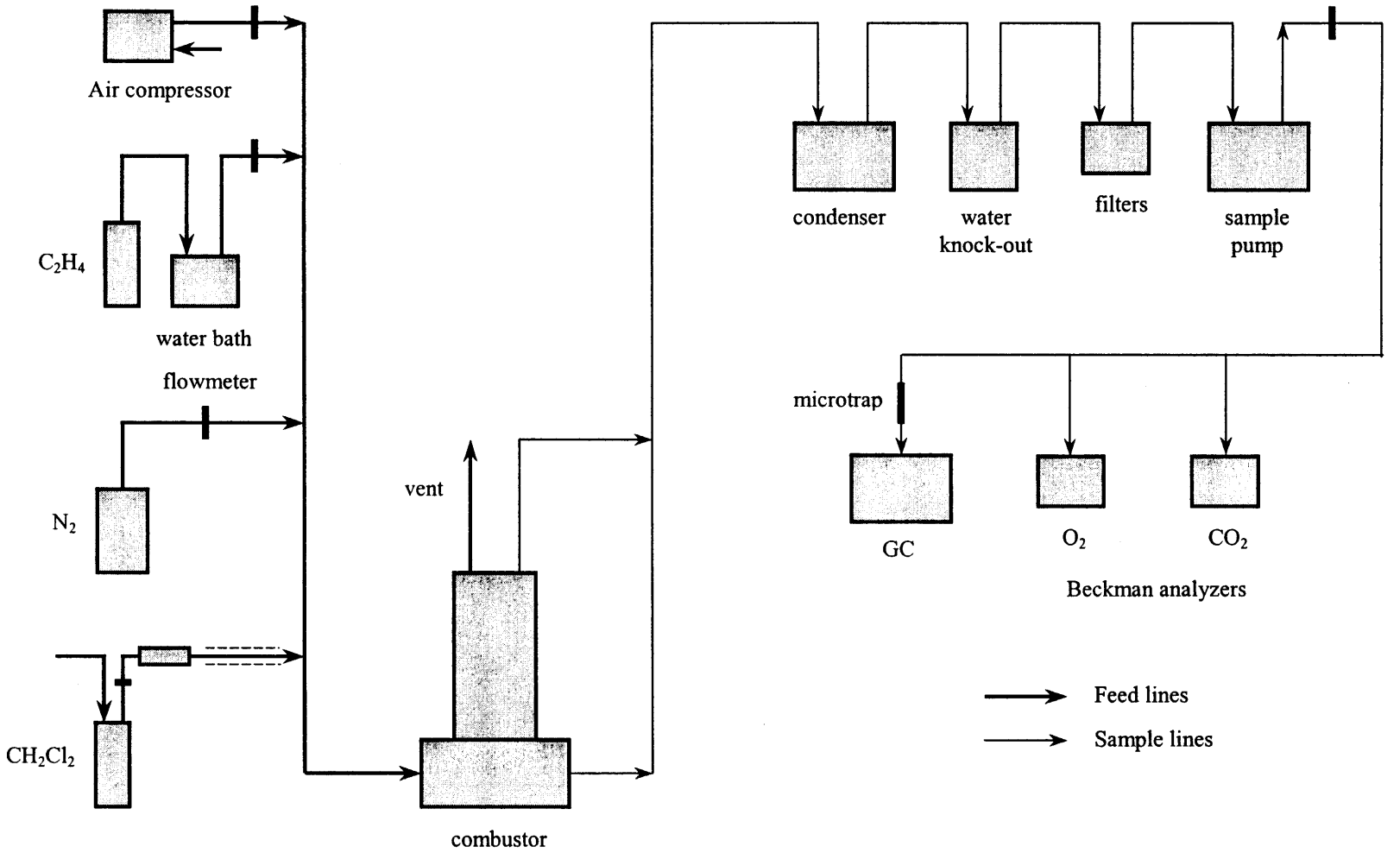


Figure 3.1 Schematic diagram of the experimental system.

ethylene fluid at cylinder pressure is preheated by a stainless steel coil immersed in a hot water bath, with control temperature 70-80°C before the regulator. After preheating and pressure letdown, the temperature of ethylene gas is about room temperature at the rotameter.

High-pressure air (120 psig) from an in-house compressor was used as the oxidant for combustion. Before entering the main line, air was cleaned by knockout filter in order to remove any oil particles and saturated moisture. Low-pressure house air (60 psig) was used for combustion ignition and the analytical instruments. The analytical instrument air is dried by flowing through an activated charcoal packed column.

Methylene chloride (CH_2Cl_2) is used as a model chlorine containing hazardous waste. It is stored as a liquid at room temperature, in a bottle, and withdrawn by pressurizing the bottle with nitrogen gas using a siphon tube. Methylene chloride feed system is shown in Figure 3.2. Flow of liquid methylene chloride is regulated by calibrated

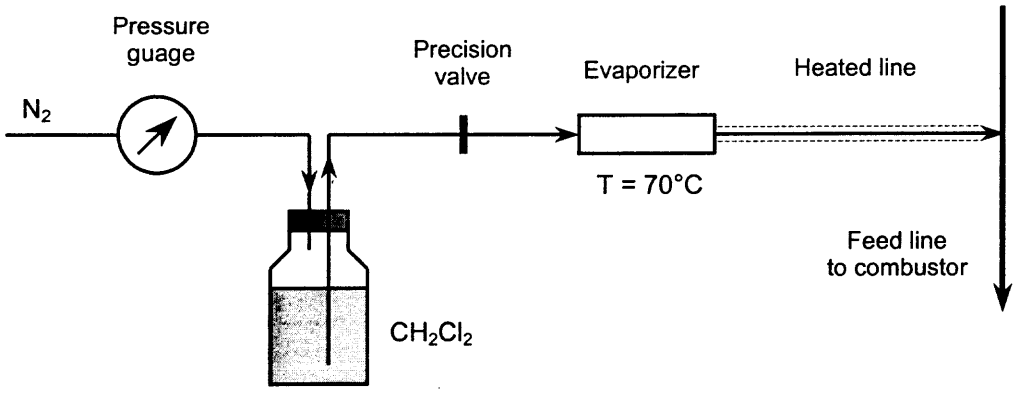


Figure 3.2 Schematic diagram of CH_2Cl_2 feed system.

precise metering valve. The metered liquid flow enters a gas-atomizing nozzle fitted into a heated tube. A metered low flow of nitrogen gas flows through the nozzle to atomize the liquid. Atomized methylene chloride becomes a vapor as it flows through the temperature controlled (70°C) heated pipe and tubing to the main feed line to the combustor.

Nitrogen gas, which is stored as a refrigerated liquid in a tank, is used for controlling the first stage combustor temperature. Addition of nitrogen gas to the main fuel-air mixture does not change its equivalence ratio, but does change the feed and product concentrations. This is considered in result analysis and modeling.

The fuel, air and nitrogen gas flow rates are measured by calibrated rotor flowmeters. The flowmeter flow rates are corrected as necessary for gas pressure, temperature, and molecular weight. The gas mixture is considered as ideal gas, and its actual flow rate is obtained from the equations

$$K = \sqrt{\left(\frac{P_a}{P_c}\right)\left(\frac{T_c}{T_a}\right)\left(\frac{W_c}{W_a}\right)} \tag{3.1}$$

$$V_a = KV_c \tag{3.2}$$

where K is a correction factor; P_a – actual metering pressure (psia); P_c – calibration pressure (psia); T_c – calibration temperature (K); T_a – actual metering temperature (K); W_c – molecular weight of gas for which meter was calibrated; W_a – molecular weight of metered gas; V_c – volumetric flow rate from flowmeter reading (standard units); V_a – actual volumetric flow rate (standard units).

After metering, the ethylene, air, dilution nitrogen and methylene chloride (when used) enter the main feeding line where they are mixed and enter the first stage of the reactor.

3.2 Two-Stage Reactor

An atmospheric pressure, two-stage reactor is used for this study. The first stage of the reactor is a jet-stirred toroidal combustion chamber. The chamber is made of castable high temperature alumina cement. In the outer torus wall, there are thirty two jets positioned 20 degrees off the radius. This is shown in Figure 3.3. Premixed combustible feed gas is introduced through these jets into the combustion chamber at subsonic velocity causing a swirling, highly turbulent, and intensely back-mixed combustion zone.

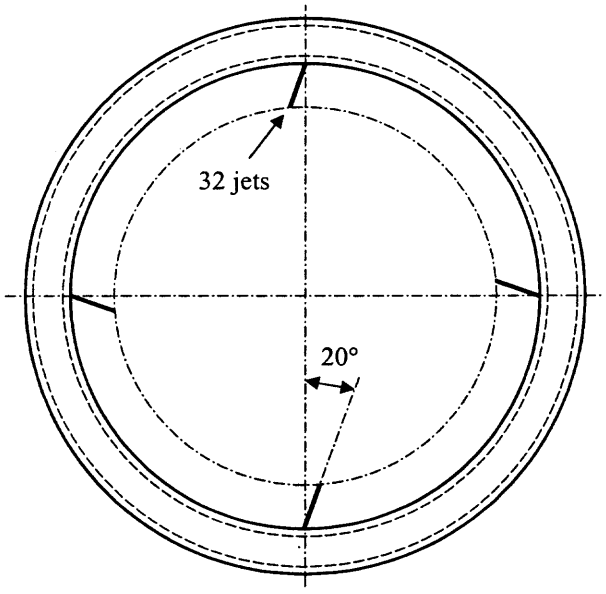


Figure 3.3 Fuel jets and jet ring in the first stage of the reactor.

The mixing in this zone has been described by Nenniger (Nenniger 1983) and Barat (Barat 1990). The first stage volume is 250 cm^3, and typical residence time ranges from 5 to 12 milliseconds, depending on feed rate and actual temperature. Typical axial bulk gas velocity is about 40-50 m/s resulting in Reynolds numbers on the order of 5×10^5. The first stage can be simulated as a perfectly stirred reactor (PSR) (Mao 1995).

Combustion gases exit the first stage pass over a flow straightener, and then enter the second stage of the reactor. The second stage is made of a precast alumina tube, 30 cm in length and 5 cm in inner diameter. Typical gas velocities in the second stage are in a range of 20-30 m/s yielding Reynolds numbers on the order of 3×10^5. The residence time in this stage is in the range of 15-25 milliseconds. This stage is simulated as a plug flow reactor (PFR) (Mao 1995). The overall schematic of a two-stage reactor used in this study is shown in Figure 3.4.

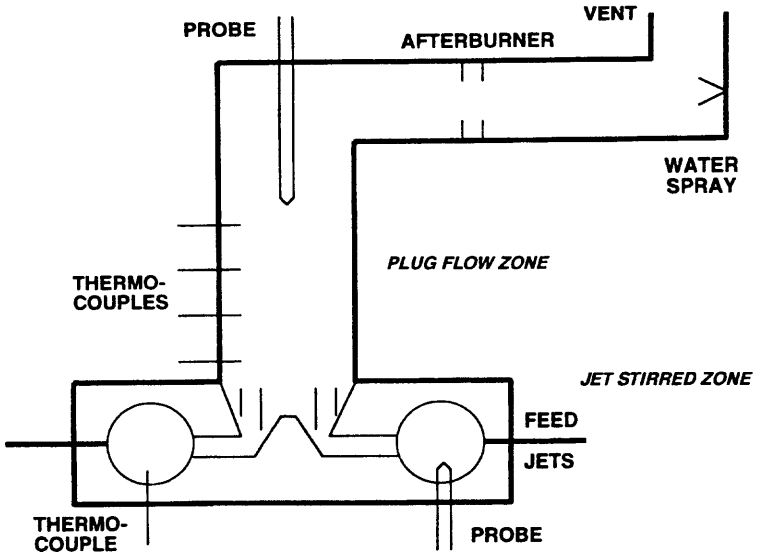


Figure 3.4 Schematic diagram of the two-stage reactor.

To reduce heat loss from the reactor, both stages are insulated with castable alumina. After the second stage outlet there is afterburner section where a large flow of air is injected in order to consume any unburned species (if fuel-rich) and to dilute the exhaust gas. Before venting, cooling water is sprayed into the hot flue gas.

The temperature in both stages is measured with uncoated type R (Pt/Pt + 13% Rh) micro-thermocouples. There is one thermocouple inserted from the bottom of the first stage, approximately 6 mm from the inside wall. Four such thermocouples are radially inserted into the second stage about 6 mm from the wall to measure temperature profile of the second stage. All thermocouples are monitored by digital thermometers.

3.3 Analytical System

3.3.1 Sampling

Sample gas is drawn from each stage by a metal bellows pump through two water-cooled stainless steel probes, the schematic of which is shown in Figure 3.5. The inner diameters of the probes are 1 mm and the outer diameters are 8 mm. The length of the PSR probe is 285 mm, and the length of the PFR probe is 590 mm. The first stage probe extends about 5-7 mm into the torus. The second stage probe is positioned at the second stage outlet,

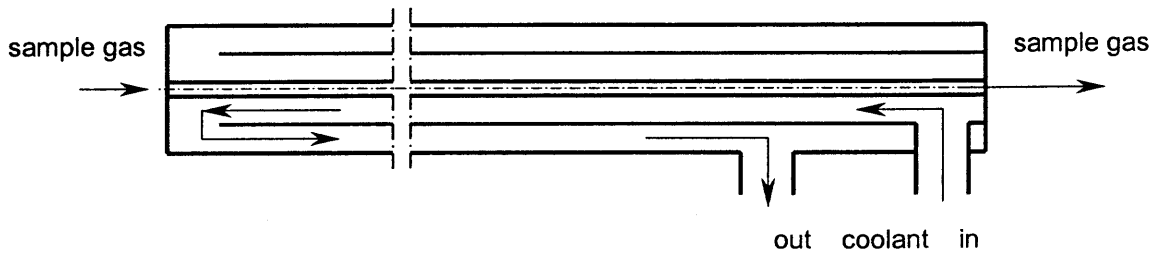


Figure 3.5 Schematic diagram of water-cooled sampling probe (not to scale).

though its position can be varied. Coolant water for the probes is preheated to about 40-50 °C by passing it through a heat removal coil at the exterior of the exhaust section. The coolant temperature is controlled by adjusting the coolant flow rate, which is monitored by a flow alarm system. In order to condense any water vapor from the sample gas before entering the analytical instruments, the sample gas is cooled in a low temperature (10°C) water bath. All droplets formed are removed in a knockout filter.

3.3.2 Hydrocarbon Analysis

The Hewlett-Packard Model 5890 gas chromatograph, which is used for hydrocarbon analysis, is equipped with two columns. One is a 6-foot long packed column (HayeSep T 80/100, stationary phase – ethyleneglycoldimethylacrylate polymer), which is used for separation of light hydrocarbons, such as methane (CH_4), ethylene (C_2H_4), acetylene (C_2H_2), and ethane (C_2H_6). This column is fed with a 6-port gas sample valve and equipped with 1 ml volume loop. The other column is a 30 m long, 0.53 mm inner diameter capillary column (AT-1, stationary phase – polydimethylsiloxane) used to separate relatively heavier volatile hydrocarbons such as benzene (C_6H_6). This capillary column is used in conjunction with the microtrap. Both columns are connected to flame ionization detectors (FIDs). For data acquisition and peak integration, two Hewlett-Packard 3396 Series II integrators are used.

The microtrap injection system used for benzene analysis, which is shown in Figure 3.6, includes the microtrap, a 14 cm long and 0.53 mm ID silica-lined stainless steel tube packed with 60 mesh Carbotrap C microsorbent. This microtrap is placed in front of GC capillary column in series with the gas sampling valve. An 8 ml sample of

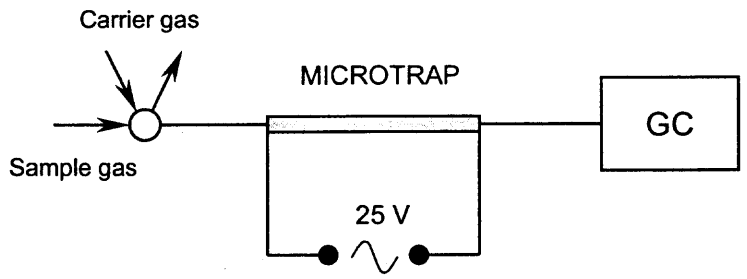


Figure 3.6 Schematic diagram of the microtrap injection system.

combustion gases from the gas-sampling valve is swept into the microtrap. The sorbent retains and focuses the heavier (e.g. benzene) and chlorinated organics while other gases pass through. Then the microtrap is rapidly heated by applying a 25 AC volt pulse of 1 second duration. This desorption results in a sharp injection band for GC separation. The focusing effect of the microtrap allows the analysis of relatively large (8 ml) volume of gas, thus lowering the detection limit. The column temperature is programmed from 30 °C to 110 °C at 15 °C/min. The retention times for each species are listed in Table 3.2.

Table 3.2 Retention Times of Investigated Compounds

Compounds		Time (min)
Methane	CH_4	0.643
Acetylene	C_2H_2	3.898
Ethylene	C_2H_4	2.382
Ethane	C_2H_6	2.645
Benzene	C_6H_6	3.637

3.3.3 CH_2Cl_2 Analysis

For analysis of CH_2Cl_2 the same gas chromatograph and AT-1 capillary column in conjunction with the same microtrap was used, but with some modifications. The only differences are that in this case microtrap was immersed in an ice-water bath, the duration of applied volt pulse was 2 seconds, and an electron capture detector (ECD) instead of an FID was used. Column temperature was kept steady at 35 °C. The retention time of methylene chloride was 1.7 min. Calibration of both columns is done using appropriate Scotty VI commercial gas standards.

3.3.4 O_2 Analysis

Oxygen concentration is determined by a Beckman Model 755 O_2 analyzer, which utilizes a paramagnetic method based on capability of the oxygen molecule to become a temporary magnet when placed in a magnetic field. The O_2 analyzer operates continuously on fresh sample gas.

3.3.5 CO_2 Analysis

In the 864/865 CO_2 analyzer, the method of non-dispersive infrared radiation produced from two separate energy sources that pass through two cells is used. One cell contains hydrogen (non-absorbing reference gas), the other cell contains the continuously flowing sample. CO_2 in the sample absorbs a portion of infrared radiation, which is related to its concentration in the sample. The difference in energy between the two cells is converted by a detector to a capacitance charge, which is proportional to the CO_2 concentration in the sample.

3.3.6 Overall Precision of Experimental Data

Precisions of experimental measurements of temperatures and concentrations are shown in the related figures by error bars. In general, after system was warmed up, which takes about 60-90 minutes, the reactor temperature fluctuated about ±10 K, and measurements of concentrations produced stable results, which are shown in Table 5.2.

CHAPTER 4

MODELING METHODS

4.1 Reactor Simulation

In order to simulate the two-stage reactor sequence, the general purpose CHEMKIN package (Glarborg, P. et al. 1989) is used.

4.1.1 Stirred Reactor Zone

In modeling of the stirred reactor zone, it is assumed that a steady premixed flow of fuel and oxidizer are introduced in such a way that highly intense turbulent mixing causes the contents of the reactor to be spatially uniform (Nenniger, J. et al. 1984). The reactor effluent conditions (temperature, composition) are assumed to be exactly the same as for the reactor contents. Therefore, the rate of conversion from reactants to products is controlled by chemical reaction rates and not by the mixing process. Another assumption is that the reactor walls are noncatalytic. Nominal residence time is deduced from the inlet volumetric flow rate and the reactor volume. A schematic representation of a perfectly stirred reactor is shown in Figure 4.1.

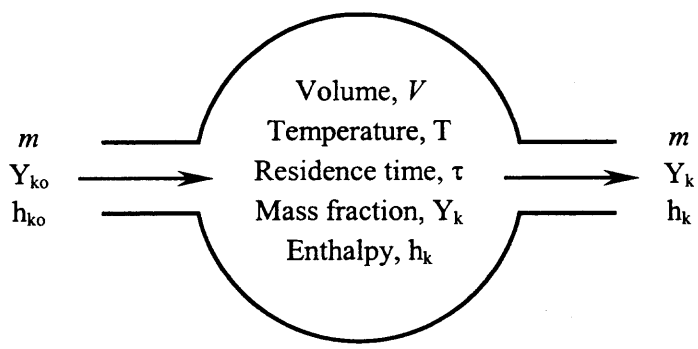


Figure 4.1 Schematic diagram of a perfectly stirred reactor.

The governing species balance equations for the PSR are:

$$m(Y_k - Y_{ko}) = \omega_k W_k V \tag{4.1}$$

where m is the mass flow rate, Y_k is the mass fraction of species k, Y_{ko} is the inlet mass fraction of species k, ω_k is the net molar rate of production by reaction of species k, W_k is the molecular weight of species k, and V is the PSR volume. For the total number of k species, there are k species balance equations.

The residence time is related to the reactor volume V and the mass flow rate as

$$\tau = \frac{\rho V}{m} \tag{4.2}$$

where the mass density ρ is calculated from the ideal gas equation of state

$$\rho = \frac{PW^*}{RT} \tag{4.3}$$

Here P is the pressure, T is the reactor temperature, R is the universal gas constant and W^* is the exiting mixture mean molecular weight.

4.1.2 Plug Flow Reactor Zone

It has been shown in previous studies that the linear turbulent flow secondary zone of the reactor can be simulated as a plug flow reactor (PFR) with high axial flow velocity (Mao et al, 1996). Schematic diagram of plug flow reactor zone used for modeling is shown in Figure 4.2.

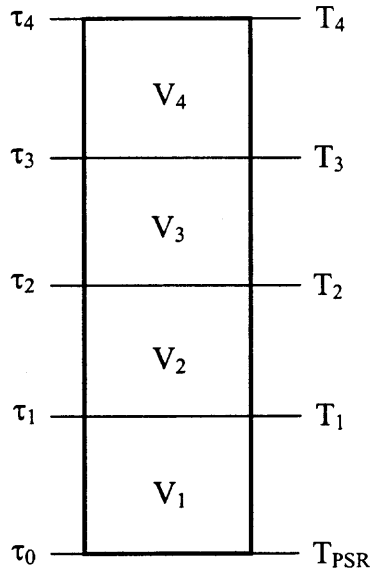


Figure 4.2 Schematic diagram PFR zone used in combustion modeling.

The governing species balance equations for species (1 to K) for the PFR are:

$$\frac{dY_k}{dt} = \frac{\omega_k W_k}{\rho} \tag{4.4}$$

The second stage has a temperature profile measured by four thermocouples. The measured temperatures are regressed using the method of least squares into the smooth form

$$T_{PFR} = T_{PSR} + B\tau + C\tau^2 + D\tau^3 \tag{4.5}$$

where T_{PSR} is observed PSR temperature, T_{PFR} is the interpolated PFR temperature, τ is PFR residence time, and B, C, D are cubic regression constants. In order to calculate residence times more accurately, real subvolumes, V_1, V_2, V_3, and V_4, between thermocouples were measured, and A, B, C, and D, cubic regression constants, are calculated from

$$M^{T} M \begin{bmatrix} A \\ B \\ C \\ D \end{bmatrix} = M^{T} \begin{bmatrix} T_{PSR} \\ T_1 \\ T_2 \\ T_3 \\ T_4 \end{bmatrix} \tag{4.6}$$

where matrix M is

$$M = \begin{bmatrix} 1 & \tau_0 & \tau_0^2 & \tau_0^3 \\ 1 & \tau_1 & \tau_1^2 & \tau_1^3 \\ 1 & \tau_2 & \tau_2^2 & \tau_2^3 \\ 1 & \tau_3 & \tau_3^2 & \tau_3^3 \\ 1 & \tau_4 & \tau_4^2 & \tau_4^3 \end{bmatrix} \tag{4.7}$$

and M^{T} is the transpose matrix. Typical temperature profile in the second stage is shown in Figure 4.3.

Residence times τ_0-τ_4 in each subvolume of PFR is calculated as

$$\tau_i = \frac{PV_i}{RMT_{iave}} \tag{4.8}$$

where V_i is an incremental PFR subvolume, P is total pressure (1 atm), R is the ideal gas constant, M is the inlet number of moles per second, and T_{iave} is the average temperature within the volume V_i. The total PFR residence time τ, used in equation (4.1) equals the sum of the incremental residence times for each PFR subvolume V_i.

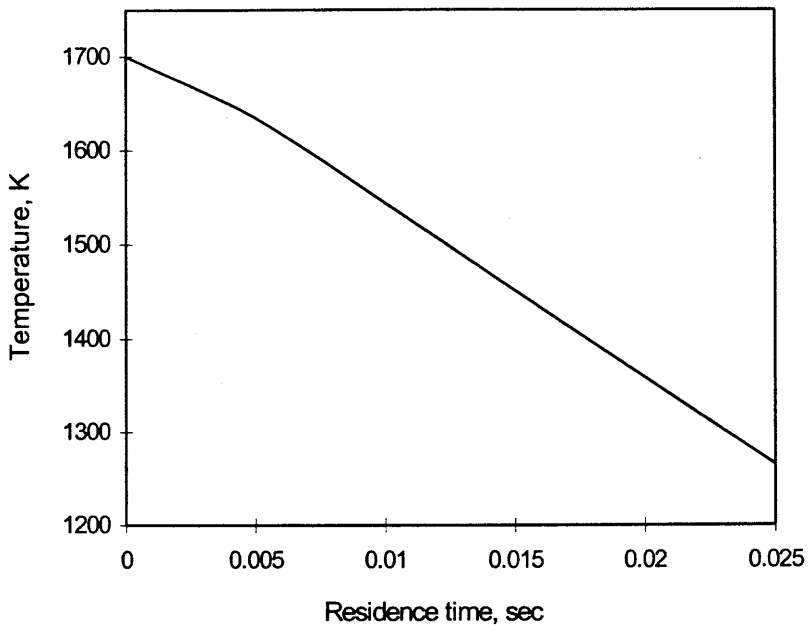


Figure 4.3 Typical temperature profile in the second stage of the reactor.

4.2 Reaction Mechanism

In conjunction with the reactor simulation, a detailed elementary reaction mechanism is necessary to generate the species net reaction rates ω_k, which results from competition between all chemical reactions involving that species. A CHEMKIN subroutine generates ω_k for species k based upon the prevailing conditions of temperature and species concentrations, and the user-supplied reaction mechanism.

A reaction mechanism is a set of reversible elementary gas phase chemical reactions with kinetic rate constants and a species thermodynamic property set. Provided with each reaction *i* is the forward kinetic rate constant, k_{fi} assumed to have the following general temperature dependence:

$$k_{fi} = A_i T^{n_i} \exp\left(\frac{-E_i}{RT}\right) \tag{4.9}$$

where A_i, n_i, and E_i are fitted parameters specific to the ith reaction that are provided with mechanism. All reactions are treated as elementary. Hence, the reverse rate constant k_{ri} is calculated by CHEMKIN from the reaction equilibrium constant, K_i according to:

$$k_{ri} = \frac{k_{fi}}{K_{ci}} \tag{4.10}$$

The equilibrium constant K_{ci} is calculated by CHEMKIN as an equilibrium constant in pressure units K_{pi} from a user-supplied database of thermodynamic properties (standard heats of formation, entropies, and heat capacities as a function of temperature)

$$K_{pi} = \exp\left(\Delta S^\circ_i / R - \Delta H^\circ_i / RT\right) \tag{4.11}$$

where

$$\Delta S^\circ_i / R = \Sigma \nu_{ki} \left(S^\circ_k / R\right) \tag{4.12}$$

$$\Delta H^\circ_i / RT = \Sigma \nu_{ki} \left(H^\circ_k / RT\right) \tag{4.13}$$

Here, the symbol Δ refers to the change that occurs in passing completely from reactants to products in the ith reaction.

Then the equilibrium constant K_{ci} is obtained from relationship

$$K_{ci} = K_{pi} \left(P_{atm} / RT\right)^{\Sigma \nu_{ki}} \tag{4.14}$$

and used in equation (4.10).

An example of the input file for the two-stage simulation program is shown in Appendix A. The thermodynamic data and reaction mechanisms used for C_2H_4/Air/CH_2Cl_2 combustion, and for C_6H_6 formation during C_2H_4/Air combustion are shown in the Appendix C and D respectively.

The reaction mechanisms, which are used for modeling are primarily drawn from literature (Ho, 1993). The elementary reaction mechanism (kinetics and thermodynamic properties) used in this work has been used successfully in similar modeling of C_2H_4/O_2 flames (Marinov et al, 1996).

4.3 Rate-of-Production Analysis

In order to determine what is the contribution of each reaction to the production or destruction of key species, rate-of-production (ROP) analysis is performed. The net generation and the destruction rates for selected species, including breakdowns of these net rates into the rates of each contributing reaction, are calculated by CHEMKIN subroutines. The net molar rate of production by reaction ω_k of species k is calculated by

$$\omega_k = \sum_{i=1}^{I} \nu_{ki} q_i \tag{4.15}$$

where ν_{ki} are the stoichiometric coefficients of species k in reaction i, and q_i is the rate of progress for the reaction i. The normalized rate-of-production C_{ki}, to the ROP of species k from reaction i is calculated from

$$C_{ki} = 100 \frac{\nu_{ki} q_i}{\sum_{i=1}^{I} \nu_{ki} q_i} \tag{4.16}$$

From C_{ki}, one can recognize how reaction i contributes to the formation or consumption of species k. The information obtained from the ROP analysis is used for identification of production and destruction pathways for species of interest, and for construction of pathways for reactant consumption and product formation.

4.4 Probe Quench Effect Calculation

When the hot gas mixture enters a cooled probe and rapidly cools down, all free radicals must combine to form stable species. In order to be able to compare concentrations of measured stable compounds with their simulated concentrations, probe quench effect calculations are performed. In this case, CHEMKIN code uses subroutine in which cooled probe tube is considered as a plug flow reactor with the residence time 0.002 sec during which temperature drops to 300K. For these probe reactions, the same thermodynamic data and reaction mechanism is used as for main reactor.

CHAPTER 5

COMBUSTOR CHARACTERIZATION AND VALIDATION

5.1 Experimental Conditions and Results

In order to validate the experimental combustion system, a series of runs with ethylene and air were made, under various feed conditions, in the two-stage combustor. These included several fuel lean and fuel rich combustion runs. Reactor temperature and species concentrations were measured in all runs, and detailed modeling with known reaction mechanisms was performed for representative fuel lean and fuel rich cases. The comparison between the measured data and model prediction served as the validation of the system.

The feed conditions are characterized by the fuel equivalence ratio, ϕ, which is defined as the actual fuel to air ratio divided by the stoichiometric fuel to air ratio:

$$\phi = \frac{(F/A)_{actual}}{(F/A)_{stoich}} \tag{5.1}$$

where F is the volumetric or molar flow rate of fuel in the feed mixture, and A is the volumetric or molar flow rate of air in the feed mixture. For a fuel-lean system, ϕ is less than 1; while for fuel-rich systems, ϕ is greater than 1. At stoichiometric conditions, $\phi = 1$. The stoichiometric condition is determined based on the assumption of complete combustion to the most thermodynamically stable products. In the case of ethylene and methylene chloride combustion, the global stoichiometry is

$$C_2H_4 + 3O_2 = 2CO_2 + 2H_2O \tag{R5.1}$$

$$CH_2Cl_2 + O_2 = CO_2 + 2HCl \tag{R5.2}$$

Using equation (5.1), and reactions (R5.1), (R5.2), the equivalence ratio equation for ethylene combustion case can be obtained as

$$\phi = \left(\frac{3}{0.21}\right)\left(\frac{\text{Ethylene}}{\text{Air}}\right)_{\text{actual}} \tag{5.2}$$

and for methylene chloride combustion

$$\phi = \left(\frac{1}{0.21}\right)\left(\frac{\text{Methylene chloride}}{\text{Air}}\right)_{\text{actual}} \tag{5.3}$$

where the name of compound in each equation stands for its volumetric or molar flow rates.

When fuel mixture containing two of these compounds is used, the equivalence ratio can be calculated as

$$\phi = \frac{\left(\dfrac{\text{Ethylene} + \text{Methylene chloride}}{\text{Air}}\right)_{\text{actual}}}{\left(\dfrac{\text{Ethylene} + \text{Methylene chloride}}{\dfrac{3}{0.21}\text{Ethylene} + \dfrac{1}{0.21}\text{Methylene chloride}}\right)_{\text{stoich.}}} \tag{5.4}$$

In cases when dilution nitrogen is used in the feed stream, it does not change the equivalence ratio, but it changes the feed composition and total flow rate. This must be considered in calculations of the concentrations of the products.

The experimental conditions for fuel-lean and fuel-rich combustion runs are shown in Tables 5.1 and 5.2. The first stage temperature was held at 1623 K with the addition of dilution N_2 gas. The total gas mass rates were typically in the range of 6.5-7.2 grams/second.

The two-stage combustor used in this study has highly turbulent gas flow and small temperature gradients, because of hot reactor walls. Therefore, heat radiation from the thermocouple bead to reactor walls can be neglected and corrections due to temperature measurement errors are not needed.

Table 5.1 Feed Conditions of Fuel-lean Runs

Feed	**Flow rate (mole/sec)**	
	Case 1	**Case 2**
C_2H_4	0.00847	0.00847
Air	0.17611	0.13467
Diluent N_2	0.05326	0.10816
Equivalence ratio	0.69	0.9

Table 5.2 Feed Conditions of Fuel-rich Runs

Feed	**Flow rate (mole/sec)**			
	Case 3	**Case 4**	**Case 5**	**Case 6**
C_2H_4	0.01131	0.01432	0.01797	0.02382
Air	0.13467	0.14503	0.15539	0.17611
Diluent N_2	0.09605	0.07990	0.05407	0.03712
Equivalence ratio	1.2	1.41	1.65	1.93

Combustion gas was sampled from both the first stage and the outlet of the second stage of the reactor. Concentrations of O_2, CO_2, CH_4, C_2H_2, C_2H_4, C_2H_6, and C_6H_6 were measured.

For hydrocarbon analysis by GC, injections from the 1 ml sample valve onto the packed column, and the 8 ml sample valve onto microtrap, were made at the same time in parallel. The analytical method is shown in Figure 5.1 for microtrap analysis.

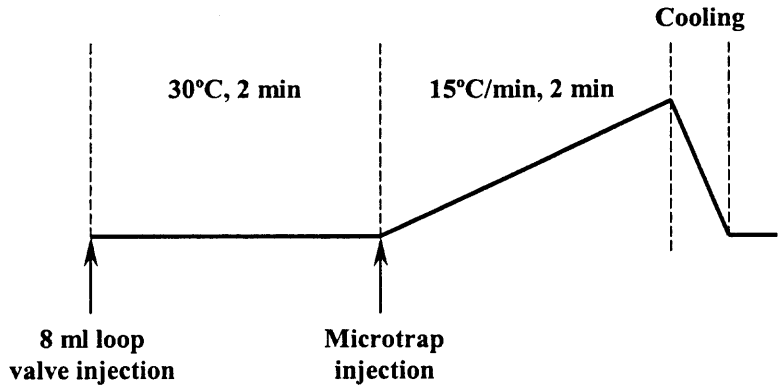
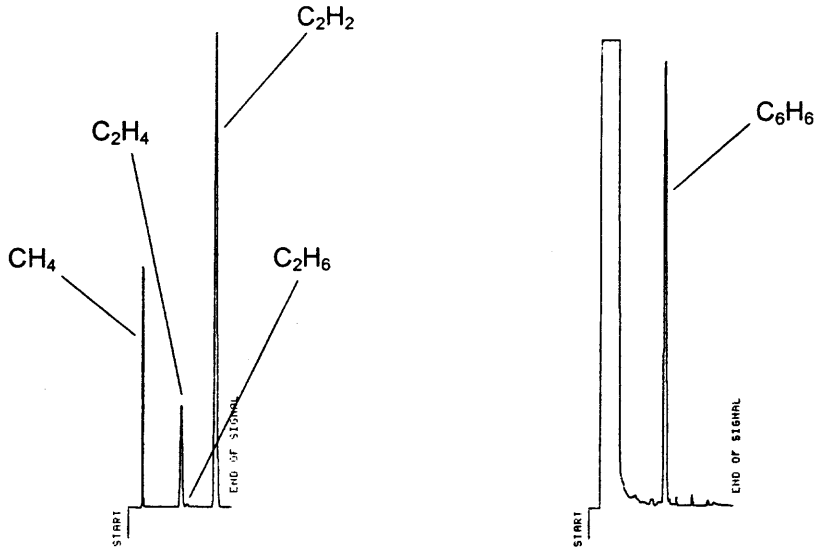


Figure 5.1 GC oven temperature programing and microtrap injections for C_6H_6 analysis.

Microtrap injection (by rapid heating) into the capillary column was made two minutes after the 8 ml loop gas sampling valve injection. This allowed all unretained compounds to clear the capillary column. The temperature program was initiated as soon as the microtrap injection was made. A typical gas chromatogram is shown in Figure 5.2. Reproducibility of retention time and peak areas are shown in the Table 5.2.



Light hydrocarbon analysis Benzene analysis

Figure 5.2 Typical gas chromatograms from combustion runs.

Table 5.2 Reproducibility of Injections

	Injection valve				Microtrap
	CH_4	C_2H_2	C_2H_4	C_2H_6	C_6H_6
Retention time, min	0.64	3.90	2.38	2.64	3.64
RSD of retention time	0.11	0.15	0.16	0.14	0.05
RSD of peak area	0.12	1.55	1.63	1.91	1.76

RSD – relative standard deviation.

The microtrap produced sharp peaks. The presence of the benzene was confirmed using an off-line analysis of a grab sample by GC-mass spectrometry (model Hewlett-Packard 5988A) equipped with a similar capillary column.

Dependencies of measured concentrations of O_2, CO_2, CH_4, C_2H_2, C_2H_4+C_2H_6, and C_6H_6 on equivalence ratio and their comparison with model predictions are shown in Figures 5.3, 5.4, 5.5, 5.6, 5.7. These gas samples were taken from the first stage and the outlet of the second stage with total residence times of approximately 7 and 25 milliseconds, respectively. Concentrations of C_2H_6 emissions in all combustion runs were very low (about 10% of the C_2H_4 concentration or less). Since the peaks elute so close together, the estimated C_2H_6 concentration is added to C_2H_4 and reported together.

Data on O_2 and CO_2 concentrations are shown on Figures 5.3 and 5.4. With increasing equivalence ratio, O_2 monotonically decreases, effectively dropping to or below

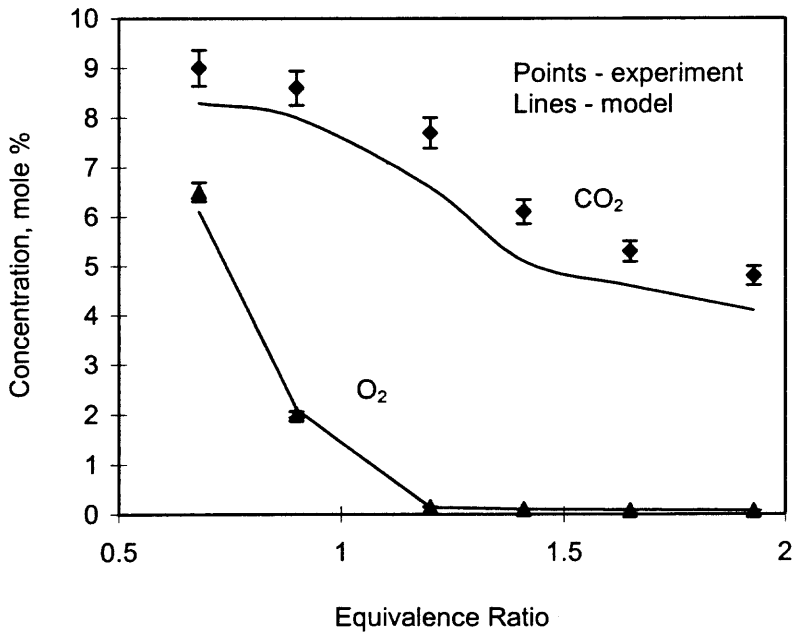


Figure 5.3 Concentrations of O_2 and CO_2 in the PSR zone of the combustor.

the detection limit for $\phi > 1.1$. For $\phi > 1.1$, CO_2 decreases slowly with increasing equivalence ratio.

With O_2 effectively consumed, not only does conversion of CO to CO_2 shut down, but carbon-based radicals undergo combination reactions to form higher molecular weight species, such as benzene (Mao, 1995). This effect is even more pronounced in the second stage outlet. The well-mixed first stage accepts the fresh feed, including O_2, while there is little or no mixing in the second stage (plug flow) with O_2 almost or totally consumed. In general, model-predicted concentration profiles for O_2 and CO_2 compare reasonably well with the observed data.

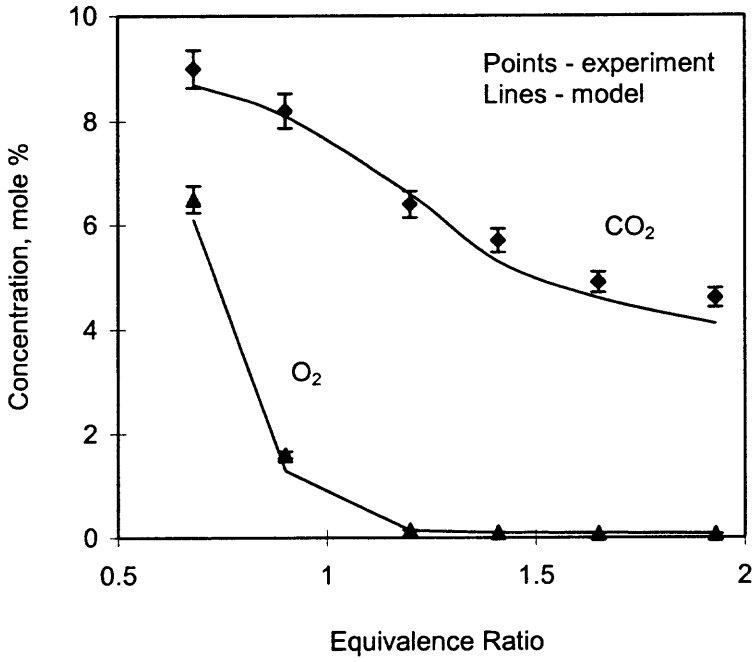


Figure 5.4 Concentrations of O_2 and CO_2 in the PFR zone of the combustor.

As shown in Figures 5.5, 5.6, and 5.7 that hydrocarbon species concentrations rise monotonically with ϕ. Hydrocarbon concentrations are negligeble for ϕ less than 1.3. There is some deviation of the model curves for CH_4 and C_2H_4+C_2H_6 from the experimental data at the higher equivalence ratios, shown in Figures 5.5 and 5.6, but the simulations of C_2H_2, which is shown in Figure 5.7, are good. The lack of a significant difference between the first stage and the second stage outlet for CH_4 suggests that there is little net production in the second stage.

There is a large decrease in C_2H_4+C_2H_6 concentrations from the first stage to the second stage outlet. The fresh feed entering the first stage keeps the C_2H_4 relatively high, but the plug flow nature of the second stage causes a rapid consumption of remaining reactant fuel, even under fuel-rich conditions. This effect is also evident, though to a much

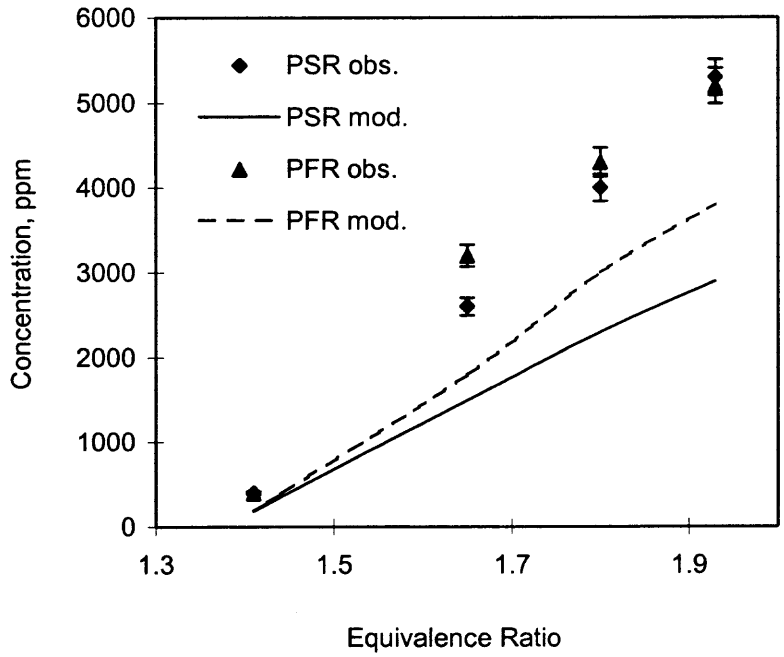


Figure 5.5 PSR zone and PFR zone CH_4 concentrations as a function of equivalence ratio.

lesser degree, with C_2H_2. Under these fuel-rich conditions, C_2H_4 rapidly converts to C_2H_2, which can either oxidize or proceed to higher hydrocarbon species (Brouwer, 1992).

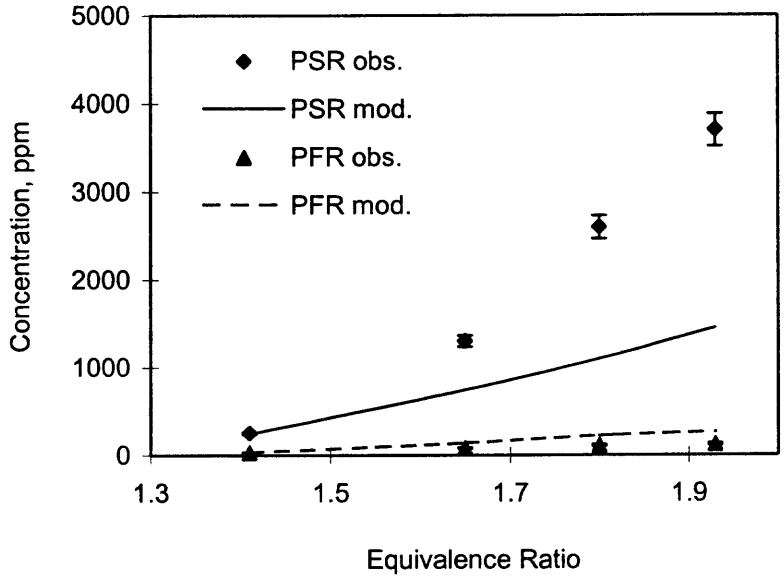


Figure 5.6 PSR zone and PFR zone C_2H_4+C_2H_6 concentrations as a function of equivalence ratio.

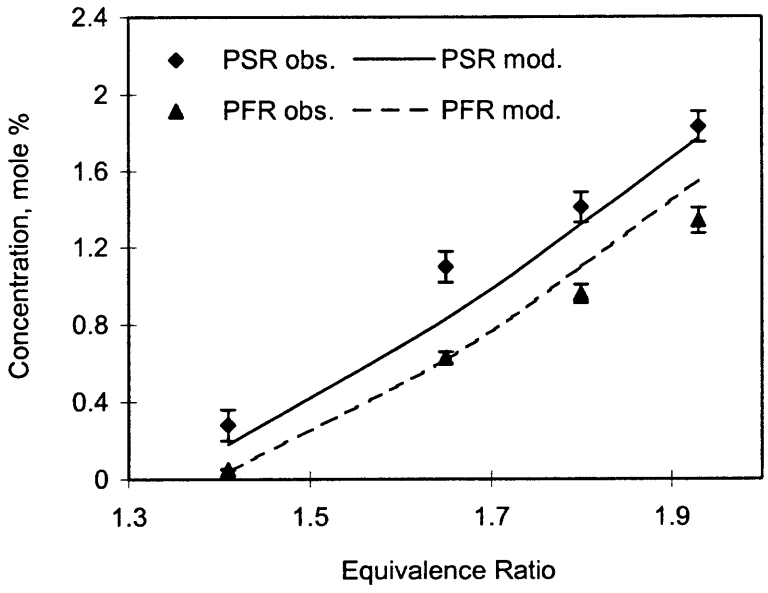


Figure 5.7 PSR zone and PFR zone C_2H_2 concentrations as a function of equivalence ratio.

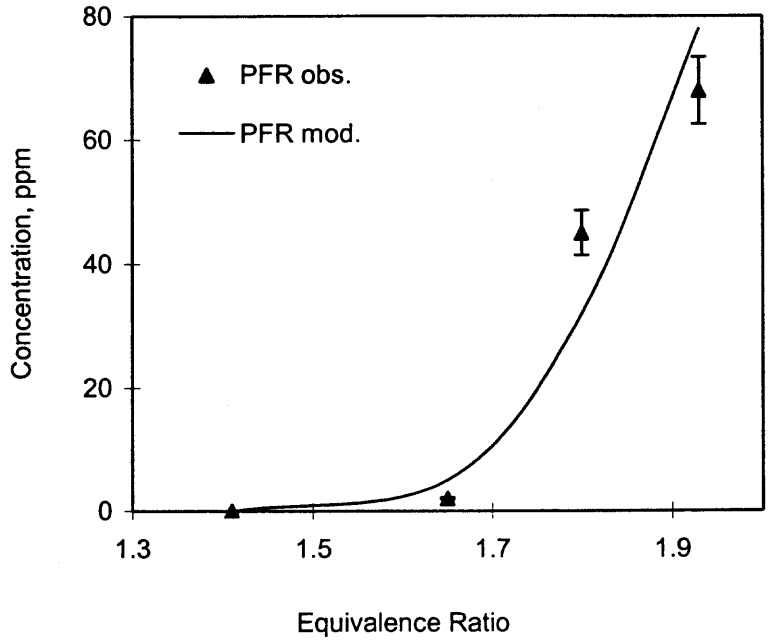


Figure 5.8 PFR zone C_6H_6 concentrations as a function of equivalence ratio.

As ϕ increases, the absence of oxygen species leads to more reactions between hydrocarbon species, especially those leading to molecular weight growth. The concentration of C_2H_2 rises rapidly, as ϕ increases. Under such fuel-rich conditions, C_2H_2 is a known precursor to benzene formation (Frenklach and Wang, 1994). As shown in Figure 5.7 benzene, detected from sub ppm to tens of ppm levels, rises sharply for $\phi >$ 1.65. The model simulations employed the Marinov mechanism (Castaldi et al., 1996). The agreement with the data is good.

5.2 Summary

A two-zone turbulent flow reactor has been validated for use in combustion studies. Microtrap gas chromatography has been demonstrated for on-line, trace monitoring of

combustion of ethylene in air. This method has shown high precision and short analysis time. In addition, light hydrocarbons (methane, ethylene, acetylene and ethane) were monitored by more conventional methods. Modeling with PSR+PFR reactor simulation code using detailed reaction mechanisms predicted reasonably well the experimental data in both the first and the second stages. These results represent an important validation of the experimental facility prior to the following studies with methylene chloride.

CHAPTER 6

BENZENE FORMATION AND DESTRUCTION PATHWAYS

Given a temperature, pressure, and complete set of species concentrations, calls to selected CHEMKIN subroutines calculate the net generation rates for selected species, including breakdowns of these net rates into the rates of each contributing elementary reaction. The contribution C_{ki} to the rate of production of species k from reaction *i* is given by:

$$C_{ki} = n_{ki} \times q_i \tag{6.1}$$

where q_i is the rate of progress of reaction *i*, and n_{ki} is the stoichiometric coefficient for species k in reaction *i*. Contributions below 5% are not reported. The normalized contribution NC_{ki} is given by:

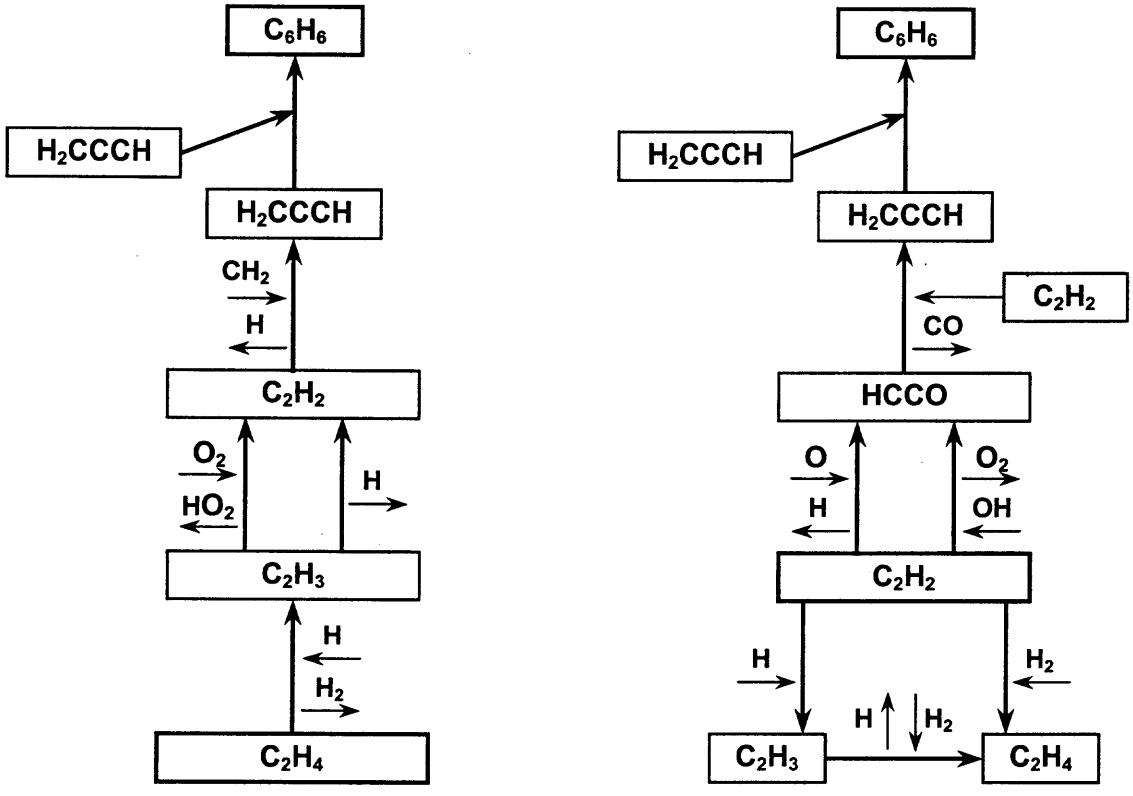
$$NC_{ki} = 100 \times \frac{n_{ki} \times q_{ki}}{\omega_k} \tag{6.2}$$

Such information is used to identify the important chemical pathways accounting for reactant, intermediate, and product formation and destruction.

Such calculations were performed for the PSR zone and for the outlet of the PFR zone at total residence times of 0.007 and 0.029 sec respectively for the ϕ = 1.93 case. The calculations have shown that the dominant routes to benzene are different in the PSR and PFR zones and are shown on Figure 6.1.

In the PSR the fuel undergoes an H abstraction to form • C_2H_3 (vinyl) radical:

$$C_2H_4 + H = \bullet C_2H_3 + H_2 \tag{R6.1}$$



First Stage (PSR)

Second Stage (PFR) outlet

Figure 6.1 Major pathways to C_6H_6 formation in the first and second stages.

The vinyl radical then forms C_2H_2 in two major ways. It undergoes an H atom elimination or it combines with molecular oxygen to form energized complex which then eliminates $\bullet HO_2$:

$$\bullet C_2H_3 = C_2H_2 + \bullet H \qquad \text{(R6.2)}$$

$$\bullet C_2H_3 + O_2 = C_2H_2 + \bullet HO_2 \qquad \text{(R6.3)}$$

A portion of C_2H_2 reacts with available $\bullet O$ atom to form a complex which decomposes to $\bullet CH_2$ and CO:

$$C_2H_2 + \bullet O = \bullet CH_2 + CO \qquad \text{(R6.4)}$$

Then C_2H_2 combines with $\bullet CH_2$ to form $\bullet H_2CCCH$, two of which combine together to form C_6H_6:

$$C_2H_2 + \bullet CH_2 = \bullet H_2CCCH + \bullet H \quad \text{(R6.5)}$$

$$\bullet H_2CCCH + \bullet H_2CCCH = C_6H_6 \quad \text{(R6.6)}$$

The importance of the C_3 species path to benzene has been suggested recently by Oulundsen and Westmoreland (2000).

The model-calculated rates of production (ROP) and consumption (ROC) of benzene are shown in Figure 6.2. In the PSR zone, ROC is close to ROP as production balances destruction. However, at outlet of the PFR zone (residence time 0.029 sec), with lower temperature and lack of oxygen species, rate of benzene production is much higher.

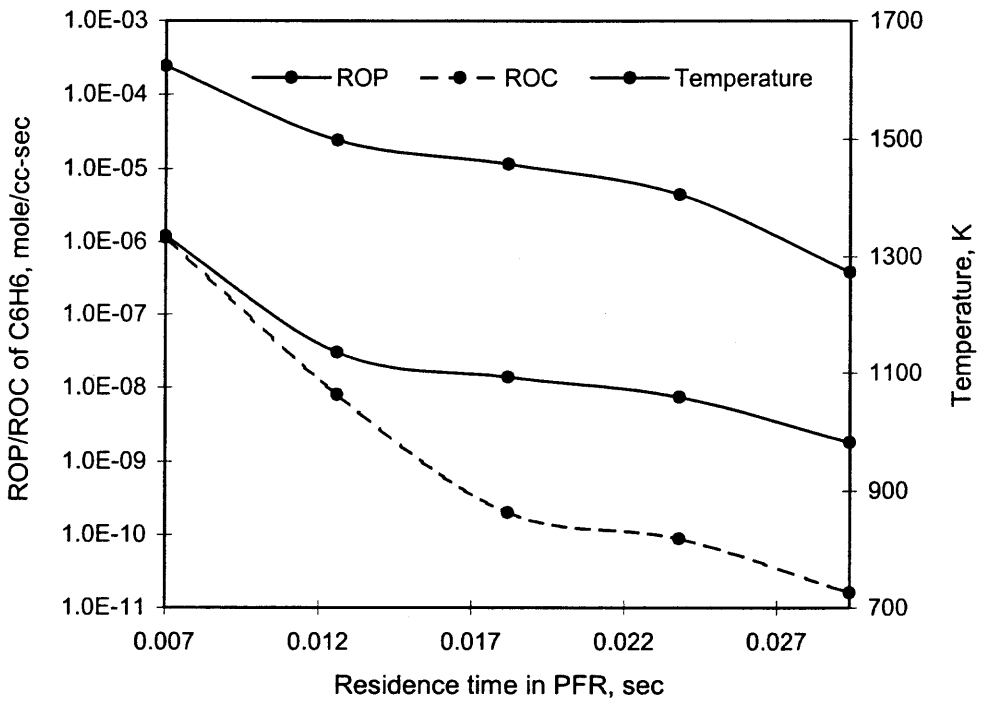


Figure 6.2 Production/consumption rates for C_6H_6.

The C_2H_2 plays a major role in benzene formation in the outlet of the PFR but in a slightly different way. C_2H_2 undergoes reactions with O and O_2 to form •HCCO radical.

$$C_2H_2 + \bullet O = \bullet HCCO + \bullet H \quad \text{(R6.7)}$$

$$C_2H_2 + O_2 = \bullet HCCO + \bullet OH \quad \text{(R6.8)}$$

Then •HCCO combines with C_2H_2 to produce $\bullet H_2CCCH$ and CO. Two $\bullet H_2CCCH$ then combine together to form C_6H_6.

$$\bullet H_2CCCH + \bullet H_2CCCH = C_6H_6 \quad \text{(R6.9)}$$

The C_2H_2 concentration in the PFR outlet, as shown in Figure 5.7, is close to its concentration in PSR but now rate of consumption of C_2H_2 is much higher. The ROP and ROC for C_2H_2 are shown in Figure 6.3.

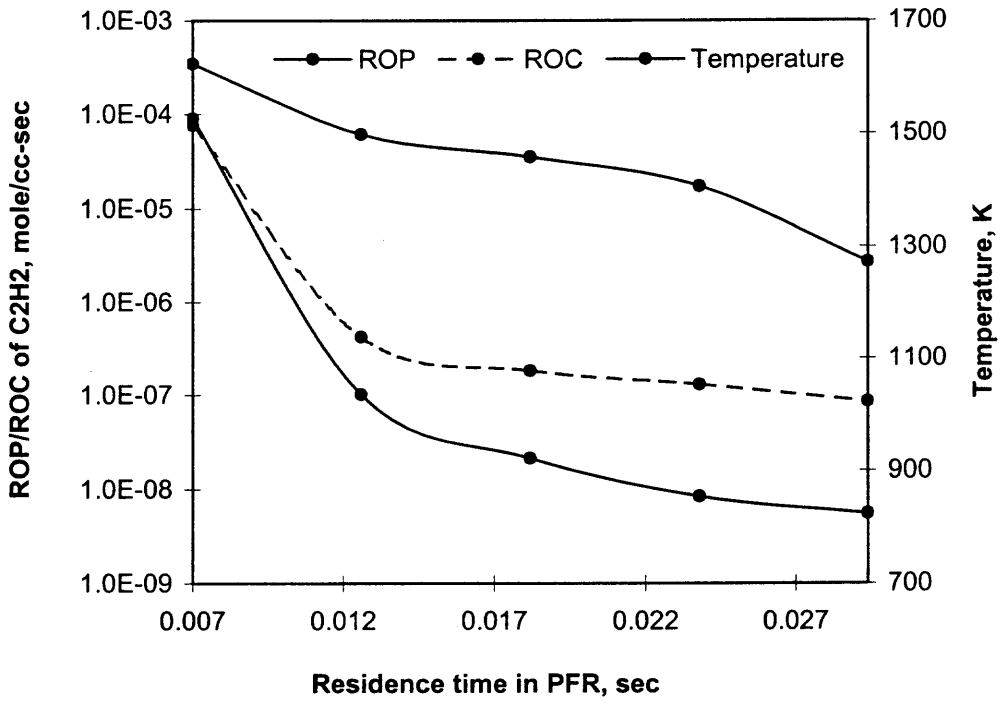


Figure 6.3 Production/consumption rates for C_2H_2 .

The C_2H_2 undergoes intensive consumption to form other hydrocarbons. In those conditions at $\tau = 0.029$ sec, the initial point to benzene formation is C_2H_2 not C_2H_4 as in PSR at $\tau = 0.007$ sec. The concentration of C_2H_2 at the outlet of PFR is much higher then C_2H_4, and C_2H_4 in these conditions is formed intensively. The ROP and ROC for C_2H_4 are shown in Figure 6.4:

$$C_2H_2 + H_2 = C_2H_4 \quad \text{(R6.10)}$$

$$\bullet C_2H_3 + H_2 = C_2H_4 + \bullet H \quad \text{(R6.11)}$$

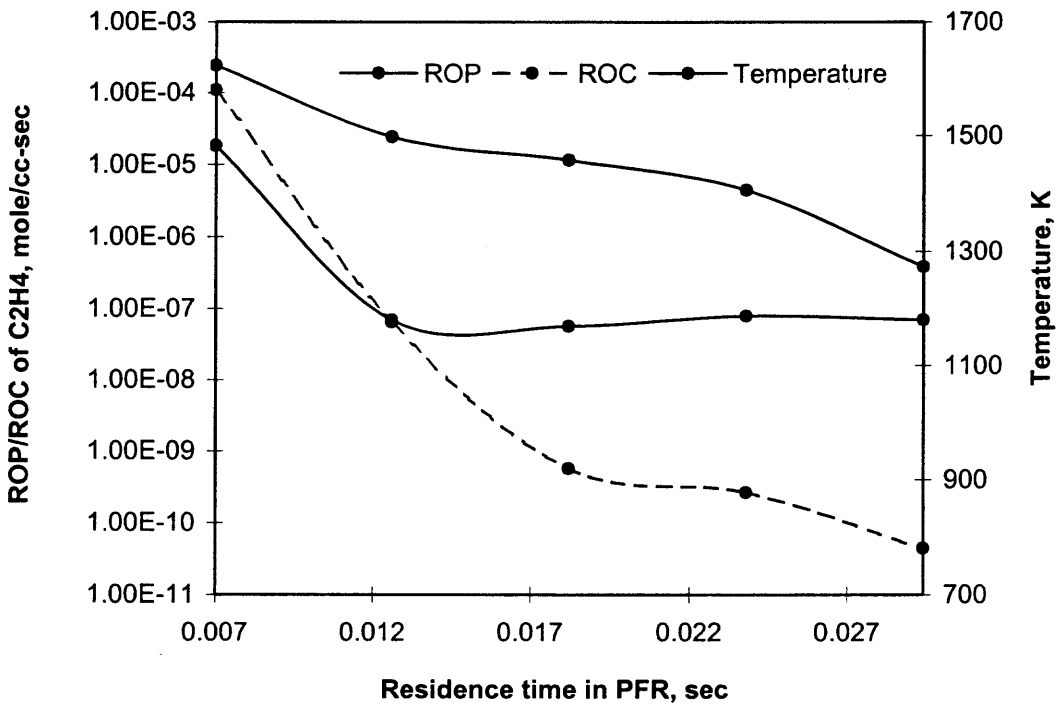


Figure 6.4 Production/consumption rates for C_2H_4.

Rate of production of benzene is higher than rate of consumption in the entire PFR zone. However, pathways to benzene consumption in the PSR and PFR are totally

different. While in PSR, major portion of benzene (normalized ROP = -0.823) undergoes the reaction of abstraction of H to form $\bullet C_6H_5$ (which then rapidly undergoes oxidation)

$$C_6H_6 + \bullet H = \bullet C_6H_5 + H_2 \qquad \text{(R6.12)}$$

large portion of benzene in the outlet of PFR (normalized ROP = -0.702) is consumed by reaction

$$C_6H_6 + \bullet H = cyC_6H_7 \qquad \text{(R6.13)}$$

to form higher molecular weight hydrocarbon radicals.

The CHEMKIN simulations show that at different combustion conditions, and species composition major pathways to C_6H_6 formation are different. At the first stage of the combustor with higher temperature and O_2 concentration, the rate of consumption of benzene is close to its production rate, while in the second stage with lower temperature and depleted O_2 the C_6H_6 is formed intensively. Initial point to C_6H_6 formation in the second stage is C_2H_2, and the major benzene consumption reaction is the addition of H atom and formation of higher hydrocarbons. In the first stage C_6H_6 eliminates H atom and undergoes destruction.

CHAPTER 7

COMBUSTION OF METHYLENE CHLORIDE

7.1 Baseline Cases

Two baseline cases were C_2H_4/air combustion without CH_2Cl_2 in the feed. The first base case was fuel-lean at fuel equivalence ratio $\phi = 0.7$. The measured temperature in the first stage was 1700 K, with a residence time of 0.010 seconds (at reaction temperature). Species concentrations were measured in the first stage and at the outlet of the second stage. The temperature at the outlet of the second stage was 1252 K. The mean second stage residence time was 0.025 seconds. The feed conditions and measured CO_2 and O_2 concentrations for this run are shown in Table 7.1.

The second base case is fuel-rich combustion run at $\phi = 1.4$. Dilution nitrogen was added in both cases to control the first stage temperature at 1700 K. Feed conditions and measured concentrations of O_2, CO_2, and light hydrocarbons are shown in Table 7.2.

7.2 CH_2Cl_2 Loaded Cases

Methylene chloride was added to the feed to examine its effect on the combustion process and the resulting emission levels. Of special interest was the destruction and removal efficiency of the CH_2Cl_2 (simulated waste). The concentrations of methylene chloride in the main feed were set at 2, 10, 50, 80, 200, 400, 580, 800, 930, 1150, 1350 ppm. Combustion runs were made at conditions as shown in Tables 7.1 and 7.2 ($\phi = 0.7$ and 1.4). The diluent nitrogen was added to keep PSR zone temperature at 1700 K. The emission stream was monitored using on-line chromatograph for organics, and the on-line

industrial stack gas analyzer (continuous) to determine the concentrations of O_2 and CO_2. Measured and predicted concentrations of these species are shown in Figures 7.1-7.5.

Table 7.1 Feed Concentration for the Fuel-lean Case (ϕ= 0.7)

Feed	Flow rate (mole/sec)
C_2H_4	0.00663
Air	0.13594
Diluent N_2	0.03252
Methylene Chloride CH_2Cl_2	0
Equivalence Ratio	0.7

Outlet Concentrations (mole fractions)

	PSR		PFR (outlet)	
	(experiment)	(model)	(experiment)	(model)
CO_2	6.0E-2	5.8E-2	6.3E-2	6.1E-2
O_2	4.6E-2	4.3E-2	4.3E-2	4.2E-2
CH_4	*		*	
C_2H_2	*		*	
C_2H_4	*		*	

* Below detection limit

Table 7.2 Feed Concentration for the Fuel-rich Case (ϕ= 1.4)

Feed	Flow rate (mole/sec)
C_2H_4	0.01046
Air	0.10615
Diluent N_2	0.58680
Methylene Chloride CH_2Cl_2	0
Equivalence Ratio	1.4

Measured Species Concentrations (mole fractions)

	PSR		PFR (outlet)	
	(experiment)	(model)	(experiment)	(model)
CO_2	3.1E-2	3.1E-2	3.3E-2	3.2E-2
O_2	1.1E-3	1.1E-3	*	1.2E-7
CH_4	3.3E-4	3.0E-4	7.3E-4	5.9E-4
C_2H_2	1.6E-3	1.6E-3	9.2E-4	7.5E-4
C_2H_4	1.4E-4	1.4E-4	1.3E-5	1.3E-5

* Below detection limit

7.3 Experimental Observations and Model Predictions

As shown in Figure 7.1, the concentration of O_2 in the first and the second stages remained essentially constant, with increasing feed concentration of CH_2Cl_2 in the fuel-lean case. This is expected since O_2 is in excess during fuel-lean combustion. However,

for fuel-rich runs at $\phi = 1.4$, where O_2 is the limiting reagent, and a good indicator of combustion efficiency, the O_2 concentrations in the first stage steadily increased with the inlet CH_2Cl_2 concentrations. This is shown in Figure 7.2. This result is consistent with data by Brouwer et al. (1992) and Mao (1995) for fuel-rich methyl chloride (CH_3Cl) combustion. The plug flow nature of the second stage resulted in complete consumption of the unreacted O_2. Under these conditions, the concentrations of unburned hydrocarbons, such as CH_4, C_2H_2, C_2H_4, which are considered as PICs, increased slightly with inlet CH_2Cl_2 concentrations. These results are shown in Figures 7.4 and 7.5, and are also consistent with those observed by Mao (1995).

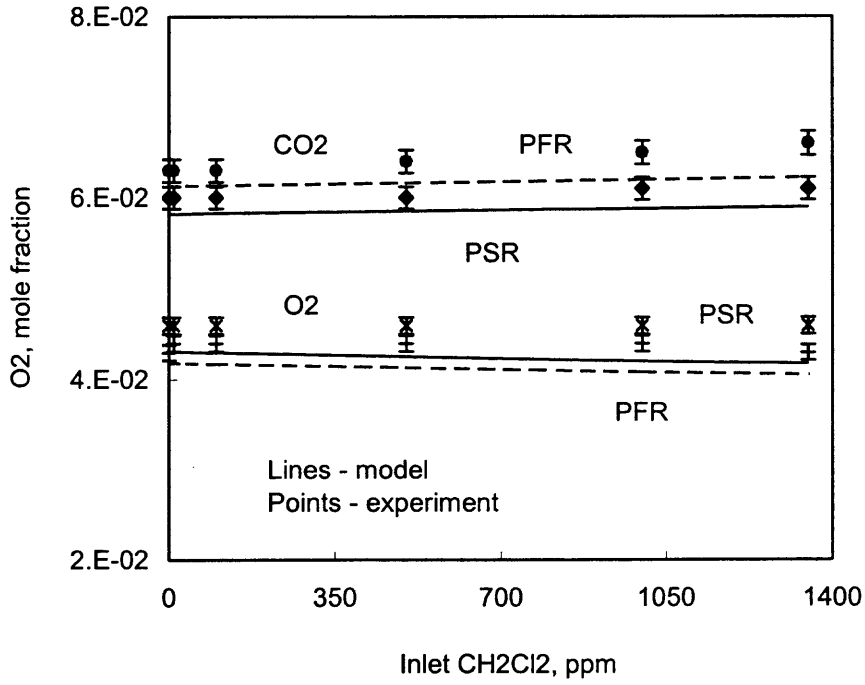


Figure 7.1 Concentrations of O_2 and CO_2 in the PSR zone and the PFR zone as a function of inlet concentration of CH_2Cl_2; fuel lean case ($\phi = 0.7$).

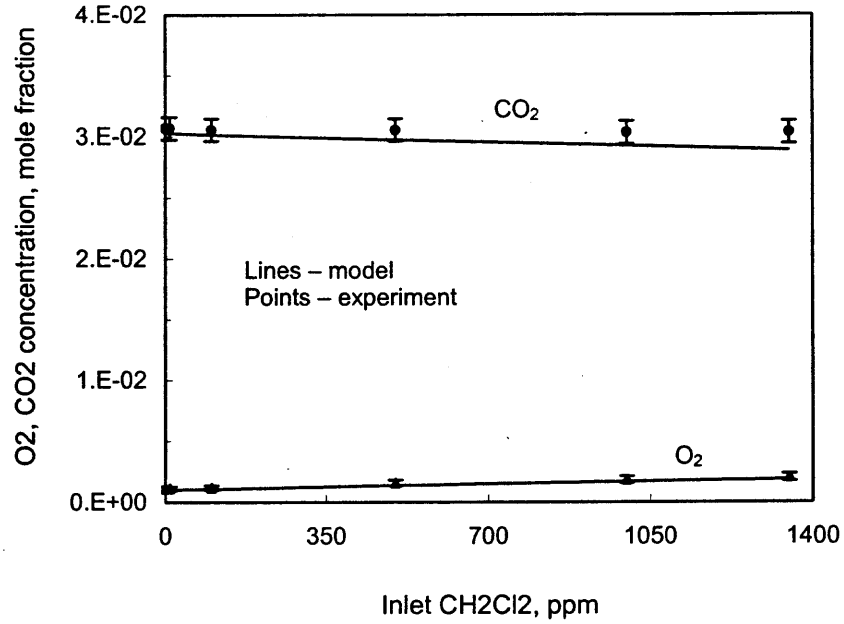


Figure 7.2 Concentrations of O_2 and CO_2 in the PSR zone as a function of inlet concentration of CH_2Cl_2; fuel rich case (ϕ = 1.4).

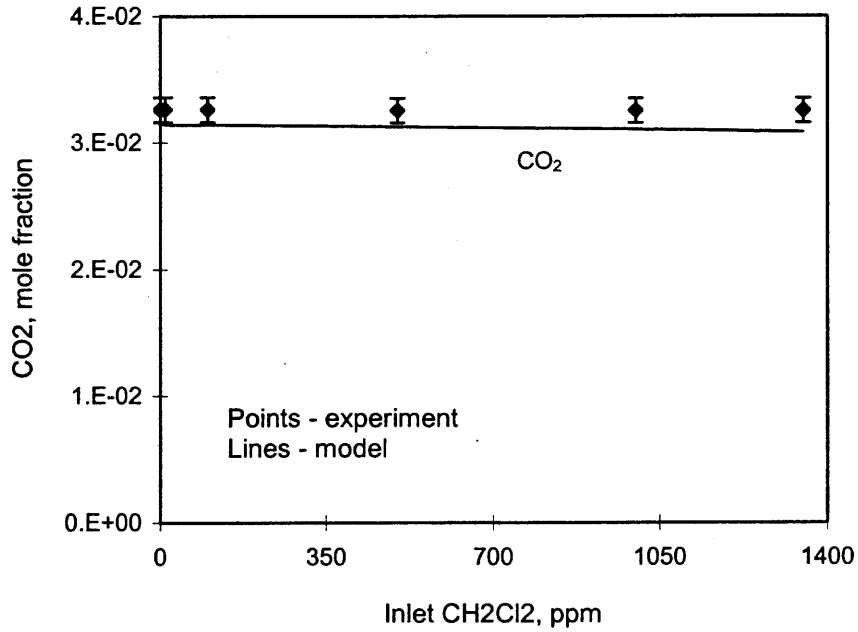


Figure 7.3 Concentrations of CO_2 in the outlet of PFR zone as a function of inlet concentration of CH_2Cl_2; fuel rich case (ϕ = 1.4).

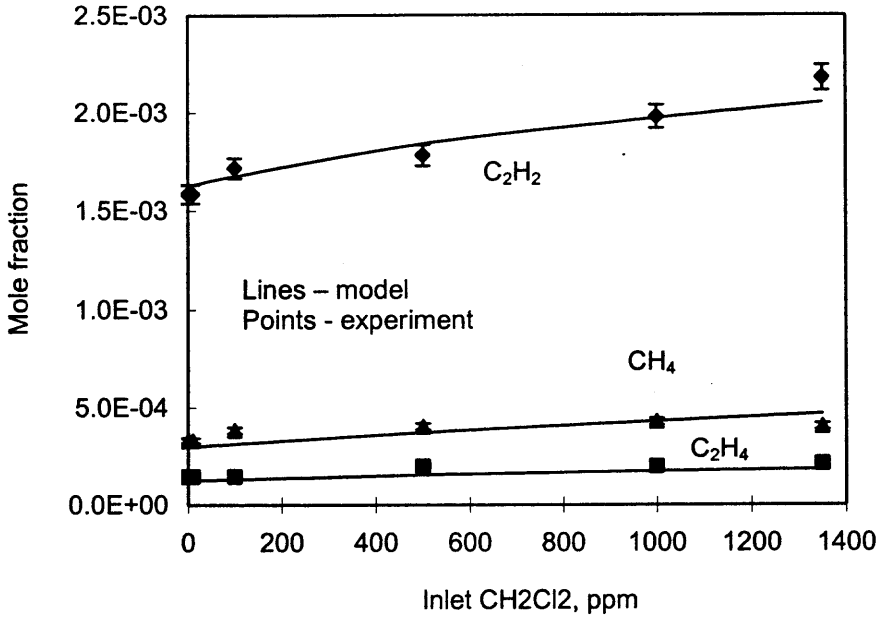


Figure 7.4 Concentrations of light hydrocarbons in the PSR zone as a function of inlet concentration of CH_2Cl_2; fuel rich case (ϕ = 1.4).

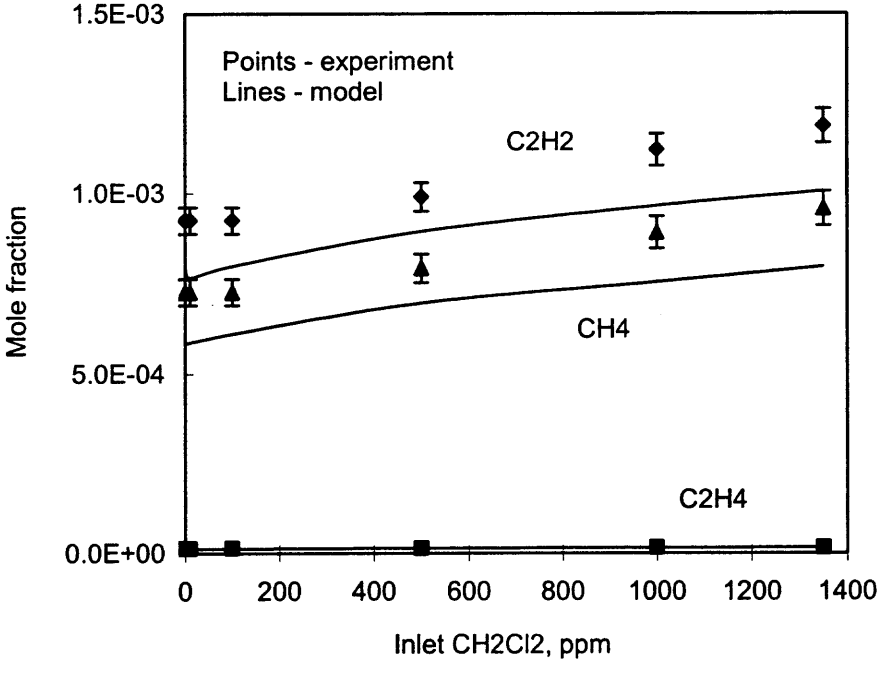


Figure 7.5 Concentrations of light hydrocarbons in the outlet of PFR zone as a function of inlet concentration of CH_2Cl_2; fuel rich case (ϕ = 1.4).

7.4 Increase of Products of Incomplete Combustion

In this section, the effects of increasing CH_2Cl_2 on products of incomplete combustion (PICs) formation is discussed and compared to those predicted by model rate-of-production (ROP) analysis results.

Recent studies (Mao 1995, Ho 1993) have suggested that chlorocarbon-induced inhibition of hydrocarbon combustion is mainly due to the competition for •OH radicals by the relatively fast reaction:

$$\bullet OH + HCl = H_2O + \bullet Cl \qquad \text{(R7.1)}$$

As predicted from ROP analysis, inhibition of hydrocarbon combustion at fuel-rich conditions occurs due to the competition for •H radicals by the relatively fast reaction:

$$\bullet H + HCl = H_2 + \bullet Cl \qquad \text{(R7.2)}$$

The ROP analysis performed for the first stage of the reactor showed that rate of consumption of •OH radicals by reaction (R7.1) and •H radicals by reaction (R7.2) increased with increasing inlet CH_2Cl_2 inlet concentration. The model predicted •OH and •H radicals concentration as a function of feed CH_2Cl_2 concentration are shown in Figures 7.6 and 7.7, which indicates that the concentrations of the active •OH and •H radicals decreased with the increase in chlorine loading. The increase in concentration of •Cl radicals is shown in Figure 7.8, where the concentration of free •Cl radicals was lower at fuel-rich conditions, when it was consumed by •H to form HCl.

The observed increase in concentrations of light hydrocarbons with higher chlorine loadings can be attributed to a reduction in the rate of •OH and •H radicals abstraction. For example the major channels to CH_4 and C_2H_2 destruction are:

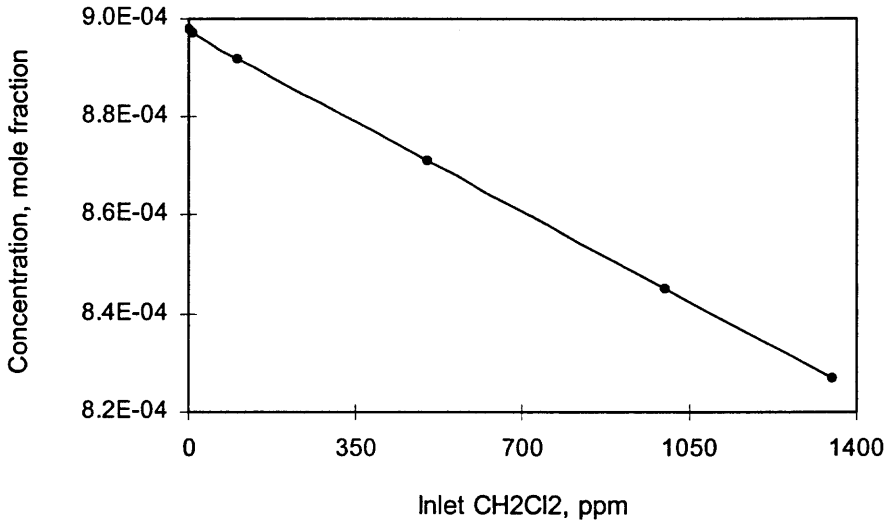


Figure 7.6 Model-predicted concentrations of •OH radical as a function of inlet CH_2Cl_2 concentrations in the PSR zone at fuel-lean combustion.

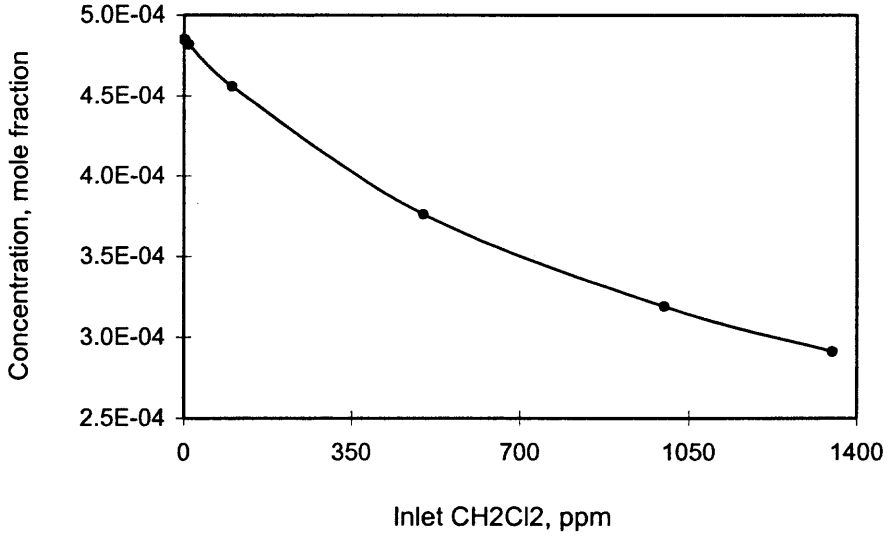


Figure 7.7 Model-predicted concentrations of •H radical as a function of inlet CH_2Cl_2 concentrations in the PSR zone at fuel-rich combustion.

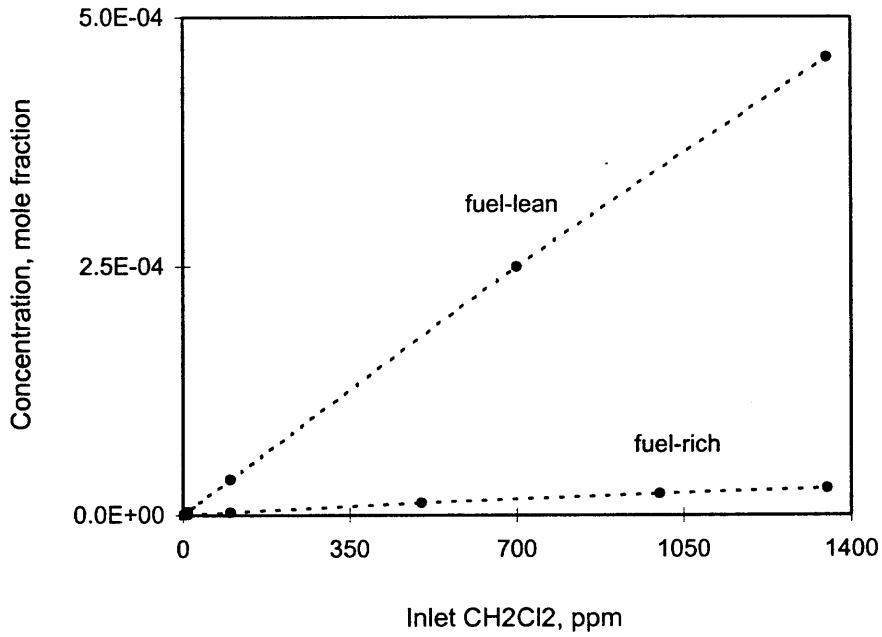


Figure 7.8 Model-predicted concentrations of •Cl radicals as a function of inlet concentration of CH_2Cl_2 at fuel-lean and fuel-rich conditions.

$$CH_4 + \bullet H = \bullet CH_3 + H_2 \qquad \text{(R7.3)}$$

$$CH_4 + \bullet OH = \bullet CH_3 + H_2O \qquad \text{(R7.4)}$$

$$C_2H_2 + \bullet OH = \bullet CH_2CO + \bullet H \qquad \text{(R7.5)}$$

The destruction rates by these reactions decreased by about 74%, 4% and 17% respectively as feed CH_2Cl_2 loading reached 1350 ppm. The difference between net CH_4 and C_2H_2 production and destruction rates increased 4% and 27% respectively. This is described in Figures 7.9 and 7.10.

At the same time, the important reaction

$$\bullet OH + H_2 = H_2O + \bullet H \qquad \text{(R7.6)}$$

is also inhibited because of a decrease in •OH concentration. This reaction is a main source of •H radicals that are needed for radical branching steps:

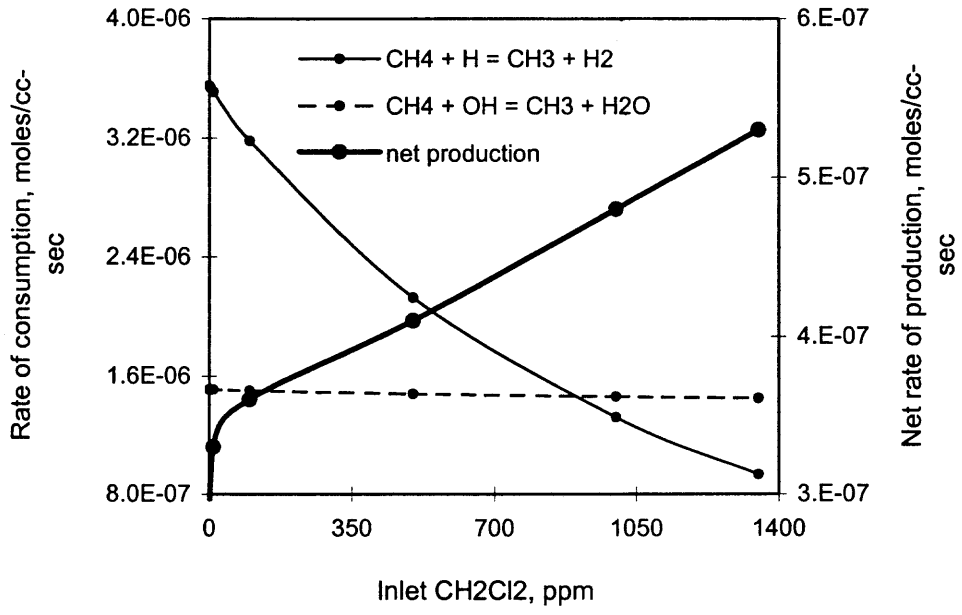


Figure 7.9 ROP analysis of CH_4 in the first stage: Destruction and production rates of CH_4 as a function of inlet CH_2Cl_2 (fuel-rich).

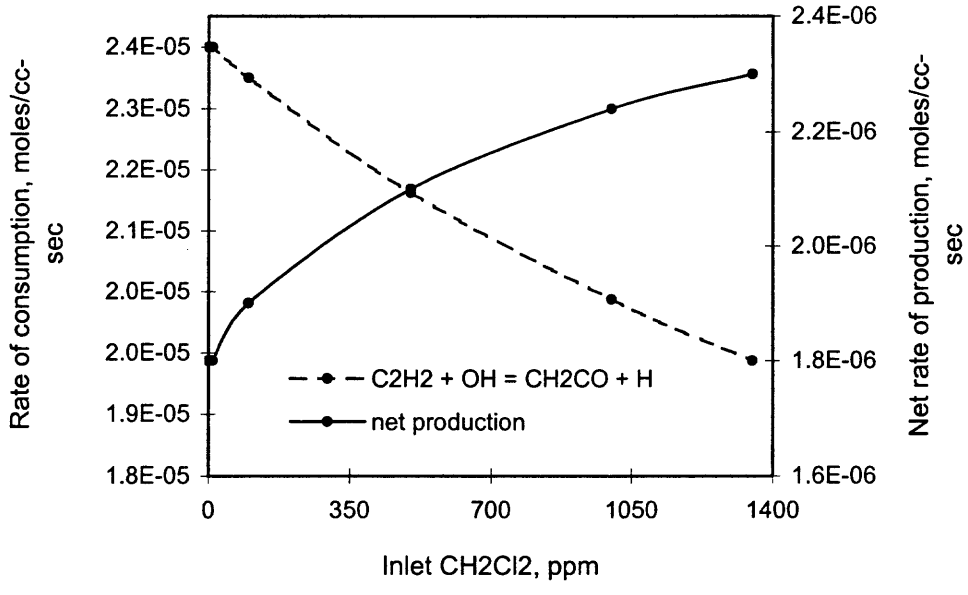


Figure 7.10 ROP analysis of C_2H_2 in the first stage: Destruction and production rates of C_2H_2 as a function of inlet CH_2Cl_2 (fuel-rich).

$$\bullet H + O_2 = \bullet OH + \bullet O \quad \text{(R7.7)}$$

$$\bullet H + O_2 = \bullet HO_2 \quad \text{(R7.8)}$$

$$\bullet H + \bullet HO_2 = \bullet OH + \bullet OH \quad \text{(R7.9)}$$

The inhibition, with its decrease in •OH radicals as shown in Figure 7.6, is illustrated in the reduced consumption of O_2 shown in Figure 7.2.

While •Cl decreases concentrations of key radicals, such as •H and •OH, it has been shown by the ROP that •Cl becomes a major radical substituting •H and •OH in performing many abstructions, such as:

$$\bullet Cl + \bullet HO_2 = HCl + O_2 \quad \text{(R7.10)}$$

This inhibits CO to CO_2 conversion since $\bullet HO_2$ is also a source of •OH. The changes in compositions of major radicals at fuel lean and fuel rich conditions are shown in Figures 7.11 and 7.12.

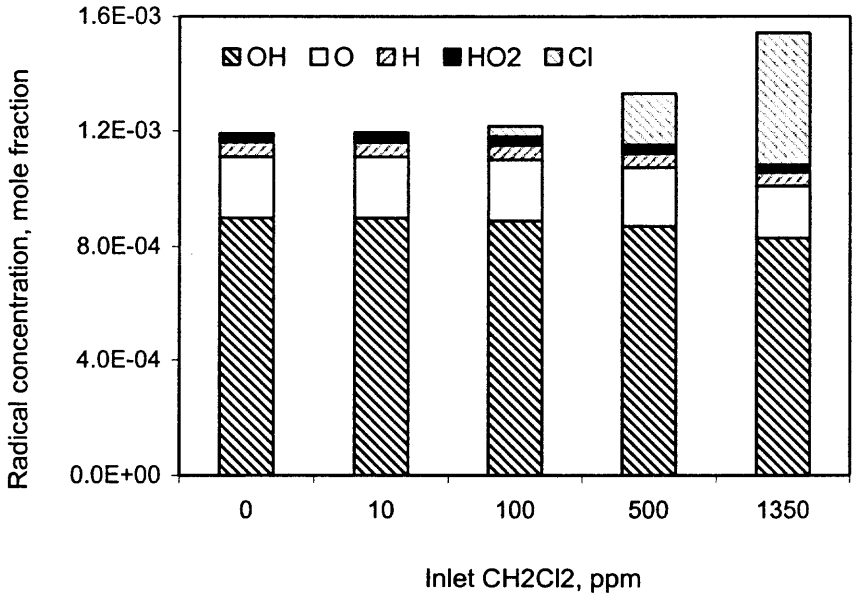


Figure 7.11 Model-predicted compositions of major radicals as a function of inlet CH_2Cl_2 at fuel-lean conditions.

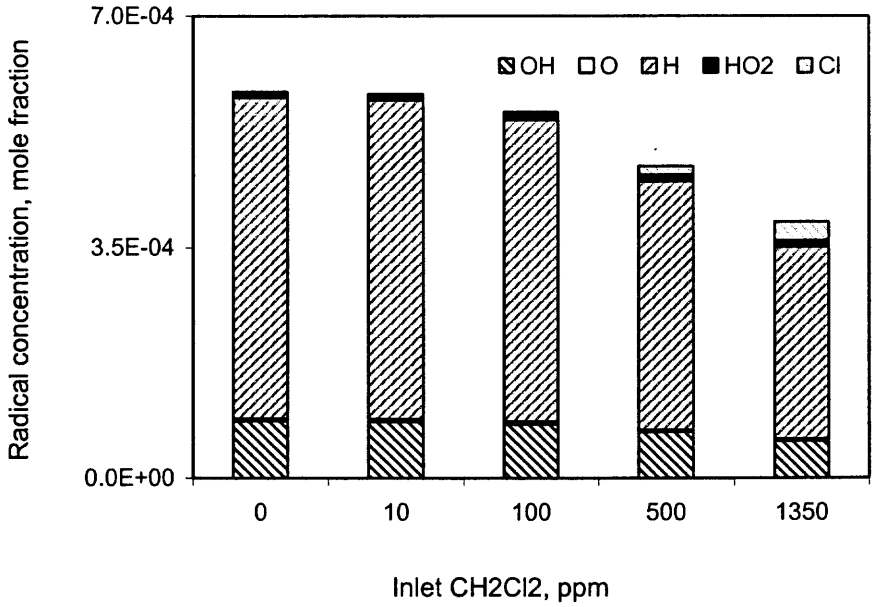


Figure 7.12 Model-predicted compositions of major radicals as a function of inlet CH_2Cl_2 at fuel-rich conditions.

7.5 Destruction Efficiency of Methylene Chloride

Figure 7.13 shows experimental data and model predicted concentrations of CH_2Cl_2 in the first stage of the combustor during fuel-lean and fuel-rich runs. The model underpredicted outlet CH_2Cl_2 concentrations, though the trend resembles the experimental data. Figure 7.14 shows the experimental and simulated CH_2Cl_2 destruction and removal efficiency (conversion) as a function of its inlet concentration. Destruction efficiency of lower inlet concentration was lower. As shown in Figure 7.15, the fraction of uncombusted CH_2Cl_2 was higher in fuel lean runs. In both cases, the outlet fraction of the original waste increased as the feed waste concentration was lowered, which is consistent with data field data by Trenholm (Trenholm, 1986). This Figure also shows data on destruction of CH_3Cl and C_6H_6 studied by Lyon (Lyon, 1990), which will be discussed later in this chapter.

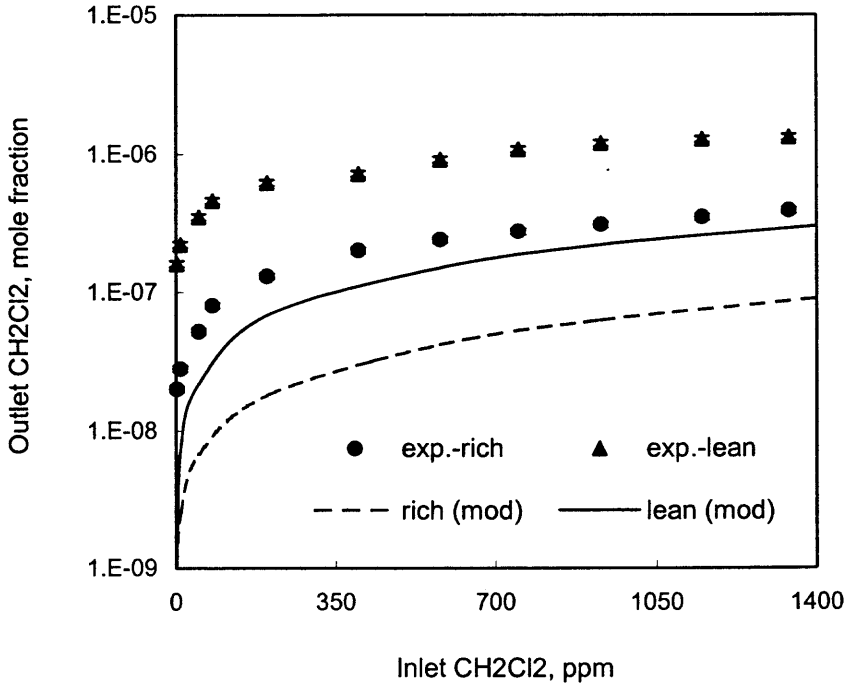


Figure 7.13 Concentrations of CH_2Cl_2 in the PSR zone during fuel-lean and fuel-rich runs.

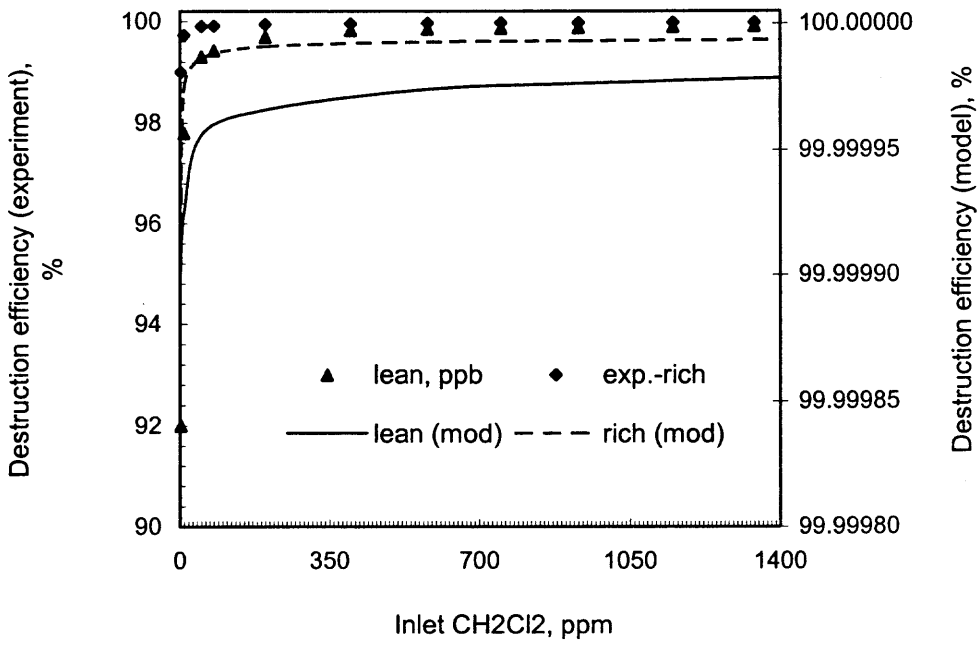


Figure 7.14 Destruction efficiency of CH_2Cl_2 as a function of its inlet concentration.

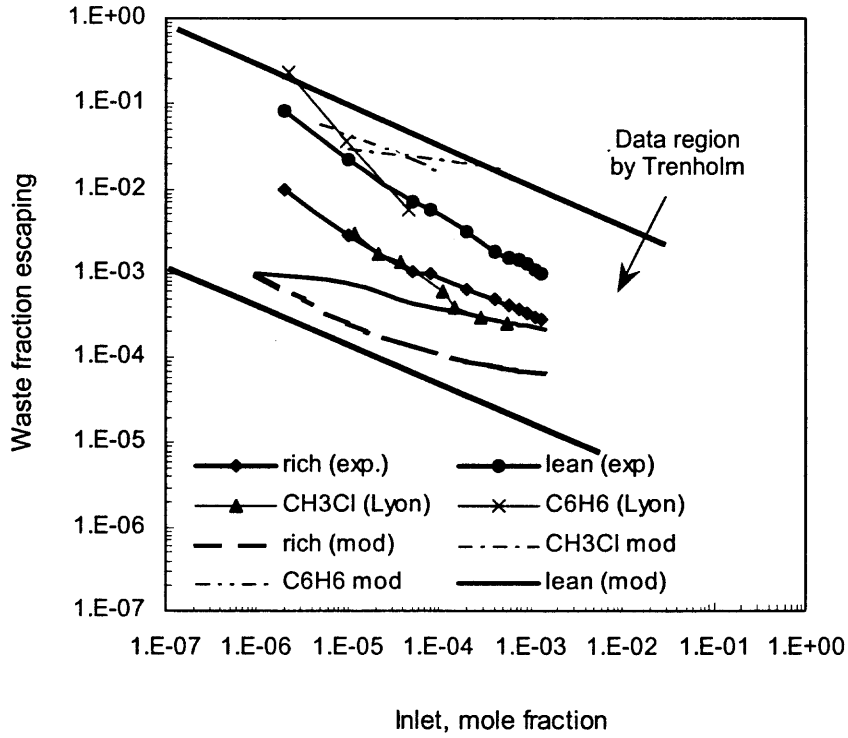
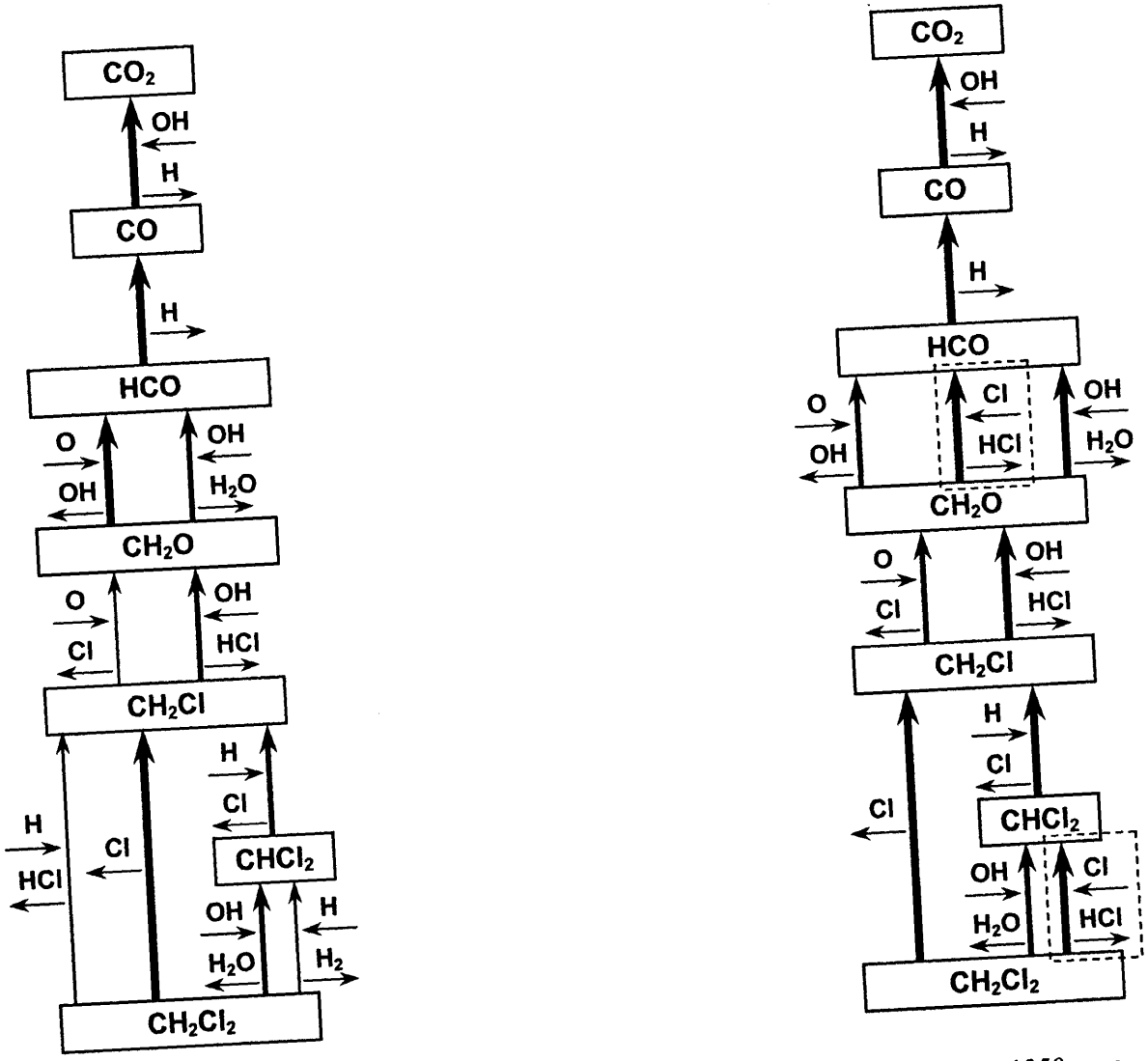


Figure 7.15 Relationship of inlet concentration of the CH_2Cl_2 and other organic compounds and their escaping fraction.

7.5.1 Methylene Chloride destruction pathways

This section discusses, the effect of feed CH_2Cl_2 concentration on its destruction efficiency, and light hydrocarbons formation. It based on rate-of-production analysis of the first stage (PSR) and second stage (PFR) of the combustor.

7.5.1.1 Fuel-lean Cases. Two fuel-lean runs, at the conditions shown in Table 7.1, were modeled with inlet CH_2Cl_2 concentrations of 10 and 1350 ppm. They are shown in Figures 7.16. The dominant pathways for CH_2Cl_2 destruction in the PSR varied with inlet concentrations. In both cases, CH_2Cl_2 underwent a unimolecular dissociation to form $\bullet CH_2Cl$ and $\bullet Cl$ radicals, or it reacted with $\bullet OH$ which abstracted $\bullet H$:



CH_2CL_2 – 10 ppm

CH_2CL_2 – 1350 ppm

Figure 7.16 Pathways to CH_2CL_2 destruction in the first stage at fuel-lean conditions ($\phi = 0.7$, $\tau = 0.010$ sec.).

	10 ppm	1350 ppm	
$CH_2Cl_2 = \bullet CH_2Cl + \bullet Cl$	-4.42E-09	-3.51E-07	(R7.11)
$CH_2Cl_2 + \bullet OH = \bullet CHCl_2 + H_2O$	-1.30E-09	-9.48E-08	(R7.12)

The values shown are rates of destruction (-) in units of moles/cc-sec.

At the lower concentration of CH_2Cl_2 (10 ppm), CH_2Cl_2 reacted with •H to abstract the Cl atom to form HCl, or to abstract H atom to form H_2. The attacks by •H were insignificant at higher CH_2Cl_2 concentrations.

	10 ppm	1350 ppm	
$CH_2Cl_2 + \bullet H = \bullet CH_2Cl + HCl$	-4.11E-10	negl.	(R7.13)
$CH_2Cl_2 + \bullet H = \bullet CHCl_2 + H_2$	-5.62E-10	negl.	(R7.14)

At higher CH_2Cl_2 inlet concentration (1350 ppm), H is abstracted by Cl atom to form $\bullet CHCl_2$ and HCl:

	10 ppm	1350 ppm	
$CH_2Cl_2 + \bullet Cl = \bullet CHCl_2 + HCl$	negl.	-4.06E-07	(R7.15)

Then, in both cases, $\bullet CHCl_2$ combined with •H atom and eliminated •Cl to form $\bullet CH_2Cl$:

	10 ppm	1350 ppm	
$\bullet CHCl_2 + \bullet H = \bullet CH_2Cl + \bullet Cl$	-2.11E-09	-5.47E-07	(R7.16)

The $\bullet CH_2Cl$ then combines with •O or •OH, then eliminates Cl atom or HCl respectively:

	10 ppm	1350 ppm	
$\bullet CH_2Cl + \bullet O = \bullet CH_2O + \bullet Cl$	-2.41E-10	-4.51E-08	(R7.17)
$\bullet CH_2Cl + \bullet OH = \bullet CH_2O + HCl$	-7.87E-10	-1.48E-07	(R7.18)

In both cases, $\bullet CH_2O$ combines with $\bullet O$ or $\bullet OH$, then eliminates $\bullet OH$ or H_2O to form $\bullet HCO$ radical:

	10 ppm	1350 ppm	
$\bullet CH_2O + \bullet O = \bullet HCO + \bullet OH$	-2.10E-06	-1.06E-06	(R7.19)
$\bullet CH_2O + \bullet OH = \bullet HCO + H_2O$	-1.48E-05	-7.77E-06	(R7.20)

At higher concentration of CH_2Cl_2, the $\bullet CH_2O$ radical combines with $\bullet Cl$, then eliminates HCl to form $\bullet HCO$:

	10 ppm	1350 ppm	
$\bullet CH_2O + \bullet Cl = \bullet HCO + HCl$	negl.	-8.25E-06	(R7.21)

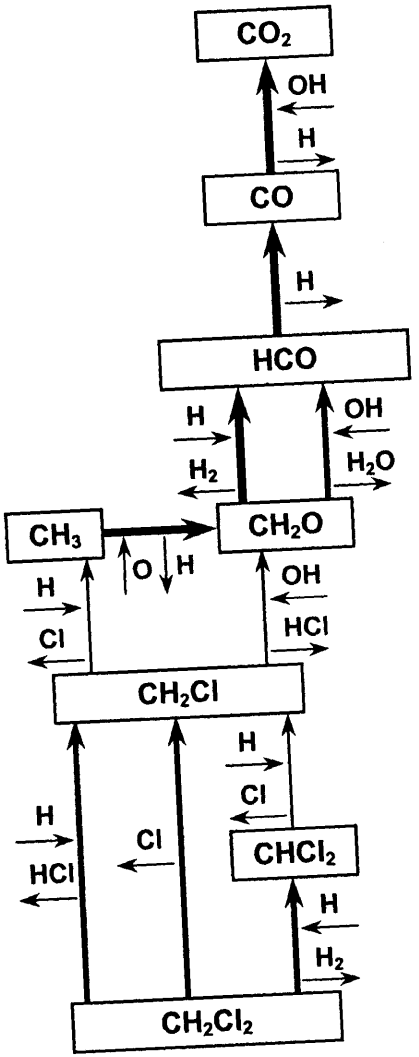
Then $\bullet HCO$ decomposes to CO and $\bullet H$:

	10 ppm	1350 ppm	
$\bullet HCO + M = \bullet H + CO + M$	-3.08E-05	-3.01E-05	(R7.22)

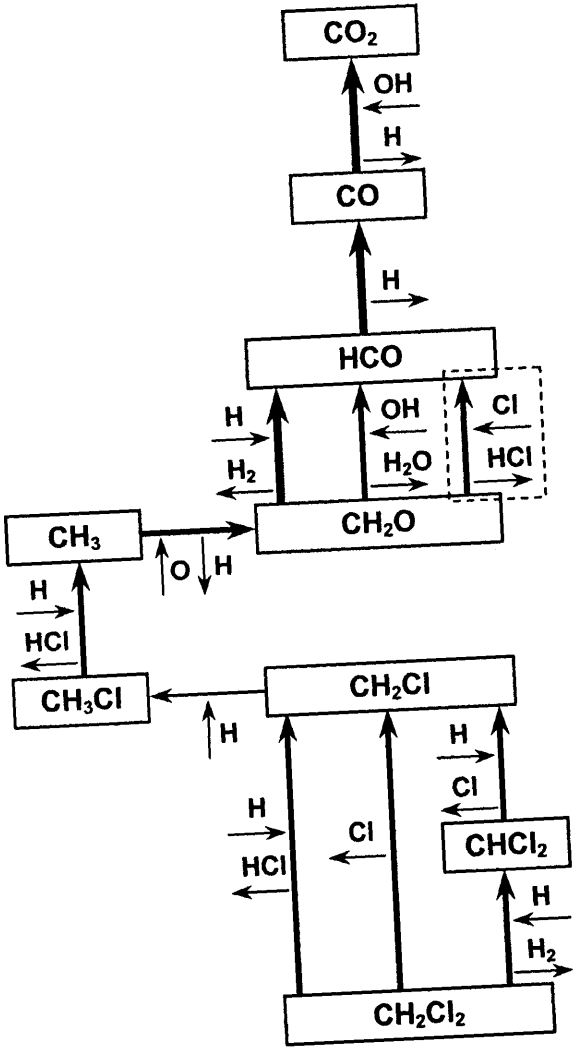
Then, CO reacts with $\bullet OH$ to form CO_2:

	10 ppm	1350 ppm	
$CO + \bullet OH = CO_2 + \bullet H$	-5.56E-05	-4.60E-05	(R7.23)

7.5.1.2 Fuel-rich Cases. Pathways to CH_2Cl_2 destruction at fuel-rich conditions are shown in Figures 7.17. In both lower (10 ppm) and higher (1350 ppm) inlet concentrations, CH_2Cl_2 underwent elimination of Cl atom or it reacted with $\bullet H$ radical to form $\bullet CH_2Cl$ or $\bullet CHCl_2$:



CH_2CL_2 – 10 ppm



CH_2CL_2 – 1350 ppm

Figure 7.17 Pathways to CH_2CL_2 destruction in the first stage at fuel-rich conditions (ϕ= 1.4, τ = 0.010 sec.).

	10 ppm	1350 ppm	
$CH_2Cl_2 = \bullet CH_2Cl + \bullet Cl$	-2.31E-09	-4.00E-07	(R7.11)
$CH_2Cl_2 + \bullet H = \bullet CH_2CL + HCl$	-1.96E-09	-2.15E-07	(R7.13)
$CH_2Cl_2 + \bullet H = \bullet CHCl_2 + H_2$	-2.66E-09	-2.86E-07	(R7.14)

Then, at lower concentrations of CH_2Cl_2, $\bullet CH_2Cl$ was attacked by $\bullet OH$ to form $\bullet CH_2O$ and HCl, or was attacked by $\bullet H$ to form $\bullet CH_3$ which then reacted with other $\bullet CH_2Cl$ to form C_2H_4 and HCl:

	10 ppm	1350 ppm	
$\bullet CH_2Cl + OH = \bullet CH_2O + HCl$	-3.41E-10	negl.	(R7.18)
$\bullet CH_2Cl + \bullet H = \bullet CH_3 + \bullet Cl$	-4.62E-10	negl.	(R7.24)
$\bullet CH_2Cl + \bullet CH_3 = C_2H_4 + HCl$	-1.46E-09	negl.	(R7.25)

In the fuel-rich combustion environment, $\bullet H$ combined with $\bullet CH_2Cl$ to form CH_3Cl which was attacked by $\bullet H$ and decomposed to $\bullet CH_3$ and HCl:

	10 ppm	1350 ppm	
$\bullet CH_2Cl + \bullet H = CH_3Cl$	negl.	-6.57E-06	(R7.26)
$CH_3Cl + \bullet H = \bullet CH_3 + HCl$	negl.	-4.15E-06	(R7.27)

In the fuel rich environment, the light hydrocarbon products of incomplete combustion resulted from reaction with $\bullet CH_3$. Major reactions to formation of light hydrocarbons, in this case were:

	10 ppm	1350 ppm	
$\bullet CH_3 + \bullet CH_3 = C_2H_6$	-1.00E-05	-1.10E-05	(R7.28)
$\bullet CH_3 + \bullet CH_2 = C_2H_4 + \bullet H$	-2.90E-06	-2.56E-06	(R7.29)
$\bullet CH_3 + \bullet H = CH_4$	-6.22E-06	-4.21E-06	(R7.30)

$\bullet CH_3 + \bullet O = \bullet CH_2O + \bullet H$	-3.58E-06	-3.34E-06	(R7.31)

Radical $\bullet CH_2O$ in both fuel-rich cases reacted with •H and •OH to form •HCO which then decomposed to CO and •H:

	10 ppm	1350 ppm	
$\bullet CH_2O + \bullet H = \bullet HCO + H_2$	-1.40E-05	-1.02E-05	(R7.32)
$\bullet CH_2O + \bullet OH = \bullet HCO + H_2O$	-6.85E-06	-5.36E-06	(R7.20)

At higher Cl concentration it also attacked •CH2O to form •HCO:

	10 ppm	1350 ppm	
$\bullet CH_2O + \bullet Cl = \bullet HCO + HCl$	negl.	-5.08E-06	(R7.21)

Then •HCO decomposes to •H and CO, some of which reacts with •OH and $\bullet HO_2$ and is oxidized to CO_2:

	10 ppm	1350 ppm	
$\bullet HCO + M = \bullet H + CO + M$	-3.31E-05	-3.26E-05	(R7.22)
$CO + \bullet OH = CO_2 + \bullet H$	-3.02E-05	-2.75E-05	(R7.23)
$CO + \bullet HO_2 = CO_2 + \bullet OH$	-3.80E-06	-4.22E-06	(R7.33)

7.6 Role of H, OH, and Cl Radicals in the Destruction of CH_2Cl_2

Based on the rate of production analysis described in the previous section, the major reactions for the primary destruction of CH_2Cl_2 were found to be unimolecular elimination of Cl atom, and the attack of CH_2Cl_2 by •H, •OH or •Cl radical which abstracts H or Cl atom:

$CH_2Cl_2 = \bullet CH_2Cl + \bullet Cl$ (R7.11)

$CH_2Cl_2 + \bullet OH = \bullet CHCl_2 + H_2O$ (R7.12)

$CH_2Cl_2 + \bullet H = \bullet CH_2Cl + HCl$ (R7.13)

$$CH_2Cl_2 + \bullet H = \bullet CHCl_2 + H_2 \quad (R7.14)$$

$$CH_2Cl_2 + \bullet Cl = \bullet CHCl_2 + HCl \quad (R7.15)$$

The relative significance of each elementary reaction varies at different CH_2Cl_2 concentrations, and at different equivalence ratios is shown in Figures 7.18 and 7.19. At low CH_2Cl_2 concentration major role plays reaction of abstraction of Cl atom (R7.11), and reaction of CH_2Cl_2 with a major radical in the combustion environment, which are •OH at fuel lean (reaction R7.12), or •H at fuel rich conditions (reactions R7.13 and R7.14). At higher CH_2Cl_2 feed concentration when there is a large supply of •Cl, the rate of CH_2Cl_2 destruction by this radical increases sharply (reaction R7.15). This rise would not be possible if •Cl radical was not donated to radical environment by CH_2Cl_2 itself. This suggests that some fragments derived from waste molecules can actively participate in the destruction of the parent species.

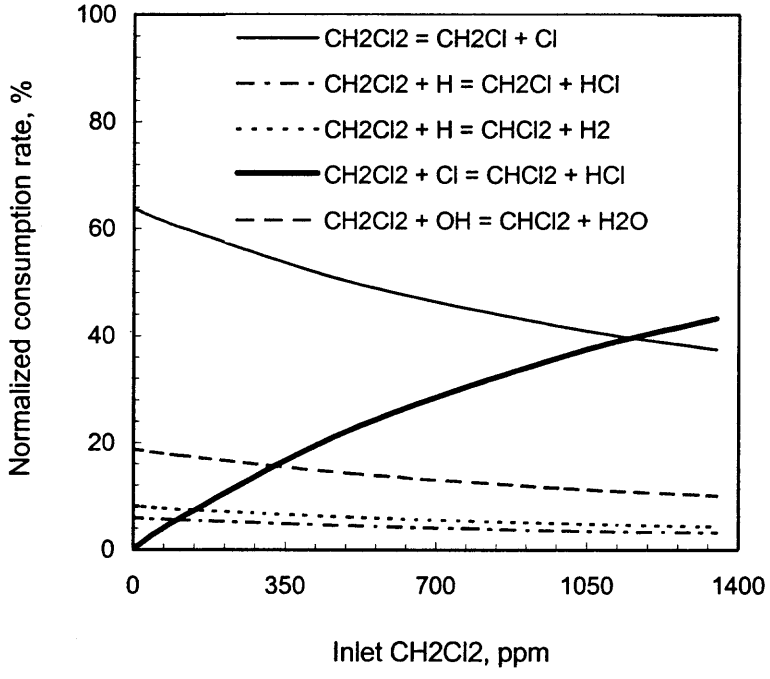


Figure 7.18 Model-predicted normalized rates of CH_2Cl_2 consumption as a function of inlet CH_2Cl_2 concentration at fuel-lean conditions ($\phi = 0.7$).

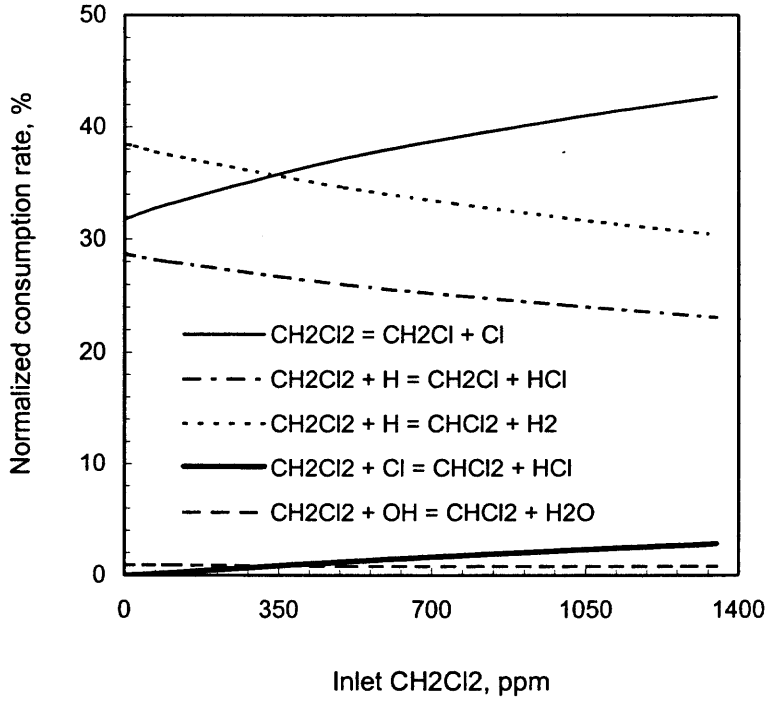


Figure 7.19 Model-predicted normalized rates of CH_2Cl_2 consumption as a function of inlet CH_2Cl_2 concentration at fuel-rich conditions ($\phi = 1.4$).

Figures 7.20 and 7.21 show calculated kinetic and equilibrium concentrations of •Cl radicals at fuel lean and fuel rich conditions. In both cases mechanism causes concentrations of •Cl much higher then their thermodynamic equilibrium, which increases rates of reactions. This supports the hypothesis by Lyon, that the injection of a compound or fuel which generate additional radicals can increase the extent to which an organic is oxidized (Lyon, 1990).

At fuel rich conditions with higher concentration of •H radicals, the effects of attacks on CH_2Cl_2 by •Cl and the rate of reaction (R7.15) is much lower, which indicates competition among •Cl and •H radicals. In a such •H rich environment they react with •Cl radicals to form a stable product, HCl. Therefore, less free •Cl radicals are available to

attack CH_2Cl_2. On the other hand, at fuel-lean •H limited conditions, •Cl abstracted H atoms from CH_2Cl_2, which increased their role in CH_2Cl_2 destruction. In a fuel-lean

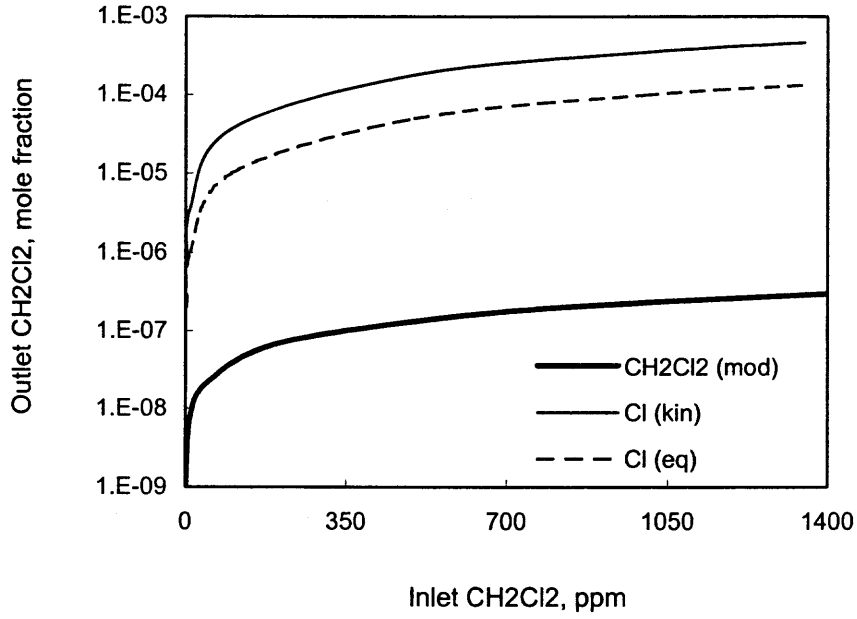


Figure 7.20 Comparison of model-predicted kinetic and equilibrium •Cl concentrations as a function of inlet CH_2Cl_2 at fuel-lean conditions ($\phi = 0.7$).

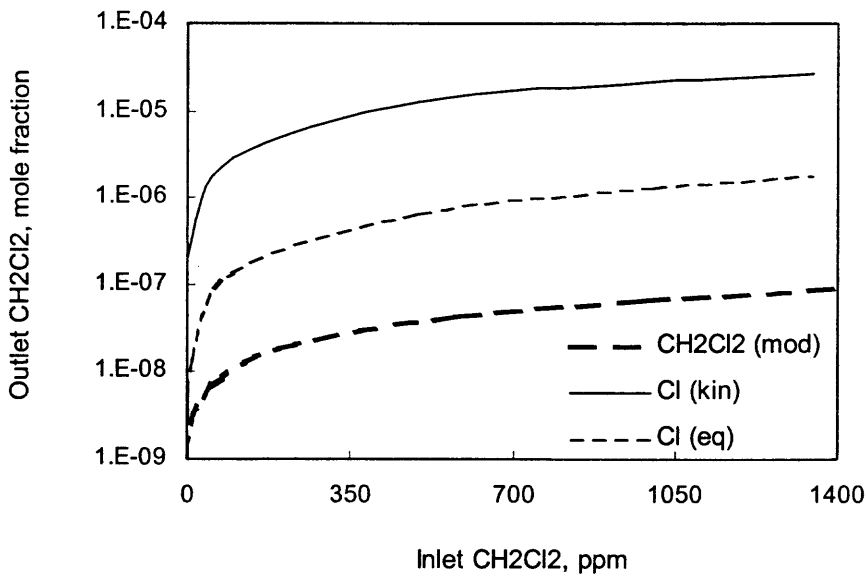


Figure 7.21 Comparison of model-predicted kinetic and equilibrium •Cl concentrations as a function of inlet CH_2Cl_2 at fuel-rich conditions ($\phi = 1.4$).

condition, there was not enough free •H to bind •Cl into HCl, which lead to significant increase in free •Cl concentration, as shown in Figure 7.8.

7.7 Effect of Concentration of an Organic Compound on its Destruction Efficiency

In order to explain the phenomena of lower destruction efficiency at lower concentrations, simulations of other available experimental data on destruction of CH_3Cl and C_6H_6 (Lyon, R., 1990) were performed.

7.7.1 Analysis of Primary Destruction of CH_3Cl

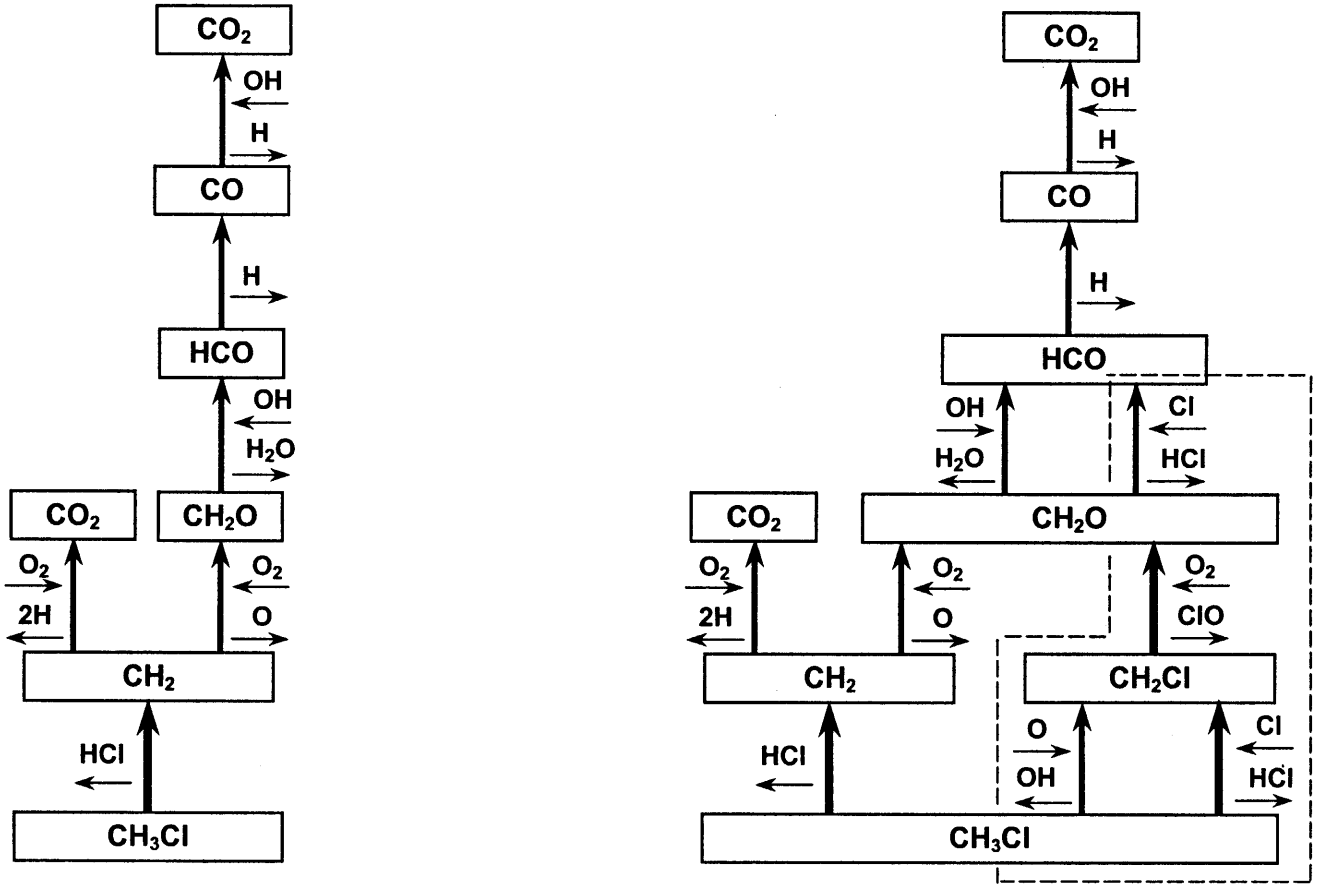
This section describes CHEMKIN simulation results and analysis, which are based on experimental data on destruction of CH_3Cl described by Lyon (Lyon R., 1990). This experimental data also showed lower destruction efficiency at low concentration. This was illustrated in Figure 7.15. Lyon studied oxidation of CH_3Cl in a quartz tube placed in an electric furnace at 951°C. Investigated gas mixture contained 4.4% of O_2, 616 ppm of H_2O and different CH_3Cl concentration ranging from 10 to 500 ppm.

Major pathways to CH_3Cl destruction at low (10 ppm) and high (500 ppm) concentration were identified and are shown in Figure 7.22. At low CH_3Cl concentration, and in the oxygen rich environment (shown in Figure 7.22a) the major channel to destruction was decomposition of CH_3Cl that resulted in formation of $\bullet CH_2$ and HCl via:

$$CH_3Cl = \bullet CH_2 + HCl \qquad \text{(R7.34)}$$

Then radical $\bullet CH_2$ was attacked by molecular O_2 to form CO_2 or $\bullet CH_2O$, which resulted in the release two •H, or one •O radical respectively:

$$\bullet CH_2 + O_2 = CO_2 + 2(\bullet H) \qquad \text{(R7.35)}$$



a) CH_3CL – 10 ppm

b) CH_3CL – 500 ppm

Figure 7.22 Pathways to CH_3CL destruction at low and high concentrations.

$$\bullet CH_2 + O_2 = \bullet CH_2O + \bullet O \qquad (R7.36)$$

At the same time HCl reacted with •OH radical to form H_2O and released •Cl:

$$HCl + \bullet OH = H_2O + \bullet Cl \qquad (R7.37)$$

This reaction, which was the main channel of production of •Cl radicals, was also the major channel to consumption of •OH radicals (79% of •OH consumption at 500 ppm of CH_2Cl).

Then H atom was eliminated from $\bullet CH_2O$ by •OH radical to form •HCO and H_2O via:

$$\bullet CH_2O + \bullet OH = \bullet HCO + H_2O \qquad (R7.38)$$

which was followed by •HCO decomposition:

$$\bullet HCO = \bullet H + CO \qquad (R7.39)$$

and CO-CO_2 conversion:

$$CO + \bullet OH = CO_2 + \bullet H \qquad (R7.40)$$

As can be seen from the above reactions, the destruction of each CH_3Cl molecule donated three active •H radicals (reactions R7.35 and R7.39), and one •Cl radical (reaction R7.34 followed by R7.37). All these (•H and •Cl) radicals entered existing radical pool. In the oxygen rich mixture •H radicals reacted with molecular O_2 via

$$\bullet H + O_2 = \bullet O + \bullet OH \qquad (R7.41)$$

$$\bullet H + O_2 = \bullet HO_2 \qquad (R7.42)$$

$$\downarrow$$

$$\bullet HO_2 + \bullet HO_2 = O_2 + H_2O_2 \qquad (R7.43)$$

$$\downarrow$$

$$H_2O_2 = \bullet OH + \bullet OH \qquad (R7.44)$$

which resulted in the generation of additional •O and •OH radicals.

However, at very low feed concentration of CH_3Cl, the concentrations of its fragments and additional number of radicals donated (•H, •Cl), or initiated (•O) by CH_3Cl were insignificant in affecting the existing CH_3Cl-free combustion environment.

At higher CH_3Cl concentration and consequently higher concentration of •Cl and •O, the latter played an important role in primary CH_3Cl destruction eliminating H atom from CH_3Cl. This is shown in Figure 7.22b. So, there are three major channels to primary CH_3Cl destruction at higher CH_3Cl concentration:

$$CH_3Cl = \bullet CH_2 + HCl \qquad \text{(R7.34)}$$

$$CH_3Cl + \bullet Cl = \bullet CH_2Cl + HCl \qquad \text{(R7.45)}$$

$$CH_3Cl + \bullet O = CH_2Cl + \bullet OH \qquad \text{(R7.46)}$$

Radicals $\bullet CH_2$ were attacked by molecular O_2 to form CO_2 or $\bullet CH_2O$:

$$\bullet CH_2 + O_2 = CO_2 + 2(\bullet H) \qquad \text{(R7.35)}$$

$$\bullet CH_2 + O_2 = \bullet CH_2O + \bullet O \qquad \text{(R7.36)}$$

and at the same time HCl (resulting from reaction R7.34) reacted with •OH to form H_2O, which released highly active •Cl radical:

$$HCl + \bullet OH = H_2O + \bullet Cl \qquad \text{(R7.37)}$$

Radical $\bullet CH_2Cl$ (resulting from reactions R7.45 and R7.46) reacted with O_2 to form $\bullet CH_2O$ and •ClO:

$$\bullet CH_2Cl + O_2 = \bullet CH_2O + \bullet ClO \qquad \text{(R7.47)}$$

At higher •Cl concentration, •Cl along with •OH reacted with $\bullet CH_2O$ eliminating H atom, which resulted in the formation of •HCO and H_2O/HCl:

$$\bullet CH_2O + \bullet OH = \bullet HCO + H_2O \qquad \text{(R7.38)}$$

$$\bullet CH_2O + \bullet Cl = \bullet HCO + HCl \qquad (R7.48)$$

These are followed by •HCO decomposition and CO-CO_2 conversion:

$$\bullet HCO = \bullet H + CO \qquad (R7.39)$$

$$CO + \bullet OH = CO_2 + \bullet H \qquad (R7.40)$$

These additional channels to CH_3Cl breakdown initiated by products of its destruction (reactions R7.45, R7.46, R7.47 and R7.48) are shown in Figure 7.22b by dashed lines.

7.7.2 Role of Radicals and Fragments Generated by CH_3Cl

The analysis of rate-of-production calculations showed that the roles of the major channels in destruction of CH_3Cl are different at low and high concentrations. Destruction of one CH_3Cl molecule donates four active radicals (one •Cl, and three •H radicals) into the existing radical pool. So, the number of donated radicals grows exponentially with the number of CH_3Cl molecules in feed mixture, which modifies the existing radical pool. The composition of major radicals are shown in Figure 7.23. Relatively lower concentration of free •Cl and •O radicals (at higher CH_3Cl concentration) could be explained by their high consumption rates by reactions with CH_3Cl (reactions R7.45 and R7.46), which were the main channels to •Cl and •O consumption (normalized consumption 72%, and 33% respectively). As shown by normalized rates in Figure 7.24, these reactions (R7.45 and R7.46) became the main channels to CH3Cl destruction.

As can be seen from Figure 7.24, at low CH_3Cl concentrations (10 ppm), when the radicals generated from its destruction could not effectively alter the radical pool, the role of additional •Cl and •O was very insignificant. The major channel to CH_3Cl

destruction (about 90%) was its decomposition via reaction R7.34. At higher CH_3Cl concentration (500 ppm), this decomposition resulted in the generation of active $\bullet CH_2$ radicals, which reacting with O_2 (reaction R7.36), formed the major channel to the production of •O (contribution about 60%). Normalized rates of •O radical production and •O radical concentration are shown in Figure 7.25. As shown in this Figure more active $\bullet CH_2$ radicals resulting from CH_3Cl destruction substituted •H radicals in reactions with molecular O_2, which result in higher production of •O radicals (reactions R7.36 and R7.41). At the same time •O radicals involved in CH_3Cl destruction via reaction R7.46, which became the main channel of •O consumption. This is shown in Figure 7.26.

The destruction of CH_3Cl provided radicals or fragments ($\bullet CH_2$, •H), which reacting with unlimited (in this case) O_2 resulted in formation of additional •O in existing environment. This suggests that in an O_2 rich environment any organic material, which donates additional •H radicals (or some other active fragments, such as $\bullet CH_2$) contributes to additional generation of •O and •OH radicals. This eventually increases further oxidation of its species.

At the same time, the destruction of CH_3Cl resulted in increased concentration of free •Cl radicals (reaction R7.34 followed by R7.37). At higher CH_3Cl concentration, elimination of H atom by •Cl attack became one of the major channels in CH_3Cl destruction, as shown in Figure 7.22b (dashed line). This reaction also was a major channel for •Cl consumption (consuming up to 71% of •Cl at concentration 500 ppm of CH_3Cl).

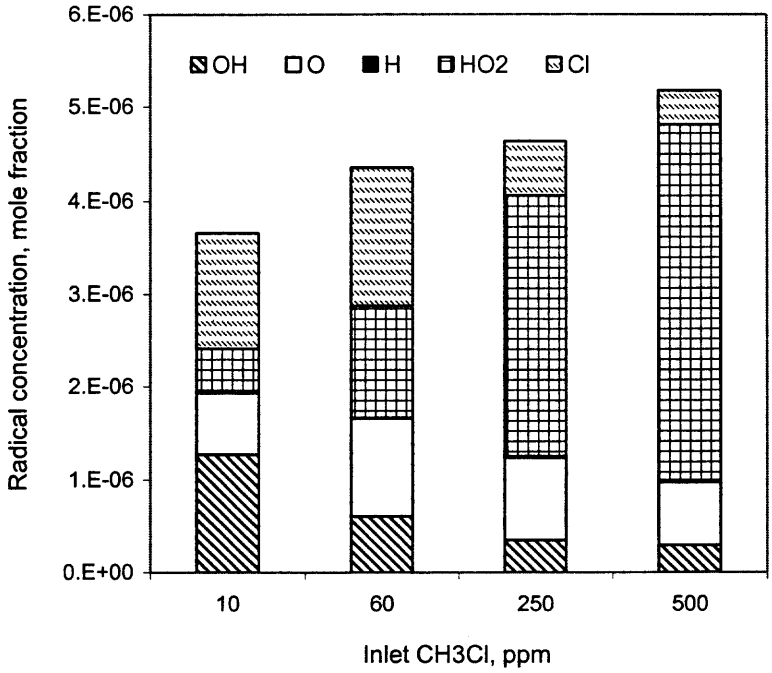


Figure 7.23 Effect of inlet CH_3Cl concentration on composition of major radicals.

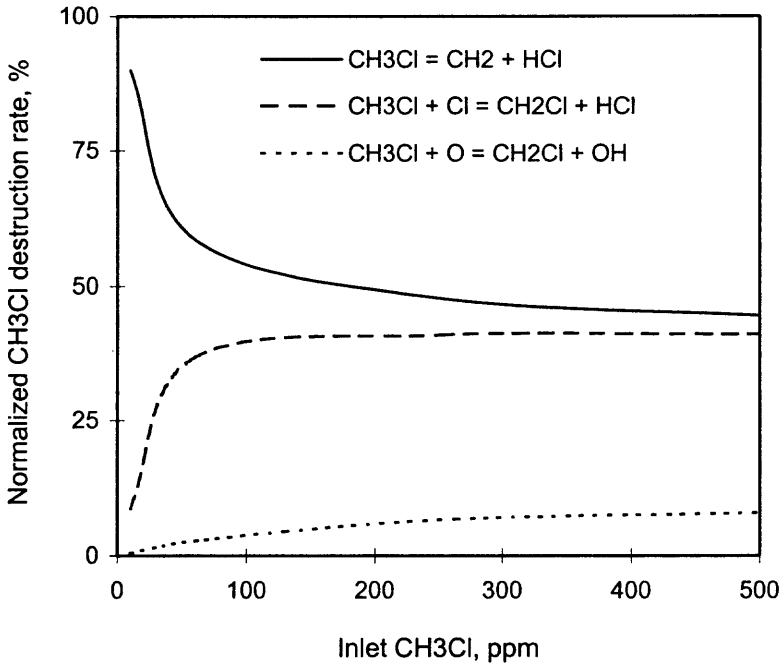


Figure 7.24 Model-predicted normalized rates of major channels to CH_3Cl destruction.

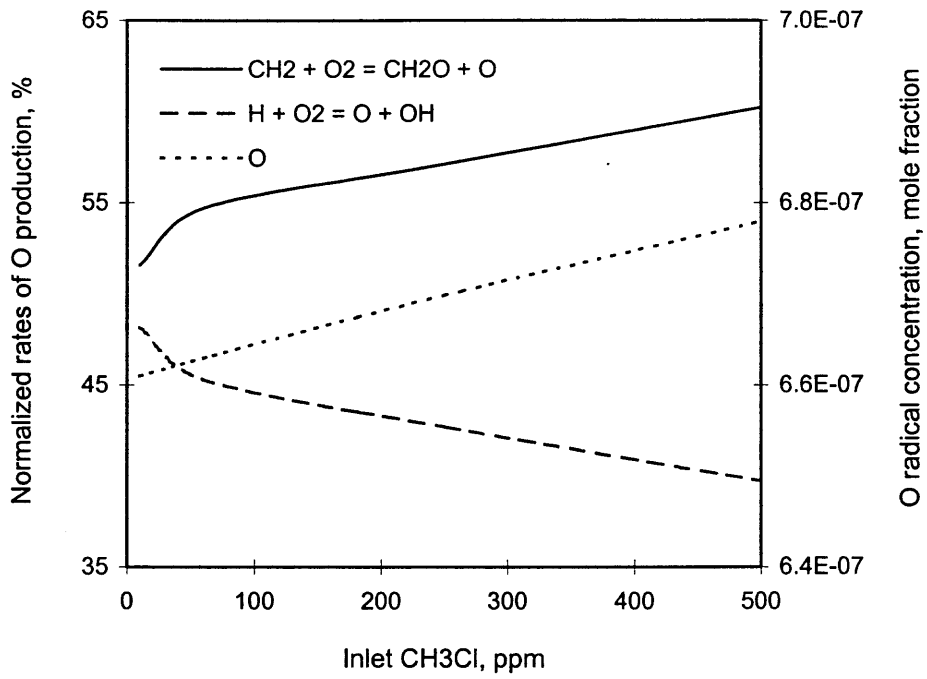


Figure 7.25 Model-predicted normalized rates of production and concentration of •O radicals.

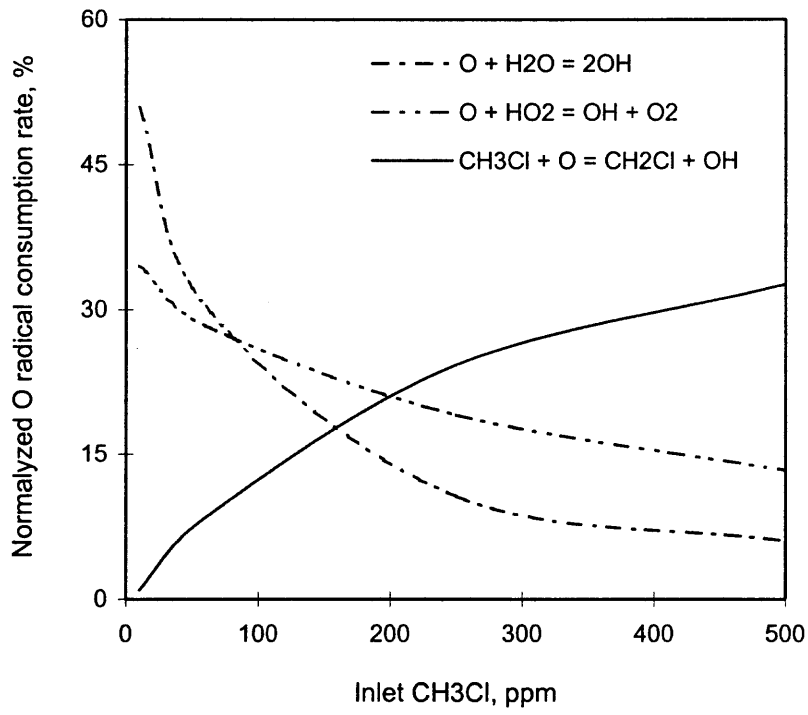


Figure 7.26 Model-predicted normalized rates of consumption of •O radicals.

As shown above, radicals resulting from destruction of one CH_3Cl molecule actively participated in the destruction of another CH_3Cl molecule. As illustrated in the rate of production analysis, addition of •Cl, •CH_2 and •H radicals to existing radical pool initiated additional (or enhanced existing) channels for CH_3Cl destruction. The presence of •Cl has originated destruction channel R7.45. Radicals •CH_2 and •H were involved in additional production of •O radicals via reactions R7.36 and R7.41, which are needed for CH_3Cl destruction via R7.46.

Thus, additional active radicals that were generated at higher CH_3Cl concentrations effectively altered the combustion environment and made available additional channels for CH_3Cl destruction. Efficiency of CH_3Cl destruction at its higher concentrations was higher. At low CH_3Cl feed concentrations, the number and efficiency of destruction channels depended only on the radicals present in the equivalent CH_3Cl free environment.

7.7.3 Analysis of Destruction of C_6H_6

Based on experimental data on C_6H_6 destruction, shown in Figure 7.15, CHEMKIN calculations were performed. Experiments on oxidation of C_6H_6 were done in the same quartz tube described in previous section at the following conditions: temperature 721°C, 4.6% O_2 and 1.42% H_2O. Concentrations of C_6H_6 ranged from 2 ppm to 100 ppm. Based on simulation results major routes of C_6H_6 destruction were identified. They are shown in Figure 7.27.

In this oxygen rich environment, C_6H_6 molecules were attacked by •OH and •O to form •C_6H_5 and •C_6H_5O via

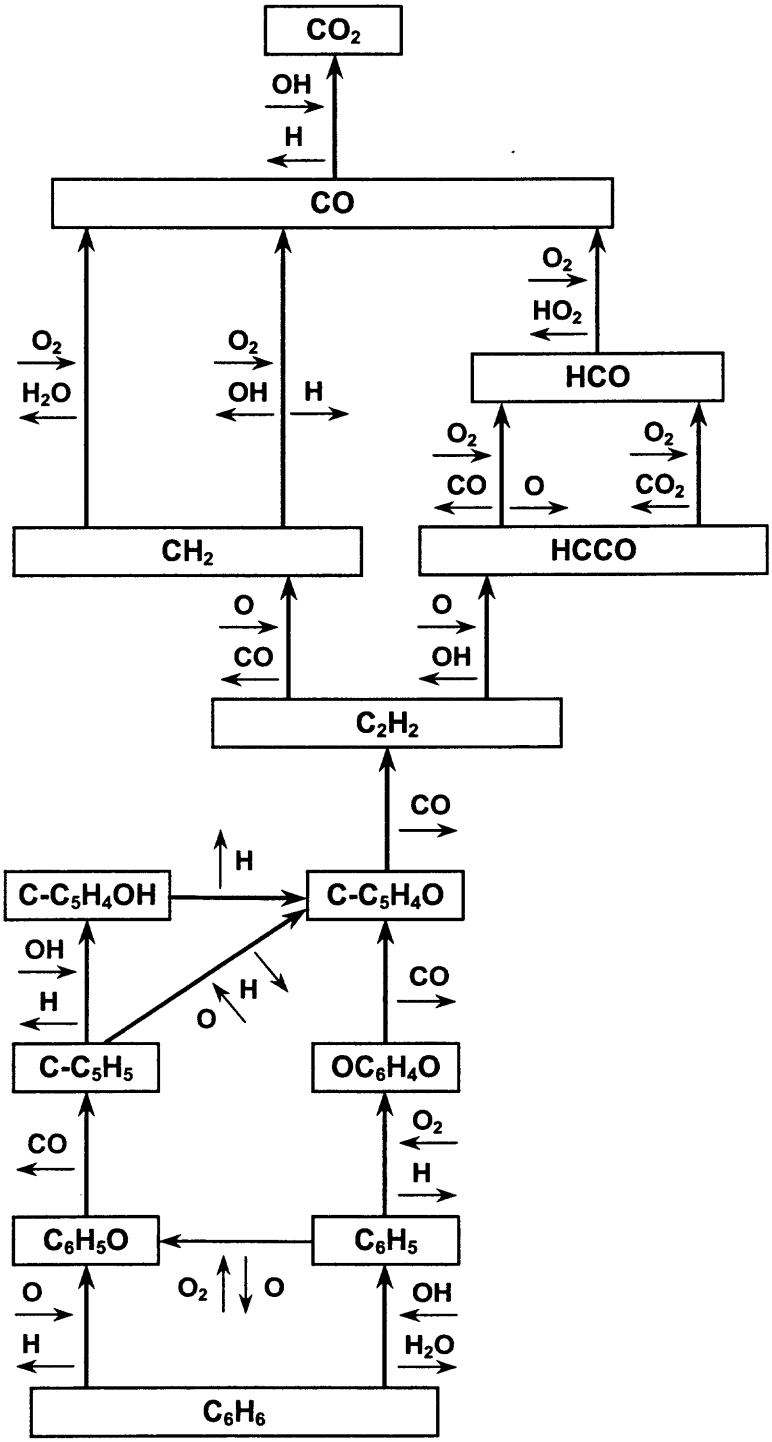


Figure 7.27 Pathways to C_6H_6 destruction.

$$C_6H_6 + \bullet OH = \bullet C_6H_5 + H_2O \quad (R7.49)$$

$$C_6H_6 + \bullet O = \bullet C_6H_5O + \bullet H \quad (R7.50)$$

Then $\bullet C_6H_5$ radicals were oxidized by molecular O_2 with formation of $\bullet C_6H_5O$ and $\bullet OC_6H_4O$ via

$$\bullet C_6H_5 + O_2 = \bullet C_6H_5O + \bullet O \quad (R7.51)$$

$$\bullet C_6H_5 + O_2 = \bullet OC_6H_4O + \bullet H \quad (R7.52)$$

which then were decomposed to form $\bullet$cyc-C_5H_5 or $\bullet$cyc-C_5H_4O radicals and CO via

$$\bullet C6H5O = \bullet cyc\text{-}C5H5 + CO \quad (R7.53)$$

$$\bullet OC6H4O = \bullet cyc\text{-}C5H4O + CO \quad (R7.54)$$

Reactions of $\bullet$cyc-C_5H_5 with $\bullet$OH and $\bullet$O resulted in substitution of H atom via

$$\bullet cyc\text{-}C_5H_5 + \bullet OH = \bullet cyc\text{-}C_5H_4OH + \bullet H \quad (R7.55)$$

$$\bullet cyc\text{-}C_5H_5 + \bullet O = \bullet cyc\text{-}C_5H_4O + \bullet H \quad (R7.56)$$

Radical $\bullet$cyc-C_5H_4OH eliminated H atom to form $\bullet$cyc-C_5H_4O via

$$\bullet cyc\text{-}C_5H_4OH = \bullet cyc\text{-}C_5H_4O + \bullet H \quad (R7.57)$$

Then the benzene ring of $\bullet$cyc-C_5H_4O breaks and the radicals decompose to form C_2H_2 and CO via

$$\bullet cyc\text{-}C_5H_4O = 2(C_2H_2) + CO \quad (R7.58)$$

Reactions of C_2H_2 with $\bullet$O resulted in substitution of H or abstraction of C atoms and formation of $\bullet$HCCO and $\bullet CH_2$ radicals via

$$C_2H_2 + \bullet O = \bullet HCCO + \bullet H \quad (R7.59)$$

$$C_2H_2 + \bullet O = \bullet CH_2 + CO \quad (R7.60)$$

Radicals $\bullet$HCCO and $\bullet CH_2$ then react in several steps with molecular O_2 and $\bullet$OH radical, which eventually result in formation of CO_2 and H_2O via

$$\bullet HCCO + O_2 = \bullet HCO + CO + \bullet O \quad (R7.61)$$

$$\bullet HCCO + O_2 = \bullet HCO + CO_2 \quad (R7.62)$$

$$\bullet HCO + O_2 = \bullet HO_2 + CO \quad (R7.63)$$

$$\bullet HO_2 + \bullet OH = H_2O + O_2 \quad (R7.64)$$

$$\bullet CH_2 + O_2 = H_2O + CO \quad (R7.65)$$

$$\bullet CH_2 + O_2 = CO + \bullet OH + \bullet H \quad (R7.66)$$

$$\bullet CO + \bullet OH = CO_2 + \bullet H \quad (R7.67)$$

Rate of production analysis performed for this case shows that though pathways to C_6H_6 destruction at its low and higher concentrations are the same, involvement and role of particular reactions are different. This is especially true for the reactions of C_6H_6 with •O and •OH radicals. ROP analysis shows that at C_6H_6-free environment these radicals (•O and •OH) are generated from existing O_2 and H_2O mainly by reactions

$$H_2O + \bullet O = 2(\bullet OH) \quad (R7.68)$$

$$\downarrow$$

$$2(\bullet OH) = \bullet HO_2 + \bullet H \quad (R7.69)$$

$$\downarrow$$

$$\bullet H + O_2 = \bullet O + \bullet OH \quad (R7.70)$$

When C_6H_6 enters that environment during destruction it eventually donates six of its H atoms, to the existing radical pool (reactions R7.50, R7.52, R7.56, R7.59, R7.66). The increase in concentration of •H radicals from inlet C_6H_6 is shown in Figure 7.28. At the same time major channel to consumption of •H radicals is their reaction with molecular O_2 (reaction R7.41), which generates additional •O and •OH radicals needed for C_6H_6 attacks (reactions R7.49 and R7.50). In this oxygen-rich mixture reaction R7.41 generated about 75% of •O and about 45% of •OH radicals. This is shown in Figure 7.29.

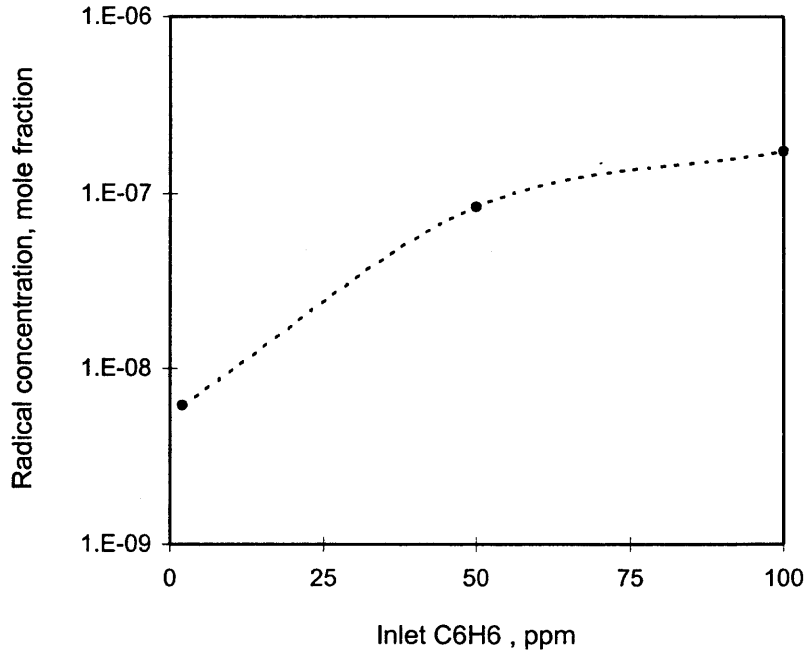


Figure 7.28 Model-predicted concentration of •H radicals as a function of inlet C_6H_6.

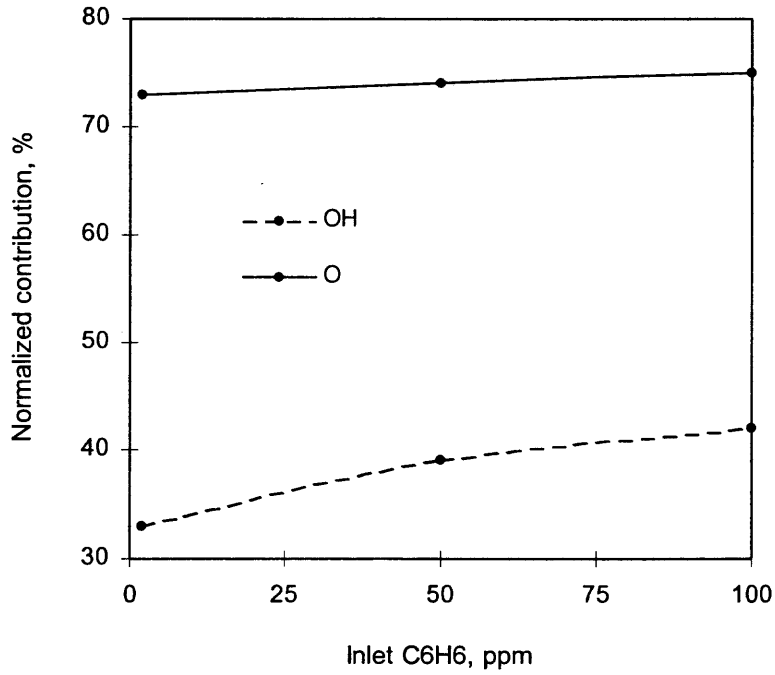


Figure 7.29 Model-predicted normalized rates of production of •H and •OH radicals by O_2 + •H = •O + •OH as a function of inlet C_6H_6.

Therefore, if each •H radical reacting with O_2 can generate two active radicals (•O and •OH), then each C_6H_6 molecule, which during destruction eventually donates six of its H atoms, can produce twelve active radicals (six •O and six •OH) to be used in destruction of next C_6H_6 molecule. So, number of •O and •OH radicals increases exponentially with number of C_6H_6 molecules in the feed. The effect of •H radicals on concentrations and composition of •O and •OH radicals is shown in Figure 7.30, and the effect of •H radical concentration on rates of destruction of C_6H_6 by these radicals are shown in Figure 7.31.

As can be seen from above discussion and Figures 7.28-7.31, H atom donated by C_6H_6 to the O_2 rich environment generates additional •O and •OH radicals needed for further C_6H_6 destruction, or destruction of other C_6H_6 molecules. This phenomena is also true for CH_3Cl destruction at O_2 rich conditions. In both these cases, where •H radicals are limited, any aditionally donated H atoms will be used by available O_2 to produce additional •O and •OH radicals, to be used for further reactions.

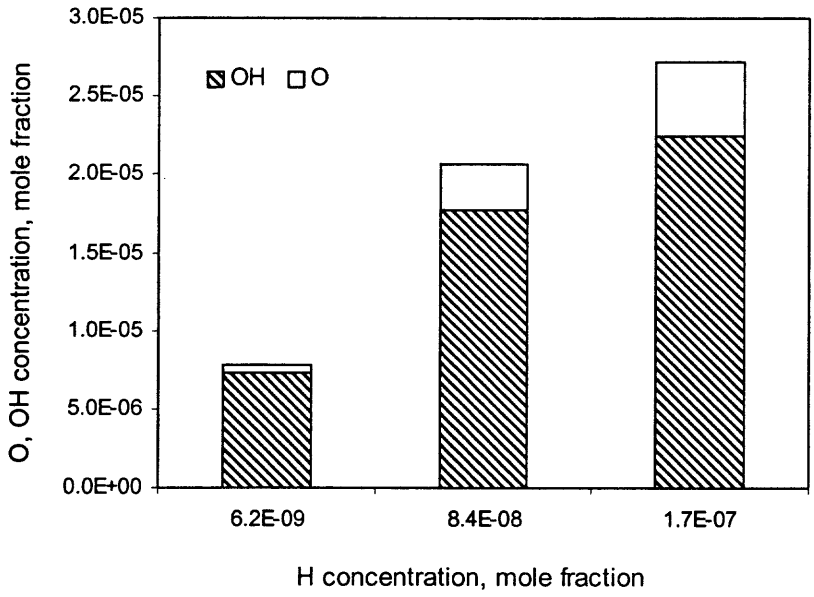


Figure 7.30 Effect of •H on concentrations of •OH and •O radicals.

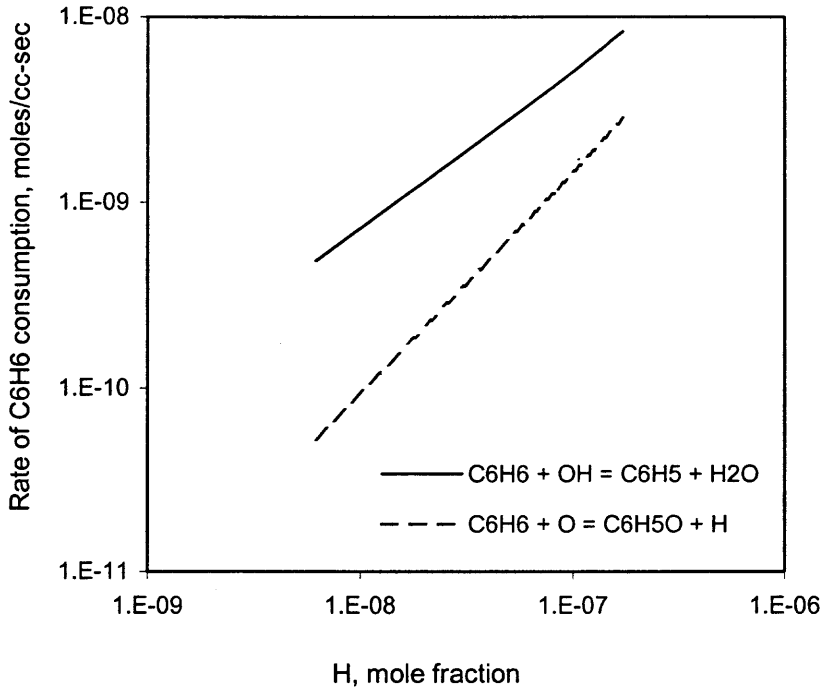


Figure 7.31 Effect of •H radical concentration on rates of C_6H_6 destruction by •O and •OH radicals.

However, the donation of H atoms to the combustion environment with limited O_2, does not contribute to C_6H_6 destruction but to the formation of higher hydrocarbons such as C_6H_6, as was shown by increased rates of formation and destruction of C_6H_6 at fuel-rich conditions in the Chapter 4. Thus, on the other side, it can be suggested that any additional O atoms donated by combustible material to the fuel-rich combustion environment will eventually contribute to the increase of •O and •OH radical concentrations and to the increase of their reaction rates, and destruction of that material if these radicals are involved in a such.

CHAPTER 8

EFFECT OF CONCENTRATION OF ORGANIC MATERIAL ON ITS DESTRUCTION EFFICIENCY

Differences in rates of destruction at low and high concentrations can be seen as follows. Consider combustion of an organic material A at low concentrations ($[A] \rightarrow 0$). The rate of destruction is determined by concentrations and activities of main radicals present in the flame and may be given as (Rose, 1961):

$$(dx/d\tau)_{\text{low}} = ([A]_{\text{o}} - x)K \tag{8.1}$$

where, $[A]_{\text{o}}$ denotes the initial concentration of A; x is the amount of A decomposed at time τ; and K is the total rate of destruction which is equal to a sum of rates of all elementary reactions and is given as

$$K = k_1 C_{\text{H}} + k_2 C_{\text{OH}} + k_3 C_{\text{O}} + \ldots. \tag{8.2}$$

where C_{H}, C_{OH}, C_{O}, etc. are the concentrations of all available active radicals H, OH, O, ets.; and k_1, k_2, k_3 ... are corresponding rate constants. The total rate of destruction K also can be given as

$$K = [\text{M}_k][\text{R}] \tag{8.2a}$$

where $[\text{M}_k]$ is the matrix containing all of rate constants k_{i}, and $[\text{R}]$ is the matrix containing concentrations of all radicals of the fuel-air waste free flame.

At a low concentration of A ($[A] \rightarrow 0$), concentrations of active species, such as H, OH, O etc. are determined by combustion conditions (fuel composition, temperature, ϕ, etc.). All active radicals result from destruction of components of the fuel-air mixture.

After separation of variables Equation (8.1) becomes:

$$dx/([A]_o - x) = Kd\tau \tag{8.3}$$

and integration Equation (8.2) yeilds to

$$- \ln([A]_o - x) = K\tau + constant\ C \tag{8.4}$$

The value of the integration constant C depends on initial A concentration, $[A]_o$. At initial conditions when A concentration is unchanged, i.e. $\tau = 0$ and $x = 0$, $-\ln [A]_o = C$. Hence

$$- \ln([A]_o - x) = K\tau - \ln [A]_o \tag{8.5}$$

Then

$$\ln [A]_o - \ln([A]_o - x) = K\tau \tag{8.6}$$

$$\ln\{[A]_o / ([A]_o - x)\} = K\tau \tag{8.7}$$

$$\frac{[A]_o}{[A]_o - x} = e^{K\tau} \tag{8.8}$$

$$[A] = [A]_o - x = [A]_o e^{-K\tau} \tag{8.9}$$

or

$$[A] = [A]_o e^{-[Mk][R]\tau} \tag{8.10}$$

However, if the concentration of A is high enough such that fragments and atoms of its destruction which enter the combustion environment, are able to alter and modify the existed composition of active species, the total rate of destruction, K, becomes

$$K^* = k_1 C^*_{\mathrm{H}} + k_2 C^*_{\mathrm{OH}} + k_3 C^*_{\mathrm{O}} + \ldots. \tag{8.11}$$

where C^*_{H}, C^*_{OH}, C^*_{O}, etc. are modified concentrations of all available active radicals, such as H, OH, ets. caused by destruction of A, so $C^*_{\mathrm{H}} = C_{\mathrm{H}} \pm \Delta C_{\mathrm{H}}$, $C^*_{\mathrm{OH}} = C_{\mathrm{OH}} \pm \Delta C_{\mathrm{OH}}$, etc. Hence, the rate of destruction, K, becomes

$$K^* = k_1(C_{\mathrm{H}} \pm \Delta C_{\mathrm{H}}) + k_2(C_{\mathrm{OH}} \pm \Delta C_{\mathrm{OH}}) + \ldots \tag{8.12}$$

$$K^* = [\mathrm{M}_k][\mathrm{R} \pm \Delta\mathrm{R}] = [\mathrm{M}_k]([\mathrm{R}] \pm [\Delta\mathrm{R}]) \tag{8.13}$$

$$K^* = [\mathrm{M}_k][\mathrm{R}] \pm [\mathrm{M}_k][\Delta\mathrm{R}] = K \pm \Delta K \tag{8.14}$$

where $[\Delta\mathrm{R}]$ is the matrix containing all differences in radical concentrations, due to the impact of the waste, and ΔK is the additional rate due to modified composition of radical pool. After substitution of Equation (8.14) into (8.9), it becomes

$$[A] = [A]_0 e^{-(K + \Delta K)\tau} \tag{8.15}$$

$$[A] = [\mathrm{A}]_0 e^{-K\tau} e^{-\Delta K\tau} \tag{8.16}$$

where the second term

$$\eta = e^{-\Delta K\tau} \tag{8.17}$$

is the additional rate function that reflects changes in radical composition and concentrations, due to the fragments of the parent waste compound. This term is the function of the ability of organic waste to contribute to the existing radical pool, as well

as the residence time during which this donation occurs; longer the residence time, larger are the number of donated species. At low A concentration, when $[A] \rightarrow 0$, $\Delta K \rightarrow 0$.

According to the above equation (8.12–8.17), if products of destruction of organic waste do not interfere with the existing radical pool such that $[\Delta R] = 0$, hence $\Delta K = 0$ and $\eta = 1$. At a constant residence time ($\tau = const$), the outlet waste concentration is proportional to its inlet concentration, thus equation (8.15) or (8.16) result in a linear relationship shown in Figure 8.1 by a solid line. However, in cases with real organic wastes, where the term η (equation 8.17) becomes a function of the contribution of a waste to the radical pool (thus, a function of waste concentration), the outlet concentration become an exponential function, as shown in Figure 8.1 by dashed lines. If fragments of the organic compound contribute to the radical pool, such that total rate of A destruction increase, $\Delta K > 0$, the relative outlet concentration of A will decrease (line α). However, if the fragments of a organic compound surpress or inhibit the activity of some active radicals, $\Delta K < 0$, the relative outlet concentration of A will increase, as shown by line β.

The existance, role and dependence of η on concentration is supported by experiments discussed in previous sections, where changes in radical concentrations and composition at higher CH_2Cl_2, CH_3Cl, C_6H_6 concentration, led to an increase of their destruction rates. In the case of CH_2Cl_2 combustion, at the same time formation of light hydrocarbons, such as CH_4, C_2H_2, C_2H_4, C_2H_6 was increased. Thus, the same change in the radical composition term η impacted charcteristic values and signs ($\pm$) for different species.

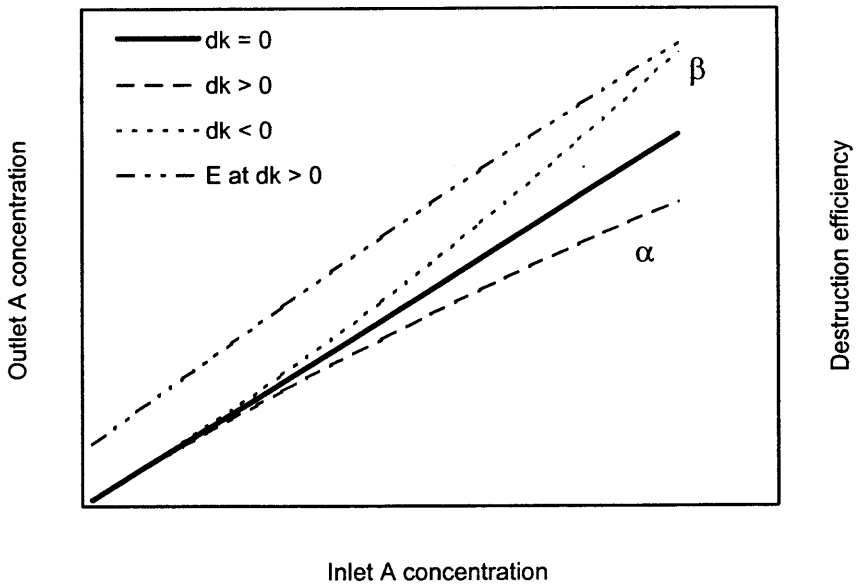


Figure 8.1 Outlet concentration and destruction efficiency as a function of ΔK, $\Delta K = f([A], \tau)$.

Based on equation (8.16), the efficiency of destruction (waste conversion) can be calculated as

$$E = 1 - [A]/[A]_o \tag{8.18}$$

$$E = 1 - [A]_o e^{-(K + \Delta K)\tau}/[A]_o = 1 - e^{-(K + \Delta K)\tau} = 1 - e^{-K\tau}\, e^{-\Delta K\tau} \tag{8.19}$$

At low concentration of A, the destruction efficiency is

$$E_{low} = 1 - e^{-K\tau} \tag{8.20}$$

The difference between destruction efficiency of A at high and low concentration:

$$\Delta E = E_{high} - E_{low} = (1 - e^{-K\tau}\, e^{-\Delta K\tau}) - (1 - e^{-K\tau}) = 1 - e^{-K\tau} e^{-\Delta K\tau} - 1 + e^{-K\tau} \tag{8.20}$$

$$\Delta E = - e^{-K\tau} e^{-\Delta K\tau} + e^{-K\tau} = e^{-K\tau}\,(1 - e^{-\Delta K\tau}) = e^{-K\tau}\,(1 - \eta) \tag{8.21}$$

or $\Delta E = \{[A]/[A]_o\}_{low}(1 - \eta) = \{[A]/[A]_o\}_{low}(1 - e^{-f([A])\tau})$ (8.22)

Thus, the difference, ΔE, depends on the effect of the compound A and products of its destruction on rates of reactions in existing waste-free flame, so $\Delta K = - f([A])$. Dependence of destruction efficiency on concentration, calculated from is (8.18), is shown in Figure 8.1.

In order to evaluate equation (8.15) with the Trenholm data, $\ln([A]/[A]_o)$ can be calculated at low feed concentration of A, ($[A] \wedge 0$ and $\Delta K \wedge 0$) as

$$\ln([A]/[A]_o)_{low} = \ln([A]_o e^{-K\tau}/[A]_o) = \ln e^{-K\tau} = -K\tau = a \quad (8.23)$$

At higher waste feed concentrations, and at constant residence time (τ = *const)*, and other combustion parameters, this computed as

$$\ln([A]/[A]_o)_{high} = \ln([A]_o e^{-(K+\Delta K)\tau}/[A]_o) = \ln e^{-(K+\Delta K)\tau} = -(K + \Delta K)\tau \quad (8.24)$$

$$= -K\tau - \Delta K\tau = a - \Delta K\tau \quad (8.24a)$$

which is a function of waste concentration, because of $\Delta K = f([A])$. Thus

$$\ln([A]/[A]_o)_{high} = a - \tau f([A]) \quad (8.25)$$

$$\ln([A]/[A]_o)_{high} = \ln([A]/[A]_o)_{low} - \tau f([A]) \quad (8.26)$$

As seen in Figure 8.2, this linear relationship matches field data by Trenholm.

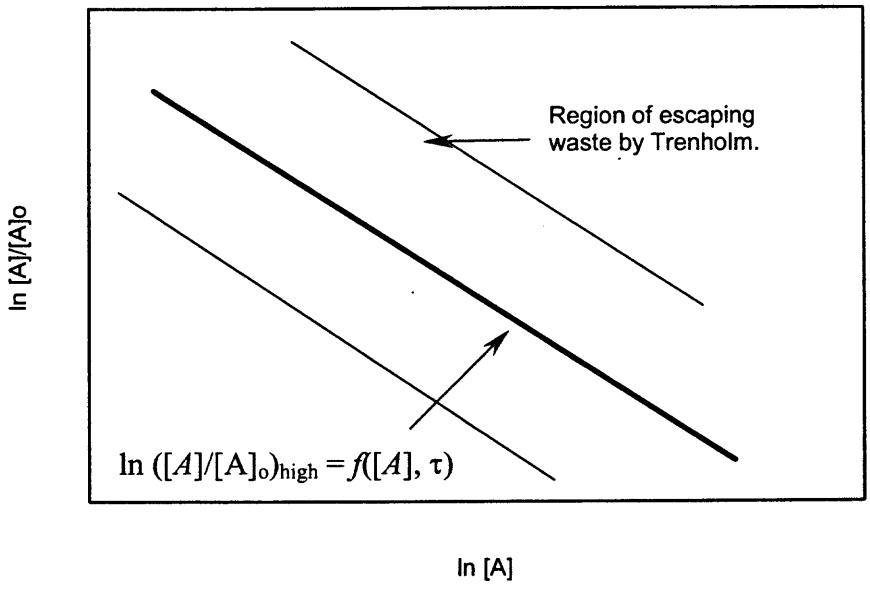


Figure 8.2 Calculated fraction of escaping waste.

8.1 Estimation of ΔK for C_2H_4/Air/CH_2Cl_2 System

Value of additional reaction rate ΔK (or f) can be estimated from equation (8.26) as

$$f([A])\tau = \ln ([A]/[A]_o)_{low} - \ln ([A]/[A]_o)_{high} \tag{8.27}$$

$$f([A])\tau = \ln \{([A]/[A]_o)_{low} / ([A]/[A]_o)_{high}\} \tag{8.27a}$$

For systems with equal residence time τ could be neglected, which makes equation (8.27a) as

$$f([A]) = \Delta K = \ln \{([A]/[A]_o)_{low} / ([A]/[A]_o)_{high}\} \tag{8.28}$$

The values of additional destruction rate, ΔK, as a functions of the inlet concentration of CH_2Cl_2 are shown in Figure 8.3.

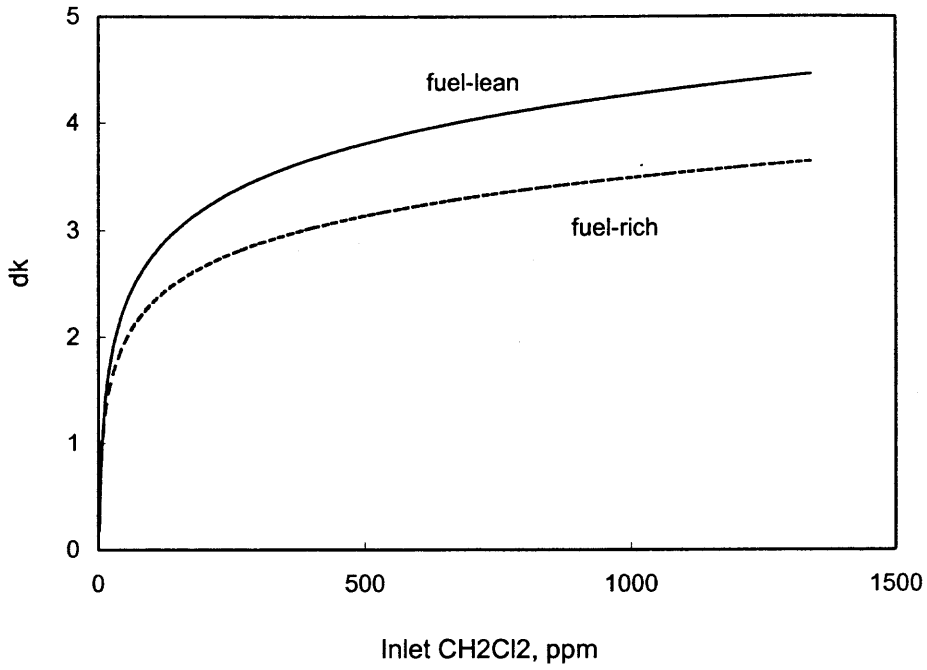


Figure 8.3 Additional rate function ΔK as a function of CH_2Cl_2 inlet concentration.

8.2 Summary

In order to evaluate effect of concentration of organic waste on its destruction efficiency, additional term $\eta = e^{-\Delta K \tau}$ was included, where ΔK was the total additional rate of destruction. It depended on the ability of atoms and fragments donated by the organic waste to alter the existing composition and concentrations of radical pool.

CHAPTER 9

FINAL CONCLUSIONS AND RECOMMENDATIONS

9.1 Conclusions

From the experimental observations and model predictions of the C_2H_4/Air/N_2 and C_2H_4/Air/CH_2Cl_2/N_2 combustion systems in a two-stage turbulent flow reactor, the following conclusions are obtained:

1) The two stage combustor that has been characterized as a PSR+PFR sequence was used successfully for studies on formation of products of incomplete combustion, such as CH_4, C_2H_2, C_2H_4, and C_6H_6 in the first and the second stages under different equivalence ratios during C_2H_4/Air combustion. Chlorocarbon (CH_2Cl_2) destruction and its effect on PICs formation has been investigated.

2) At different combustion conditions, and species composition in the first and the second stages of the combustor major pathways to C_6H_6 formation are different. At the first stage of the combustor with higher temperature and O_2 concentration the rate of consumption of C_6H_6 is close to its production rate, while in the second stage with lower temperature and depleted O_2 the C_6H_6 is formed intensively. Initial point to C_6H_6 formation in the second stage is C_2H_2, and the major benzene consumption reaction is the addition of H atom and formation of higher hydrocarbons. In the first stage C_6H_6 eliminates H atom and undergoes destruction.

3) At a fuel-rich conditions ($\phi = 1.4$), the combustion inhibition of CH_2Cl_2 was observed in the first stage. The emissions of PICs (CH_4, C_2H_2, C_2H_4) increased and the CO_2 decreased, as the feed CH_2Cl_2 concentration was increased from 0 to 1350 ppm.

4) Modeling with a detailed reaction mechanism (measured temperature used as input) satisfactorily predicted the observed concentration profiles of light hydrocarbons and CO_2 and O_2 in the CH_2Cl_2 combustion, while concentrations of outlet CH_2Cl_2 were underestimated. Rate-of production analysis (ROP) based on the modeling indicated that reaction

$$\cdot OH + HCl = H_2O + \cdot Cl \qquad \text{(R9.1)}$$

is a major channel of ·OH consumption under fuel-lean conditions. The decreased ·OH concentration level in the combustion limited the CH_4 and C_2H_2 burnout rates of the reactions

$$CH_4 + \cdot OH = \cdot CH_3 + H_2O \qquad \text{(R9.2)}$$

$$C_2H_2 + \cdot OH = \cdot CH_2CO + \cdot H \qquad \text{(R9.3)}$$

While ·Cl decreases concentrations of key radicals, such as ·H and ·OH, at higher CH_2Cl_2 concentrations, it has been shown by the ROP that ·Cl becomes a major radical substituting ·H and ·OH in performing many abstractions, such as

$$Cl + HO_2 = HCl + O_2 \qquad \text{(R9.4)}$$

which inhibits CO-CO_2 conversion since $\cdot HO_2$ is also a source of ·OH.

5) Experimental and modeling studies on CH_2Cl_2 destruction has been shown that destruction efficiency is lower at fuel-lean conditions, due to lower concentration of ·H radicals needed for ·Cl radical consumption via formation of HCl. ROP analysis indicates that pathways to CH_2Cl_2 destruction are different at fuel-lean and fuel-rich conditions, as

well as at lower and higher CH_2Cl_2 concentrations. Fraction of escaping CH_2Cl_2 is higher at its lower inlet concentration, which is consistent with field data collected on waste incinerators by Trenholm.

6) At low CH_2Cl_2 concentration major channel to its primary destruction is CH_2Cl_2 decomposition via

$$CH_2Cl_2 = \cdot CH_2Cl + \cdot Cl \qquad \text{(R9.5)}$$

and reactions with ·OH radicals at fuel-lean or with ·H radicals at fuel-rich conditions:

$$CH_2Cl_2 + \cdot OH = \cdot CHCl_2 + H_2O \qquad \text{(fuel-lean)} \qquad \text{(R9.6)}$$

$$CH_2Cl_2 + \cdot H = \cdot CHCl_2 + H_2 \qquad \text{(fuel-rich)} \qquad \text{(R9.7)}$$

At high CH_2Cl_2 concentrations with higher concentration of ·Cl radicals reaction

$$CH_2Cl_2 + \cdot Cl = \cdot CHCl_2 + HCl \qquad \text{(R9.8)}$$

becomes a major channel to CH_2Cl_2 destruction. Destruction of CH_2Cl_2 by ·Cl is more significant at fuel-lean conditions.

7) Simulation of CH_2Cl_2, CH_3Cl, and C_6H_6 destruction and ROP analysis has shown that their atoms and fragments, such as ·H and $\cdot CH_2$, intensively react with molecular O_2 that result in generation of additional ·O and ·OH radicals, involved in major destruction pathways. Released during CH_2Cl_2 and CH_3Cl destruction ·Cl radical forms additional channel to destruction of chlorinated wastes.

8) Analysis of the effect of concentration of organic wastes on their destruction efficiency shows that outlet and inlet waste concentrations are related by expression

$$[A] = [A]_o e^{-(k + \Delta k)\tau} \tag{9.1}$$

where ΔK is the additional destruction rate that reflects the effect of atoms and fragments donated by organic waste on the existing radical pool. This additional rate function, is calculated as

$$\Delta K = f([A]) = \ln\{([A]/[A]_o)_{low}/([A]/[A]_o)_{high}\} \tag{9.2}$$

9.2 Recommendations

According to the capability of using the two stage reactor for studies of hazardous waste incineration, some recommendations in specific areas are offered for the future work.

For the chlorocarbon combustion, a higher concentrations in the feed should be used to observe the effect of atoms and fragments donated by organic waste on the combustion process.

In order to incinerate the organic wastes, it will be usefull to use fuel-rich first stage combustion, followed by delution by air in the second stage.

Model that reflects effect of donated by waste species and their interaction more accurately (additional rate function ΔK) must be improved. This probably can be achieved by deviding a reactor volume to subsections, and multiple integrations and calculations of concentrations of all species during entire reactor residence time.

To get better understanding of the interaction of active species, more detailed identification of product species and determination of their concentrations are recommended.

APPENDIX A

FORTRAN CODE USED IN MODELING STUDIES

This appendix contains the FORTRAN code that was used for the combustion modeling in a PSR and PFR reaction zones. The code utilizes the copyrited library subroutines, which are not shown here.

```
C     PROGRAM chemkin2.for
C             LAST REVISED:     AUGUST 2002 BY ROMAN BRUKH
C//////////////////////////////////////////////////////////
C
C     PSR/PFR REACTOR MODEL BY RBB
C     MODIFIED ROP ROUTINE FOR PFR (single species ONLY)
C     INPUT PFR RESIDENCE TIMES, GUESS psr temp
C     INPUT PSR RESID. TIME OR MASS FEED RATE
C     INJECTION AFTER PSR
C
C\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\
C LAST REVISED:  12/20/1992,     BY MAO
C
C   1. PROBLEM TYPE: 0 = ENERGY BALANCE (ENRG)
C                    1 = TEMPERATURE GIVEN (TGIV)
C   2. HEAT LOSS IN PSR (ENRG)
C   3. HEAT LOSS IN PFR (ENRG)
C   4. PFR TEMP. PROFILE (TGIV): TEMP =AAAA+BBBB*TIME+CCCC*TIME**2
C                                +DDDD*TIME**3
C   5. PRINT OUT SPECIFICATION : 0 = PRINT ALL SPECIES
C                                1 = PRINT SPECIFIED SPECIES
C   6. EXTENTION OF WORK SPACE. CAN HANDLE 440 RXNS & 100 SPECIES.
C
C  REVISED:  2/1 1993,      BY MAO
C   1. RATE OF PRODUCTION IN PSR AND PFR
C   2  SENSITIVITY ANALASIS IN PSR
C            3/10/1993      BY MAO
C   1. PROBE QUENCH(NEED FURTHER WORK IN PFR PROBE)
C            3/20/1993      BY MAO
C     MIXING TEMP. IN SUBROUTINE MIX.
c            5/21/93   by Mao
c     reset parameters in LSODE after  PFR probe quench.
C            5/21/93   BY MAO
C
C\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\
C
c*****double precision
    IMPLICIT DOUBLE PRECISION(A-H,O-Z), INTEGER(I-N)
c*****IMPLICIT REAL*8 (A-H,O-Z)
    PARAMETER (LENIWK=20000, LENRWK=60000, LENCWK=1500,
   1  LIW=500,LRW=60000,NLMAX=55,KMAX=200)
```

```
      CHARACTER*80 KEYWORD,KEYWORD2(70)
      CHARACTER*16 DUMMY
      DIMENSION X(200),Y(200),Z(200),XP(200),YP(200),XINJ(200),YY(200),
     1  YINJ(200),XINP(200),VAL(20),XMIX(200),YMIX(200),KPRT(200),
     2  KROP(200),KSEN(200),cik(1500),cikn(1500),ROP(1000),D(5),
     3  UML(200),GML(200),TQ(10),VQ(10)
      DIMENSION ELWRK(60000),IELWRK(300),TAVC(10),VPFR1(10),DSTEP(10)
      COMMON/WRK/ICKWRK(14000),RCKWRK(38000)
      COMMON/PARAM/KK,P,RU,WT(200)
      COMMON/DUM/WDOT(160),H(200)
      COMMON/DTF/MFLAG,BBBB,CCCC,DDDD,CPB
      DIMENSION XFEED(200),XPFR(200),TPFR(9),VPFR(9),TAV(9),TAUPFR(9)
      DIMENSION TPS(10),PPS(10),TPF(10),PPF(10),XSQ(200),XFQ(200)
      CHARACTER CCKWRK(14000)*16, LINE*80, KSYM(KMAX)*16
      LOGICAL KERR,IERR
      DATA KERR/.FALSE./,X/KMAX*0.0/,VPSR1/250.0/
      DATA LIN/5/, LPSRINP2/10/, IFLAG/0/
      DATA LPSRBIN/15/, LFINAL/12/, LINCK/25/
      DATA A11/0.0/,A12/0.0/,A13/0.0/,A14/0.0/,A21/0.0/,A22/0.0/,
     1 A23/0.0/,A24/0.0/,A31/0.0/,A32/0.0/,A33/0.0/,A34/0.0/,
     2 A41/0.0/,A42/0.0/,A43/0.0/,A44/0.0/,B1/0.0/,B2/0.0/,B3/0.0/,
     3 B4/0.0/,AAAA/0.0/,BBBB/0.0/,CCCC/0.0/,DDDD/0.0/
C
      EXTERNAL FUN
C
C*******OPEN THE CHEMKIN LINK FILE
C
      OPEN(UNIT=LINCK, STATUS='OLD', FORM='UNFORMATTED')
C
C*******INITIALIZE CHEMKIN
C
      CALL CKINIT(LENIWK,LENRWK,LENCWK,LINCK,LFINAL,ICKWRK,
     1 RCKWRK,CCKWRK)
      CALL CKINDX(ICKWRK,RCKWRK,MM,KK,II,NFIT)
      CALL CKSYMS(CCKWRK,LFINAL,KSYM,IERR)
      IF (IERR) KERR=.TRUE.
      CALL CKWT(ICKWRK,RCKWRK,WT)
      CALL CKRP(ICKWRK,RCKWRK,RU,RUC,PATM)
      CLOSE(LINCK)
C
C*******INPUT A FLAG No. FOR PROBLEM TYPE  (0=ENRG, 1=TGIV)
```

```
C
      LINE=' '
      READ(LIN,'(A)')LINE
      ILEN=INDEX(LINE,'!')
      IF(ILEN.EQ.1)CONTINUE
      READ(LIN,*) MFLAG
C
C*******READ PSR VOLUME (CM3)
C
      LINE=' '
      READ(LIN,'(A)')LINE
      ILEN=INDEX(LINE,'!')
      IF(ILEN.EQ.1)CONTINUE
      READ(LIN,*)VPSR1
c
C*******READ HEAT LOSE IN BOTH PSR AND PFR (CAL/SEC)
C
      IF(MFLAG.EQ.0) THEN
        WRITE (LPSRINP2,2224)
 2224 FORMAT ('ENRG')
      ELSE
        WRITE (LPSRINP2,2225)
 2225 FORMAT ('TGIV')
      ENDIF
C
      LINE=' '
      READ(LIN,'(A)')LINE
      ILEN=INDEX(LINE,'!')
      IF(ILEN.EQ.1)CONTINUE
      READ(LIN,*)QLOS1,QLOS2
C
C*******READ PRESSURE AND FEED TEMPERATURE
C
      LINE=' '
      READ(LIN,'(A)')LINE
      ILEN=INDEX(LINE,'!')
      IF(ILEN.EQ.1)CONTINUE
      READ(LIN,*) PA,TFEED
      P=PA*PATM
C
C*******READ THE INITIAL NON-ZERO MOLES
```

```
C
  40 CONTINUE
    LINE=' '
    READ(LIN,'(A)',END=45) LINE
     ILEN=INDEX(LINE,'!')
     IF (ILEN.EQ.1)GOTO 40
     IF (ILEN.NE.1)THEN
      ILEN=ILEN-1
      IF (ILEN.LE.0) ILEN=LEN(LINE)
      IF (INDEX(LINE(:ILEN),'END').EQ.0) THEN
       IF (LINE(:ILEN).NE.' ')THEN
        CALL CKSNUM(LINE(:ILEN),1,LFINAL,KSYM,KK,KNUM,NVAL,VAL,IERR)
         IF (IERR) THEN
          WRITE (LFINAL,*) 'Error reading moles...'
          KERR=.TRUE.
        ELSE
          XFEED(KNUM)=VAL(1)
        END IF
      ENDIF
      GOTO 40
     ENDIF
     ENDIF
  45 CONTINUE
c
    XTOT=0.0E0
    DO 555 K=1, KK
    XTOT=XTOT+XFEED(K)
 555 CONTINUE
C
C*******INPUT LSODE PRINTOUT INCREMENT, PFR TAU
C
    LINE=' '
    READ(LIN,'(A)')LINE
    ILEN=INDEX(LINE,'!')
    IF(ILEN.EQ.1)CONTINUE
c
    READ(LIN,*) DELT,TPFR1
C
C*******INPUT PSR GUESS/GIVEN TEMPERATURE
C
    LINE=' '
```

```
      READ(LIN,'(A)')LINE
      ILEN=INDEX(LINE,'!')
      IF(ILEN.EQ.1)CONTINUE
      READ(LIN,*) TGUESS
C
C*******INPUT PFR VOLUMES AND TEMPERATURE MEASUREMENTS
C
      LINE=' '
      READ(LIN,'(A)')LINE
      ILEN=INDEX(LINE,'!')
      IF(ILEN.EQ.1)CONTINUE
      DO 489 J=1,5
       READ (LIN,*) VPFR(J)
 489 CONTINUE
      LINE=' '
      READ(LIN,'(A)')LINE
      ILEN=INDEX(LINE,'!')
      IF(ILEN.EQ.1)CONTINUE
      DO 490 J=1,5
       READ (LIN,*) TPFR(J)
 490 CONTINUE
C
C***INPUT PSR TAU OR MASS FEED RATE, START WITH A LOGIC SWITCH
C
      LINE=' '
      READ(LIN,'(A)')LINE
      ILEN=INDEX(LINE,'!')
      IF(ILEN.EQ.1)CONTINUE
c
      READ (LIN,*) ISWITCH,FEEDTAU
      IF (ISWITCH.EQ.0) THEN
       FEEDRATE=FEEDTAU
      ELSE
       PSRTAU=FEEDTAU
      ENDIF
 492 CONTINUE
C
      WRITE (LPSRINP2,3003) TGUESS
      WRITE (LPSRINP2,3005) TFEED
      WRITE (LPSRINP2,2229) PA
      IF (ISWITCH.EQ.0) GOTO 54
```

```
      WRITE (LPSRINP2,2302) PSRTAU
      GOTO 541
   54 CONTINUE
      WRITE (LPSRINP2,2231) FEEDRATE
  541 CONTINUE
      WRITE (LPSRINP2,2226) VPSR1
C
      DO 55 K=1, KK
      XFEED(K)=XFEED(K)/XTOT
      IF (XFEED(K).NE.0) WRITE (LPSRINP2,2223) KSYM(K),XFEED(K)
   55 CONTINUE
C
C*******INPUT THE COMPOSITION OF INJECTION MATERIAL
C
  493 CONTINUE
      LINE=' '
      READ (LIN,'(A)',END=740) LINE
      ILEN=INDEX(LINE,'!')
      IF (ILEN.EQ.1) GOTO 493
      IF (ILEN.NE.1) THEN
       ILEN=ILEN-1
       IF (ILEN.LE.0) ILEN=LEN(LINE)
       IF (INDEX(LINE(:ILEN),'END').EQ.0) THEN
        IF (LINE(:ILEN).NE.' ') THEN
         CALL CKSNUM(LINE(:ILEN),1,LFINAL,KSYM,KK,KNUM,NVAL,VAL,IERR)
         IF (IERR) THEN
          WRITE (LFINAL,*) 'Error reading moles of injection material'
          KERR=.TRUE.
         ELSE
          XINJ(KNUM)=VAL(1)
         END IF
        END IF
        GOTO 493
       END IF
       END IF
  740 CONTINUE
C
C*******INPUT THE MASS RATE AND TEMPERATURE OF INJECTION
C
      LINE=' '
      READ(LIN,'(A)')LINE
```

```
      ILEN=INDEX(LINE,'!')
      IF(ILEN.EQ.1)CONTINUE
c
      READ (LIN,*) RINJ, TINJ
      IF (RINJ.EQ.0) GOTO 960
      IFLAG=1
C
C*******NORMALIZE THE INJECTION MOLE FRACTIONS
C
      XTOTINJ=0
C
      DO 741 K=1, KK
      XTOTINJ=XTOTINJ+XINJ(K)
  741 CONTINUE
      XINJ(K)=XINJ(K)/XTOTINJ
  955 CONTINUE
       CALL CKXTY(XINJ,ICKWRK,RCKWRK,YINJ)
  960 CONTINUE
C
C*******INPUT A FLAG No. FOR PRINT OUT SPECIFICATION
C            (0=PRINT OUT ALL SPECIESS; 1=SPECIFIED SPECIES)
C            (0=PROBE OFF, 1=PROBE ON)
C
      LINE=' '
      READ(LIN,'(A)')LINE
      ILEN=INDEX(LINE,'!')
      IF(ILEN.EQ.1)CONTINUE
      READ(LIN,*) KFLAG, PROBE
      WRITE (LPSRINP2,2009) KFLAG
 2009 FORMAT ('PRNT',1X,I1)
C
C*******READ PRINTING SPECIES
C
  961 CONTINUE
c
      LINE=' '
      READ (LIN,'(A)',END=17) LINE
       ILEN=INDEX(LINE,'!')
       IF (ILEN.EQ.1) GOTO 961
       IF (ILEN.NE.1) THEN
        ILEN=ILEN-1
```

```
      IF (ILEN.LE.0) ILEN=LEN(LINE)
      IF (INDEX(LINE(:ILEN),'END').EQ.0) THEN
       IF (LINE(:ILEN).NE.' ') THEN
        CALL CKSNUM(LINE(:ILEN),1,LFINAL,KSYM,KK,KNUM,NVAL,VAL,IERR)
        IF (IERR) THEN
         WRITE (LFINAL,*) 'Error reading printing species...'
         KERR=.TRUE.
       ELSE
         KPRT(KNUM)=KNUM
       ENDIF
       GOTO 961
      ENDIF
     ENDIF
     ENDIF
 17  CONTINUE
C
C*******INPUT A FLAG No. FOR R-O-P****(0=NO ; 1=ALL ; 2=SELECTED)
C
     LINE=' '
     READ(LIN,'(A)')LINE
     ILEN=INDEX(LINE,'!')
     IF(ILEN.EQ.1)CONTINUE
     READ(LIN,*) NFLAG
C
C**INPUT A THRESHOLD VALUE FOR R-O-P and single species # for pfr/rop
C
     LINE=' '
     READ(LIN,'(A)')LINE
     ILEN=INDEX(LINE,'!')
     IF(ILEN.EQ.1)CONTINUE
c
      READ (LIN, *) THRP, KSPNUM
     IF (NFLAG. NE. 0) THEN
      WRITE (LPSRINP2, 2004)
      WRITE (LPSRINP2, 2002) THRP
     ENDIF
C
C*******INPUT SELECTED SPECIES FOR R-O-P
C
  19 CONTINUE
     LINE=' '
```

```
      READ (LIN,'(A)',END=170) LINE
      ILEN=INDEX(LINE,'!')
      IF (ILEN.EQ.1) GOTO 19
      IF (ILEN.NE.1) THEN
       ILEN=ILEN-1
       IF (ILEN.LE.0) ILEN=LEN(LINE)
       IF (INDEX(LINE(:ILEN),'END').EQ.0) THEN
        IF (LINE(:ILEN).NE.' ') THEN
         CALL CKSNUM(LINE(:ILEN),1,LFINAL,KSYM,KK,KNUM,NVAL,VAL,IERR)
         IF (IERR) THEN
          WRITE (LFINAL,*) 'Error reading ROP species...'
          KERR=.TRUE.
          ELSE
          KROP(KNUM)=KNUM
           IF (NFLAG.EQ.2) WRITE (LPSRINP2,2005) KSYM(KNUM)
         ENDIF
        ENDIF
        GOTO 19
       ENDIF
      ENDIF
 170 CONTINUE
C
C*******INPUT A FLAG FOR SENSITIVITY ANALYSIS
C      (0=NO; 1=ALL; 2=SELECTED SPECIES; 3=TEMP.)
C
      READ (LIN, *) JFLAG
C
C*******INPUT TWO THRESHOLD VALUES FOR SENS. OF SPECIES & TEMP.
C
      READ (LIN, *) THSES, THSET
      IF (JFLAG .NE. 0) THEN
       WRITE (LPSRINP2, 2006)
       WRITE (LPSRINP2, 2003) THSES
       WRITE (LPSRINP2, 2001) THSET
      ENDIF
C
C*******INPUT SELECTED SPECIES FOR SENS.
C
C1     IF (JFLAG. EQ. 2) THEN
C
 171 CONTINUE
```

```
      READ(LIN,'(A)',END=181) LINE
       ILEN=INDEX(LINE,'!')
       IF (ILEN.EQ.1) GOTO 171
       IF (ILEN.NE.1) THEN
        ILEN=ILEN-1
        IF (ILEN.LE.0) ILEN=LEN(LINE)
        IF (INDEX(LINE(:ILEN),'END').EQ.0) THEN
         IF (LINE(:ILEN).NE.' ') THEN
          CALL CKSNUM(LINE(:ILEN),1,LFINAL,KSYM,KK,KNUM,NVAL,VAL,IERR)
          IF (IERR) THEN
           WRITE (LFINAL, *) ' Error reading SENS species...'
           KERR = .TRUE.
           ELSE
           KSEN(KNUM) = KNUM
           IF (JFLAG. EQ. 2) WRITE (LPSRINP2, 2008) KSYM(KNUM)
          ENDIF
         ENDIF
         GOTO 171
        ENDIF
        ENDIF
 181 CONTINUE
C
      CLOSE(LIN)
C
C*******WRITE FILE FOR PSR INPUT
C
c1      IF(JFLAG .EQ. 1) THEN
c1        WRITE (LPSRINP2, 2006)
c1      ENDIF
c1      IF(JFLAG .NE. 0) THEN
c1        WRITE (LPSRINP2, 2003) THSES
c1        WRITE (LPSRINP2, 2001) THSET
c1      ENDIF
      IF(JFLAG .EQ. 3) THEN
       WRITE (LPSRINP2, 2007)
      ENDIF
      IF(JFLAG .EQ. 2) THEN
      ENDIF
C//////////////////////////////////////
      IF(MFLAG .EQ. 0 ) THEN
       PSRHL = QLOS1
```

```
       PFRHL = QLOS2
       WRITE (LPSRINP2,2227) PSRHL
      ENDIF
C////////////////////////////////////
      WRITE (LPSRINP2,2228)
      CLOSE (LPSRINP2,STATUS='KEEP')
      CONTINUE
      WRITE (LFINAL,*) '              '
C\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\
C
C    ****** PSR CALCULATION ******
C
      CALL PSRDRIVER
C
      OPEN (LPSRBIN,STATUS='OLD',FORM='UNFORMATTED')
      REWIND (LPSRBIN)
      READ (LPSRBIN) DUMMY
      READ (LPSRBIN) NNP
      KKP=NNP-1
      READ (LPSRBIN) EQUIVP1,PP1,TAUP1,FLRTP1,VP1,QP1
      READ (LPSRBIN) TINP1,(XINP(K),K=1,KK)
      READ (LPSRBIN) TP,(YP(K),K=1,KK)
      CLOSE (LPSRBIN,STATUS='keep')
C/////
      CLOSE (LPSRINP2,STATUS='KEEP')
C/////
      CALL CKYTX(YP,ICKWRK,RCKWRK,XP)
      WRITE(LFINAL,1519)
      WRITE(LFINAL,4543) PA,TFEED
      WRITE(LFINAL,7020)
C\\\\\\\\\\\\\\\\\\\\\\\\\\
C
C*******OUTPUT NON-ZERO FEED COMPOSITION
C
       DO 189 K=1,KK
        IF(XFEED(K).GT.0.0) THEN
         WRITE(LFINAL,2203) KSYM(K),XFEED(K)
        ENDIF
c
  189 CONTINUE
      WRITE(LFINAL,1517)
```

```
      WRITE(LFINAL,1514)
C\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\
      WRITE(24,499) TAUP1
      WRITE(LFINAL,1515) VPSR1
      WRITE(LFINAL,1518) TAUP1
      WRITE(LFINAL,9752) FLRTP1
      IF(MFLAG.EQ.0) THEN
        WRITE(LFINAL,9770) TP
      ELSE
        WRITE(LFINAL,9771) TP
      ENDIF
C\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\
      IF(PROBE.EQ.1)THEN
       WRITE(LFINAL,*)'PROBE QUENCH CALCULATION PERFORMED'
       WRITE(LFINAL,*)' '
      ENDIF
      WRITE(LFINAL,1520)
C\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\
c
      CALL CKUML (TP,ICKWRK,RCKWRK,UML)
      CALL CKGML (TP,ICKWRK,RCKWRK,GML)
c
C*******OUTPUT SPECIFIED SPECIES MOLE FRACTIONS OF PSR
C
      IF(KFLAG.EQ.1)THEN
       DO 191 K=1,KK
        KP = KPRT(K)
         IF(K.EQ.KP)THEN
          WRITE(LFINAL,2203)KSYM(K),XP(K)
c, UML(K), GML(K)
c 911 FORMAT(2X,'Internal energy',5X,E11.4,3X,'ergs/mole'
c    1       /,2X,'Gibbs free energy',3X,E11.4,3X,'ergs/mole')
         ENDIF
  191  CONTINUE
      ENDIF
      IF(KFLAG.EQ.2) THEN
       DO 192 K=1,KK
        WRITE (LFINAL,2203) KSYM(K), XP(K)
c, UML(K), GML(K)
  192  continue
      ENDIF
```

```
      WRITE(LFINAL,1517)
C
C\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\
C
      CALL CKMMWX (XP,ICKWRK,RCKWRK,WTM)
c       write (lfinal,*)WTM,' =WTM'
c
      IF(PROBE.EQ.1)THEN
       VQ(1)=0
       VQ(2)=5
       VQ(3)=15
       VQ(4)=25
       VQ(5)=45
       TQ(1)=TP
       TQ(2)=(TP+300)*0.67
       TQ(3)=(TP+300)*0.5
       TQ(4)=(TP+300)*0.33
       TQ(5)=300
      ENDIF
C
      VPF=0
c
      A11=5
      DO 30 J=1,5
c1-2   D(J)=DELT*(J-1)
       IF (J.EQ.1) D(J)=0
       IF (PROBE.EQ.0)THEN
      D(J)=D(J-1)+(VPFR(J)-VPFR(J-1))*WTM/
     1        (82.056*FLRTP1*((TPFR(J)+TPFR(J-1))/2))
      ELSE
       D(J)=D(J-1)+(VQ(J)-VQ(J-1))*WTM/
     1        (82.056*FLRTP1*((TQ(J)+TQ(J-1))/2))
      ENDIF
c
       taupf=D(J)
c
   30 CONTINUE
c
      DO 1 J=1,5
        A12=A12+D(J)
        A13=A13+D(J)**2
```

```
      A14=A14+D(J)**3
      A24=A24+D(J)**4
      A34=A34+D(J)**5
      A44=A44+D(J)**6
    1 CONTINUE
      A21=A12
      A22=A13
      A23=A14
      A31=A22
      A32=A23
      A33=A24
      A41=A32
      A42=A33
      A43=A34
      DO 2 J=1,5
       IF(PROBE.EQ.0)THEN
        B1=B1+TPFR(J)
        B2=B2+D(J)*TPFR(J)
        B3=B3+(D(J)**2)*TPFR(J)
        B4=B4+(D(J)**3)*TPFR(J)
       ELSE
        B1=B1+TQ(J)
        B2=B2+D(J)*TQ(J)
        B3=B3+(D(J)**2)*TQ(J)
        B4=B4+(D(J)**3)*TQ(J)
       ENDIF
    2 CONTINUE
C eliminating A41
      A42=A32-A42*A31/A41
      A43=A33-A43*A31/A41
      A44=A34-A44*A31/A41
      B4=B3-B4*A31/A41
C eliminating A31
      A32=A22-A32*A21/A31
      A33=A23-A33*A21/A31
      A34=A24-A34*A21/A31
      B3=B2-B3*A21/A31
C eliminating A21
      A22=A12-A22*A11/A21
      A23=A13-A23*A11/A21
      A24=A14-A24*A11/A21
```

```
      B2=B1-B2*A11/A21
C eliminating A42
      A43=A33-A43*A32/A42
      A44=A34-A44*A32/A42
      B4=B3-B4*A32/A42
C eliminating A32
      A33=A23-A33*A22/A32
      A34=A24-A34*A22/A32
      B3=B2-B3*A22/A32
C eliminating A43
      A44=A34-A44*A33/A43
      B4=B3-B4*A33/A43
C
      DDDD=B4/A44
      CCCC=(B3-A34*DDDD)/A33
      BBBB=(B2-A23*CCCC-A24*DDDD)/A22
      AAAA=(B1-BBBB*A12-CCCC*A13-DDDD*A14)/A11
C
c      write (lfinal,*) AAAA,'=aaaa     ',BBBB,'=bbbb     '
c      write (lfinal,*) CCCC,'=cccc     ',DDDD,'=dddd     '
c
      IF(PROBE.EQ.1)THEN
       DELTA=1
      ELSE
       DELTA=INT(taupf*1000)
      ENDIF
      DEL=DELTA/1000
c
      IF (IFLAG.EQ.0) GOTO 433
C\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\
C
C*******DESCRIPTION OF INJECTION MATERIALS
C
      WRITE(LFINAL,4004)
      WRITE(LFINAL,4006)TINJ,RINJ
      DO 281 K=1,KK
        IF(XINJ(K) .GT. 0.0) THEN
c           WRITE(LFINAL,2203) (KSYM(I,IJ),I=1,KK),XINJ(IJ)
        ENDIF
  281 continue
      WRITE(LFINAL,*)'     '
```

```
C
C*******MIXING THE INJECTION MATERIAL INTO THE PSR OUTLET GAS
C
   CALL MIX(KK,ICKWRK,RCKWRK,FLRTP1,RINJ,XP,XINJ,
  1   TP,TINJ,YP,YINJ,TMIX,YMIX,RMIX)
   CALL CKYTX (YMIX,ICKWRK,RCKWRK,XMIX)
   WRITE(LFINAL,4000)
   WRITE(LFINAL,4002) TMIX,RMIX
C\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\
c
   IF (KFLAG .EQ. 0) GOTO 29
   DO 29 K=1,KK
     KP=KPRT(K)
      IF(K.EQ.KP) THEN
         WRITE(LFINAL,2203) KSYM(K),XMIX(K)
      ENDIF
c       END DO
c       GO TO 29
c     ENDIF
c     WRITE(LFINAL,2203) (KSYM(I,IJ),I=1,KK),XMIX(IJ)
 29   CONTINUE
C
c   END DO
   WRITE(LFINAL,*)'   '
C
C*******INITIAL VALUES OF LSODE
C
   IF(MFLAG .EQ. 1) THEN
    Z(1) = TP
    TEMPFR = TP
   ELSE
    Z(1) = TMIX
    TEMPFR = TMIX
   ENDIF
C
   DO 431 K=1,KK
    Z(K+1) = YMIX(K)
    XPFR(K) = XMIX(K)
 431 CONTINUE
   goto 481
 433 continue
```

```
      Z(1) = TP
      TEMPFR = TP
      DO 481 K=1,KK
        Z(K+1) = YP(K)
        XPFR(K) = XP(K)
 481 CONTINUE
      P=PA*PATM
C
C*******SET THE INTEGRATION CONTROL PARAMETERS FOR LSODE
C
 8222 CONTINUE
      NEQ=KK+1
      TT1=0.0
      NLINES=NLMAX+1
      IF(PROBE.EQ.0)THEN
      WRITE(LFINAL,250) taupf
 250   FORMAT('****** PFR RESULTS * TOTAL PFR RESIDENCE
     1 TIME (SEC): ', F6.4)
      ENDIF
C
C*******INTEGRATION LOOP FOR PFR
c
      DE=0.001
c
      DO 999 J=0,DELTA
c
      MF=22
      ITOL=1
      IOPT=0
      RTOL=1.0E-6
      ITASK=1
      ATOL=1.0E-15
      ISTATE=1
C
C*******PRINT THE SOLUTION
c
c     WRITE(LFINAL,7100)
c     IF(MFLAG .EQ. 0) THEN
c       WRITE(LFINAL,7102)
c     ELSE
c       WRITE(LFINAL,7101)
```

```
c     ENDIF
C
C*******CALCULATE TEMPERATURE DROP DUE TO HEAT LOSS IN PFR
C
      IF(MFLAG .EQ. 0) THEN
       IF(TT1 .GT. 0.0) THEN
        call tdec(tempfr,pfrhl,flrtp1,cpb,de)
c         CALL TDEC(TEMPFR,PFRHL,FLRTP1,CPB,DELT)
        Z(1) = TEMPFR
       ENDIF
      ENDIF
C
c     IF(MFLAG.EQ.1)THEN
c       Z(1)=AAAA+BBBB*DE+CCCC*DE**2+DDDD*DE**3
c     write(lfinal,*)Z(1), ' = Z(1)'
c       Z(1)=TEMPFR
c     ENDIF
c
      VPF=(TT1*82.056*FLRTP1*TEMPFR)/WTM
c
      CALL CKUML(TEMPFR,ICKWRK,RCKWRK,UML)
      CALL CKGML(TEMPFR,ICKWRK,RCKWRK,GML)
c
      IF(PROBE.EQ.1)THEN
       IF(TT1.EQ.0)GOTO 993
       IF(TT1.EQ.0.001)GOTO 995
      ENDIF
c
      IF(MFLAG.EQ.1) THEN
      WRITE (LFINAL,7105) TT1, TEMPFR
 7105 FORMAT(/,'** TIME (SEC) = ',F6.4,5x,
     1'TEMPERATURE GIVEN (K) = ',F6.1)
      WRITE (LFINAL,*) ' '
       ELSE
      WRITE (LFINAL,7106) TT1, TEMPFR
 7106 FORMAT(/,'** TIME (SEC) = ',F6.4,5x,
     1'TEMPERATURE CALC. (K) = ',F6.1)
      WRITE (LFINAL,*) ' '
      ENDIF
  995 CONTINUE
      IF(KFLAG.EQ.1)THEN
```

```
      DO 991 K=1,KK
      KP=KPRT(K)
      IF(K.EQ.KP)THEN
       IF(PROBE.EQ.1)THEN
        IF(TT1.EQ.0.001)THEN
         WRITE(LFINAL,*)' '
         WRITE(LFINAL,994) KSYM(K), XPFR(K)
 994      FORMAT(1x,'Probe ',A10,' = ',E11.4)
        ENDIF
        IF(PROBE.EQ.1) GOTO 996
         WRITE (LFINAL,2203) KSYM(K), XPFR(K)
c, UML(K), GML(K)
 996     continue
       ENDIF
      ENDIF
 991  CONTINUE
     ELSE
      DO 992 K=1,KK
      WRITE (LFINAL,2203) KSYM(K), XPFR(K)
c, UML(K), GML(K)
 992  CONTINUE
     ENDIF
C
     IF(PROBE.EQ.1)THEN
      IF(TT1.EQ.0.001)GOTO 999
     ENDIF
c
 993 CONTINUE
c
C*******CALCULATION OF PFR R-O-P
C
     IF(NFLAG .EQ. 0) GO TO 49
     IF(NFLAG .EQ. 1) GO TO 49
C
C    ***************************INSERT BY BARAT**********************
C
c     write (lfinal,1021) TT1
c 1021 format (/,'** PFR time (sec):',F6.3)
     do 201 k=1,kk
     yy(k) = z(k+1)
 201  continue
```

```
      pfrtemper = z(1)
      epsr = thrp
      cneps=1.0E-30
      call ckqyp(p,pfrtemper,yy,ickwrk,rckwrk,rop)
c22     call ckcont(kspnum,rop,ickwrk,rckwrk,cik)
      do 202 k=1,kk
       call ckcont(k,rop,ickwrk,rckwrk,cik)
       KR=KROP(K)
       IF (K.EQ.KR) THEN
c       if (krop(k)) then
       write (lfinal,203) ksym(k)
 203   format(/1x,'Normalized and absolute R-O-P of ',
     1          A10,2x,'NORMALIZED',2x,
     2                '(MOLES/CC-SEC)')
c                                  normalization
       cnorm1=0.0
       cnorm2=0.0
       do 301 I=1,II
        if(cik(I) .lt. 0.0) then
         cnorm1=cnorm1-cik(I)
        else
         cnorm2=cnorm2+cik(I)
        endif
       forma=cnorm2-cnorm1
 301  continue
c22     cneps = 1.0E-30
      do 302 I=1,II
      cikn(I)=0.0
       if(cik(I) .lt. 0.0) then
      cikn(I) = cik(I)/(max(cneps,cnorm1))
       else
      cikn(I) = cik(I)/(max(cneps,cnorm2))
       endif
       if(abs(cikn(I)).GE.epsr) then
c       call cksymr(I,LFINAL,ICKWRK,RCKWRK,CCKWRK,LT,ISYM,IERR)
        write (lfinal,204) I,cikn(I),cik(I)
 204   format(5x,'Reaction #:',I4,24x,F9.3,5x,'(',1PE9.2,')')
c 204   format(I4,'. ',/,A80,/,F9.4,'(',1PE9.2,')')
       endif
 302  continue
      write(lfinal,205)cnorm2,cnorm1,forma
```

```
 205  format(1x,'NET RATE-OF-PRODUCTION (MOLES/CC-SEC)  = ',1PE9.2,
    1  /1x,'NET RATE-OF-CONSUMPTION (MOLES/CC-SEC) = ',1PE9.2,
    2  /1x,'NET CONTRIBUTION RATE (MOLES/CC-SEC)   = ',1PE9.2)
      endif
 202  continue
C
C     **********************END OF INSERT***************************
C
 49   CONTINUE
C
C*******CALL DIFFERENTIAL EQUATION SOLVER LSODE
C
      TT2=TT1+0.001
c
      CALL dvode(FUN,NEQ,Z,TT1,TT2,ITOL,RTOL,ATOL,ITASK,ISTATE,IOPT,
    1  ELWRK,LRW,IELWRK,LIW,JAC,MF)
      IF (ISTATE.EQ.2) GOTO 67
      WRITE(LFINAL,1212) ISTATE
      STOP
  67  TEMPFR=Z(1)
      DO 420 K=1,KK
      Y(K)=Z(K+1)
 420  CONTINUE
C
      CALL CKYTX(Y,ICKWRK,RCKWRK,XPFR)
C
      TT1=TT2
c
      IF (TT2.GT.DELTA) GOTO 999
c 998 continue
c     GOTO 250
C
 999  CONTINUE
      WRITE (LFINAL,1081) KK
 1081 FORMAT (/,2X,'TOTAL # OF SPECIES:   ',I6)
      WRITE (LFINAL,1082) II
 1082 FORMAT (2X,'TOTAL # OF REACTIONS: ',I6)
C
      CLOSE(LFINAL)
C
C*******FORMATS
```

```
C
 111 FORMAT(1X,//)
 115 FORMAT(1X,'ELAPSED PFR TIME:',E10.3,5X,'CUM. PFR VOL:',F5.1)
 702 FORMAT(1x,'MOLE FRACTIONS')
 888 FORMAT(1x,'Temp:',F8.1)
 498 FORMAT(/////,23X,'RATE-OF-PRODUCTION OF PSR')
 499 FORMAT(//,20X,'RESIDENT TIME OF PSR = ',E10.3,'  SEC.')
1212 FORMAT('ISTATE=',I4)
1378 FORMAT(1X,'PFR residence time (sec)')
cccc          'DELT (sec):',E10.3,10X,'TPFR1 (sec):',E10.3,/)
1514 FORMAT(1X,'****** PSR RESULTS ******',/)
1517 FORMAT(1X,'    ')
1515 FORMAT(1X,'PSR VOLUME (cm3):',2X,F7.2)
1518 FORMAT(1X,'PSR TAU (sec):',2X,E10.3)
1519 FORMAT(1X,'****** FEED CONDITIONS ******',/)
1520 FORMAT(1X,'CALCULATED PSR MOLE FRACTIONS',/)
2203 FORMAT(2X, A10, 1X, E11.4)
c,/
c, 20X, A10, E11.4)
c    1    5X,'Internal energy',5X,E11.4,3X,'ergs/mole',/,
c    2    5X,'Gibbs free energy',3X,E11.4,3X,'ergs/mole')
2223 FORMAT('REAC',1X,A8,1X,E11.4)
2002 FORMAT('EPSR',F6.3)
2003 FORMAT('EPSS',F7.4)
2001 FORMAT('EPST',F7.4)
2004 FORMAT('AROP')
2005 FORMAT(('ROP ',4(1X,A10)))
2006 FORMAT('ASEN')
2007 FORMAT('SENT')
2008 FORMAT(('SEN ',6(1X,A10)))
2226 FORMAT('VOL ',1X,E11.4)
2227 FORMAT('QLOS',1X,E11.4)
2228 FORMAT('END')
2229 FORMAT('PRES',1X,E11.4)
2231 FORMAT('FLRT',1X,E11.4)
2302 FORMAT('TAU',1X,E11.4)
3003 FORMAT('TEMP',1X,E11.4)
3005 FORMAT('TINL',1X,E11.4)
4000 FORMAT(1X,'****** RESULTS OF MIXING - INTO PFR ******',/)
4002 FORMAT(1X,'TEMP (K): ',F6.1,10X,'MASS RATE (g/s): ',F5.1)
4004 FORMAT(1X,'****** DESCRIPTION OF INJ. MATERIAL ******',/)
```

```
 4006 FORMAT(1X,'TEMP (K): ',F6.1,10X,'MASS RATE (g/s): ',F5.1)
 4543 FORMAT(1X,'PRES (atm):',F5.1,10X,'TFEED (K):',F7.1,/)
 7003 FORMAT('1')
 7020 FORMAT(1X,'****** INPUT MOLE FRACTIONS ******',/)
 7100 FORMAT(/,'** T(SEC)      TMP(K)      VOL(CC)')
 7101 FORMAT(3X,'     ',7X,'(TGIV)',3X,'      ')
 7102 FORMAT(3X,'     ',7X,'(CALC)',3X,'      ')
c 7105 FORMAT(E10.2,6X,F6.1,6X,F6.1,/)
 7110 FORMAT(34X,4(1X,10A1))
 7115 FORMAT(31X,10E11.3)
 7600 FORMAT(80A1)
 8400 FORMAT(1X,'ERROR IN INPUT FILE')
 9752 FORMAT(1X,'MASS RATE (g/s):',3X,F7.2)
 9770 FORMAT(1X,'CALC. PSR TEMP (K):',F7.1,/)
 9771 FORMAT(1X,'GIVEN PSR TEMP (K):',F7.1,/)
      END
C
C
      SUBROUTINE FUN(N,TIME,Z,ZP)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z), INTEGER(I-N)
c      IMPLICIT REAL*8(A-H,O-Z)
      DIMENSION Z(N),ZP(N)
      COMMON/WRK/ICKWRK(14000),RCKWRK(38000)
      COMMON/PARAM/KK,P,RU,WT(160)
      COMMON/DUM/WDOT(160),H(160)
C
      COMMON/DTF/MFLAG, BBBB, CCCC, DDDD, CPB
C
C       VARIABLES IN Z ARE
C          Z(1)=T
C          Z(K+1)=Y(K)
C
C*******CALL CHEMKIN SUBROUTINES
C
      CALL CKWYP(P,Z(1),Z(2),ICKWRK,RCKWRK,WDOT)
      CALL CKHMS(Z(1),ICKWRK,RCKWRK,H)
      CALL CKRHOY(P,Z(1),Z(2),ICKWRK,RCKWRK,RHO)
      CALL CKCPBS(Z(1),Z(2),ICKWRK,RCKWRK,CPB)
C
C*******FORM GOVERNING EQUATIONS
C
```

```
      IF(MFLAG .EQ. 0) THEN
        SUM=0.0
        DO 100 K=1,KK
          SUM=SUM+H(K)*WDOT(K)*WT(K)
          ZP(K+1)=WDOT(K)*WT(K)/RHO
 100    CONTINUE
        ZP(1)=-1.0*SUM/(RHO*CPB)
c
c       DO 202 K=1,KK
c         ZP(K+1)=WDOT(K)*WT(K)/RHO
c 202   CONTINUE
      ELSE
        ZP(1)= BBBB+2.0*CCCC*TIME+3.0*DDDD*TIME*TIME
        DO 203 K=1,KK
          ZP(K+1)=WDOT(K)*WT(K)/RHO
 203  CONTINUE
      ENDIF
C
      RETURN
      END
C
c/////////////////////////////////////////////////////////////////
c
      SUBROUTINE PSRDRIVER
c
      IMPLICIT DOUBLE PRECISION (A-H,O-Z),INTEGER (I-N)
c     IMPLICIT REAL*8 (A-H,O-Z)
      PARAMETER (LENLWK=30000,LENIWK=20000,LENRWK=60000,LENCWK=1500)
      LOGICAL LWORK(LENLWK)
      CHARACTER CWORK(LENCWK)*16
      DIMENSION IWORK(LENIWK), RWORK(LENRWK)
      DATA LIN/10/, LOUT/6/, LRSTRT/14/, LSAVE/15/, LRECOV/16/,
     1    LINKCK/25/
      OPEN(UNIT=LIN, STATUS='OLD', FORM='FORMATTED',READONLY)
      OPEN(UNIT=LOUT, STATUS='NEW', FORM='FORMATTED')
      OPEN(UNIT=LRSTRT, STATUS='OLD', FORM='UNFORMATTED', READONLY)
      OPEN(UNIT=LSAVE,STATUS='NEW',FORM='UNFORMATTED')
      OPEN(UNIT=LRECOV,STATUS='NEW',FORM='UNFORMATTED')
      OPEN(UNIT=LINKCK, STATUS='OLD', FORM='UNFORMATTED', READONLY)
C
      CALL PSR (LIN,LOUT,LINKCK,LRSTRT,LSAVE,LRECOV,LENLWK,LWORK,
```

```
     1        LENIWK,IWORK,LENRWK,RWORK,LENCWK,CWORK)
      RETURN
      END
C
      SUBROUTINE MIX(KK,ICKWRK,RCKWRK,SMDOT1,SMDOT2,X1,X2,T1,T2,Y1,Y2,
     1            TI,YTOL,SMDOTTOL)
C
C*******THIS SUBROUTINE CALCULATES THE MIX TEMPERATURE OF TWO STREAMS
C      ?TOL ARE THE PARAMETERS RETURNED ALONG WITH TI
C
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
c     IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION X1(160),X2(160),HMS1(160),RCKWRK(38000),ICKWRK(14000),
     1        HMS2(160),HMLTOL(160),Y1(160),Y2(160),YTOL(160),
     2        XTOL(160)
      CALL CKHMS(T1,ICKWRK,RCKWRK,HMS1)
      CALL CKHMS(T2,ICKWRK,RCKWRK,HMS2)
      CALL CKCPBS(T1,Y1,ICKWRK,RCKWRK,CPAV1)
      CALL CKCPBS(T2,Y2,ICKWRK,RCKWRK,CPAV2)
      DATA LFINAL/12/
      SMDOTTOL=SMDOT1+SMDOT2
      HTOL=0.
      DO I=1,KK
        YTOL(I)=0.
      END DO
C
C*******CALCULATE TOTAL ENTHALPY AND MASS FRACTIONS
C
      DO 100 I=1,KK
        HTOL=HTOL+Y1(I)*HMS1(I)*SMDOT1+Y2(I)*HMS2(I)*SMDOT2
        YTOL(I)=(Y1(I)*SMDOT1+Y2(I)*SMDOT2)/(SMDOT1+SMDOT2)
  100 CONTINUE
C
C*******CALCULATE FIRST GUESS FOR MIX TEMPERATURE
C
      TI=(SMDOT1*CPAV1*T1+SMDOT2*CPAV2*T2)/(SMDOT1*CPAV1+SMDOT2*CPAV2)
      write(*,*)'TI1=',ti
      CALL CKCPBS(TI,Y1,ICKWRK,RCKWRK,CPAV1I)
      CALL CKCPBS(TI,Y2,ICKWRK,RCKWRK,CPAV2I)
      CPAV1=(CPAV1+CPAV1I)/2.
      CPAV2=(CPAV2+CPAV2I)/2.
```

```
      TI=(SMDOT1*CPAV1*T1+SMDOT2*CPAV2*T2)/(SMDOT1*CPAV1+SMDOT2*CPAV2)
      write(*,*)'TI2=',ti
C
C*******INTERPOLATE TO GET FINAL MIXING TEMPERATURE
C
c     DO 120 IJ=1,100000
c       HTOLG=0.
c     CALL CKHMS(TI,ICKWRK,RCKWRK,HMLTOL)
c     DO 110 I=1,KK
c       HTOLG=HTOLG+HMLTOL(I)*YTOL(I)*SMDOTTOL
c 110 CONTINUE
c     DIFF=(HTOL-HTOLG)/HTOL
c     IF (ABS(DIFF).LE.0.05) GOTO 130
c     TI=(1.+0.005*DIFF)*TI
c     if(ti .gt. 10000.0 .or. ti .lt. 0.0) then
c       write(*,*) 'ij, diff,ti',ij,diff,ti
c       stop
c     endif
c 120 CONTINUE
c     WRITE(LFINAL,90)
c  90 FORMAT(1X,'TEMPERATURE NOT CONVERGED IN MIX')
c     STOP
c 130 CONTINUE
      RETURN
      END
C\\\\\
C
CC      SUBROUTINE INTP (DELT,TPFR,AAAA,BBBB,CCCC,DDDD)
C
CC      IMPLICIT REAL*8 (A-H,O-Z)
CC      DIMENSION D(10),TPFR(10)
CC      DATA A11/0.0/,A12/0.0/,A13/0.0/,A14/0.0/,A21/0.0/,A22/0.0/,
CC     1 A23/0.0/,A24/0.0/,A31/0.0/,A32/0.0/,A33/0.0/,A34/0.0/,
CC     2 A41/0.0/,A42/0.0/,A43/0.0/,A44/0.0/
C     3 AAAA/0.0/,BBBB/0.0/,CCCC/0.0/,DDDD/0.0/
CC      A11=5
CC      DO 30 J=1,5
CC       D(J)=DELT*(J-1)
CC   30 CONTINUE
CC      DO 1 J=1,5
CC       A12=A12+D(J)
```

```
CC      A13=A13+D(J)**2
CC      A14=A14+D(J)**3
CC      A24=A24+D(J)**4
CC      A34=A34+D(J)**5
CC      A44=A44+D(J)**6
CC    1 CONTINUE
CC     A21=12
CC     A22=A13
CC     A31=A22
CC     A23=A14
CC     A32=A23
CC     A33=A24
CC     A41=A32
CC     A42=A33
CC     A43=A34
CC     DO 2 J=1,5
CC      B1=B1+TPFR(J)
CC      B2=B2+D(J)*TPFR(J)
CC      B3=B3+(D(J)**2)*TPFR(J)
CC      B4=B4+(D(J)**3)*TPFR(J)
CC    2 CONTINUE
C                          eliminating  A41
CC     A42=A32-A42*A31/A41
CC     A43=A33-A43*A31/A41
CC     A44=A34-A44*A31/A41
CC     B4=B3-B4*A31/A41
C                          eliminating  A31
CC     A32=A22-A32*A21/A31
CC     A33=A23-A33*A21/A31
CC     A34=A24-A34*A21/A31
CC     B3=B2-B3*A21/A31
C                          eliminating  A21
CC     A22=A12-A22*A11/A21
CC     A23=A13-A23*A11/A21
CC     A24=A14-A24*A11/A21
CC     B2=B1-B2*A11/A21
C                          eliminating  A42
CC     A43=A33-A43*A32/A42
CC     A44=A34-A44*A32/A42
CC     B4=B3-B4*A32/A42
C                          eliminating  A32
```

```
CC    A33=A23-A33*A22/A32
CC    A34=A24-A34*A22/A32
CC    B3=B2-B3*A22/A32
CC    A44=A34-A44*A33/A43
CC    B4=B3-B4*A33/A43
CC    DD=B4/A44
CC    CC=(B3-A34*DD)/A33
CC    BB=(B2-A23*CC-A24*DD)/A22
CC    AA=(B1-BB*A12-CC*A13-DD*A14)/A11
CC    AAAA=AA
CC    BBBB=BB
CC    CCCC=CC
CC    DDDD=DD
CC    RETURN
CC    END
C
   SUBROUTINE TDEC(TEMP, QLOS, FLOW, CP, DELT)
C
C*******THIS SUBROUTINE CALCULATES THE TEMPERATURE OF DECREMENT IN PFR
C     DUE TO THE HEAT LOSS (NEW FILE BY FUHE MAO)
C
   IMPLICIT DOUBLE PRECISION (A-H,O-Z)
c   IMPLICIT REAL*8 (A-H,O-Z)
c
C   DESCRIPTION OF VARIABLES
C
C   NAME       I/O      DESCRIPTION
C   ---------------------------------------------------
C   TEMP       I/O      TEMP. AT PRINTOUT POINTS OF PFR (K)
C   QLOS        I       TOTAL HEAT LOSS IN PFR  (CAL/S)
C   FLOW        I       MASS FLOW RATE (G/S)
C   CP          I       MEAN SPECIFIC HEAT  (ERGS/G.K)
C   DELT        I       PRINT STEP  (S)
C   ---------------------------------------------------
   QERG = QLOS * 4.18 * 10.0E7
   Q123 = QERG * DELT
   TDRO = Q123 / (CP * FLOW)
   TEMP = TEMP - TDRO
   RETURN
   END
C\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\
```

APPENDIX B

REACTION MECHANISM USED FOR C_6H_6 MODELING

This appendix contains the reaction mechanism used for modeling studies of benzene formation.

CHEMKIN INTERPRETER OUTPUT: CHEMKIN-II Version 3.4 Mar. 1994

DOUBLE PRECISION

ELEMENTS CONSIDERED	ATOMIC WEIGHT
1. h	1.00797
2. o	15.9994
3. c	12.0112
4. n	14.0067
5. ar	39.9480

SPECIES CONSIDERED	C P H A R	S E	G E	MOLECULAR WEIGHT	TEMPERATURE LOW	HIGH	ELEMENT COUNT h	o	c	n	ar
1. h2		G	0	2.01594	300.0	5000.0	2	0	0	0	0
2. h		G	0	1.00797	300.0	5000.0	1	0	0	0	0
3. ch4		G	0	16.04303	300.0	5000.0	4	0	1	0	0
4. ch3		G	0	15.03506	300.0	5000.0	3	0	1	0	0
5. ch2		G	0	14.02709	300.0	5000.0	2	0	1	0	0
6. ch		G	0	13.01912	300.0	5000.0	1	0	1	0	0
7. ch2o		G	0	30.02649	300.0	5000.0	2	1	1	0	0
8. hco		G	0	29.01852	300.0	5000.0	1	1	1	0	0
9. co2		G	0	44.00995	300.0	5000.0	0	2	1	0	0
10. co		G	0	28.01055	300.0	5000.0	0	1	1	0	0
11. o2		G	0	31.99880	300.0	5000.0	0	2	0	0	0
12. o		G	0	15.99940	300.0	5000.0	0	1	0	0	0
13. oh		G	0	17.00737	300.0	5000.0	1	1	0	0	0
14. ho2		G	0	33.00677	300.0	5000.0	1	2	0	0	0
15. h2o2		G	0	34.01474	300.0	5000.0	2	2	0	0	0
16. h2o		G	0	18.01534	300.0	5000.0	2	1	0	0	0

```
17. c2h          G 0  25.03027  300.0 4000.0  1  0  2  0  0
18. hcco         G 0  41.02967  300.0 4000.0  1  1  2  0  0
19. c2h2         G 0  26.03824  300.0 5000.0  2  0  2  0  0
20. c2h3         G 0  27.04621  300.0 5000.0  3  0  2  0  0
21. c2h4         G 0  28.05418  300.0 5000.0  4  0  2  0  0
22. c2h5         G 0  29.06215  300.0 5000.0  5  0  2  0  0
23. c2h6         G 0  30.07012  300.0 4000.0  6  0  2  0  0
24. ch2oh        G 0  31.03446  250.0 4000.0  3  1  1  0  0
25. ch3o         G 0  31.03446  300.0 3000.0  3  1  1  0  0
26. hccoh        G 0  42.03764  300.0 4000.0  2  1  2  0  0
27. h2ccch       G 0  39.05736  300.0 4000.0  3  0  3  0  0
28. c3h2         G 0  38.04939  150.0 4000.0  2  0  3  0  0
29. ch2(s)       G 0  14.02709  300.0 5000.0  2  0  1  0  0
30. ch2co        G 0  42.03764  300.0 5000.0  2  1  2  0  0
31. c4h2         G 0  50.06054  300.0 5000.0  2  0  4  0  0
32. c5h2         G 0  62.07169  300.0 5000.0  2  0  5  0  0
33. c5h3         G 0  63.07966  300.0 5000.0  3  0  5  0  0
34. c6h2         G 0  74.08284  300.0 5000.0  2  0  6  0  0
35. c2           G 0  24.02230  300.0 5000.0  0  0  2  0  0
36. c2o          G 0  40.02170  300.0 5000.0  0  1  2  0  0
37. c            G 0  12.01115  300.0 5000.0  0  0  1  0  0
38. hcoh         G 0  30.02649  300.0 5000.0  2  1  1  0  0
39. ch2chcch     G 0  52.07648  300.0 4000.0  4  0  4  0  0
40. hcchcch      G 0  51.06851  300.0 4000.0  3  0  4  0  0
41. h2cccch      G 0  51.06851  300.0 4000.0  3  0  4  0  0
42. c6h5         G 0  77.10675  300.0 4000.0  5  0  6  0  0
43. c6h6         G 0  78.11472  300.0 5000.0  6  0  6  0  0
44. c6h5o        G 0  93.10615  300.0 4000.0  5  1  6  0  0
45. ch2chchch    G 0  53.08445  300.0 4000.0  5  0  4  0  0
46. ch2chcch2    G 0  53.08445  300.0 4000.0  5  0  4  0  0
47. h2c4o        G 0  66.05994  300.0 4000.0  2  1  4  0  0
48. ch2chchch2   G 0  54.09242  300.0 4000.0  6  0  4  0  0
49. ch3oh        G 0  32.04243  300.0 5000.0  4  1  1  0  0
50. ch2hco       G 0  43.04561  300.0 5000.0  3  1  2  0  0
51. c-c5h5       G 0  65.09560  300.0 5000.0  5  0  5  0  0
52. c-c5h5o      G 0  81.09500  300.0 5000.0  5  1  5  0  0
53. c-c5h6       G 0  66.10357  300.0 5000.0  6  0  5  0  0
```

```
54. c6h5oh        G 0  94.11412  300.0 4000.0  6  1  6  0  0
55. c10h8         G 0 128.17526  300.0 5000.0  8  0 10  0  0
56. c-c5h4oh      G 0  81.09500  300.0 5000.0  5  1  5  0  0
57. c-c5h4o       G 0  80.08703  300.0 5000.0  4  1  5  0  0
58. c4h10         G 0  58.12430  300.0 4000.0 10  0  4  0  0
59. pc4h9         G 0  57.11633  300.0 5000.0  9  0  4  0  0
60. sc4h9         G 0  57.11633  300.0 5000.0  9  0  4  0  0
61. c4h8-1        G 0  56.10836  300.0 5000.0  8  0  4  0  0
62. c4h8-2        G 0  56.10836  300.0 5000.0  8  0  4  0  0
63. c4h7          G 0  55.10039  300.0 5000.0  7  0  4  0  0
64. c3h6          G 0  42.08127  300.0 5000.0  6  0  3  0  0
65. ac3h5         G 0  41.07330  300.0 4000.0  5  0  3  0  0
66. pc3h5         G 0  41.07330  300.0 4000.0  5  0  3  0  0
67. sc3h5         G 0  41.07330  300.0 4000.0  5  0  3  0  0
68. ch2chcho      G 0  56.06473  300.0 5000.0  4  1  3  0  0
69. pc3h4         G 0  40.06533  300.0 4000.0  4  0  3  0  0
70. ac3h4         G 0  40.06533  300.0 4000.0  4  0  3  0  0
71. ch3co         G 0  43.04561  300.0 5000.0  3  1  2  0  0
72. c6h5ch2       G 0  91.13384  300.0 5000.0  7  0  7  0  0
73. c6h5ch3       G 0  92.14181  300.0 5000.0  8  0  7  0  0
74. ch2chco       G 0  55.05676  300.0 5000.0  3  1  3  0  0
75. ch3chco       G 0  56.06473  300.0 5000.0  4  1  3  0  0
76. ch3hco        G 0  44.05358  300.0 5000.0  4  1  2  0  0
77. chocho        G 0  58.03704  300.0 5000.0  2  2  2  0  0
78. c3h8          G 0  44.09721  300.0 5000.0  8  0  3  0  0
79. ic3h7         G 0  43.08924  300.0 5000.0  7  0  3  0  0
80. nc3h7         G 0  43.08924  300.0 5000.0  7  0  3  0  0
81. ch3chcch2     G 0  54.09242  300.0 5000.0  6  0  4  0  0
82. ch3ccch2      G 0  53.08445  300.0 4000.0  5  0  4  0  0
83. c6h5c2h5      G 0 106.16890  300.0 5000.0 10  0  8  0  0
84. c10h10        G 0 130.19120  300.0 5000.0 10  0 10  0  0
85. c10h9         G 0 129.18323  300.0 5000.0  9  0 10  0  0
86. c10h7         G 0 127.16729  300.0 5000.0  7  0 10  0  0
87. c6h4c2h3      G 0 103.14499  300.0 5000.0  7  0  8  0  0
88. c6h4c2h       G 0 101.12905  300.0 5000.0  5  0  8  0  0
89. c6h5c2h3      G 0 104.15296  300.0 5000.0  8  0  8  0  0
90. c6h5c2h       G 0 102.13702  300.0 5000.0  6  0  8  0  0
```

```
91. c10h7o        G 0 143.16669  300.0 5000.0  7  1 10  0  0
92. c6h5cho       G 0 106.12527  300.0 5000.0  6  1  7  0  0
93. c6h5co        G 0 105.11730  300.0 5000.0  5  1  7  0  0
94. hoc6h4ch3     G 0 108.14121  300.0 5000.0  8  1  7  0  0
95. c6h5ch2oh     G 0 108.14121  300.0 5000.0  8  1  7  0  0
96. oc6h4o        G 0 108.09758  300.0 5000.0  4  2  6  0  0
97. oc6h4ch3      G 0 107.13324  300.0 5000.0  7  1  7  0  0
98. c10h7ch2      G 0 141.19438  300.0 5000.0  9  0 11  0  0
99. c10h7ch3      G 0 142.20235  300.0 5000.0 10  0 11  0  0
100. ch3c6h4ch3   G 0 106.16890  300.0 5000.0 10  0  8  0  0
101. indene       G 0 116.16411  300.0 5000.0  8  0  9  0  0
102. indenyl      G 0 115.15614  300.0 5000.0  7  0  9  0  0
103. acenphthln   G 0 152.19756  300.0 5000.0  8  0 12  0  0
104. phnthrn      G 0 178.23580  300.0 5000.0 10  0 14  0  0
105. ch3chcch     G 0  53.08445  300.0 5000.0  5  0  4  0  0
106. ch3ch2cch    G 0  54.09242  300.0 4000.0  6  0  4  0  0
107. ch3c6h4ch2   G 0 105.16093  300.0 5000.0  9  0  8  0  0
108. phnthryl-1   G 0 177.22783  300.0 5000.0  9  0 14  0  0
109. phnthryl-9   G 0 177.22783  300.0 5000.0  9  0 14  0  0
110. flrnthn      G 0 202.25810  300.0 5000.0 10  0 16  0  0
111. ch3c6h4c2h3  G 0 118.18005  300.0 5000.0 10  0  9  0  0
112. ch3c6h4c2h5  G 0 120.19599  300.0 5000.0 12  0  9  0  0
113. c-2*4c6h6o   G 0  94.11412  300.0 5000.0  6  1  6  0  0
114. c-c5h7       G 0  67.11154  300.0 5000.0  7  0  5  0  0
115. l-c5h8       G 0  68.11951  298.1 3000.0  8  0  5  0  0
116. l-c5h7       G 0  67.11154  298.1 3000.0  7  0  5  0  0
117. c10h7c2h5    G 0 156.22944  300.0 5000.0 12  0 12  0  0
118. c10h7c2h3    G 0 154.21350  300.0 5000.0 10  0 12  0  0
119. c10h7oh      G 0 144.17466  300.0 5000.0  8  1 10  0  0
120. c6h5cco      G 0 117.12845  300.0 5000.0  5  1  8  0  0
121. c6h5chch     G 0 103.14499  300.0 5000.0  7  0  8  0  0
122. c6h5cch2     G 0 103.14499  300.0 5000.0  7  0  8  0  0
123. c10h7cch2    G 0 153.20553  300.0 5000.0  9  0 12  0  0
124. c10h7cch     G 0 152.19756  300.0 5000.0  8  0 12  0  0
125. c10h6cch     G 0 151.18959  300.0 5000.0  7  0 12  0  0
126. anthracn     G 0 178.23580  300.0 5000.0 10  0 14  0  0
127. ch3indene    G 0 130.19120  300.0 5000.0 10  0 10  0  0
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128. ch3indenyl      G 0 129.18323  300.0 5000.0  9  0 10  0  0
129. ch3phnthrn      G 0 192.26289  300.0 5000.0 12  0 15  0  0
130. pyrene          G 0 202.25810  300.0 5000.0 10  0 16  0  0
131. fluoryl         G 0 165.21668  300.0 5000.0  9  0 13  0  0
132. fluorene        G 0 166.22465  300.0 5000.0 10  0 13  0  0
133. h2cccch2        G 0  52.07648  300.0 4000.0  4  0  4  0  0
134. chchcho         G 0  55.05676  300.0 5000.0  3  1  3  0  0
135. hcccho          G 0  54.04879  300.0 5000.0  2  1  3  0  0
136. hccco           G 0  53.04082  300.0 5000.0  1  1  3  0  0
137. hc4-p(def)pthn  G 0 190.24695  300.0 5000.0 10  0 15  0  0
138. hc4-p(def)pthyl G 0 189.23898  300.0 5000.0  9  0 15  0  0
139. phnthroxy-1     G 0 193.22723  300.0 5000.0  9  1 14  0  0
140. phnthroxy-9     G 0 193.22723  300.0 5000.0  9  1 14  0  0
141. bz(a)ndene      G 0 166.22465  300.0 5000.0 10  0 13  0  0
142. bz(a)ndnyl      G 0 165.21668  300.0 5000.0  9  0 13  0  0
143. phnthrol-1      G 0 194.23520  300.0 5000.0 10  1 14  0  0
144. phnthrol-9      G 0 194.23520  300.0 5000.0 10  1 14  0  0
145. biphenyl        G 0 154.21350  300.0 5000.0 10  0 12  0  0
146. bz(a)phnthrn    G 0 228.29634  300.0 5000.0 12  0 18  0  0
147. bz(ghi)fln      G 0 226.28040  300.0 5000.0 10  0 18  0  0
148. fulvene         G 0  78.11472  300.0 3000.0  6  0  6  0  0
149. ch3cy24pd       G 0  80.13066  300.0 5000.0  8  0  6  0  0
150. ch3cy24pd1      G 0  79.12269  300.0 5000.0  7  0  6  0  0
151. ch3dcy24pd      G 0  79.12269  300.0 5000.0  7  0  6  0  0
152. cyc6h7          G 0  79.12269  300.0 5000.0  7  0  6  0  0
153. bnzofulv        G 0 128.17526  300.0 5000.0  8  0 10  0  0
154. adhfulv         G 0 130.19120  300.0 5000.0 10  0 10  0  0
155. adhflvyl        G 0 129.18323  300.0 5000.0  9  0 10  0  0
156. fulvenyl        G 0  77.10675  300.0 5000.0  5  0  6  0  0
157. ar              G 0  39.94800  300.0 5000.0  0  0  0  0  1
158. n2              G 0  28.01340  300.0 5000.0  0  0  0  2  0
-----------------------------------------------------------------------------
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(k = A T**b exp(-E/RT))

REACTIONS CONSIDERED	A	b	E
1. oh+h2=h+h2o	2.14E+08	1.5	3449.0
2. o+oh=o2+h	2.02E+14	-0.4	0.0
3. o+h2=oh+h	5.06E+04	2.7	6290.0
4. h+o2(+m)=ho2(+m)	4.52E+13	0.0	0.0
Low pressure limit: 0.10500E+20 -0.12570E+01 0.00000E+00			
h2o Enhanced by 0.000E+00			
h2 Enhanced by 0.000E+00			
n2 Enhanced by 0.000E+00			
ch4 Enhanced by 1.000E+01			
co2 Enhanced by 3.800E+00			
co Enhanced by 1.900E+00			
5. h+o2(+n2)=ho2(+n2)	4.52E+13	0.0	0.0
Low pressure limit: 0.20300E+21 -0.15900E+01 0.00000E+00			
6. h+o2(+h2)=ho2(+h2)	4.52E+13	0.0	0.0
Low pressure limit: 0.15200E+20 -0.11330E+01 0.00000E+00			
7. h+o2(+h2o)=ho2(+h2o)	4.52E+13	0.0	0.0
Low pressure limit: 0.21000E+24 -0.24370E+01 0.00000E+00			
8. oh+ho2=h2o+o2	2.13E+28	-4.8	3500.0
Declared duplicate reaction...			
9. oh+ho2=h2o+o2	9.10E+14	0.0	10964.0
Declared duplicate reaction...			
10. h+ho2=oh+oh	1.50E+14	0.0	1000.0
11. h+ho2=h2+o2	8.45E+11	0.7	1241.0
12. h+ho2=o+h2o	3.01E+13	0.0	1721.0
13. o+ho2=o2+oh	3.25E+13	0.0	0.0
14. oh+oh=o+h2o	3.57E+04	2.4	-2112.0
15. h+h+m=h2+m	1.00E+18	-1.0	0.0
h2o Enhanced by 0.000E+00			
h2 Enhanced by 0.000E+00			
16. h+h+h2=h2+h2	9.20E+16	-0.6	0.0
17. h+h+h2o=h2+h2o	6.00E+19	-1.3	0.0
18. h+oh+m=h2o+m	2.21E+22	-2.0	0.0
h2o Enhanced by 6.400E+00			
19. h+o+m=oh+m	4.71E+18	-1.0	0.0

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    h2o          Enhanced by   6.400E+00
20. o+o+m=o2+m                          1.89E+13   0.0   -1788.0
21. ho2+ho2=h2o2+o2                      4.20E+14   0.0   11982.0
  Declared duplicate reaction...
22. ho2+ho2=h2o2+o2                      1.30E+11   0.0   -1629.0
  Declared duplicate reaction...
23. oh+oh(+m)=h2o2(+m)                   1.24E+14  -0.4       0.0
  Low pressure limit:  0.30400E+31 -0.46300E+01  0.20490E+04
  TROE centering:     0.47000E+00  0.10000E+03  0.20000E+04  0.10000E+16
24. h2o2+h=ho2+h2                        1.98E+06   2.0    2435.0
25. h2o2+h=oh+h2o                        3.07E+13   0.0    4217.0
26. h2o2+o=oh+ho2                        9.55E+06   2.0    3970.0
27. h2o2+oh=h2o+ho2                      2.40E+00   4.0   -2162.0
28. ch3+ch3(+m)=c2h6(+m)                 9.22E+16  -1.2     636.0
  Low pressure limit:  0.11400E+37 -0.52460E+01  0.17050E+04
  TROE centering:     0.40500E+00  0.11200E+04  0.69600E+02  0.10000E+16
    h2o          Enhanced by   5.000E+00
    h2           Enhanced by   2.000E+00
    co2          Enhanced by   3.000E+00
    co           Enhanced by   2.000E+00
29. ch3+h(+m)=ch4(+m)                    2.14E+15  -0.4       0.0
  Low pressure limit:  0.33100E+31 -0.40000E+01  0.21080E+04
  TROE centering:     0.00000E+00  0.10000E-14  0.10000E-14  0.40000E+02
    h2o          Enhanced by   5.000E+00
    h2           Enhanced by   2.000E+00
    co2          Enhanced by   3.000E+00
    co           Enhanced by   2.000E+00
30. ch4+h=ch3+h2                         2.20E+04   3.0    8750.0
31. ch4+oh=ch3+h2o                       4.19E+06   2.0    2547.0
32. ch4+o=ch3+oh                         6.92E+08   1.6    8485.0
33. ch4+ho2=ch3+h2o2                     1.12E+13   0.0   24640.0
34. ch3+ho2=ch3o+oh                      7.00E+12   0.0       0.0
35. ch3+ho2=ch4+o2                       3.00E+12   0.0       0.0
36. ch3+o=ch2o+h                         8.00E+13   0.0       0.0
37. ch3+o2=ch3o+o                        1.45E+13   0.0   29209.0
38. ch3+o2=ch2o+oh                       2.51E+11   0.0   14640.0
39. ch3o+h=ch3+oh                        1.00E+14   0.0       0.0
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40. ch3+oh=ch2(s)+h2o                    2.65E+13   0.0    2186.0
41. ch3+oh=ch2+h2o                       3.00E+06   2.0    2500.0
42. ch3+oh=hcoh+h2                       5.48E+13   0.0    2981.0
43. ch3+oh=ch2o+h2                       2.25E+13   0.0    4300.0
44. ch3+h=ch2+h2                         9.00E+13   0.0   15100.0
45. ch3+m=ch+h2+m                        6.90E+14   0.0   82469.0
46. ch3+m=ch2+h+m                        1.90E+16   0.0   91411.0
47. ch3+oh(+m)=ch3oh(+m)                 5.65E+13   0.1       0.0
   Low pressure limit:  0.57500E+42 -0.74000E+01  0.62600E+03
   TROE centering:     0.25000E-01  0.10000E-14  0.80000E+04  0.30000E+04
     h2o          Enhanced by   1.600E+01
     h2           Enhanced by   2.000E+00
     co2          Enhanced by   3.000E+00
     co           Enhanced by   2.000E+00
48. ch3oh(+m)=hcoh+h2(+m)                4.15E+16  -0.1   92285.0
   Low pressure limit:  0.42300E+45 -0.76500E+01  0.92911E+05
   TROE centering:     0.25000E-01  0.10000E-14  0.80000E+04  0.30000E+04
     h2o          Enhanced by   1.600E+01
     h2           Enhanced by   2.000E+00
     co2          Enhanced by   3.000E+00
     co           Enhanced by   2.000E+00
49. ch3oh+oh=ch2oh+h2o                   2.61E+05   2.2   -1344.0
50. ch3oh+oh=ch3o+h2o                    2.62E+06   2.1     916.0
51. ch3oh+o=ch2oh+oh                     3.88E+05   2.5    3080.0
52. ch3oh+h=ch2oh+h2                     1.70E+07   2.1    4868.0
53. ch3oh+h=ch3o+h2                      4.24E+06   2.1    4868.0
54. ch3oh+ho2=ch2oh+h2o2                 9.64E+10   0.0   12578.0
55. ch2o+h(+m)=ch3o(+m)                  5.40E+11   0.5    2600.0
   Low pressure limit:  0.15000E+31 -0.48000E+01  0.55600E+04
   TROE centering:     0.75800E+00  0.94000E+02  0.15550E+04  0.42000E+04
     h2o          Enhanced by   5.000E+00
56. ch2o+h(+m)=ch2oh(+m)                 5.40E+11   0.5    3600.0
   Low pressure limit:  0.91000E+32 -0.48200E+01  0.65300E+04
   TROE centering:     0.71870E+00  0.10300E+03  0.12910E+04  0.41600E+04
     h2o          Enhanced by   5.000E+00
57. ch3o+h=ch2o+h2                       2.00E+13   0.0       0.0
58. ch2oh+h=ch2o+h2                      2.00E+13   0.0       0.0
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59. ch3o+oh=ch2o+h2o	1.00E+13	0.0	0.0
60. ch2oh+oh=ch2o+h2o	1.00E+13	0.0	0.0
61. ch3o+o=ch2o+oh	1.00E+13	0.0	0.0
62. ch2oh+o=ch2o+oh	1.00E+13	0.0	0.0
63. ch3o+o2=ch2o+ho2	6.30E+10	0.0	2600.0
64. ch2oh+o2=ch2o+ho2	1.57E+15	-1.0	0.0
Declared duplicate reaction...			
65. ch2oh+o2=ch2o+ho2	7.23E+13	0.0	3577.0
Declared duplicate reaction...			
66. hcoh+oh=hco+h2o	2.00E+13	0.0	0.0
67. hcoh+h=ch2o+h	2.00E+14	0.0	0.0
68. hcoh+o=co2+h+h	5.00E+13	0.0	0.0
69. hcoh+o=co+oh+h	3.00E+13	0.0	0.0
70. hcoh+o2=co2+h+oh	5.00E+12	0.0	0.0
71. hcoh+o2=co2+h2o	3.00E+13	0.0	0.0
72. ch2+h=ch+h2	1.00E+18	-1.6	0.0
73. ch2+oh=ch+h2o	1.13E+07	2.0	3000.0
74. ch2+oh=ch2o+h	2.50E+13	0.0	0.0
75. ch2+co2=ch2o+co	1.10E+11	0.0	1000.0
76. ch2+o=co+h+h	5.00E+13	0.0	0.0
77. ch2+o=co+h2	3.00E+13	0.0	0.0
78. ch2+o2=ch2o+o	3.29E+21	-3.3	2868.0
79. ch2+o2=co2+h+h	3.29E+21	-3.3	2868.0
80. ch2+o2=co2+h2	1.01E+21	-3.3	1508.0
81. ch2+o2=co+h2o	7.28E+19	-2.5	1809.0
82. ch2+o2=hco+oh	1.29E+20	-3.3	284.0
83. ch2+ch3=c2h4+h	4.00E+13	0.0	0.0
84. ch2+ch2=c2h2+h+h	4.00E+13	0.0	0.0
85. ch2+hcco=c2h3+co	3.00E+13	0.0	0.0
86. ch2+c2h2=h2ccch+h	1.20E+13	0.0	6600.0
87. ch2(s)+m=ch2+m	1.00E+13	0.0	0.0
h Enhanced by 1.200E+01			
c2h2 Enhanced by 4.000E+00			
h2o Enhanced by 3.000E+00			
88. ch2(s)+ch4=ch3+ch3	4.00E+13	0.0	0.0
89. ch2(s)+c2h6=ch3+c2h5	1.20E+14	0.0	0.0
90. ch2(s)+o2=co+oh+h	7.00E+13	0.0	0.0

91. ch2(s)+h2=ch3+h 7.00E+13 0.0 0.0
92. ch2(s)+c2h2=h2ccch+h 1.50E+14 0.0 0.0
93. ch2(s)+c2h4=ac3h5+h 1.30E+14 0.0 0.0
94. ch2(s)+o=co+h+h 3.00E+13 0.0 0.0
95. ch2(s)+oh=ch2o+h 3.00E+13 0.0 0.0
96. ch2(s)+h=ch+h2 3.00E+13 0.0 0.0
97. ch2(s)+co2=ch2o+co 3.00E+12 0.0 0.0
98. ch2(s)+ch3=c2h4+h 2.00E+13 0.0 0.0
99. ch2(s)+ch2co=c2h4+co 1.60E+14 0.0 0.0
100. ch+o2=hco+o 3.30E+13 0.0 0.0
101. ch+o=co+h 5.70E+13 0.0 0.0
102. ch+oh=hco+h 3.00E+13 0.0 0.0
103. ch+oh=c+h2o 4.00E+07 2.0 3000.0
104. ch+co2=hco+co 3.40E+12 0.0 690.0
105. ch+h=c+h2 1.50E+14 0.0 0.0
106. ch+h2o=ch2o+h 1.17E+15 -0.8 0.0
107. ch+ch2o=ch2co+h 9.46E+13 0.0 -515.0
108. ch+c2h2=c3h2+h 1.00E+14 0.0 0.0
109. ch+ch2=c2h2+h 4.00E+13 0.0 0.0
110. ch+ch3=c2h3+h 3.00E+13 0.0 0.0
111. ch+ch4=c2h4+h 6.00E+13 0.0 0.0
112. c+o2=co+o 2.00E+13 0.0 0.0
113. c+oh=co+h 5.00E+13 0.0 0.0
114. c+ch3=c2h2+h 5.00E+13 0.0 0.0
115. c+ch2=c2h+h 5.00E+13 0.0 0.0
116. ch2o+oh=hco+h2o 3.43E+09 1.2 -447.0
117. ch2o+h=hco+h2 2.19E+08 1.8 3000.0
118. ch2o+m=hco+h+m 3.31E+16 0.0 81000.0
119. ch2o+o=hco+oh 1.80E+13 0.0 3080.0
120. hco+o2=ho2+co 7.58E+12 0.0 410.0
121. hco+m=h+co+m 1.86E+17 -1.0 17000.0
    h2o Enhanced by 5.000E+00
    h2 Enhanced by 1.870E+00
    co2 Enhanced by 3.000E+00
    co Enhanced by 1.870E+00
    ch4 Enhanced by 2.810E+00
122. hco+oh=h2o+co 1.00E+14 0.0 0.0

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123. hco+h=co+h2                    1.19E+13  0.3     0.0
124. hco+o=co+oh                    3.00E+13  0.0     0.0
125. hco+o=co2+h                    3.00E+13  0.0     0.0
126. co+oh=co2+h                    9.42E+03  2.3   -2351.0
127. co+o+m=co2+m                     6.17E+14  0.0   3000.0
128. co+o2=co2+o                    2.53E+12  0.0  47688.0
129. co+ho2=co2+oh                   5.80E+13  0.0  22934.0
130. c2h6+ch3=c2h5+ch4                 5.50E-01  4.0   8300.0
131. c2h6+h=c2h5+h2                  5.40E+02  3.5   5210.0
132. c2h6+o=c2h5+oh                  3.00E+07  2.0   5115.0
133. c2h6+oh=c2h5+h2o                 7.23E+06  2.0    864.0
134. c2h5+h=c2h4+h2                  1.25E+14  0.0   8000.0
135. c2h5+h=ch3+ch3                  3.00E+13  0.0      0.0
136. c2h5+h=c2h6                    7.00E+13  0.0      0.0
137. c2h5+oh=c2h4+h2o                 4.00E+13  0.0      0.0
138. c2h5+o=ch3+ch2o                 1.00E+14  0.0      0.0
139. c2h5+ho2=ch3+ch2o+oh               3.00E+13  0.0      0.0
140. c2h5+o2=c2h4+ho2                 3.00E+20 -2.9   6760.0
   Declared duplicate reaction...
141. c2h5+o2=c2h4+ho2                 2.12E-06  6.0   9484.0
   Declared duplicate reaction...
142. c2h4+h=c2h3+h2                  3.36E-07  6.0   1692.0
143. c2h4+oh=c2h3+h2o                 2.02E+13  0.0   5936.0
144. c2h4+o=ch3+hco                  1.02E+07  1.9    179.0
145. c2h4+o=ch2hco+h                 3.39E+06  1.9    179.0
146. c2h4+ch3=c2h3+ch4                6.62E+00  3.7   9500.0
147. c2h4+h(+m)=c2h5(+m)               1.08E+12  0.5   1822.0
   Low pressure limit:  0.11120E+35 -0.50000E+01  0.44480E+04
   TROE centering:     0.10000E+01  0.10000E-14  0.95000E+02  0.20000E+03
     h2o          Enhanced by   5.000E+00
     h2           Enhanced by   2.000E+00
     co2          Enhanced by   3.000E+00
     co           Enhanced by   2.000E+00
148. c2h4(+m)=c2h2+h2(+m)              1.80E+13  0.0  76000.0
   Low pressure limit:  0.15000E+16  0.00000E+00  0.55443E+05
149. c2h3+h(+m)=c2h4(+m)               6.10E+12  0.3    280.0
   Low pressure limit:  0.98000E+30 -0.38600E+01  0.33200E+04
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   TROE centering:     0.78200E+00  0.20800E+03  0.26630E+04  0.60950E+04
     h2o          Enhanced by    5.000E+00
150. c2h3+h=c2h2+h2                    4.00E+13   0.0      0.0
151. c2h3+o=ch2co+h                    3.00E+13   0.0      0.0
152. c2h3+o2=ch2o+hco                  1.70E+29  -5.3    6500.0
153. c2h3+o2=ch2hco+o                  3.50E+14  -0.6    5260.0
154. c2h3+o2=c2h2+ho2                  2.12E-06   6.0    9484.0
155. c2h3+oh=c2h2+h2o                  2.00E+13   0.0      0.0
156. c2h3+c2h=c2h2+c2h2                3.00E+13   0.0      0.0
157. c2h3+ch=ch2+c2h2                  5.00E+13   0.0      0.0
158. c2h3+ch3=ac3h5+h                  4.73E+02   3.7    5677.0
159. c2h3+ch3=c3h6                     4.46E+56 -13.0   13865.0
160. c2h3+ch3=c2h2+ch4                 2.00E+13   0.0      0.0
161. c2h3+c2h2=ch2chcch+h              2.00E+12   0.0    5000.0
162. c2h3+c2h4=ch2chchch2+h            5.00E+11   0.0    7304.0
163. c2h3+c2h3=ch2chcch2+h             7.00E+13   0.0      0.0
164. c2h3+c2h3=c2h4+c2h2               1.45E+13   0.0      0.0
165. c2h2+oh=c2h+h2o                   3.37E+07   2.0   14000.0
166. c2h2+oh=hccoh+h                   5.04E+05   2.3   13500.0
167. c2h2+oh=ch2co+h                   2.18E-04   4.5   -1000.0
   Declared duplicate reaction...
168. c2h2+oh=ch2co+h                   2.00E+11   0.0      0.0
   Declared duplicate reaction...
169. c2h2+oh=ch3+co                    4.83E-04   4.0   -2000.0
170. hccoh+h=ch2co+h                   1.00E+13   0.0      0.0
171. c2h2+o=ch2+co                     6.12E+06   2.0    1900.0
172. c2h2+o=hcco+h                     1.43E+07   2.0    1900.0
173. c2h2+o=c2h+oh                     3.16E+15  -0.6   15000.0
174. c2h2+ch3=c2h+ch4                  1.81E+11   0.0   17289.0
175. c2h2+o2=hcco+oh                   4.00E+07   1.5   30100.0
176. c2h2+m=c2h+h+m                    4.20E+16   0.0  107000.0
177. c2h2+h(+m)=c2h3(+m)               3.11E+11   0.6    2589.0
   Low pressure limit:  0.22500E+41 -0.72690E+01  0.65770E+04
   TROE centering:     0.10000E+01  0.10000E-14  0.67500E+03  0.10000E+16
     h2o          Enhanced by    5.000E+00
     h2           Enhanced by    2.000E+00
     co2          Enhanced by    3.000E+00
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    co          Enhanced by   2.000E+00
178. ch3hco+oh=ch3co+h2o                  5.37E+10   0.7   -1110.0
179. ch3hco+h=ch3co+h2                    4.09E+09   1.2    2400.0
180. ch3hco+o=ch3co+oh                    5.89E+12   0.0    1810.0
181. ch3hco+ho2=ch3co+h2o2                1.70E+12   0.0   10700.0
182. ch3hco+o2=ch3co+ho2                  2.00E+13   0.5   42200.0
183. ch3hco+ch3=ch3co+ch4                 2.00E-06   5.6    2464.0
184. ch2hco+h=ch2co+h2                    4.00E+13   0.0       0.0
185. ch2hco+o=ch2o+hco                    1.00E+14   0.0       0.0
186. ch2hco+oh=ch2co+h2o                  3.00E+13   0.0       0.0
187. ch2hco+o2=ch2o+co+oh                 3.00E+10   0.0       0.0
188. ch2hco+ch3=>c2h5+co+h                4.90E+14  -0.5       0.0
189. ch2hco=ch2co+h                       3.95E+38  -7.6   45115.0
190. chocho(+m)=ch2o+co(+m)               4.27E+12   0.0   50600.0
   Low pressure limit:  0.89100E+17  0.00000E+00  0.49200E+05
191. chocho=co+co+h2                      4.07E+42  -8.5   69278.0
192. chocho+oh=hco+co+h2o                 1.00E+13   0.0       0.0
193. chocho+o=hco+co+oh                   7.24E+12   0.0    1970.0
194. chocho+h=ch2o+hco                    1.00E+12   0.0       0.0
195. chocho+ho2=hco+co+h2o2               1.70E+12   0.0   10700.0
196. chocho+ch3=hco+co+ch4                1.74E+12   0.0    8440.0
197. chocho+o2=hco+co+ho2                 1.00E+14   0.0   37000.0
198. ch3co(+m)=ch3+co(+m)                 3.00E+12   0.0   16722.0
   Low pressure limit:  0.12000E+16  0.00000E+00  0.12518E+05
199. ch2co+o=co2+ch2                      1.75E+12   0.0    1350.0
200. ch2co+h=ch3+co                       7.00E+12   0.0    3011.0
201. ch2co+h=hcco+h2                      2.00E+14   0.0    8000.0
202. ch2co+o=hcco+oh                      1.00E+13   0.0    8000.0
203. ch2co+oh=hcco+h2o                    1.00E+13   0.0    2000.0
204. ch2co+oh=ch2oh+co                    3.73E+12   0.0   -1013.0
205. ch2+co(+m)=ch2co(+m)                 8.10E+11   0.5    4510.0
   Low pressure limit:  0.19000E+34 -0.51100E+01  0.71000E+04
   TROE centering:     0.59070E+00  0.27500E+03  0.12260E+04  0.51850E+04
    h2o         Enhanced by   5.000E+00
206. c2h+h2=c2h2+h                        4.09E+05   2.4     864.3
207. c2h+o=ch+co                          5.00E+13   0.0       0.0
208. c2h+oh=hcco+h                        2.00E+13   0.0       0.0
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209. c2h+oh=c2+h2o                    4.00E+07   2.0    8000.0
210. c2h+o2=co+co+h                   9.04E+12   0.0    -457.0
211. c2h+c2h2=c4h2+h                  9.64E+13   0.0       0.0
212. c2h+c2h4=ch2chcch+h              1.20E+13   0.0       0.0
213. hcco+c2h2=h2ccch+co              1.00E+11   0.0    3000.0
214. hcco+h=ch2(s)+co                 1.00E+14   0.0       0.0
215. hcco+o=h+co+co                   8.00E+13   0.0       0.0
216. hcco+o=ch+co2                    2.95E+13   0.0    1113.0
217. hcco+o2=hco+co+o                 2.50E+08   1.0       0.0
218. hcco+o2=co2+hco                  2.40E+11   0.0    -854.0
219. hcco+ch=c2h2+co                  5.00E+13   0.0       0.0
220. hcco+hcco=c2h2+co+co             1.00E+13   0.0       0.0
221. hcco+oh=c2o+h2o                  3.00E+13   0.0       0.0
222. c2o+h=ch+co                      1.00E+13   0.0       0.0
223. c2o+o=co+co                      5.00E+13   0.0       0.0
224. c2o+oh=co+co+h                   2.00E+13   0.0       0.0
225. c2o+o2=co+co+o                   2.00E+13   0.0       0.0
226. c2+h2=c2h+h                      4.00E+05   2.4    1000.0
227. c2+o2=co+co                      5.00E+13   0.0       0.0
228. c2+oh=c2o+h                      5.00E+13   0.0       0.0
229. c3h8(+m)=c2h5+ch3(+m)            7.90E+22  -1.8   88629.0
   Low pressure limit:  0.72370E+28 -0.28800E+01  0.67448E+05
   TROE centering:      0.10000E+01  0.10000E-14  0.15000E+04  0.10000E+16
     h2o          Enhanced by   5.000E+00
     co2          Enhanced by   3.000E+00
     co           Enhanced by   2.000E+00
     h2           Enhanced by   2.000E+00
230. c3h8+o2=ic3h7+ho2                4.00E+13   0.0   48610.0
231. c3h8+o2=nc3h7+ho2                4.00E+13   0.0   51360.0
232. c3h8+ho2=nc3h7+h2o2              4.76E+04   2.5   16492.0
233. c3h8+ho2=ic3h7+h2o2              9.64E+03   2.6   13909.0
234. c3h8+oh=nc3h7+h2o                3.16E+07   1.8     934.0
235. c3h8+oh=ic3h7+h2o                7.08E+06   1.9    -159.0
236. c3h8+o=nc3h7+oh                  3.73E+06   2.4    5504.0
237. c3h8+o=ic3h7+oh                  5.48E+05   2.5    3139.0
238. c3h8+h=ic3h7+h2                  1.30E+06   2.4    4471.0
239. c3h8+h=nc3h7+h2                  1.33E+06   2.5    6756.0
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240. c3h8+ch3=nc3h7+ch4                    9.04E-01   3.6    7153.0
241. c3h8+ch3=ic3h7+ch4                    1.51E+00   3.5    5480.0
242. c3h8+c2h3=ic3h7+c2h4                  1.00E+03   3.1    8830.0
243. c3h8+c2h3=nc3h7+c2h4                  6.00E+02   3.3   10500.0
244. c3h8+c2h5=ic3h7+c2h6                  1.51E+00   3.5    7470.0
245. c3h8+c2h5=nc3h7+c2h6                  9.03E-01   3.6    9140.0
246. c3h8+ac3h5=c3h6+nc3h7                 2.35E+02   3.3   19842.0
247. c3h8+ac3h5=c3h6+ic3h7                 7.83E+01   3.3   18169.0
248. nc3h7(+m)=c2h4+ch3(+m)                1.23E+13  -0.1   30202.0
   Low pressure limit:  0.54850E+50 -0.10000E+02  0.35766E+05
   TROE centering:     0.21700E+01  0.10000E-14  0.25100E+03  0.11850E+04
     h2o          Enhanced by   5.000E+00
     h2           Enhanced by   2.000E+00
     co2          Enhanced by   3.000E+00
     co           Enhanced by   2.000E+00
249. nc3h7+o2=c3h6+ho2                     3.58E+09   0.0   -3532.0
250. ic3h7+o2=c3h6+ho2                     6.10E+20  -2.9    7910.0
251. c3h6+h(+m)=ic3h7(+m)                  5.70E+09   1.2     874.0
   Low pressure limit:  0.16400E+55 -0.11100E+02  0.93640E+04
   TROE centering:     0.10000E+01  0.10000E-14  0.26000E+03  0.30000E+04
     h2o          Enhanced by   5.000E+00
     h2           Enhanced by   2.000E+00
     co2          Enhanced by   3.000E+00
     co           Enhanced by   2.000E+00
252. ic3h7+h=c2h5+ch3                      5.00E+13   0.0       0.0
253. nc3h7+h=c2h5+ch3                      1.00E+14   0.0       0.0
254. pc3h5+h=c3h6                          1.00E+14   0.0       0.0
255. sc3h5+h=c3h6                          5.00E+13   0.0       0.0
256. c3h6=c2h2+ch4                         2.50E+12   0.0   70000.0
257. c3h6=ac3h4+h2                         3.00E+13   0.0   80000.0
258. c3h6+ho2=ac3h5+h2o2                   9.64E+03   2.6   13910.0
259. c3h6+oh+o2=ch3hco+ch2o+oh             3.00E+10   0.0   -8280.0
260. c3h6+oh=ac3h5+h2o                     3.12E+06   2.0    -298.0
261. c3h6+oh=sc3h5+h2o                     1.11E+06   2.0    1451.0
262. c3h6+oh=pc3h5+h2o                     2.11E+06   2.0    2778.0
263. c3h6+o=ch3chco+h+h                    5.01E+07   1.8      76.0
264. c3h6+o=c2h5+hco                       1.58E+07   1.8   -1216.0
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265. c3h6+o=ac3h5+oh	5.24E+11	0.7	5884.0
266. c3h6+o=pc3h5+oh	1.20E+11	0.7	8959.0
267. c3h6+o=sc3h5+oh	6.03E+10	0.7	7632.0
268. c3h6+h=c2h4+ch3	7.23E+12	0.0	1302.0
269. c3h6+h=ac3h5+h2	1.73E+05	2.5	2492.0
270. c3h6+h=sc3h5+h2	4.09E+05	2.5	9794.0
271. c3h6+h=pc3h5+h2	8.04E+05	2.5	12284.0
272. pc3h5+ho2=c3h6+o2	2.00E+12	0.0	0.0
273. sc3h5+ho2=c3h6+o2	1.00E+12	0.0	0.0
274. ac3h5+ho2=c3h6+o2	3.00E+12	0.0	0.0
275. c3h6+ch3=ac3h5+ch4	2.22E+00	3.5	5675.0
276. c3h6+ch3=sc3h5+ch4	8.43E-01	3.5	11656.0
277. c3h6+ch3=pc3h5+ch4	1.35E+00	3.5	12848.0
278. c3h6+hco=ac3h5+ch2o	1.08E+07	1.9	17010.0
279. ch3chco+oh=ch2chco+h2o	4.00E+06	2.0	0.0
280. ch3chco+o=ch2chco+oh	7.60E+08	1.5	8500.0
281. ch3chco+h=ch2chco+h2	2.00E+05	2.5	2500.0
282. ch3chco+h=c2h5+co	2.00E+13	0.0	2000.0
283. ch3chco+o=ch3+hco+co	3.00E+07	2.0	0.0
284. ch2chcho+oh=ch2chco+h2o	1.00E+13	0.0	0.0
285. ch2chcho+o=ch2chco+oh	7.24E+12	0.0	1970.0
286. ch2chcho+o=ch2co+hco+h	5.01E+07	1.8	76.0
287. ch2chcho+h=ch2chco+h2	3.98E+13	0.0	4200.0
288. ch2chcho+h=c2h4+hco	2.00E+13	0.0	3500.0
289. ch2chcho+o2=ch2chco+ho2	3.00E+13	0.0	36000.0
290. ch2chco=c2h3+co	1.00E+14	0.0	34000.0
291. ch2chco+o=c2h3+co2	1.00E+14	0.0	0.0
292. ac3h5+o2=ch2chcho+oh	1.82E+13	-0.4	22859.0
293. ac3h5+o2=ac3h4+ho2	4.99E+15	-1.4	22428.0
294. ac3h5+o2=ch2hco+ch2o	1.06E+10	0.3	12838.0
295. ac3h5+o2=c2h2+ch2o+oh	2.78E+25	-4.8	15468.0
296. ac3h5+ho2=ch2chcho+h+oh	1.00E+13	0.0	0.0
297. ac3h5+oh=ac3h4+h2o	1.00E+13	0.0	0.0
298. ac3h5+h=ac3h4+h2	5.00E+13	0.0	0.0
299. ac3h5+h=c3h6	1.88E+26	-3.6	5468.0
300. ac3h5+o=ch2chcho+h	1.81E+14	0.0	0.0
301. ac3h5+ch3=ac3h4+ch4	3.02E+12	-0.3	-131.0

302. ac3h5+c2h2=c-c5h6+h 2.95E+32 -5.8 25733.0
303. ac3h5+ch3=c4h8-1 1.76E+50 -11.0 18600.0
304. ac3h5+c2h3=c-c5h6+h+h 1.59E+65 -14.0 61265.0
305. fulvene=c6h6 9.84E+37 -7.4 76979.0
306. fulvene+h=c6h6+h 3.00E+12 0.5 2000.0
307. pc3h5+o2=ch3hco+hco 1.09E+23 -3.3 3892.0
308. pc3h5+o2=ch3chco+h+o 1.60E+15 -0.8 3135.0
309. pc3h5+o=ch3chco+h 1.00E+14 0.0 0.0
310. pc3h5+h=pc3h4+h2 2.00E+13 0.0 0.0
311. pc3h5+oh=pc3h4+h2o 1.00E+13 0.0 0.0
312. pc3h5+h=ac3h5+h 1.00E+14 0.0 0.0
313. sc3h5+h=ac3h5+h 1.00E+14 0.0 0.0
314. sc3h5+o2=ch3co+ch2o 1.09E+22 -3.3 3892.0
315. sc3h5+o=ch2co+ch3 1.00E+14 0.0 0.0
316. sc3h5+h=pc3h4+h2 4.00E+13 0.0 0.0
317. sc3h5+oh=pc3h4+h2o 2.00E+13 0.0 0.0
318. ac3h4+h=h2ccch+h2 2.00E+07 2.0 5000.0
319. ac3h4+o=c2h4+co 1.34E+07 1.9 179.0
320. ac3h4+oh=h2ccch+h2o 1.00E+07 2.0 1000.0
321. ac3h4+ch3=h2ccch+ch4 1.50E+00 3.5 5600.0
322. ac3h4=pc3h4 1.48E+13 0.0 60401.0
323. pc3h4+h=h2ccch+h2 2.00E+07 2.0 5000.0
324. pc3h4+o=c2h4+co 1.50E+13 0.0 2102.0
325. pc3h4+oh=h2ccch+h2o 1.00E+07 2.0 1000.0
326. pc3h4+ch3=h2ccch+ch4 1.50E+00 3.5 5600.0
327. pc3h4+h=ch3+c2h2 5.12E+10 1.0 2060.0
328. pc3h4+h(+m)=sc3h5(+m) 6.50E+12 0.0 2000.0
Low pressure limit: 0.84500E+40 -0.72700E+01 0.65770E+04
329. ac3h4+h(+m)=ac3h5(+m) 1.20E+11 0.7 3007.0
Low pressure limit: 0.55600E+34 -0.50000E+01 0.44480E+04
330. ac3h4+h(+m)=sc3h5(+m) 8.49E+12 0.0 2000.0
Low pressure limit: 0.11100E+35 -0.50000E+01 0.44480E+04
331. h2ccch+o2=ch2co+hco 3.00E+10 0.0 2868.0
332. h2ccch+o=ch2o+c2h 2.00E+13 0.0 0.0
333. h2ccch+h=c3h2+h2 5.00E+13 0.0 3000.0
334. h2ccch+oh=c3h2+h2o 2.00E+13 0.0 0.0
335. h2ccch+c2h3=c-c5h5+h 9.63E+40 -7.8 28820.0

336. h2ccch+ch3=ch3chcch2 5.00E+12 0.0 0.0
337. h2ccch+ch3=ch3ch2cch 5.00E+12 0.0 0.0
338. h2ccch+ch=hcchcch+h 7.00E+13 0.0 0.0
339. h2ccch+ch=h2cccch+h 7.00E+13 0.0 0.0
340. h2ccch+h(+m)=ac3h4(+m) 1.66E+15 -0.4 0.0
Low pressure limit: 0.33600E+46 -0.85200E+01 0.62930E+04
h2o Enhanced by 5.000E+00
h2 Enhanced by 2.000E+00
co2 Enhanced by 3.000E+00
co Enhanced by 2.000E+00
o2 Enhanced by 2.000E+00
c2h2 Enhanced by 2.000E+00
341. h2ccch+h(+m)=pc3h4(+m) 1.66E+15 -0.4 0.0
Low pressure limit: 0.87800E+46 -0.89000E+01 0.79740E+04
h2o Enhanced by 5.000E+00
h2 Enhanced by 2.000E+00
co2 Enhanced by 3.000E+00
co Enhanced by 2.000E+00
o2 Enhanced by 2.000E+00
c2h2 Enhanced by 2.000E+00
342. h2ccch+h2ccch=c6h6 5.56E+20 -2.5 1692.0
343. h2ccch+ac3h5=fulvene+h+h 5.56E+20 -2.5 1692.0
344. h2ccch+h2ccch=c6h5+h 2.00E+12 0.0 0.0
345. c3h2+o2=hcco+co+h 5.00E+13 0.0 0.0
346. c3h2+oh=c2h2+hco 5.00E+13 0.0 0.0
347. chchcho+o2=c2h2+co+ho2 3.00E+12 0.0 0.0
348. chchcho=c2h2+hco 1.00E+14 0.0 33000.0
349. chchcho+h=ch2chco+h 1.00E+14 0.0 0.0
350. chchcho+oh=hcccho+h2o 1.00E+13 0.0 0.0
351. chchcho+h=hcccho+h2 2.00E+13 0.0 0.0
352. hcccho+h=c2h2+hco 1.00E+14 0.0 3000.0
353. hcccho+oh=hccco+h2o 1.00E+13 0.0 0.0
354. hcccho+h=hccco+h2 4.00E+13 0.0 4200.0
355. hccco+o2=hco+co+co 1.40E+09 1.0 0.0
356. hccco+h=c2h2+co 1.00E+14 0.0 0.0
357. c4h10=c2h5+c2h5 2.00E+16 0.0 81300.0
358. c4h10=nc3h7+ch3 1.74E+17 0.0 85700.0

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359. c4h10=pc4h9+h                    1.00E+14   0.0   100000.0
360. c4h10=sc4h9+h                    1.00E+14   0.0   100000.0
361. c4h10+o2=pc4h9+ho2               2.50E+13   0.0    49000.0
362. c4h10+o2=sc4h9+ho2               4.00E+13   0.0    47600.0
363. c4h10+ac3h5=pc4h9+c3h6           7.94E+11   0.0    20500.0
364. c4h10+ac3h5=sc4h9+c3h6           3.16E+11   0.0    16400.0
365. c4h10+ch3=pc4h9+ch4              5.00E+11   0.0    13600.0
366. c4h10+ch3=sc4h9+ch4              4.30E+11   0.0    10500.0
367. c4h10+h=pc4h9+h2                 2.84E+05   2.5     6050.0
368. c4h10+h=sc4h9+h2                 5.68E+05   2.4     3765.0
369. c4h10+oh=pc4h9+h2o               4.13E+07   1.7      753.0
370. c4h10+oh=sc4h9+h2o               7.23E+07   1.6     -247.0
371. c4h10+o=pc4h9+oh                 1.13E+14   0.0     7850.0
372. c4h10+o=sc4h9+oh                 5.62E+13   0.0     5200.0
373. c4h10+ho2=pc4h9+h2o2             1.70E+13   0.0    20460.0
374. c4h10+ho2=sc4h9+h2o2             1.12E+13   0.0    17700.0
375. sc4h9(+m)=c3h6+ch3(+m)           2.14E+12   0.7    30856.0
   Low pressure limit:  0.63230E+59 -0.12850E+02  0.35567E+05
     h2o          Enhanced by   5.000E+00
     h2           Enhanced by   2.000E+00
     co2          Enhanced by   3.000E+00
     co           Enhanced by   2.000E+00
376. sc4h9=c4h8-1+h                   2.00E+13   0.0    40400.0
377. sc4h9=c4h8-2+h                   5.01E+12   0.0    37900.0
378. pc4h9(+m)=c2h5+c2h4(+m)          1.06E+13   0.0    27828.0
   Low pressure limit:  0.18970E+56 -0.11910E+02  0.32263E+05
     h2o          Enhanced by   5.000E+00
     h2           Enhanced by   2.000E+00
     co2          Enhanced by   3.000E+00
     co           Enhanced by   2.000E+00
379. pc4h9=c4h8-1+h                   1.26E+13   0.0    38600.0
380. c4h8-1=c2h3+c2h5                 1.00E+19  -1.0    96770.0
381. c4h8-1=h+c4h7                    4.11E+18  -1.0    97350.0
382. c4h8-1+ch3=c4h7+ch4              1.00E+11   0.0     7300.0
383. c4h8-1+h=c4h7+h2                 5.00E+13   0.0     3900.0
384. c4h8-1+o=nc3h7+hco               1.80E+05   2.5    -1029.0
385. c4h8-1+o=ch2chcho+ch3+h          9.67E+04   2.5    -1029.0
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386. c4h8-1+oh=c4h7+h2o	2.25E+13	0.0	2217.0
387. c4h8-1+ac3h5=c4h7+c3h6	7.90E+10	0.0	12400.0
388. c4h8-1+o2=c4h7+ho2	4.00E+12	0.0	33200.0
389. c4h8-2=h+c4h7	4.11E+18	-1.0	97350.0
390. c4h8-2+ch3=c4h7+ch4	1.00E+11	0.0	8200.0
391. c4h8-2+h=c4h7+h2	5.00E+13	0.0	3800.0
392. c4h8-2+o=ic3h7+hco	2.79E+06	2.1	-1775.0
393. c4h8-2+oh=c4h7+h2o	3.90E+13	0.0	2217.0
394. c4h8-2+o=ch3co+c2h5	1.53E+07	1.9	-1476.0
395. c4h8-2+o=ch3+ch3chco+h	8.22E+06	1.9	-1476.0
396. c4h8-2+o2=c4h7+ho2	8.00E+13	0.0	37400.0
397. c4h7=ch2chchch2+h	1.00E+14	0.0	55000.0
398. c4h7+oh=ch2chchch2+h2o	1.00E+13	0.0	0.0
399. c4h7+ch3=ch2chchch2+ch4	8.00E+12	0.0	0.0
400. c4h7+ac3h5=c3h6+ch2chchch2	6.31E+12	0.0	0.0
401. c4h7+o2=ch2chchch2+ho2	1.00E+09	0.0	0.0
402. c4h7+h=ch2chchch2+h2	3.16E+13	0.0	0.0
403. ch2chchch2+oh=ch2chchch+h2o	2.00E+07	2.0	5000.0
404. ch2chchch2+oh=ch2chcch2+h2o	2.00E+07	2.0	2000.0
405. ch2chchch2+o=hco+ac3h5	6.02E+08	1.4	-858.0
406. ch2chchch2+o=ch2hco+c2h3	1.00E+12	0.0	0.0
407. ch2chchch2+h=ch2chchch+h2	3.00E+07	2.0	13000.0
408. ch2chchch2+h=ch2chcch2+h2	3.00E+07	2.0	6000.0
409. ch3ch2cch+oh=ch3chcch+h2o	1.00E+07	2.0	2000.0
410. ch3ch2cch+h=c2h5+c2h2	1.00E+14	0.0	3000.0
411. ch3chcch2+oh=ch2chcch2+h2o	2.00E+07	2.0	1000.0
412. ch3chcch2+oh=ch3ccch2+h2o	1.00E+07	2.0	2000.0
413. ch3chcch2+oh=ch3chcch+h2o	2.00E+07	2.0	2500.0
414. ch3chcch2+h=ch2chcch2+h2	5.00E+07	2.0	5000.0
415. ch3chcch2+h=ch3ccch2+h2	1.50E+07	2.0	6000.0
416. ch3chcch2+h=ch3chcch+h2	3.00E+07	2.0	6500.0
417. ch3chcch2+h=ch3+ac3h4	2.00E+12	0.0	2000.0
418. ch3chcch+h=ch3+h2ccch	5.00E+13	0.0	0.0
419. ch3chcch+o2=ch3chco+hco	4.16E+10	0.0	2510.0
420. ch3chcch+oh=ch2chcch+h2o	3.00E+13	0.0	0.0
421. ch2chcch2+h=ch3+h2ccch	2.50E+13	0.0	0.0
422. ch2chcch2+h=ch3ccch2+h	3.00E+13	0.0	0.0

423. ch2chcch2+c2h2=c6h6+h 3.00E+11 0.0 14900.0
424. ch3ccch2+h=ch3+h2ccch 1.00E+14 0.0 0.0
425. ch3ccch2+o2=ch3co+ch2co 4.16E+10 0.0 2510.0
426. ch3ccch2+h=h2cccch2+h2 1.00E+14 0.0 8000.0
427. ch3ccch2+oh=h2cccch2+h2o 1.00E+13 0.0 0.0
428. ch2chchch+h=ch2chcch2+h 1.00E+14 0.0 0.0
429. ch2chchch+oh=ch2chcch+h2o 2.00E+07 2.0 1000.0
430. ch2chchch+h=ch2chcch+h2 3.00E+07 2.0 1000.0
431. ch2chchch+c2h2=c6h6+h 1.60E+16 -1.3 5400.0
432. ch3chcch(+m)=ch2chcch+h(+m) 1.00E+13 0.0 49000.0
Low pressure limit: 0.20000E+15 0.00000E+00 0.41000E+05
433. ch3ccch2(+m)=h2cccch2+h(+m) 1.00E+13 0.0 56000.0
Low pressure limit: 0.20000E+15 0.00000E+00 0.48000E+05
434. ch2chcch2(+m)=ch2chcch+h(+m) 1.00E+14 0.0 50000.0
Low pressure limit: 0.20000E+16 0.00000E+00 0.42000E+05
435. ch2chchch(+m)=ch2chcch+h(+m) 1.00E+14 0.0 37000.0
Low pressure limit: 0.10000E+15 0.00000E+00 0.30000E+05
436. ch2chchch+o2=chchcho+ch2o 1.00E+12 0.0 0.0
437. ch2chchch+o2=ch2chcch+ho2 1.00E+07 2.0 10000.0
438. ch3ccch2+h2ccch=c6h5ch2+h 1.00E+11 0.0 0.0
439. ch3chcch+h2ccch=c6h5ch2+h 1.00E+11 0.0 0.0
440. ch3ccch2+ch3ccch2=ch3c6h4ch2+h 1.00E+08 0.0 0.0
441. ch3chcch+ch3chcch=ch3c6h4ch2+h 1.00E+08 0.0 0.0
442. h2cccch2+oh=h2cccch+h2o 2.00E+07 2.0 2000.0
443. h2cccch2+h=h2cccch+h2 3.00E+07 2.0 6000.0
444. ch2chcch+oh=hcchcch+h2o 7.50E+06 2.0 5000.0
445. ch2chcch+h=hcchcch+h2 2.00E+07 2.0 15000.0
446. ch2chcch+oh=h2cccch+h2o 1.00E+07 2.0 2000.0
447. ch2chcch+h=h2cccch+h2 3.00E+07 2.0 5000.0
448. hcchcch+h=h2cccch+h 1.00E+14 0.0 0.0
449. hcchcch+c2h2=c6h5 9.60E+70 -17.8 31300.0
450. hcchcch+o2=hcccho+hco 3.00E+12 0.0 0.0
451. h2cccch+o2=ch2co+hcco 1.00E+12 0.0 0.0
452. h2cccch+oh=c4h2+h2o 3.00E+13 0.0 0.0
453. h2cccch+o=ch2co+c2h 2.00E+13 0.0 0.0
454. h2cccch+o=h2c4o+h 2.00E+13 0.0 0.0
455. h2cccch+h=c4h2+h2 5.00E+13 0.0 0.0

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456. h2cccch+ch2=ac3h4+c2h                    2.00E+13   0.0      0.0
457. h2cccch+c2h2=c6h5                        3.00E+11   0.0   14900.0
458. h2cccch(+m)=c4h2+h(+m)                   1.00E+14   0.0   47000.0
   Low pressure limit:  0.20000E+16  0.00000E+00  0.40000E+05
459. hcchcch(+m)=c4h2+h(+m)                   1.00E+14   0.0   36000.0
   Low pressure limit:  0.10000E+15  0.00000E+00  0.30000E+05
460. c4h2+ch2=c5h3+h                          1.30E+13   0.0    4326.0
461. c4h2+ch=c5h2+h                           1.00E+14   0.0       0.0
462. c4h2+ch2(s)=c5h3+h                       3.00E+13   0.0       0.0
463. c4h2+c2h=c6h2+h                          9.60E+13   0.0       0.0
464. c4h2+oh=h2c4o+h                          6.66E+12   0.0    -410.0
465. c4h2+o=c3h2+co                           1.20E+12   0.0       0.0
466. h2c4o+h=c2h2+hcco                        5.00E+13   0.0    3000.0
467. h2c4o+oh=ch2co+hcco                      1.00E+07   2.0    2000.0
468. l-c5h8+oh=l-c5h7+h2o                     7.00E+06   2.0       0.0
469. l-c5h8+h=l-c5h7+h2                       7.00E+06   2.0    5000.0
470. l-c5h8+h=ac3h5+c2h4                      3.35E+08   1.5    2000.0
471. c-c5h7=c-c5h6+h                          3.16E+15   0.0   36000.0
472. c-c5h7=l-c5h7                            3.16E+15   0.0   39500.0
473. l-c5h7+o=ch2chcho+c2h3                   2.00E+14   0.0       0.0
474. l-c5h7+h=l-c5h8                          1.00E+14   0.0       0.0
475. c-c5h6+o2=c-c5h5+ho2                     5.00E+13   0.0   35400.0
476. c-c5h6+ho2=c-c5h5+h2o2                   1.99E+12   0.0   11660.0
477. c-c5h6+oh=c-c5h5+h2o                     3.43E+09   1.2    -447.0
478. c-c5h6+o=c-c5h5+oh                       1.81E+13   0.0    3080.0
479. c-c5h6+h=c-c5h5+h2                       2.19E+08   1.8    3000.0
480. c-c5h6+ch3=c-c5h5+ch4                    3.11E+11   0.0    5500.0
481. c-c5h6+c2h3=c-c5h5+c2h4                  6.00E+12   0.0       0.0
482. c-c5h6+ch2chchch=c-c5h5+ch2chchch2       6.00E+12   0.0       0.0
483. c-c5h6+c6h5o=c-c5h5+c6h5oh               3.16E+11   0.0    8000.0
484. c-c5h5+h=c-c5h6                          2.00E+14   0.0       0.0
485. c-c5h5+o=c-c5h4o+h                       1.00E+14   0.0       0.0
486. c-c5h5+ho2=c-c5h5o+oh                    3.00E+13   0.0       0.0
487. c-c5h5+oh=c-c5h4oh+h                     3.00E+13   0.0       0.0
488. c-c5h5+c-c5h5=c10h8+h+h                  2.00E+13   0.0    8000.0
489. c-c5h5o=ch2chchch+co                     2.51E+11   0.0   43900.0
490. c-c5h4oh=c-c5h4o+h                       2.10E+13   0.0   48000.0
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491. c-c5h4o=co+c2h2+c2h2 1.00E+15 0.0 78000.0
492. c6h6+o2=c6h5+ho2 6.30E+13 0.0 60000.0
493. c6h6+oh=c6h5+h2o 1.63E+08 1.4 1454.0
494. c6h6+oh=c6h5oh+h 6.70E+12 0.0 10592.0
495. c6h6+o=c6h5o+h 2.40E+13 0.0 4670.0
496. c6h6+h=c6h5+h2 3.03E+02 3.3 5690.0
497. c6h5+h=c6h6 8.00E+13 0.0 0.0
498. c6h5+c2h4=c6h5c2h3+h 7.23E+01 3.5 8345.0
499. c6h5+c2h2=c6h5c2h+h 3.98E+13 0.0 10099.0
500. c6h5+oh=c6h5o+h 5.00E+13 0.0 0.0
501. c6h5+o=c-c5h5+co 1.00E+14 0.0 0.0
502. c6h5+o2=c6h5o+o 2.60E+13 0.0 6120.0
503. c6h5+o2=oc6h4o+h 3.00E+13 0.0 8981.0
504. c6h5+c6h5=biphenyl 5.00E+12 0.0 0.0
505. c6h5+c6h6=biphenyl+h 4.00E+11 0.0 4000.0
506. oc6h4o=c-c5h4o+co 1.00E+15 0.0 78000.0
507. c6h5o=co+c-c5h5 7.40E+11 0.0 43850.0
508. c6h5o+h=c6h5oh 1.00E+14 0.0 0.0
509. c6h5o+h=c-2*4c6h6o 1.00E+14 0.0 0.0
510. c6h5oh+oh=c6h5o+h2o 2.95E+06 2.0 -1310.0
511. c6h5oh+ch3=c6h5o+ch4 1.81E+11 0.0 7716.0
512. c6h5oh+h=c6h5o+h2 1.58E+13 0.0 6100.0
513. c6h5oh+o=c6h5o+oh 2.81E+13 0.0 7352.0
514. c6h5oh+c2h3=c2h4+c6h5o 6.00E+12 0.0 0.0
515. c6h5oh+c6h5=c6h6+c6h5o 4.91E+12 0.0 4400.0
516. c-2*4c6h6o+h=c-c5h7+co 2.51E+13 0.0 4700.0
517. c6h5ch3=c6h5+ch3 1.40E+16 0.0 99800.0
518. c6h5ch3+o2=c6h5ch2+ho2 2.00E+12 0.0 39080.0
519. c6h5ch3+oh=c6h5ch2+h2o 1.26E+13 0.0 2583.0
520. c6h5ch3+o=c6h5ch2+oh 5.00E+08 1.5 8000.0
521. c6h5ch3+h=c6h5ch2+h2 3.98E+02 3.4 3120.0
522. c6h5ch3+h=c6h6+ch3 1.20E+13 0.0 5148.0
523. c6h5ch3+o=oc6h4ch3+h 1.63E+13 0.0 3418.0
524. c6h5ch3+ch3=ch4+c6h5ch2 3.16E+11 0.0 9500.0
525. c6h5ch3+c6h5=c6h6+c6h5ch2 2.10E+12 0.0 4400.0
526. c6h5ch2+h=c6h5ch3 1.80E+14 0.0 0.0
527. c6h5ch2+c6h5oh=c6h5o+c6h5ch3 1.05E+11 0.0 9500.0

528. c6h5ch2+hoc6h4ch3=oc6h4ch3+c6h5ch3 1.05E+11 0.0 9500.0
529. c6h5ch2+o=c6h5cho+h 2.50E+14 0.0 0.0
530. c6h5ch2+o=c6h5+ch2o 8.00E+13 0.0 0.0
531. c6h5ch2+ho2=c6h5cho+h+oh 2.50E+14 0.0 0.0
532. c6h5ch2+ho2=c6h5+ch2o+oh 8.00E+13 0.0 0.0
533. c6h5ch2+ch3=c6h5c2h5 1.19E+13 0.0 221.0
534. c6h5ch2+h2ccch=adhflvyl+h 2.00E+12 0.0 0.0
535. c6h5ch2+c2h2=indene+h 3.20E+11 0.0 7000.0
536. c6h5ch2+c6h5cho=c6h5ch3+c6h5co 2.77E+03 2.8 5773.0
537. c6h5ch2+oh=c6h5ch2oh 6.00E+13 0.0 0.0
538. c6h5ch2oh+oh=c6h5cho+h2o+h 8.43E+12 0.0 2583.0
539. c6h5ch2oh+h=c6h5cho+h2+h 8.00E+13 0.0 8235.0
540. c6h5ch2oh+h=c6h6+ch2oh 1.20E+13 0.0 5148.0
541. c6h5ch2oh+c6h5ch2=c6h5cho+c6h5ch3+h 2.11E+11 0.0 9500.0
542. c6h5ch2oh+c6h5=c6h5cho+c6h6+h 1.40E+12 0.0 4400.0
543. c6h5cho+o2=c6h5co+ho2 1.02E+13 0.0 38950.0
544. c6h5cho+oh=c6h5co+h2o 1.71E+09 1.2 -447.0
545. c6h5cho+h=c6h5co+h2 5.00E+13 0.0 4928.0
546. c6h5cho+h=c6h5+ch2o 2.00E+13 0.0 2000.0
547. c6h5cho+h=c6h6+hco 1.20E+13 0.0 5148.0
548. c6h5cho+o=c6h5co+oh 9.04E+12 0.0 3080.0
549. c6h5cho+ch3=ch4+c6h5co 2.77E+03 2.8 5773.0
550. c6h5cho+c6h5=c6h6+c6h5co 7.01E+11 0.0 4400.0
551. c6h5co=c6h5+co 3.98E+14 0.0 29400.0
552. oc6h4ch3+h=hoc6h4ch3 2.50E+14 0.0 0.0
553. oc6h4ch3=c6h6+h+co 2.51E+11 0.0 43900.0
554. hoc6h4ch3+oh=oc6h4ch3+h2o 6.00E+12 0.0 0.0
555. hoc6h4ch3+h=oc6h4ch3+h2 1.15E+14 0.0 12400.0
556. hoc6h4ch3+h=c6h5ch3+oh 2.21E+13 0.0 7910.0
557. hoc6h4ch3+h=c6h5oh+ch3 1.20E+13 0.0 5148.0
558. c6h5c2h5+oh=c6h5c2h3+h2o+h 8.43E+12 0.0 2583.0
559. c6h5c2h5+h=c6h5c2h3+h2+h 8.00E+13 0.0 8235.0
560. c6h5c2h3+oh=c6h4c2h3+h2o 1.63E+08 1.4 1454.0
561. c6h5c2h3+h=c6h4c2h3+h2 3.03E+02 3.3 5690.0
562. c6h5c2h3+oh=c6h5cch2+h2o 1.00E+07 2.0 2000.0
563. c6h5c2h3+h=c6h5cch2+h2 2.00E+07 2.0 6000.0
564. c6h5chch+h=c6h5cch2+h 1.00E+14 0.0 0.0

565. c6h5cch2+oh=c6h5c2h+h2o 2.00E+13 0.0 0.0
566. c6h5cch2+h=c6h5c2h+h2 5.00E+13 0.0 0.0
567. c6h5c2h+o=c6h5cco+h 4.80E+09 1.0 0.0
568. c6h5cco+o2=c6h5co+co2 1.00E+12 0.0 0.0
569. c6h5c2h+oh=c6h4c2h+h2o 1.63E+08 1.4 1454.0
570. c6h5c2h+h=c6h4c2h+h2 3.03E+02 3.3 5690.0
571. c6h5c2h+ch3=c6h4c2h+ch4 1.67E+12 0.0 15057.0
572. c6h4c2h+c2h2=c10h7 1.07E+04 2.3 -657.3
573. c6h4c2h3+ch3=indene+h+h 1.00E+13 0.0 0.0
574. ch3c6h4ch3+oh=ch3c6h4ch2+h2o 2.95E+13 0.0 2623.0
575. ch3c6h4ch3+o=ch3c6h4ch2+oh 5.00E+08 1.5 8000.0
576. ch3c6h4ch3+h=ch3c6h4ch2+h2 3.98E+02 3.4 3120.0
577. ch3c6h4ch2+c2h2=c10h10+h 3.20E+11 0.0 7000.0
578. ch3c6h4ch2+c2h2=ch3indene+h 3.20E+11 0.0 7000.0
579. ch3c6h4ch2+h=ch3c6h4ch3 7.46E+13 0.0 78.0
580. ch3c6h4ch2+ch3=ch3c6h4c2h5 6.00E+12 0.0 221.0
581. indene+oh=indenyl+h2o 3.43E+09 1.2 -447.0
582. indene+o=indenyl+oh 1.81E+13 0.0 3080.0
583. indene+h=indenyl+h2 2.19E+08 1.8 3000.0
584. indenyl+h=indene 2.00E+14 0.0 0.0
585. indenyl+o=c6h5chch+co 1.00E+14 0.0 0.0
586. indenyl+ho2=c6h5chch+co+oh 1.00E+13 0.0 0.0
587. indenyl+c-c5h5=phnthrn+h+h 1.00E+13 0.0 8000.0
588. ch3c6h4c2h5+oh=ch3c6h4c2h3+h2o+h 8.43E+12 0.0 2583.0
589. ch3c6h4c2h5+h=ch3c6h4c2h3+h2+h 8.00E+13 0.0 8235.0
590. ch3c6h4c2h3+oh=indene+h+h2o 1.26E+13 0.0 2583.0
591. ch3c6h4c2h3+h=indene+h+h2 3.98E+02 3.4 3120.0
592. ch3indene+oh=ch3indenyl+h2o 3.43E+09 1.2 -447.0
593. ch3indene+o=ch3indenyl+oh 1.81E+13 0.0 3080.0
594. ch3indene+h=ch3indenyl+h2 2.19E+08 1.8 3000.0
595. ch3indene+h=indene+ch3 1.20E+13 0.0 5200.0
596. ch3indenyl+h=ch3indene 2.00E+14 0.0 0.0
597. ch3indenyl+c-c5h5=ch3phnthrn+h+h 1.00E+13 0.0 8000.0
598. adhfulv+oh=adhflvyl+h2o 5.00E+06 2.0 0.0
599. adhfulv+o=adhflvyl+oh 7.00E+11 0.7 6000.0
600. adhfulv+h=adhflvyl+h2 2.00E+05 2.5 2500.0
601. adhflvyl+h=adhfulv 1.00E+14 0.0 0.0

602. bnzofulv+h=adhflvyl 2.00E+13 0.0 1500.0
603. bnzofulv+h=c10h8+h 3.00E+12 0.5 0.0
604. bnzofulv=c10h8 5.00E+37 -7.4 76979.0
605. c10h10+oh=c10h9+h2o 5.00E+06 2.0 0.0
606. c10h10+o=c10h9+oh 7.00E+11 0.7 6000.0
607. c10h10+h=c10h9+h2 2.00E+05 2.5 2500.0
608. c10h9+h=c10h10 1.00E+14 0.0 0.0
609. c10h8+h=c10h9 5.00E+14 0.0 5000.0
610. c10h8+oh=c10h7+h2o 2.44E+08 1.4 1454.0
611. c10h8+oh=c10h7oh+h 9.00E+12 0.0 10592.0
612. c10h8+o=c10h7o+h 1.40E+13 0.0 1792.0
613. c10h8+h=c10h7+h2 4.55E+02 3.3 5690.0
614. c10h7+h=c10h8 1.00E+14 0.0 0.0
615. c10h7+o2=c10h7o+o 1.00E+13 0.0 0.0
616. c10h7+oh=c10h7o+h 5.00E+13 0.0 0.0
617. c10h7+ch3=c10h7ch3 1.00E+13 0.0 0.0
618. c10h7+ch3=c10h7ch2+h 1.00E+13 0.0 0.0
619. c10h7+c2h2=acenphthln+h 1.00E+20 -2.1 12000.0
620. c10h7+c2h2=c10h7cch+h 1.17E-07 5.2 -9482.0
621. c10h7+c6h5=flrnthn+h+h 5.00E+12 0.0 0.0
622. c10h7+c6h6=flrnthn+h+h2 4.00E+11 0.0 4000.0
623. c10h7o+h=c10h7oh 1.00E+14 0.0 0.0
624. c10h7oh+oh=c10h7o+h2o 2.95E+06 2.0 -1312.0
625. c10h7oh+h=c10h7o+h2 1.58E+13 0.0 6100.0
626. c10h7o=indenyl+co 7.40E+11 0.0 43850.0
627. c10h7ch3+oh=c10h7ch2+h2o 1.27E+13 0.0 2583.0
628. c10h7ch3+o=c10h7ch2+oh 5.00E+08 1.5 8000.0
629. c10h7ch3+h=c10h7ch2+h2 3.98E+02 3.4 3120.0
630. c10h7ch3+h=c10h8+ch3 1.20E+13 0.0 5148.0
631. c10h7ch2+h=c10h7ch3 1.00E+14 0.0 0.0
632. c10h7ch2+o=c10h7+ch2o 1.00E+14 0.0 0.0
633. c10h7ch2+ho2=>c10h7+ch2o+oh 1.00E+13 0.0 0.0
634. c10h7ch2+c2h2=bz(a)ndene+h 3.20E+11 0.0 7000.0
635. c10h7ch2+ch3=c10h7c2h5 1.19E+13 0.0 221.0
636. c10h7c2h5+oh=c10h7c2h3+h2o+h 8.44E+12 0.0 2583.0
637. c10h7c2h5+h=c10h7c2h3+h2+h 8.00E+13 0.0 8235.0
638. c10h7c2h3+oh=c10h7cch2+h2o 1.00E+07 2.0 2000.0

639. c10h7c2h3+h=c10h7cch2+h2 2.00E+07 2.0 6000.0
640. c10h7cch2+oh=c10h7cch+h2o 2.00E+13 0.0 0.0
641. c10h7cch2+h=c10h7cch+h2 5.00E+13 0.0 0.0
642. c10h7cch+oh=c10h6cch+h2o 1.63E+08 1.4 1454.0
643. c10h7cch+h=c10h6cch+h2 3.03E+02 3.3 5690.0
644. c10h7cch+h=acenphthln+h 8.46E+21 -2.6 7062.6
645. c10h6cch+c2h2=phnthryl-1 1.07E+04 2.3 -657.3
646. fluorene+oh=fluoryl+h2o 3.43E+09 1.2 -447.0
647. fluorene+o=fluoryl+oh 1.81E+13 0.0 3080.0
648. fluorene+h=fluoryl+h2 2.19E+08 1.8 3000.0
649. fluoryl+h=fluorene 2.00E+14 0.0 0.0
650. bz(a)ndnyl+h=bz(a)ndene 2.00E+14 0.0 0.0
651. bz(a)ndene+oh=bz(a)ndnyl+h2o 3.43E+09 1.2 -447.0
652. bz(a)ndene+o=bz(a)ndnyl+oh 1.81E+13 0.0 3080.0
653. bz(a)ndene+h=bz(a)ndnyl+h2 2.19E+08 1.8 3000.0
654. bz(a)ndnyl+c-c5h5=bz(a)phnthrn+h+h 1.00E+13 0.0 8000.0
655. phnthrn+oh=phnthryl-1+h2o 2.17E+08 1.4 1454.0
656. phnthrn+oh=phnthryl-9+h2o 5.43E+07 1.4 1454.0
657. phnthrn+oh=phnthrol-1+h 9.00E+12 0.0 10592.0
658. phnthrn+oh=phnthrol-9+h 9.00E+12 0.0 10592.0
659. phnthrn+h=phnthryl-1+h2 4.04E+02 3.3 5690.0
660. phnthrn+h=phnthryl-9+h2 1.01E+02 3.3 5690.0
661. anthracn=phnthrn 8.00E+12 0.0 65000.0
662. phnthryl-1+h=phnthrn 8.00E+13 0.0 0.0
663. phnthryl-9+h=phnthrn 8.00E+13 0.0 0.0
664. phnthryl-1+o2=phnthroxy-1+o 1.00E+13 0.0 0.0
665. phnthryl-9+o2=phnthroxy-9+o 1.00E+13 0.0 0.0
666. phnthrol-1+oh=phnthroxy-1+h2o 2.95E+06 2.0 -1310.0
667. phnthrol-1+h=phnthroxy-1+h2 1.59E+13 0.0 6100.0
668. phnthroxy-1+h=phnthrol-1 1.00E+14 0.0 0.0
669. phnthrol-9+oh=phnthroxy-9+h2o 2.95E+06 2.0 -1310.0
670. phnthrol-9+h=phnthroxy-9+h2 1.59E+13 0.0 6100.0
671. phnthroxy-9+h=phnthrol-9 1.00E+14 0.0 0.0
672. phnthroxy-1=bz(a)ndnyl+co 7.40E+11 0.0 43850.0
673. phnthroxy-9=fluoryl+co 7.40E+11 0.0 43850.0
674. phnthryl-1+c2h2=pyrene+h 3.49E+10 0.6 5658.0
675. phnthryl-1+ch3=hc4-p(def)pthn+h+h 5.00E+13 0.0 0.0

676. ch3phnthrn+oh=hc4-p(def)pthn+h2o+h 1.27E+13 0.0 2583.0
677. ch3phnthrn+h=hc4-p(def)pthn+h2+h 3.98E+02 3.4 3120.0
678. ch3phnthrn+h=phnthrn+ch3 1.20E+13 0.0 5148.0
679. hc4-p(def)pthn+oh=hc4-p(def)pthyl+h2o 3.43E+09 1.2 -447.0
680. hc4-p(def)pthn+o=hc4-p(def)pthyl+oh 1.81E+13 0.0 3080.0
681. hc4-p(def)pthn+h=hc4-p(def)pthyl+h2 2.19E+08 1.8 3000.0
682. hc4-p(def)pthyl+h=hc4-p(def)pthn 2.00E+14 0.0 0.0
683. bz(a)phnthrn+h=bz(ghi)fln+h2+h 3.03E+02 3.3 5690.0
684. bz(a)phnthrn+oh=bz(ghi)fln+h2o+h 1.63E+08 1.4 1454.0
685. h2ccch+ch2=ch2chcch+h 4.00E+13 0.0 0.0
686. c-c5h5+ch3=ch3cy24pd 1.76E+50 -11.0 18600.0
687. ch3cy24pd+h=c-c5h6+ch3 1.00E+13 0.0 1300.0
688. c6h6+h=ch3cy24pd1 2.39E+27 -3.9 29200.0
689. cyc6h7=ch3cy24pd1 5.00E+12 0.0 38100.0
690. ch3cy24pd1+h=ch3cy24pd 1.00E+14 0.0 0.0
691. ch3cy24pd1+h=c-c5h5+ch3 1.00E+14 0.0 0.0
692. cyc6h7=ch3dcy24pd 5.50E+10 0.0 23500.0
693. c6h6+h=cyc6h7 4.87E+56 -12.7 26800.0
694. ch3dcy24pd+h2=ch3cy24pd+h 4.00E+12 0.0 15000.0
695. fulvene+h=fulvenyl+h2 3.03E+02 3.3 5690.0
696. fulvene+oh=fulvenyl+h2o 1.63E+08 1.4 1454.0
697. fulvenyl+h=c6h5+h 1.00E+14 0.0 0.0
698. fulvenyl+o2=c-c5h4o+hco 1.00E+12 0.0 0.0

NOTE: A units mole-cm-sec-K, E units cal/mole

NO ERRORS FOUND ON INPUT...CHEMKIN LINKING FILE WRITTEN.

WORKING SPACE REQUIREMENTS ARE

INTEGER: 11643

REAL: 11156

CHARACTER: 163

APPENDIX C

REACTION MECHANISM USED FOR CH_2Cl_2 MODELING

This appendix contains the reaction mechanism used for modeling of methylene chloride combustion.

```
CHEMKIN INTERPRETER OUTPUT: CHEMKIN-II Version 3.4 Mar. 1994
                    DOUBLE PRECISION

                    --------------------
                    ELEMENTS    ATOMIC
                    CONSIDERED  WEIGHT
                    --------------------
                     1. H      1.00797
                     2. O      15.9994
                     3. C      12.0112
                     4. CL     35.4530
                     5. N      14.0067
                    --------------------
-------------------------------------------------------------------------------
                  C
                 P H
                 H A
                 A R
SPECIES            S G MOLECULAR TEMPERATURE   ELEMENT COUNT
CONSIDERED           E E WEIGHT   LOW    HIGH   H  O  C  CL N
-------------------------------------------------------------------------------
 1. OH            G 0  17.00737  300.0 5000.0  1  1  0  0  0
 2. CH            G 0  13.01912  300.0 5000.0  1  0  1  0  0
 3. O            G 0  15.99940  300.0 5000.0  0  1  0  0  0
 4. CH3           G 0  15.03506  300.0 5000.0  3  0  1  0  0
 5. C2H6          G 0  30.07012  300.0 5000.0  6  0  2  0  0
 6. CH4           G 0  16.04303  300.0 5000.0  4  0  1  0  0
 7. CH3O          G 0  31.03446  300.0 5000.0  3  1  1  0  0
 8. CH2OH         G 0  31.03446  300.0 5000.0  3  1  1  0  0
 9. H2O2          G 0  34.01474  300.0 5000.0  2  2  0  0  0
10. CH2           G 0  14.02709  300.0 5000.0  2  0  1  0  0
11. CH2S          G 0  14.02709  300.0 5000.0  2  0  1  0  0
12. C2H3          G 0  27.04621  300.0 5000.0  3  0  2  0  0
13. C2H4          G 0  28.05418  300.0 5000.0  4  0  2  0  0
14. C2H           G 0  25.03027  300.0 5000.0  1  0  2  0  0
15. CH2O          G 0  30.02649  300.0 5000.0  2  1  1  0  0
16. C2H5          G 0  29.06215  300.0 5000.0  5  0  2  0  0
```

```
17. C2H2        G 0  26.03824  300.0 5000.0  2  0  2  0  0
18. CH2CO       G 0  42.03764  300.0 5000.0  2  1  2  0  0
19. C           G 0  12.01115  300.0 5000.0  0  0  1  0  0
20. C4H2        G 0  50.06054  300.0 5000.0  2  0  4  0  0
21. C3H3        G 0  39.05736  300.0 5000.0  3  0  3  0  0
22. C3H2        G 0  38.04939  300.0 5000.0  2  0  3  0  0
23. C4H3        G 0  51.06851  300.0 5000.0  3  0  4  0  0
24. O2          G 0  31.99880  300.0 5000.0  0  2  0  0  0
25. H           G 0   1.00797  300.0 5000.0  1  0  0  0  0
26. HO2         G 0  33.00677  300.0 5000.0  1  2  0  0  0
27. H2          G 0   2.01594  300.0 5000.0  2  0  0  0  0
28. H2O         G 0  18.01534  300.0 5000.0  2  1  0  0  0
29. CO2         G 0  44.00995  300.0 5000.0  0  2  1  0  0
30. CO          G 0  28.01055  300.0 5000.0  0  1  1  0  0
31. HCO         G 0  29.01852  300.0 5000.0  1  1  1  0  0
32. HCCO        G 0  41.02967  300.0 5000.0  1  1  2  0  0
33. HCCOH       G 0  42.03764  300.0 5000.0  2  1  2  0  0
34. CH3CL       G 0  50.48806  300.0 2000.0  3  0  1  1  0
35. HCL         G 0  36.46097  300.0 5000.0  1  0  0  1  0
36. C2H3CL      G 0  62.49921  300.0 2000.0  3  0  2  1  0
37. CH2CL2      G 0  84.93309  300.0 2000.0  2  0  1  2  0
38. CL2         G 0  70.90600  300.0 5000.0  0  0  0  2  0
39. CCLO        G 0  63.46355  300.0 2000.0  0  1  1  1  0
40. COCL2       G 0  98.91655  300.0 2000.0  0  1  1  2  0
41. CLO         G 0  51.45240  300.0 5000.0  0  1  0  1  0
42. HOCL        G 0  52.46037  300.0 2000.0  1  1  0  1  0
43. CL          G 0  35.45300  300.0 5000.0  0  0  0  1  0
44. C2H5CL      G 0  64.51515  300.0 2000.0  5  0  2  1  0
45. CHCLO       G 0  64.47152  300.0 2000.0  1  1  1  1  0
46. CH2CCL2     G 0  96.94424  300.0 2000.0  2  0  2  2  0
47. CHCLCHCL    G 0  96.94424  300.0 2000.0  2  0  2  2  0
48. CHCL3       G 0 119.37812  300.0 2000.0  1  0  1  3  0
49. C2HCL3      G 0 131.38927  300.0 2000.0  1  0  2  3  0
50. C2H3CL3     G 0 133.40521  300.0 2000.0  3  0  2  3  0
51. CHCL2       G 0  83.92512  300.0 2000.0  1  0  1  2  0
52. CH2CL       G 0  49.48009  300.0 2000.0  2  0  1  1  0
53. CH2CLCCL2   G 0 132.39724  300.0 2000.0  2  0  2  3  0
```

```
54. CH2CLCHCL      G 0  97.95221  300.0 2000.0  3  0  2  2  0
55. CH3CCL3        G 0 133.40521  300.0 2000.0  3  0  2  3  0
56. CH3CCL2        G 0  97.95221  300.0 2000.0  3  0  2  2  0
57. CCL3CH2        G 0 132.39724  300.0 2000.0  2  0  2  3  0
58. CH3CHCL2       G 0  98.96018  300.0 2000.0  4  0  2  2  0
59. CH3CHCL        G 0  63.50718  300.0 2000.0  4  0  2  1  0
60. CCL            G 0  47.46415  300.0 5000.0  0  0  1  1  0
61. CCL2           G 0  82.91715  300.0 2000.0  0  0  1  2  0
62. CCL3           G 0 118.37015  300.0 2000.0  0  0  1  3  0
63. CCL4           G 0 153.82315  300.0 2000.0  0  0  1  4  0
64. CH2CCL         G 0  61.49124  300.0 2000.0  2  0  2  1  0
65. CHCL2CH2       G 0  97.95221  300.0 2000.0  3  0  2  2  0
66. CH2CLCH2       G 0  63.50718  300.0 2000.0  4  0  2  1  0
67. CH2CLOO        G 0  81.47889  300.0 2000.0  2  2  1  1  0
68. C2HCL          G 0  60.48327  300.0 2000.0  1  0  2  1  0
69. CHCL           G 0  48.47212  300.0 2000.0  1  0  1  1  0
70. C2H2CL3        G 0 132.39724  300.0 2000.0  2  0  2  3  0
71. C2CL2          G 0  94.92830  300.0 2000.0  0  0  2  2  0
72. C2H2CL4        G 0 167.85024  300.0 2000.0  2  0  2  4  0
73. C2H4CL2        G 0  98.96018  300.0 2000.0  4  0  2  2  0
74. CH2CLO         G 0  65.47949  300.0 2000.0  2  1  1  1  0
75. N2             G 0  28.01340  300.0 5000.0  0  0  0  0  2
-----------------------------------------------------------------------------
```

```
                                  (k = A T**b exp(-E/RT))
  REACTIONS CONSIDERED                          A       b       E

 1. CH3+CH3=C2H6                          4.00E+57  -13.0   24800.0
 2. CH3+CH3=H+C2H5                         4.00E+18   -1.6   16080.0
 3. CH3+CH3=H2+C2H4                        5.60E+35   -7.1   20050.0
 4. CH3+H+M=CH4+M                          6.00E+16   -1.0       0.0
     H2          Enhanced by    2.000E+00
 5. CH2OH+H=CH3+OH                         1.00E+14    0.0       0.0
 6. CH2OH+H=CH2O+H2                        2.00E+13    0.0       0.0
 7. CH2OH+OH=CH2O+H2O                        1.00E+13    0.0       0.0
```

8. CH2OH+O=CH2O+OH	1.00E+13	0.0	0.0
9. CH2OH+O2=CH2O+HO2	1.48E+13	0.0	1500.0
10. CH2+H=CH+H2	5.00E+13	0.0	0.0
11. CH2+OH=CH+H2O	1.13E+07	2.0	3000.0
12. CH2+OH=CH2O+H	2.50E+13	0.0	0.0
13. CH+O2=HCO+O	3.30E+13	0.0	0.0
14. CH+O=CO+H	5.70E+13	0.0	0.0
15. CH+OH=HCO+H	3.00E+13	0.0	0.0
16. CH+CO2=HCO+CO	3.40E+12	0.0	690.0
17. CH+H2O=CH3O	5.71E+12	0.0	-750.0
18. CH+H=C+H2	1.50E+14	0.0	0.0
19. CH+CH2O=CH2CO+H	9.46E+13	0.0	-515.0
20. CH+C2H2=C3H2+H	1.00E+14	0.0	0.0
21. CH+CH2=C2H2+H	4.00E+13	0.0	0.0
22. CH+CH3=C2H3+H	3.00E+13	0.0	0.0
23. CH+CH4=C2H4+H	6.00E+13	0.0	0.0
24. C+O2=CO+O	2.00E+13	0.0	0.0
25. C+OH=CO+H	5.00E+13	0.0	0.0
26. C+CH3=C2H2+H	5.00E+13	0.0	0.0
27. C+CH2=C2H+H	5.00E+13	0.0	0.0
28. CH2+CO2=CH2O+CO	1.10E+11	0.0	1000.0
29. CH2+O=CO+2H	5.00E+13	0.0	0.0
30. CH2+O=CO+H2	3.00E+13	0.0	0.0
31. CH2+O2=CO2+2H	1.60E+12	0.0	1000.0
32. CH2+O2=CH2O+O	5.00E+13	0.0	9000.0
33. CH2+O2=CO2+H2	6.90E+11	0.0	500.0
34. CH2+O2=CO+H2O	1.90E+10	0.0	-1000.0
35. CH2+O2=CO+OH+H	8.60E+10	0.0	-500.0
36. CH2+O2=HCO+OH	4.30E+10	0.0	-500.0
37. C2H4+O=CH3+HCO	1.60E+09	1.2	746.0
38. CH2+CH3=C2H4+H	3.00E+13	0.0	0.0
39. H+C2H4=C2H5	3.20E+47	-10.1	20070.0
40. H+C2H2+M=C2H3+M	5.54E+12	0.0	2410.0
H2 Enhanced by 2.000E+00			
41. C2H3+O=CH2CO+H	3.00E+13	0.0	0.0
42. C2H3+OH=C2H2+H2O	5.00E+12	0.0	0.0
43. C2H3+CH2=C2H2+CH3	3.00E+13	0.0	0.0

44. C2H3+C2H=2C2H2	3.00E+13	0.0	0.0
45. C2H3+CH=CH2+C2H2	5.00E+13	0.0	0.0
46. OH+C2H2=HCCOH+H	5.04E+05	2.3	13500.0
47. HCCOH+H=CH2CO+H	1.00E+13	0.0	0.0
48. C2H+O2=2CO+H	5.00E+13	0.0	1500.0
49. C2H+C2H2=C4H2+H	3.00E+13	0.0	0.0
50. H+HCCO=CH2+CO	1.00E+14	0.0	0.0
51. O+HCCO=H+2CO	1.00E+14	0.0	0.0
52. O2+HCCO=OH+2CO	1.60E+12	0.0	854.0
53. CH+HCCO=C2H2+CO	5.00E+13	0.0	0.0
54. CH2S+C2H6=CH3+C2H5	1.20E+14	0.0	0.0
55. CH2S+O2=CO+OH+H	3.00E+13	0.0	0.0
56. CH2S+H=CH2+H	2.00E+14	0.0	0.0
57. 2HCCO=C2H2+2CO	1.00E+13	0.0	0.0
58. C2H+O=CH+CO	5.00E+13	0.0	0.0
59. C2H+OH=HCCO+H	2.00E+13	0.0	0.0
60. 2CH2=C2H2+H2	4.00E+13	0.0	0.0
61. CH2+HCCO=C2H3+CO	3.00E+13	0.0	0.0
62. CH2+C2H2=C3H3+H	1.20E+13	0.0	6600.0
63. C4H2+OH=C3H2+HCO	6.66E+12	0.0	-410.0
64. C3H2+O2=HCO+HCCO	1.00E+13	0.0	0.0
65. C3H3+O2=CH2CO+HCO	3.00E+10	0.0	2868.0
66. C3H3+O=CH2O+C2H	2.00E+13	0.0	0.0
67. C3H3+OH=C3H2+H2O	2.00E+13	0.0	0.0
68. 2C2H2=C4H3+H	2.00E+12	0.0	45900.0
69. C4H3+M=C4H2+H+M	1.00E+16	0.0	59700.0
70. CH2S+C2H2=C3H3+H	3.00E+13	0.0	0.0
71. C4H2+O=C3H2+CO	1.20E+12	0.0	0.0
72. C2H2+O2=HCCO+OH	2.00E+08	1.5	30100.0
73. C2H2+M=C2H+H+M	4.20E+16	0.0	107000.0
74. C2H4+M=C2H2+H2+M	1.50E+15	0.0	55800.0
75. C2H4+M=C2H3+H+M	1.40E+15	0.0	82360.0
76. H2+O2=2OH	1.70E+13	0.0	47780.0
77. 2H+M=H2+M	1.00E+18	-1.0	0.0
H2 Enhanced by 0.000E+00			
78. 2H+H2=2H2	9.20E+16	-0.6	0.0
79. 2H+H2O=H2+H2O	6.00E+19	-1.3	0.0

80. 2H+CO2=H2+CO2	5.49E+20	-2.0	0.0
81. C2H6+CH3=C2H5+CH4	2.70E-01	4.0	8280.0
82. CH3+C2H5=CH4+C2H4	5.50E+11	0.0	0.0
83. CH2CL2=CHCL+HCL	8.73E+37	-7.7	86730.0
84. CH2CL2=CH2CL+CL	7.40E+40	-7.9	84990.0
85. CH2CL+H=CH3+CL	5.20E+14	-0.4	830.0
86. CH3CL=CH2S+HCL	1.40E+12	0.0	35050.0
87. CH3CL=CH2CL+H	7.40E+08	1.2	2140.0
88. CH2CL2+H=CH2CL+HCL	7.00E+13	0.0	7100.0
89. CHCL2+H2=CH2CL2+H	4.63E+12	0.0	15295.0
90. CH2CL+H2=CH3CL+H	3.90E+12	0.0	14059.0
91. CH2CL2+CL=CHCL2+HCL	2.79E+13	0.0	2940.0
92. CH3CL+H=CH3+HCL	6.64E+13	0.0	7620.0
93. CH4=CH3+H	1.03E+33	-5.6	111810.0
94. CH4+H=CH3+H2	1.55E+14	0.0	11000.0
95. CH4+CL=CH3+HCL	3.09E+13	0.0	3600.0
96. CH3CL+CL=CH2CL+HCL	3.16E+13	0.0	3300.0
97. CH2CL2+CH3=CH4+CHCL2	6.76E+10	0.0	7200.0
98. CH2CL2+CH3=CH3CL+CH2CL	1.40E+11	0.0	4900.0
99. CH3CL+CH3=CH4+CH2CL	3.30E+11	0.0	9400.0
100. CHCL2+CHCL2=C2H2CL4	9.08E+45	-10.6	13170.0
101. CHCL2+CHCL2=C2H2CL3+CL	1.36E+30	-5.2	14180.0
102. CHCL2+CHCL2=C2HCL3+HCL	6.72E+35	-7.1	13210.0
103. CH2CL+CH2CL=C2H4CL2	7.84E+45	-10.2	13150.0
104. CH2CL+CH2CL=CH2CLCH2+CL	9.34E+29	-4.9	14070.0
105. CH2CL+CH2CL=C2H3CL+HCL	3.75E+35	-6.7	13160.0
106. CH2CL+CHCL2=C2H3CL3	6.41E+33	-10.2	12910.0
107. CH2CL+CHCL2=CH2CCL2+HCL	3.75E+36	-7.2	13620.0
108. CH2CL+CHCL2=CHCLCHCL+HCL	1.22E+37	-7.2	13640.0
109. CH2CL+CH3=C2H5CL	3.27E+40	-8.5	10590.0
110. CH2CL+CH3=C2H4+HCL	1.48E+21	-2.2	5207.0
111. CH2CL+CH3=C2H5+CL	9.27E+19	-2.1	10130.0
112. CHCL2+CH3=CH3CHCL2	2.28E+41	-8.7	11620.0
113. CHCL2+CH3=C2H3CL+HCL	1.35E+30	-5.0	11550.0
114. CHCL2+CH3=CH3CHCL+CL	2.74E+25	-3.5	12810.0
115. CHCL2+H=CH2CL2	4.81E+26	-4.8	3810.0
116. CHCL2+H=CH2CL+CL	1.25E+14	0.0	570.0

117. C2H3CL+H=CH2CLCH2	5.01E+23	-4.2	8470.0
118. C2H3CL+H=C2H4+CL	1.55E+13	0.0	5840.0
119. C2H3CL+H=C2H3+HCL	1.20E+12	0.0	15000.0
120. C2HCL3+H=CH2CLCCL2	1.51E+23	-4.2	7520.0
121. C2HCL3+H=C2H2CL3	2.87E+22	-4.1	10890.0
122. C2HCL3+H=CH2CCL2+CL	1.45E+13	0.0	5830.0
123. C2HCL3+H=CHCLCHCL+CL	7.37E+12	0.0	9220.0
124. C2H3CL3=CHCLCHCL+HCL	1.39E+20	-2.0	60450.0
125. C2H3CL3=CH2CCL2+HCL	3.13E+19	-2.0	60330.0
126. CH3CHCL2=C2H3CL+HCL	2.94E+21	-2.4	59460.0
127. CH3CHCL2=CH3CHCL+CL	3.17E+42	-8.1	92670.0
128. C2H2CL4=C2HCL3+HCL	8.62E+21	-2.6	51870.0
129. C2H4CL2=C2H3CL+HCL	6.76E+19	-1.9	58710.0
130. C2H5CL=C2H4+HCL	7.81E+19	-2.0	60660.0
131. C2H5CL=C2H5+CL	2.35E+43	-8.5	96980.0
132. C2H5CL+CL=HCL+CH3CHCL	3.55E+13	0.0	1500.0
133. C2H5CL+CL=HCL+CH2CLCH2	1.12E+13	0.0	1500.0
134. C2H5CL+H=HCL+C2H5	1.00E+14	0.0	7900.0
135. C2H3CL=C2H2+HCL	1.62E+28	-4.3	75780.0
136. C2H3CL=C2H3+CL	1.71E+38	-7.1	96370.0
137. C2H4=C2H2+H2	8.52E+43	-8.3	121240.0
138. C2H4=C2H3+H	8.53E+30	-5.9	118240.0
139. CH2CCL2+H=C2H3CL+CL	7.21E+12	0.0	7510.0
140. CHCLCHCL+H=C2H3CL+CL	3.44E+13	0.0	5890.0
141. C2H6+H=C2H5+H2	5.40E+02	3.6	5210.0
142. C2H6+CL=C2H5+HCL	4.60E+13	0.0	179.0
143. C2H6+O=C2H5+OH	2.51E+13	0.0	6400.0
144. C2H6+OH=C2H5+H2O	6.30E+06	2.0	645.0
145. C2H5+O=CH2O+CH3	1.00E+13	0.0	0.0
146. C2H5+O2=C2H4+HO2	2.00E+12	0.0	4992.0
147. C2H5+HO2=C2H4+H2O2	3.01E+11	0.0	0.0
148. C2H4+OH=C2H3+H2O	3.50E+13	0.0	3012.0
149. C2H4+CH3=CH4+C2H3	4.20E+11	0.0	11113.0
150. C2H4+O2=C2H3+HO2	4.22E+13	0.0	57623.0
151. C2H4+H=C2H3+H2	6.92E+14	0.0	14500.0
152. C2H4+CL=C2H3+HCL	1.00E+14	0.0	7000.0
153. C2H3=C2H2+H	9.30E+22	-3.7	37255.0

154. C2H3+O2=C2H2+HO2	1.60E+13	0.0	10400.0
155. C2H3+O2=HCO+CH2O	3.97E+12	0.0	-250.0
156. C2H3+H=C2H2+H2	1.00E+13	0.0	0.0
157. C2H3+CL=C2H2+HCL	1.00E+13	0.0.	0.0
158. C2H2+CL=C2H+HCL	1.58E+14	0.0	16900.0
159. C2H2+O2=C2H+HO2	1.21E+13	0.0	74520.0
160. C2H2+O=CO+CH2	4.10E+08	1.5	1697.0
161. C2H2+O=HCCO+H	4.00E+14	0.0	10660.0
162. C2H2+OH=C2H+H2O	1.45E+04	2.7	12040.0
163. C2H2+OH=CH2CO+H	3.00E+12	0.0	1100.0
164. C2H+O2=CO+HCO	2.41E+12	0.0	0.0
165. C2H+H2=C2H2+H	1.15E+13	0.0	2880.0
166. C2H+CH4=C2H2+CH3	1.81E+12	0.0	500.0
167. C2H+OH=CH2+CO	1.81E+13	0.0	0.0
168. C2H+OH=C2H2+O	1.81E+13	0.0	0.0
169. HCCO+H=CH2S+CO	3.00E+13	0.0	0.0
170. CH2CO+O=CH2+CO2	1.74E+12	0.0	1350.0
171. CH2CO+H=HCCO+H2	5.00E+13	0.0	8000.0
172. CH2CO+O=HCCO+OH	1.00E+13	0.0	8000.0
173. CH2CO+OH=HCCO+H2O	7.50E+12	0.0	2000.0
174. CH2CO+M=CH2+CO+M	3.00E+15	0.0	75980.0
175. CH2CO+OH=HCO+CH2O	2.80E+13	0.0	0.0
176. CH2CO+H=CH3+CO	1.50E+04	2.8	672.8
177. CH2S+M=CH2+M	1.00E+13	0.0	0.0
178. CH2S+O2=CO+H2O	2.41E+11	0.0	0.0
179. CH2S+CH4=C2H5+H	9.43E+12	-0.1	6620.0
180. CH2S+CH4=CH3+CH3	3.45E+22	-2.5	7460.0
181. CH2S+CH4=C2H6	5.78E+46	-10.3	12830.0
182. CH2S+CH3CL=C2H5CL	7.85E+31	-6.2	5830.0
183. CH2S+CH3CL=C2H4+HCL	1.60E+18	-1.5	2710.0
184. CH2S+CH3CL=C2H5+CL	3.09E+07	1.7	520.0
185. CH2S+H2=CH4	3.82E+25	-4.5	3770.0
186. CH2S+H2=CH3+H	1.27E+14	-0.1	130.0
187. CH2+CH4=CH3+CH3	1.82E+05	0.0	0.0
188. CH2+CH3CL=CH3+CH2CL	9.10E+04	0.0	0.0
189. CH2+H2=CH3+H	3.01E+09	0.0	0.0
190. CH2+H2O=CH3+OH	9.64E+07	0.0	0.0

191. CH4+O2=CH3+HO2	4.04E+13	0.0	56910.0
192. CH4+O=CH3+OH	1.02E+09	1.5	8600.0
193. CH4+OH=CH3+H2O	1.93E+05	2.4	2110.0
194. CH4+HO2=CH3+H2O2	2.00E+13	0.0	18000.0
195. CH3+O2=CH2O+OH	3.59E+09	-0.1	10150.0
196. CH3+O2=CH3O+O	2.88E+15	-1.1	30850.0
197. CH3+O=CH2O+H	7.00E+13	0.0	0.0
198. CH3+OH=CH3O+H	3.87E+12	-0.2	13741.0
199. CH3+HO2=CH3O+OH	2.00E+13	0.0	0.0
200. CH3O+O2=CH2O+HO2	6.62E+10	0.0	2600.0
201. CH3O+M=CH2O+H+M	1.00E+14	0.0	25100.0
202. CH3O+CO=CO2+CH3	1.57E+13	0.0	11800.0
203. CH3O+HO2=CH2O+H2O2	3.01E+11	0.0	0.0
204. CH3O+CH3=CH4+CH2O	2.41E+13	0.0	0.0
205. CH3O+O=OH+CH2O	6.03E+12	0.0	0.0
206. CH3O+OH=H2O+CH2O	1.81E+13	0.0	0.0
207. CH3O+H=CH2O+H2	1.99E+13	0.0	0.0
208. CH3O+CH2=CH3+CH2O	1.81E+13	0.0	0.0
209. CH3O+C2H5=C2H6+CH2O	2.41E+13	0.0	0.0
210. CH3O+CLO=HOCL+CH2O	2.41E+13	0.0	0.0
211. CH3O+CL=HCL+CH2O	4.00E+14	0.0	0.0
212. CH2O+CLO=HCO+HOCL	5.50E+03	2.8	5860.0
213. CH2O+C2H5=HCO+C2H6	5.50E+03	2.8	5860.0
214. CH2O+CH3=CH4+HCO	1.00E+11	0.0	6090.0
215. CH2O+H=HCO+H2	2.50E+13	0.0	3990.0
216. CH2O+O=HCO+OH	3.50E+13	0.0	3510.0
217. CH2O+OH=HCO+H2O	3.00E+13	0.0	1190.0
218. CH2O+HO2=HCO+H2O2	1.00E+12	0.0	8000.0
219. CH2O+CL=HCO+HCL	5.00E+13	0.0	500.0
220. CH2O+M=HCO+H+M	5.00E+16	0.0	76200.0
221. CH2O+O2=HCO+HO2	2.05E+13	0.0	38945.0
222. HCO+M=H+CO+M	7.10E+14	0.0	16802.0
223. HCO+H=CO+H2	2.00E+14	0.0	0.0
224. HCO+O2=CO+HO2	3.00E+12	0.0	0.0
225. HCO+O=CO+OH	3.01E+13	0.0	0.0
226. HCO+O=H+CO2	3.01E+13	0.0	0.0
227. HCO+OH=CO+H2O	3.01E+13	0.0	0.0

228. CO+OH=CO2+H	4.40E+06	1.5	-740.0
229. CO+HO2=CO2+OH	1.50E+14	0.0	23573.0
230. CO+O2=CO2+O	2.50E+12	0.0	47800.0
231. CO+O+M=CO2+M	6.17E+14	0.0	3000.0
232. H+O2=O+OH	1.20E+17	-0.9	16504.0
233. H+O2=HO2	7.00E+17	-0.8	0.0
234. O+H2O=OH+OH	1.50E+10	1.1	17244.0
235. H+OH+M=H2O+M	7.50E+23	-2.6	0.0
236. O2+M=O+O+M	1.20E+14	0.0	107552.0
237. H+O+M=OH+M	2.29E+14	0.0	3900.0
238. H+HO2=OH+OH	1.69E+14	0.0	870.0
239. H+HO2=H2+O2	6.62E+13	0.0	2130.0
240. O+HO2=OH+O2	2.00E+13	0.0	0.0
241. OH+HO2=H2O+O2	2.00E+13	0.0	0.0
242. OH+H2O2=HO2+H2O	1.75E+12	0.0	320.0
243. O+H2O2=HO2+OH	9.63E+06	2.0	3970.0
244. H+H2O2=H2+HO2	4.82E+13	0.0	7950.0
245. H+H2O2=OH+H2O	2.41E+13	0.0	3970.0
246. O2+H2O2=HO2+HO2	5.42E+13	0.0	39740.0
247. H2O2+M=OH+OH+M	1.29E+33	-4.9	53250.0
248. O+HCL=OH+CL	5.24E+12	0.0	6400.0
249. OH+HCL=CL+H2O	1.58E+13	0.0	1000.0
250. H2+OH=H2O+H	1.00E+08	1.6	3296.0
251. H2+O=H+OH	1.50E+07	2.0	7547.0
252. CL+CL+M=CL2+M	2.34E+14	0.0	-1800.0
253. H+CL+M=HCL+M	1.00E+17	0.0	0.0
254. H+O2+M=HO2+M	7.00E+17	-0.8	0.0
255. H+HCL=H2+CL	7.90E+12	0.0	3400.0
256. CL+HO2=HCL+O2	1.08E+13	0.0	-338.0
257. CL+HO2=CLO+OH	2.47E+13	0.0	894.0
258. CLO+CO=CL+CO2	6.03E+11	0.0	17400.0
259. CHCLO+H=HCO+HCL	8.33E+13	0.0	7400.0
260. CHCLO+H=CH2O+CL	6.99E+14	-0.6	6360.0
261. CH3+CLO=CH3O+CL	3.33E+11	0.5	30.0
262. CH3+CLO=CH2O+HCL	3.47E+18	-1.8	2070.0
263. CH2CL2+O2=CHCL2+HO2	1.35E+13	0.0	51800.0
264. CH2CL2+HO2=CHCL2+H2O2	6.67E+12	0.0	18270.0

265. CH2CL2+OH=CHCL2+H2O	2.83E+12	0.0	2090.0
266. CH2CL2+O=CHCL2+OH	6.00E+12	0.0	5760.0
267. CH2CL+O2=CH2CLOO	2.73E+33	-7.5	4440.0
268. CH2CL+O2=CH2O+CLO	1.91E+14	-1:3	3810.0
269. CH2CL+O2=CHCLO+OH	4.00E+13	0.0	34000.0
270. CH2CL+O=CH2CLO	1.29E+15	-2.0	1100.0
271. CH2CL+O=CH2O+CL	5.59E+13	-0.1	710.0
272. CH2CL+OH=CH2O+HCL	3.41E+18	-1.5	3370.0
273. CH2CL+OH=CH2OH+CL	2.10E+10	0.8	5980.0
274. CH2CL+HO2=CH2CLO+OH	1.00E+13	0.0	0.0
275. CH2CLO=CHCLO+H	1.83E+27	-5.1	21170.0
276. CH2CLO=CH2O+CL	4.53E+31	-6.4	22560.0
277. CHCLO=HCO+CL	8.86E+29	-5.2	92920.0
278. CHCLO=CO+HCL	1.10E+30	-5.2	92960.0
279. CH2CL+CLO=CH2CLO+CL	4.15E+12	0.1	1110.0
280. CH2CL+CLO=CHCLO+HCL	4.13E+19	-2.2	2360.0
281. CH2CL+CH2O=CH3CL+HCO	2.00E+11	0.0	6000.0
282. CH3CL+O2=CH2CL+HO2	2.02E+13	0.0	54000.0
283. CH3CL+O=CH2CL+OH	1.70E+13	0.0	7300.0
284. CH3CL+OH=CH2CL+H2O	2.45E+12	0.0	2700.0
285. CH3CL+HO2=CH2CL+H2O2	1.00E+13	0.0	21660.0
286. H2O2+CL=HCL+HO2	6.62E+12	0.0	1950.0
287. CLO+CH4=CH3+HOCL	6.03E+11	0.0	15000.0
288. CLO+CH3CL=CH2CL+HOCL	3.03E+11	0.0	10700.0
289. CLO+H2=HOCL+H	6.03E+11	0.0	14100.0
290. OH+HOCL=H2O+CLO	1.81E+12	0.0	990.0
291. H+HOCL=HCL+OH	9.55E+13	0.0	7620.0
292. CL+HOCL=CL2+OH	1.81E+12	0.0	260.0
293. CL+HOCL=HCL+CLO	7.28E+12	0.0	100.0
294. O+HOCL=OH+CLO	6.03E+12	0.0	4370.0
295. HOCL=CL+OH	1.76E+20	-3.0	56720.0
296. HOCL=H+CLO	8.12E+14	-2.1	93690.0
297. O+CL2=CL+CLO	2.51E+12	0.0	2720.0
298. H+CL2=HCL+CL	8.59E+13	0.0	1170.0
299. C2H3+CL2=C2H3CL+CL	5.25E+12	0.0	-480.0
300. CHCLO+OH=CCLO+H2O	7.50E+12	0.0	1200.0
301. CHCLO+O=CCLO+OH	8.80E+12	0.0	3500.0

302. CHCLO+O2=CCLO+HO2	4.50E+12	0.0	41800.0
303. CHCLO+CL=CCLO+HCL	1.25E+13	0.0	500.0
304. CHCLO+CH3=CCLO+CH4	2.50E+13	0.0	6000.0
305. CHCLO+CH3=HCO+CH3CL	1.50E+13	0.0	8800.0
306. CHCLO+CLO=CCLO+HOCL	1.10E+13	0.0	500.0
307. CCLO+OH=CO+HOCL	3.30E+12	0.0	0.0
308. CCLO+O2=CO2+CLO	1.00E+13	0.0	0.0
309. CCLO+CL=CO+CL2	4.00E+14	0.0	800.0
310. COCL2+M=CCLO+CL+M	1.20E+16	0.0	75500.0
311. COCL2+OH=CCLO+HOCL	1.00E+13	0.0	23300.0
312. COCL2+O=CCLO+CLO	2.00E+13	0.0	17000.0
313. COCL2+H=CCLO+HCL	5.00E+13	0.0	6300.0
314. COCL2+CL=CCLO+CL2	3.20E+14	0.0	23500.0
315. COCL2+CH3=CCLO+CH3CL	1.90E+13	0.0	12900.0
316. CHCL3=CHCL2+CL	5.70E+12	0.0	67700.0
317. CHCL3=CCL2+HCL	5.20E+12	0.0	51500.0
318. CHCL3+OH=H2O+CCL3	3.30E+12	0.0	2300.0
319. CHCL3+O2=HO2+CCL3	1.00E+13	0.0	47200.0
320. CHCL3+HO2=H2O2+CCL3	4.50E+10	0.0	14200.0
321. CHCL3+H=HCL+CHCL2	3.60E+12	0.0	6200.0
322. CHCL3+O=OH+CCL3	3.00E+12	0.0	4900.0
323. CHCL3+CH3=CH3CL+CHCL2	2.40E+13	0.0	12000.0
324. CHCL3+CL=HCL+CCL3	1.60E+13	0.0	3300.0
325. CCL3+H2=CHCL3+H	5.01E+12	0.0	14300.0
326. CCL3+CH4=CHCL3+CH3	5.00E+12	0.0	14900.0
327. CCL2+O2=COCL2+O	5.78E+10	0.0	4100.0
328. CHCLCHCL=C2HCL+HCL	7.26E+13	0.0	69090.0
329. CH2CCL2=C2HCL+HCL	1.45E+14	0.0	69220.0
330. C2HCL3=C2CL2+HCL	7.26E+13	0.0	74440.0
331. C2HCL+H=HCL+C2H	1.00E+13	0.0	17030.0
332. C2HCL+H=C2H2+CL	2.00E+13	0.0	2100.0
333. CCL3+CH3=C2H3CL3	9.54E+46	-10.7	11740.0
334. CCL3+CH3=CH2CCL2+HCL	1.62E+30	-5.3	8640.0
335. CCL3+CH3=CH3CCL2+CL	3.98E+22	-2.6	7090.0
336. CCL3+CH2CL=C2H2CL4	4.01E+45	-10.2	10670.0
337. CCL3+CH2CL=C2HCL3+HCL	4.74E+30	-5.1	8810.0
338. CCL3+CH2CL=C2H2CL3+CL	5.90E+23	-2.8	8960.0

```
339. CHCL+CHCL=CHCLCHCL                    4.00E+12   0.0      0.0
340. CHCL+O2=CHCLO+O                       1.50E+13   0.0   2860.0
341. CHCL+O=CHCLO                          1.00E+13   0.0      0.0
342. CHCL+O2=CO+HOCL                       1.20E+11   0.0      0.0

 NOTE:  A units mole-cm-sec-K, E units cal/mole


NO ERRORS FOUND ON INPUT...CHEMKIN LINKING FILE WRITTEN.

WORKING SPACE REQUIREMENTS ARE
  INTEGER:    5641
  REAL:       5288
  CHARACTER:    80
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APPENDIX D

THERMODYNAMIC DATA USED IN MODELING STUDIES

This appendix contains the thermodynamic data in NASA format usedfor the combustion modeling studies.

```
THERMO
  300.000  1500.000  5000.000
AR            120186AR 1   0   0   0G  300.000  5000.000 1000.000   01
 2.50104422E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00   2
-7.45686320E+02 4.36103012E+00 2.50104422E+00 0.00000000E+00 0.00000000E+00   3
 0.00000000E+00 0.00000000E+00-7.45686320E+02 4.36103012E+00                  4
C             121086C  1   0   0   0G  300.000  5000.000 1000.000   01
 2.50104422E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00   2
 8.54747470E+04 4.75358171E+00 2.50104422E+00 0.00000000E+00 0.00000000E+00   3
 0.00000000E+00 0.00000000E+00 8.54747470E+04 4.75358171E+00                  4
C(S)          121286C  1   0   0   0S  300.000  5000.000 1000.000   01
 2.01291286E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00   2
-6.00149955E+02-1.07792840E+01 2.01291286E+00 0.00000000E+00 0.00000000E+00   3
 0.00000000E+00 0.00000000E+00-6.00149955E+02-1.07792840E+01                  4
C2            121286C  2   0   0   0G  300.000  5000.000 1365.000   01
 1.75087700E+00 2.17821466E-03-5.02393150E-07 4.43367660E-11-9.61938275E-16   2
 1.00578269E+05 1.41898316E+01 3.54370009E+00 6.26080510E-05-9.54499947E-07   3
 1.33851188E-09-3.91027750E-13 9.97317394E+04 3.79797435E+00                  4
C2H           20387C  2H  1   0   0G  300.000  5000.000 1676.000   01
 4.70512615E+00 2.18053473E-03-8.14031977E-07 1.34394768E-10-8.14750090E-15   2
 6.57335930E+04-2.96169080E+00 3.17251474E+00 5.10333807E-03-2.51022358E-06   3
 3.70351877E-10 2.83115320E-14 6.62971349E+04 5.45813034E+00                  4
C2H2          121386C  2H  2   0   0G  300.000  5000.000 1400.000   01
 5.32804348E+00 4.21578830E-03-1.41488586E-06 2.16740885E-10-1.24532782E-14   2
 2.52001339E+04-8.03643654E+00 2.63015149E+00 1.15991429E-02-9.53866936E-06   3
 4.37631793E-09-8.27219600E-13 2.60535932E+04 6.11019332E+00                  4
C2H3           12787C  2H  3   0   0G  300.000  5000.000 1361.000   01
 4.54901573E+00 7.25010896E-03-2.51760018E-06 3.94770712E-10-2.30604434E-14   2
 3.21580682E+04-1.33454895E+00 2.72824220E+00 7.07857135E-03 2.39922202E-06   3
-3.76405776E-09 9.76970409E-13 3.32965877E+04 1.01208182E+01                  4
C2H4          121286C  2H  4   0   0G  300.000  5000.000 1394.000   01
 5.11559901E+00 9.00813091E-03-3.05532070E-06 4.71519699E-10-2.72376649E-14   2
 3.66320840E+03-6.86533909E+00 5.58887914E-01 1.82723404E-02-9.95033950E-06   3
 2.69314606E-09-2.85954569E-13 5.41496476E+03 1.81481649E+01                  4
C2H5           12387C  2H  5   0   0G  300.000  5000.000 1992.000   01
 4.43775354E+00 1.25341458E-02-4.40322779E-06 6.99006928E-10-4.12650206E-14   2
 1.16034582E+04 4.74248931E-02 1.28283253E+00 1.58385744E-02-2.53378618E-06   3
-2.24063844E-09 7.45640247E-13 1.30416717E+04 1.83713738E+01                  4
C2H6          121686C  2H  6   0   0G  300.000  5000.000 1370.000   01
 6.20258185E+00 1.29577778E-02-4.37747121E-06 6.74393362E-10-3.89295188E-14   2
-1.36342663E+04-1.37999913E+01 5.38489603E-01 2.14952010E-02-6.89355460E-06   3
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-6.39159968E-10 5.48076256E-13-1.11395921E+04 1.83831383E+01 4
C2N 121286C 2N 1 0 0G 300.000 5000.000 1557.000 01
2.34507880E+07-4.91431199E+04 3.44632119E+01-9.35210982E-03 8.19825237E-07 2
-8.06613340E+09-1.27071061E+08-6.83993441E-02 2.94177674E-02-4.12511910E-05 3
2.46345803E-08-5.30147230E-12 6.59762810E+04 2.10156312E+01 4
C2N2 121286C 2N 2 0 0G 300.000 5000.000 1391.000 01
7.42521354E+00 2.61993376E-03-9.06701642E-07 1.41926171E-10-8.28276782E-15 2
3.44992823E+04-1.47552640E+01 4.51496879E+00 9.84970328E-03-7.90184061E-06 3
3.26720151E-09-5.48646636E-13 3.54664022E+04 7.21153194E-01 4
C2O 121286C 2O 1 0 0G 300.000 5000.000 1713.000 01
3.67614538E+04-6.74761607E+01 4.25830184E-02-1.07054928E-05 8.93133253E-10 2
-1.48664453E+07-2.04561605E+05-4.96747980E+00 4.80511329E-02-6.71074998E-05 3
3.99340383E-08-8.56658449E-12 3.43474958E+04 4.46502610E+01 4
C3 121286C 3 0 0 0G 300.000 5000.000 1447.000 01
3.49154205E+00 2.50335453E-03-7.59903114E-07 1.07953068E-10-5.85813672E-15 2
9.75643163E+04 8.04041316E+00 4.01653253E+00 1.22027396E-03 3.44753022E-07 3
-2.82986570E-10 4.04788066E-14 9.74019942E+04 5.26410514E+00 4
C3H2 121686C 3H 2 0 0G 300.000 5000.000 1395.000 01
7.59711354E+00 5.02341324E-03-1.73631018E-06 2.71494986E-10-1.58306808E-14 2
5.04982418E+04-1.77671242E+01 2.31581883E+00 1.84362492E-02-1.50904192E-05 3
6.42697006E-09-1.11233756E-12 5.22297730E+04 1.02237117E+01 4
C3H3 121686C 3H 3 0 0G 300.000 5000.000 1408.000 01
7.45639322E+00 6.77756243E-03-2.23489210E-06 3.38347612E-10-1.92829268E-14 2
3.54031341E+04-1.55251838E+01 2.07997008E+00 2.11371300E-02-1.71906853E-05 3
7.47152176E-09-1.31782735E-12 3.70833980E+04 1.26987811E+01 4
C*C*C 40687C 3H 4 0 0G 300.000 5000.000 1394.000 01
7.85694307E+00 9.09615964E-03-3.06033419E-06 4.69955088E-10-2.70606569E-14 2
1.91251007E+04-2.16364912E+01 7.65311814E-01 2.63997950E-02-1.95349508E-05 3
7.73750067E-09-1.27232660E-12 2.15243264E+04 1.62055091E+01 4
C3H4C 121686C 3H 4 0 0G 300.000 5000.000 1407.000 01
7.88990676E+00 8.99806678E-03-3.01248313E-06 4.61143025E-10-2.64968493E-14 2
2.95420149E+04-2.04492520E+01-1.05605115E+00 3.16975545E-02-2.51679503E-05 3
1.03014713E-08-1.69555276E-12 3.24303953E+04 2.68927219E+01 4
C#CC 40687C 3H 4 0 0G 300.000 5000.000 1387.000 01
7.59018781E+00 9.29723037E-03-3.12413427E-06 4.79339527E-10-2.75839503E-14 2
1.86250438E+04-2.27418395E+01 1.80636930E+00 2.20984630E-02-1.39343060E-05 3
4.65899495E-09-6.56547989E-13 2.07273058E+04 8.61077836E+00 4
C3H5 120186C 3H 5 0 0G 300.000 5000.000 1395.000 01
9.81659934E+00 9.98373269E-03-3.37584661E-06 5.20827704E-10-3.01084413E-14 2
1.13070381E+04-3.09881181E+01-2.06140915E+00 3.85305230E-02-2.92808536E-05 3
1.10520418E-08-1.64673646E-12 1.52795886E+04 3.24003387E+01 4

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C3H6            120186C  3H  6   0   0G  300.000 5000.000 1374.000   01
 8.58512074E+00 1.34382370E-02-4.53667644E-06 6.98813474E-10-4.03417296E-14   2
-2.08952899E+03-2.46972522E+01-2.74700111E-02 3.01891412E-02-1.56860259E-05   3
 3.43267099E-09-1.65481873E-13 1.25925396E+03 2.27890949E+01                 4
C3H8            120186C  3H  8   0   0G  300.000 5000.000 1370.000   01
 9.83592018E+00 1.74275867E-02-5.90596682E-06 9.12067971E-10-5.27464347E-14   2
-1.80115147E+04-3.22871071E+01-7.81023311E-01 3.68517225E-02-1.71795088E-05   3
 2.62886628E-09 1.60331260E-13-1.37497646E+04 2.67039045E+01                 4
C3O2            121286C  3O  2   0   0G  300.000 5000.000 1394.000   01
 9.44182085E+00 3.53422022E-03-1.24066780E-06 1.96079469E-10-1.15206234E-14   2
-1.48525395E+04-2.29158705E+01 4.23736508E+00 1.65616049E-02-1.37909217E-05   3
 5.71230024E-09-9.41118855E-13-1.31516952E+04 4.69458600E+00                 4
C4              121286C  4   0   0   0G  300.000 5000.000 1409.000   01
 8.03325902E+00 1.82929475E-03-6.68953167E-07 1.08594497E-10-6.49919739E-15   2
 1.13693316E+05-2.01604068E+01 2.00593957E+00 1.81310635E-02-1.75186052E-05   3
 7.96270213E-09-1.39195090E-12 1.15514822E+05 1.13397493E+01                 4
C4H             121686C  4H  1   0   0G  300.000 5000.000 1678.000   01
 6.59733532E+00 5.95017417E-03-2.18996240E-06 3.58135598E-10-2.15675474E-14   2
 7.54557160E+04-9.44062892E+00 5.00826916E+00 6.71577778E-03 5.44751245E-07   3
-2.27973224E-09 6.17613147E-13 7.62650637E+04 1.11553723E-01                 4
C4H2            121686C  4H  2   0   0G  300.000 5000.000 1412.000   01
 9.63105982E+00 5.39340675E-03-1.76557585E-06 2.65915150E-10-1.50980215E-14   2
 5.26185281E+04-2.74214396E+01 3.91321080E+00 2.23550725E-02-2.11910975E-05   3
 1.02823335E-08-1.95229788E-12 5.42329530E+04 1.98945189E+00                 4
C4H3            121686C  4H  3   0   0G  300.000 5000.000 1402.000   01
 9.41736121E+00 7.63518588E-03-2.52700902E-06 3.83695192E-10-2.19175047E-14   2
 4.74574992E+04-2.45507164E+01 2.85410816E+00 2.49546776E-02-2.03728577E-05   3
 8.82793606E-09-1.55187997E-12 4.95318069E+04 9.98233570E+00                 4
C4H4            121686C  4H  4   0   0G  300.000 5000.000 1399.000   01
 1.01825800E+01 9.44213031E-03-3.13401943E-06 4.77045415E-10-2.73054690E-14   2
 3.25677588E+04-2.94018018E+01 9.89041349E-01 3.33283940E-02-2.72458924E-05   3
 1.16324090E-08-2.00511117E-12 3.54983126E+04 1.90831953E+01                 4
C4H6            120186C  4H  6   0   0G  300.000 5000.000 1369.000   01
 1.03665505E+01 1.43212322E-02-4.81036261E-06 7.38524031E-10-4.25385432E-14   2
 1.23573768E+04-3.20141771E+01 1.14238985E+00 3.16059748E-02-1.51408308E-05   3
 2.40358124E-09 1.42580104E-13 1.59829576E+04 1.90322810E+01                 4
C4H8            120386C  4H  8   0   0G  300.000 5000.000 1389.000   01
 1.06909822E+01 1.86947863E-02-6.21692721E-06 9.47204203E-10-5.42419883E-14   2
-5.68386525E+03-3.26061047E+01-7.17996157E-01 4.43474894E-02-2.82580728E-05   3
 9.61267834E-09-1.37604102E-12-1.59114962E+03 2.90731219E+01                 4
C5              121286C  5   0   0   0G  300.000 5000.000 1410.000   01
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1.03412231E+01 2.47709538E-03-9.06783005E-07 1.47302562E-10-8.81994830E-15    2
1.13742013E+05-3.23924410E+01 1.63274391E+00 2.63998782E-02-2.60337342E-05    3
1.20423067E-08-2.13709600E-12 1.16337662E+05 1.29903178E+01                   4
C5H          20387C  5H  1   0   0G  300.000  5000.000 1416.000   01
9.50783238E+00 5.06989741E-03-1.65553987E-06 2.49081868E-10-1.41372899E-14    2
8.98964465E+04-2.58085220E+01 1.15856130E+00 3.03895137E-02-3.09527108E-05    3
1.53878007E-08-2.93488558E-12 9.21718513E+04 1.68974900E+01                   4
C5H12        20387C  5H 12   0   0G  300.000  5000.000 2010.000   01
1.37480383E+01 3.09568899E-02-1.10260261E-05 1.76718897E-09-1.05037594E-13    2
-2.51976359E+04-4.98400338E+01-4.69541845E-01 5.63758351E-02-2.35587964E-05    3
2.00252241E-09 6.20801710E-13-1.97662731E+04 2.89231818E+01                   4
C5H2         20587C  5H  2   0   0G  300.000  5000.000 1405.000   01
1.30904744E+01 5.60151846E-03-1.97140358E-06 3.12145906E-10-1.83652413E-14    2
7.78651788E+04-4.66231787E+01 2.24496675E+00 3.43776526E-02-3.13363678E-05    3
1.39102877E-08-2.41321861E-12 8.12237982E+04 1.02974753E+01                   4
C5H3         20387C  5H  3   0   0G  300.000  5000.000 1399.000   01
1.19929964E+01 8.11493250E-03-2.71964885E-06 4.16654878E-10-2.39555922E-14    2
6.32799052E+04-3.71783077E+01 3.49582577E+00 3.04022206E-02-2.54548557E-05    3
1.10444659E-08-1.92592647E-12 6.59684391E+04 7.56117727E+00                   4
C5H6         20387C  5H  6   0   0G  300.000  5000.000 1397.000   01
1.23399128E+01 1.52194879E-02-5.12993874E-06 7.89730085E-10-4.55833645E-14    2
9.57503215E+03-4.68840745E+01-5.38333192E+00 5.78755167E-02-4.38823793E-05    3
1.65531884E-08-2.46503395E-12 1.54934851E+04 4.76714253E+01                   4
C6H         121686C  6H  1   0   0G  300.000  5000.000 1376.000   01
1.38594796E+01 4.69118857E-03-1.69523864E-06 2.73042901E-10-1.62523490E-14    2
1.01882345E+05-4.52686310E+01 5.66659054E+00 2.37199122E-02-1.82701980E-05    3
6.70534179E-09-9.55202894E-13 1.04697247E+05-1.29584157E+00                   4
C6H10        20387C  6H 10   0   0G  300.000  5000.000 1378.000   01
1.77386547E+01 2.36259919E-02-8.09145440E-06 1.25889962E-09-7.31955102E-14    2
-1.01467313E+04-7.71682391E+01-5.64276703E+00 7.46195738E-02-4.88244624E-05    3
1.52717735E-08-1.79467471E-12-1.73545783E+03 4.95757239E+01                   4
C6H14        20387C  6H 14   0   0G  300.000  5000.000 1385.000   01
2.07106560E+01 2.96885644E-02-9.83998565E-06 1.49705765E-09-8.56831139E-14    2
-3.08260945E+04-8.66502974E+01-2.57972076E+00 8.02776355E-02-4.95724215E-05    3
1.46039128E-08-1.54812395E-12-2.24696285E+04 3.95997360E+01                   4
C6H2        121686C  6H  2   0   0G  300.000  5000.000 1409.000   01
1.36292994E+01 7.05235241E-03-2.32980961E-06 3.53240406E-10-2.01551944E-14    2
8.02815750E+04-4.55994476E+01 5.46735692E+00 3.07737654E-02-2.90101579E-05    3
1.39136610E-08-2.61462245E-12 8.26322525E+04-3.44724566E+00                   4
C6H3         20387C  6H  3   0   0G  300.000  5000.000 1400.000   01
1.40927601E+01 8.81312877E-03-2.94820931E-06 4.51237596E-10-2.59306528E-14    2
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7.40515709E+04-4.68052605E+01 3.88825685E+00 3.57677165E-02-3.05423544E-05 3
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C6H4 20387C 6H 4 0 0G 300.000 5000.000 1398.000 01
1.37708808E+01 1.18583767E-02-4.05541852E-06 6.30538395E-10-3.66501419E-14 2
5.46206598E+04-5.12511889E+01-4.56542598E+00 5.92874553E-02-5.12268310E-05 3
2.19595742E-08-3.71600026E-12 6.04303912E+04 4.54331535E+01 4
C6H6 20387C 6H 6 0 0G 300.000 5000.000 1393.000 01
1.46901611E+01 1.64429216E-02-5.69172226E-06 8.91322774E-10-5.20418295E-14 2
2.35863241E+03-6.13351242E+01-5.48865251E+00 6.53894651E-02-5.10956888E-05 3
2.00290908E-08-3.14065763E-12 9.11321724E+03 4.62771561E+01 4
C8H 121686C 8H 1 0 0G 300.000 5000.000 1402.000 01
1.77162121E+01 6.39890807E-03-2.26011237E-06 3.58753991E-10-2.11453322E-14 2
1.38394905E+05-6.64349661E+01 3.31113732E+00 4.61605439E-02-4.46341688E-05 3
2.08504636E-08-3.77944515E-12 1.42716114E+05 8.64534610E+00 4
C8H2 121686C 8H 2 0 0G 300.000 5000.000 1410.000 01
1.81755662E+01 8.40560020E-03-2.82547033E-06 4.33826164E-10-2.49842898E-14 2
1.06739154E+05-7.06116213E+01 3.39180980E+00 5.16722082E-02-5.15141182E-05 3
2.50914196E-08-4.71691622E-12 1.10934757E+05 5.57956585E+00 4
CH 121286C 1H 1 0 0G 300.000 5000.000 1364.000 01
2.42269870E+00 1.92179277E-03-5.10813942E-07 5.88798221E-11-2.42599641E-15 2
7.08263486E+04 7.96841131E+00 3.41603784E+00-1.45912064E-04 1.06094420E-06 3
-4.57686926E-10 5.93014732E-14 7.04540821E+04 2.54008835E+00 4
CH+ 121286C 1H 1E -1 0G 300.000 5000.000 1000.000 01
3.68866281E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 2
1.94602290E+05-3.77358395E-01 3.68866281E+00 0.00000000E+00 0.00000000E+00 3
0.00000000E+00 0.00000000E+00 1.94602290E+05-3.77358395E-01 4
CH2 120186C 1H 2 0 0G 300.000 5000.000 1519.000 01
3.45921986E+00 2.30956152E-03-5.29345053E-07 5.72572751E-11-2.44283211E-15 2
4.54256416E+04 3.14357932E+00 3.48359761E+00 2.24662042E-03-4.68769918E-07 3
3.13254484E-11 1.75502387E-15 4.54181813E+04 3.01542450E+00 4
CH2S 31287C 1H 2 0 0G 300.000 5000.000 1358.000 01
3.09430986E+00 2.81267684E-03-7.15487247E-07 8.45237612E-11-3.86441463E-15 2
5.00812506E+04 4.32408003E+00 3.32234548E+00 2.28242411E-03-2.47495952E-07 3
-1.02891310E-10 2.50553870E-14 5.00024734E+04 3.09950464E+00 4
CH2CO 121686C 2H 2O 1 0G 300.000 5000.000 1400.000 01
6.76810865E+00 4.96358429E-03-1.64312625E-06 2.49582774E-10-1.42623983E-14 2
-8.97401838E+03-1.19600914E+01 2.38699001E+00 1.63268077E-02-1.31153977E-05 3
5.56599995E-09-9.59182011E-13-7.57259306E+03 1.11567934E+01 4
C4H2O 120186O 1H 2C 4 0G 300.000 2000.000 1000.000 01
4.83104182E+00 2.03670265E-02-2.89531976E-06-1.19611155E-08 5.58233101E-12 2
1.74946142E+04-5.50829650E+00 4.83104182E+00 2.03670265E-02-2.89531976E-06 3

-1.19611155E-08 5.58233101E-12 1.74946142E+04-5.50829650E+00 4
CH2O 121286C 1H 2O 1 0G 300.000 5000.000 1674.000 01
3.39729331E+00 5.91137002E-03-2.12410628E-06 3.41836853E-10-2.03568759E-14 2
-1.54575156E+04 4.72540368E+00 2.80307594E+00 4.51235772E-03 2.27297982E-06 3
-2.82676369E-09 6.77260178E-13-1.49917261E+04 8.90237672E+00 4
CH2OH 120186H 3C 1O 1 0G 300.000 5000.000 1395.000 01
6.05802372E+00 5.09626439E-03-1.84855973E-06 3.22094807E-10-2.06491882E-14 2
-4.57928914E+03-7.36360183E+00 2.10424627E+00 1.49281038E-02-1.14023865E-05 3
4.61913086E-09-7.69204081E-13-3.26232633E+03 1.36651945E+01 4
CH3 121286C 1H 3 0 0G 300.000 5000.000 1398.000 01
3.47621322E+00 5.13899064E-03-1.68260795E-06 2.53167404E-10-1.43547385E-14 2
1.61608701E+04 1.87748541E+00 3.28263038E+00 5.03774474E-03-1.34244601E-06 3
1.48151323E-10-2.55361677E-14 1.63328573E+04 3.19502269E+00 4
CH3CO 120186C 2H 3O 1 0G 300.000 5000.000 1369.000 01
6.27257917E+00 8.28535195E-03-2.86454186E-06 4.47920242E-10-2.61161840E-14 2
-5.73390303E+03-7.60131061E+00 2.63832904E+00 1.30852724E-02-3.13811972E-06 3
-1.27693854E-09 5.43668282E-13-4.05588970E+03 1.33047534E+01 4
CH3CHO 120186C 2O 1H 4 0G 300.000 5000.000 1370.000 01
6.96488741E+00 1.00331682E-02-3.42404663E-06 5.31008319E-10-3.07907419E-14 2
-2.33942691E+04-1.28523468E+01 1.58380439E+00 1.90568021E-02-7.53658836E-06 3
3.61824354E-10 3.02042361E-13-2.11377461E+04 1.73618053E+01 4
CH3O 121686C 1H 3O 1 0G 300.000 5000.000 1682.000 01
3.80354755E+00 8.17961115E-03-2.92839659E-06 4.70256328E-10-2.79667095E-14 2
4.29628033E+01 2.53701157E+00 1.52972845E+00 1.07882118E-02-2.00272171E-06 3
-1.39399635E-09 4.89077567E-13 1.04738539E+03 1.56517263E+01 4
CH3OH 121686C 1H 4O 1 0G 300.000 5000.000 1370.000 01
4.58943624E+00 9.45160636E-03-3.20826439E-06 4.95443876E-10-2.86343757E-14 2
-2.66166326E+04-1.30358955E+00 2.31483366E+00 1.06357626E-02 1.10481922E-07 3
-2.81058603E-09 8.01462623E-13-2.53459107E+04 1.24907060E+01 4
CH4 121286C 1H 4 0 0G 300.000 5000.000 1687.000 01
2.10177666E+00 9.38497696E-03-3.28522587E-06 5.19264800E-10-3.05294801E-14 2
-1.02311834E+04 7.33830071E+00 2.70645318E+00 3.96642840E-03 5.86334566E-06 3
-5.01985843E-09 1.09223790E-12-1.00341771E+04 5.55918782E+00 4
CN 121286C 1N 1 0 0G 300.000 5000.000 1401.000 01
3.17790974E+00 1.14698546E-03-3.48392105E-07 4.87496423E-11-2.60635565E-15 2
5.13372401E+04 5.89589688E+00 3.10536655E+00 1.24540239E-03-3.73527286E-07 3
3.59006292E-11 2.41065710E-15 5.13722859E+04 6.31519919E+00 4
CN+ 121286C 1N 1E -1 0G 300.000 5000.000 1000.000 01
3.97047061E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 2
2.15700956E+05 3.03966165E+00 3.97047061E+00 0.00000000E+00 0.00000000E+00 3
0.00000000E+00 0.00000000E+00 2.15700956E+05 3.03966165E+00 4

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CN-          121286C  1N  1E  1   0G  300.000  5000.000 1406.000   01
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 5.80681289E+03-1.20850322E+00 3.17960795E+00 1.05248697E-03-4.69823312E-07   3
 1.80410870E-10-1.82736808E-14 6.30645656E+03 5.14752958E+00                 4
CN2          121686C  1N  2   0   0G  300.000  5000.000 1397.000   01
 6.10578043E+00 1.28191611E-03-4.65447584E-07 7.52050844E-11-4.48635361E-15   2
 5.46471806E+04-8.72547397E+00 2.84313868E+00 9.81481657E-03-9.02694107E-06   3
 3.97087053E-09-6.79309575E-13 5.56680247E+04 8.43891324E+00                 4
CNN          121286C  1N  2   0   0G  300.000  5000.000 1402.000   01
 5.31762866E+00 1.78856645E-03-6.03058005E-07 9.27227267E-11-5.34308729E-15   2
 6.84664874E+04-3.34269646E+00 3.62405254E+00 6.30531552E-03-5.32435990E-06   3
 2.36245990E-09-4.22977985E-13 6.89988700E+04 5.55442513E+00                 4
CO           121286C  1O  1   0   0G  300.000  5000.000 1417.000   01
 3.19552608E+00 1.05191879E-03-2.99568155E-07 3.81992286E-11-1.80344014E-15   2
-1.43114638E+04 5.21809447E+00 3.14404115E+00 1.07605456E-03-2.40844519E-07   3
-1.34754226E-11 9.70526182E-15-1.42795000E+04 5.53593694E+00                 4
CO2          121286C  1O  2   0   0G  300.000  5000.000 1382.000   01
 5.23356573E+00 2.02480173E-03-7.22002738E-07 1.15269224E-10-6.81945307E-15   2
-4.93616732E+04-5.46905393E+00 2.47221170E+00 8.40592751E-03-6.30465344E-06   3
 2.31888857E-09-3.38902391E-13-4.84021564E+04 9.37560816E+00                 4
CO2-         121286C  1O  2E  1   0G  300.000  5000.000 1376.000   01
 2.83136467E+00 4.56103496E-03-1.12988241E-06 1.27210518E-10-5.43713181E-15   2
-5.40179354E+04 1.17517288E+01 3.65275866E+00 2.78241903E-03 3.21657116E-07   3
-4.08851424E-10 7.10733183E-14-5.43199908E+04 7.28574892E+00                 4
COS          121286C  1O  1S  1   0G  300.000  5000.000 1385.000   01
 5.60404412E+00 1.69949255E-03-6.07299045E-07 9.70949945E-11-5.74997228E-15   2
-1.87228699E+04-5.25594309E+00 3.01607101E+00 7.91127266E-03-6.31352241E-06   3
 2.48477066E-09-3.89744465E-13-1.78480331E+04 8.57239597E+00                 4
CS           121686C  1S  1   0   0G  300.000  5000.000 1391.000   01
 3.75694271E+00 7.70142906E-04-2.71372366E-07 4.30800166E-11-2.51582074E-15   2
 3.24710335E+04 3.46727587E+00 2.87970663E+00 2.99673217E-03-2.47540271E-06   3
 1.04930129E-09-1.79763240E-13 3.27573417E+04 8.11477056E+00                 4
CS2          121286C  1S  2   0   0G  300.000  5000.000 1406.000   01
 6.46734862E+00 9.56853535E-04-3.49123819E-07 5.65936748E-11-3.38375053E-15   2
 1.17768566E+04-9.19526829E+00 3.09636195E+00 1.04518387E-02-1.06106375E-05   3
 5.05920780E-09-9.24107636E-13 1.27628826E+04 8.29677019E+00                 4
E            120186E  1   0   0   0G  300.000  5000.000 1000.000   01
 2.50104422E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00   2
-7.45686320E+02-1.17386177E+01 2.50104422E+00 0.00000000E+00 0.00000000E+00   3
 0.00000000E+00 0.00000000E+00-7.45686320E+02-1.17386177E+01                 4
F            121286F  1   0   0   0G  300.000  5000.000 1000.000   01
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2.62685128E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
8.70850039E+03 4.11730726E+00 2.62685128E+00 0.00000000E+00 0.00000000E+00    3
0.00000000E+00 0.00000000E+00 8.70850039E+03 4.11730726E+00                   4
F2            121286F  2   0   0   0G  300.000  5000.000 1391.000    01
4.02107835E+00 6.38110523E-04-2.29662559E-07 3.67225527E-11-2.13797804E-15    2
-1.32501246E+03 1.08114548E+00 3.15705752E+00 2.88726518E-03-2.51097920E-06    3
1.10029451E-09-1.92589146E-13-1.04950570E+03 5.63727893E+00                   4
FNO3          121286F  1N  1O  3   0G  300.000  5000.000 1405.000    01
1.04004497E+01 2.41268144E-03-8.81119178E-07 1.42911826E-10-8.54788763E-15    2
-2.72745311E+03-2.64040548E+01 2.69717552E+00 2.33447855E-02-2.26781344E-05    3
1.03992097E-08-1.83680748E-12-4.02911317E+02 1.38311131E+01                   4
FO            121286F  1O  1   0   0G  300.000  5000.000 1391.000    01
3.92395514E+00 7.16934780E-04-2.55879106E-07 4.08244652E-11-2.38341207E-15    2
1.17778993E+04 3.26698497E+00 3.00985569E+00 3.07283488E-03-2.62293231E-06    3
1.13553510E-09-1.97193405E-13 1.20721091E+04 8.09618227E+00                   4
FO2           121286F  1O  2   0   0G  300.000  5000.000 1403.000    01
6.10195495E+00 8.29218583E-04-3.01878414E-07 4.88618064E-11-2.91839222E-15    2
-5.96721524E+02-4.38561229E+00 3.67295340E+00 7.36423211E-03-7.04492370E-06    3
3.19688010E-09-5.60484147E-13 1.43594058E+02 8.32589188E+00                   4
H             120186H  1   0   0   0G  300.000  5000.000 1000.000    01
2.50104422E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
2.54747466E+04-4.65341317E-01 2.50104422E+00 0.00000000E+00 0.00000000E+00    3
0.00000000E+00 0.00000000E+00 2.54747466E+04-4.65341317E-01                   4
H+            120186H  1E -1   0   0G  300.000  5000.000 1000.000    01
2.50104422E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
1.84065588E+05-1.15985566E+00 2.50104422E+00 0.00000000E+00 0.00000000E+00    3
0.00000000E+00 0.00000000E+00 1.84065588E+05-1.15985566E+00                   4
H-            120186H  1E  1   0   0G  300.000  5000.000 1000.000    01
2.50104422E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
1.59629197E+04-1.15482295E+00 2.50104422E+00 0.00000000E+00 0.00000000E+00    3
0.00000000E+00 0.00000000E+00 1.59629197E+04-1.15482295E+00                   4
H2            121286H  2   0   0   0G  300.000  5000.000 1371.000    01
2.87740693E+00 9.88605992E-04-2.66313661E-07 3.11722995E-11-1.30965211E-15    2
-7.93629768E+02-7.53700282E-01 3.51740247E+00-2.83646315E-04 6.35052089E-07    3
-2.32621082E-10 2.41073419E-14-1.04126858E+03-4.27529382E+00                   4
H2CN          41687H  2C  1N  1   0G  300.000  5000.000 1677.000    01
4.55113116E+00 4.74156719E-03-1.67742679E-06 2.67533908E-10-1.58446870E-14    2
2.78648205E+04-1.03219796E+00 2.21303039E+00 9.22194771E-03-4.29554047E-06    3
6.40585607E-10 3.82810326E-14 2.87203626E+04 1.18020493E+01                   4
H2CNH         41687C  1H  3N  1   0G  300.000  5000.000 1989.000    01
3.54660554E+00 8.47103210E-03-3.04591759E-06 4.90433705E-10-2.92171362E-14    2
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 9.19732680E+03 4.50208767E+00 2.39573312E+00 7.54972939E-03 1.84802753E-06    3
-3.27784212E-09 8.18892068E-13 9.93639182E+03 1.19607859E+01                   4
H2CNNO2          41687H  2C  1N  2O  2G  300.000  5000.000 1398.000    01
 1.03454548E+01 7.36086379E-03-2.54324138E-06 3.97561755E-10-2.31770715E-14    2
 1.25596874E+04-2.63387892E+01 1.30191521E+00 3.20731783E-02-2.90975481E-05    3
 1.35162740E-08-2.49722040E-12 1.53529030E+04 2.09774721E+01                   4
H2O              20387H  2O  1   0   0G  300.000  5000.000 1400.000    01
 2.84320234E+00 3.20572219E-03-1.03211054E-06 1.53282024E-10-8.60392078E-15    2
-2.99952638E+04 5.77799501E+00 3.95351146E+00 1.97126594E-04 1.74735583E-06    3
-8.68805820E-10 1.10773628E-13-3.02903531E+04 4.30394008E-02                   4
H2O2             120186H  2O  2   0   0G  300.000  5000.000 1415.000    01
 4.97596591E+00 3.77082472E-03-1.19453599E-06 1.75667533E-10-9.80008474E-15    2
-1.82131265E+04-1.83431177E+00 3.07292451E+00 9.02282736E-03-6.85279987E-06    3
 2.95715103E-09-5.28595494E-13-1.76336933E+04 8.09817456E+00                   4
H2S              121286H  2S  1   0   0G  300.000  5000.000 1682.000    01
 3.35560772E+00 3.26113369E-03-1.17070497E-06 1.88226178E-10-1.11998476E-14    2
-3.67804332E+03 4.55164634E+00 3.91615125E+00-6.65453137E-05 3.93190829E-06    3
-2.77356996E-09 5.75349811E-13-3.66020038E+03 2.29157895E+00                   4
H2SINH3          121386SI 1H  5N  1   0G  300.000  5000.000 1406.000    01
 7.71930068E+00 8.58444193E-03-2.75260067E-06 4.08837040E-10-2.29899579E-14    2
 8.66424030E+03-1.42451124E+01 2.26538259E+00 2.18173760E-02-1.49754575E-05    3
 5.50601435E-09-8.30661509E-13 1.04847333E+04 1.48300742E+01                   4
H2SISIH2         121386SI 2H  4   0   0G  300.000  5000.000 1362.000    01
 9.81259576E+00 5.51908293E-03-1.96575268E-06 3.13577079E-10-1.85402211E-14    2
 3.04474822E+04-2.56115036E+01 4.65406636E+00 1.50156117E-02-7.44714586E-06    3
 1.08103482E-09 1.13225139E-13 3.24977785E+04 3.00624251E+00                   4
H3SISIH3         121386SI 2H  6   0   0G  300.000  5000.000 1475.000    01
 1.17266900E+01 9.27711627E-03-3.33006433E-06 5.33962293E-10-3.16839610E-14    2
 4.12053564E+03-3.85033397E+01 4.50244244E+00 1.63739156E-02 2.45743672E-06    3
-8.01643678E-09 2.41977435E-12 7.56046096E+03 3.68957265E+00                   4
HCCO             32387H  1C  2O  1   0G  300.000  5000.000 1394.000    01
 6.46186812E+00 2.97631506E-03-1.09718076E-06 1.92367955E-10-1.23023748E-14    2
 1.90472084E+04-7.64444624E+00 4.31669952E+00 8.34124371E-03-6.33308216E-06    3
 2.55353271E-09-4.24098750E-13 1.97572055E+04 3.75173794E+00                   4
HCCOH            32387H  2C  2O  1   0G  300.000  5000.000 1682.000    01
 6.76401777E+00 5.57934916E-03-2.00918721E-06 3.24227308E-10-1.93578450E-14    2
 7.58768714E+03-1.15409698E+01 3.69263978E+00 1.14114965E-02-5.36249378E-06    3
 7.70758245E-10 5.85674907E-14 8.71949281E+03 5.34199914E+00                   4
HCN              121286H  1C  1N  1   0G  300.000  5000.000 1394.000    01
 4.17832212E+00 2.72588988E-03-9.18977922E-07 1.41208785E-10-8.13109382E-15    2
 1.47110246E+04-6.87213613E-01 2.93991835E+00 5.63922898E-03-3.72053635E-06    3
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 1.44921345E-09-2.52264438E-13 1.51586052E+04 5.98899612E+00              4
HCNH          41687C  1H  2N  1   0G  300.000  5000.000 1378.000   01
 4.78769793E+00 4.43394016E-03-1.53172679E-06 2.39382982E-10-1.39521547E-14   2
 3.12045794E+04-1.32572456E+00 2.33974837E+00 8.54024037E-03-3.37863657E-06   3
 1.26873722E-10 1.49923928E-13 3.22286419E+04 1.24144662E+01              4
HCNO          120186H  1C  1N  1O  1G  300.000  5000.000 1392.000   01
 7.06632520E+00 2.61382968E-03-9.30612430E-07 1.48436186E-10-8.77637859E-15   2
 1.66023344E+04-1.50345257E+01 2.67776550E+00 1.36951228E-02-1.17253453E-05   3
 4.95424900E-09-8.29764191E-13 1.80278275E+04 8.21498928E+00              4
HCO           121286H  1C  1O  1   0G  300.000  5000.000 1367.000   01
 3.76230764E+00 3.12438324E-03-1.06638030E-06 1.65248642E-10-9.57245663E-15   2
 3.79782609E+03 4.33652045E+00 3.49156127E+00 2.12295493E-03 1.50847283E-06   3
-1.61023278E-09 3.80907139E-13 4.08832874E+03 6.42549568E+00              4
HCO+          121286H  1C  1O  1E -1G  300.000  5000.000 1391.000   01
 4.14002984E+00 2.67478901E-03-8.43649800E-07 1.23153635E-10-6.83155157E-15   2
 9.87257892E+04-1.97043195E-01 3.15265127E+00 4.85291729E-03-2.69482804E-06   3
 8.52706574E-10-1.20118416E-13 9.90879604E+04 5.16203108E+00              4
HE            120186HE 1   0   0   0G  300.000  5000.000 1000.000   01
 2.50104422E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00   2
-7.45686320E+02 9.08589239E-01 2.50104422E+00 0.00000000E+00 0.00000000E+00   3
 0.00000000E+00 0.00000000E+00-7.45686320E+02 9.08589239E-01              4
HE+           120186HE 1E -1   0   0G  300.000  5000.000 1000.000   01
 2.50104422E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00   2
 2.85394225E+05 1.60310359E+00 2.50104422E+00 0.00000000E+00 0.00000000E+00   3
 0.00000000E+00 0.00000000E+00 2.85394225E+05 1.60310359E+00              4
HF            121286H  1F  1   0   0G  300.000  5000.000 1375.000   01
 2.86310069E+00 9.98169571E-04-2.76803196E-07 3.40214883E-11-1.54559489E-15   2
-3.35765129E+04 4.52136056E+00 3.52838453E+00-3.06781216E-04 6.30735277E-07   3
-2.23855996E-10 2.18371271E-14-3.38366484E+04 8.52845426E-01              4
HNCO           31287H  1N  1C  1O  1G  300.000  5000.000 1372.000   01
 6.11028139E+00 3.37624017E-03-1.18200022E-06 1.86416756E-10-1.09353111E-14   2
-1.49465579E+04-7.97883695E+00 3.45489519E+00 8.30220158E-03-4.06808973E-06   3
 6.14756565E-10 5.21308909E-14-1.38958364E+04 6.73706953E+00              4
HNO           121286H  1N  1O  1   0G  300.000  5000.000 1363.000   01
 4.04798680E+00 2.51948532E-03-8.71913867E-07 1.36402556E-10-7.95485215E-15   2
 1.04589897E+04 2.35610853E+00 3.44741798E+00 2.42807408E-03 8.32354492E-07   3
-1.29920153E-09 3.38048223E-13 1.08371424E+04 6.14538089E+00              4
HNO3          121286H  1N  1O  3   0G  300.000  5000.000 1400.000   01
 8.69610538E+00 3.73161528E-03-1.30923515E-06 2.07062833E-10-1.21786399E-14   2
-1.97553000E+04-2.03835293E+01 1.33760471E+00 2.22171403E-02-1.89148142E-05   3
 7.74004709E-09-1.23168104E-12-1.73889001E+04 1.85778966E+01              4
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HO2             20387H  1O  2   0   0G  300.000 5000.000 1383.000   01
 4.06240582E+00 2.44692472E-03-8.33284067E-07 1.28936188E-10-7.46135551E-15   2
-2.29509945E+02 3.35875090E+00 3.32486530E+00 3.33930460E-03-7.70146036E-07   3
-2.73221789E-10 1.14573029E-13 1.25738135E+02 7.64109911E+00                 4
HOCN            120186H  1O  1C  1N  1G  300.000 5000.000 1395.000   01
 5.38887279E+00 3.34045663E-03-1.22726864E-06 2.16968719E-10-1.40345949E-14   2
-3.19465381E+03-2.45650006E+00 2.99533645E+00 9.28681871E-03-6.99919245E-06   3
 2.81002170E-09-4.65236554E-13-2.39678404E+03 1.02759562E+01                 4
HONO            31787H  1N  1O  2   0G  300.000 5000.000 1402.000   01
 6.47878463E+00 2.87527131E-03-9.70243817E-07 1.49507164E-10-8.63624735E-15   2
-1.17529956E+04-8.74585245E+00 2.25983596E+00 1.38168659E-02-1.18507203E-05   3
 5.05465084E-09-8.50316937E-13-1.04227687E+04 1.34835850E+01                 4
HSICL           121986SI 1H  1CL 1   0G  300.000 5000.000 1391.000   01
 5.48836809E+00 1.33860238E-03-4.74724212E-07 7.55221578E-11-4.45713461E-15   2
 6.61598320E+03-2.06731773E+00 3.45346080E+00 6.43184587E-03-5.40382878E-06   3
 2.26200017E-09-3.77689189E-13 7.28353744E+03 8.73255034E+00                 4
I*C3H7          120186C  3H  7   0   0G  300.000 5000.000 1384.000   01
 9.57508960E+00 1.44778776E-02-4.75253418E-06 7.18004504E-10-4.08832662E-14   2
 4.37901197E+03-3.11540804E+01 8.33463843E-01 3.28536474E-02-1.86310084E-05   3
 5.06956115E-09-4.88623857E-13 7.60561465E+03 1.64968781E+01                 4
N               120186N  1   0   0   0G  300.000 5000.000 1000.000   01
 2.50104422E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00   2
 5.61088686E+04 4.17481976E+00 2.50104422E+00 0.00000000E+00 0.00000000E+00   3
 0.00000000E+00 0.00000000E+00 5.61088686E+04 4.17481976E+00                 4
N*C3H7          120186C  3H  7   0   0G  300.000 5000.000 1385.000   01
 9.43768625E+00 1.45204271E-02-4.75103054E-06 7.16099879E-10-4.07052195E-14   2
 6.68128400E+03-2.82534485E+01 1.04207340E+00 3.21326586E-02-1.80109063E-05   3
 4.85038921E-09-4.60754609E-13 9.78479840E+03 1.75257707E+01                 4
N2              121286N  2   0   0   0G  300.000 5000.000 1471.000   01
 3.09006692E+00 1.10067175E-03-3.09545765E-07 3.87477136E-11-1.78076873E-15   2
-9.55841328E+02 5.14097547E+00 3.22491438E+00 7.32462027E-04 6.12092935E-08   3
-1.25644770E-10 2.55131910E-14-9.94368295E+02 4.44041983E+00                 4
N2H2            121286N  2H  2   0   0G  300.000 5000.000 1386.000   01
 4.12536220E+00 4.86477025E-03-1.65044979E-06 2.54741717E-10-1.47161586E-14   2
 2.38199582E+04 6.62833553E-01 2.46629942E+00 7.06523406E-03-1.77203926E-06   3
-5.53951687E-10 2.55166285E-13 2.45837831E+04 1.02004650E+01                 4
N2H3            120186N  2H  3   0   0G  300.000 5000.000 1379.000   01
 5.64262924E+00 5.85977019E-03-1.94196938E-06 2.95376897E-10-1.69009253E-14   2
 1.60021649E+04-7.53473812E+00 1.95702173E+00 1.31303297E-02-6.74723751E-06   3
 1.37561198E-09-2.66849181E-14 1.74051676E+04 1.27163733E+01                 4
N2H4            121286N  2H  4   0   0G  300.000 5000.000 1412.000   01
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6.30066655E+00 7.57120861E-03-2.46758565E-06 3.70428040E-10-2.09803008E-14    2
8.70731371E+03-1.05557951E+01 8.50661271E-01 2.26904838E-02-1.88360641E-05    3
8.45396640E-09-1.53553148E-12 1.03578405E+04 1.78602483E+01                   4
N2O             121286N  2O  1   0   0G  300.000  5000.000 1404.000    01
5.75893487E+00 1.14883857E-03-4.18874485E-07 6.78654455E-11-4.05615211E-15    2
7.75660662E+03-7.43882557E+00 2.68876907E+00 8.93519553E-03-7.89562220E-06    3
3.28782094E-09-5.27800680E-13 8.73386065E+03 8.78628553E+00                   4
N2O+            121286N  2O  1E -1   0G  300.000  5000.000 1391.000    01
5.61139420E+00 1.83650930E-03-6.55253461E-07 1.05508184E-10-6.24134890E-15    2
1.58403739E+05-4.92788898E+00 3.37630581E+00 7.57488573E-03-6.39974088E-06    3
2.75394943E-09-4.76404517E-13 1.59125714E+05 6.88857610E+00                   4
N2O4            121286N  2O  4   0   0G  300.000  5000.000 1396.000    01
1.20628315E+01 3.60914385E-03-1.30799705E-06 2.11083132E-10-1.25815721E-14    2
-3.62784647E+03-3.52252896E+01 3.40668821E+00 2.59376905E-02-2.33639790E-05    3
1.00840604E-08-1.69546797E-12-8.89163041E+02 1.04224404E+01                   4
N3              121286N  3   0   0   0G  300.000  5000.000 1412.000    01
6.11405659E+00 8.33418973E-04-3.06893010E-07 5.00452485E-11-3.00445061E-15    2
4.76334798E+04-8.59659140E+00 2.21317577E+00 1.21947363E-02-1.29405878E-05    3
6.35040106E-09-1.18275506E-12 4.87343825E+04 1.15077650E+01                   4
NCO             121286N  1C  1O  1   0G  300.000  5000.000 1384.000    01
5.60992166E+00 1.70316738E-03-6.10638960E-07 9.78445603E-11-5.80324488E-15    2
1.70774358E+04-5.26448546E+00 2.87969870E+00 8.17952622E-03-6.43973961E-06    3
2.46619201E-09-3.72697037E-13 1.80046957E+04 9.34560895E+00                   4
NF              121286N  1F  1   0   0G  300.000  5000.000 1391.000    01
3.88372393E+00 7.18121408E-04-2.56895127E-07 4.10525266E-11-2.39854697E-15    2
2.86533685E+04 3.32232207E+00 2.95616709E+00 3.11428599E-03-2.66978049E-06    3
1.15908460E-09-2.01653227E-13 2.89512636E+04 8.22049039E+00                   4
NFO             121286N  1F  1O  1   0G  300.000  5000.000 1390.000    01
5.64513976E+00 1.22175559E-03-4.38271747E-07 7.02532026E-11-4.16799625E-15    2
-9.90463516E+03-3.24244294E+00 3.42933312E+00 6.70262706E-03-5.62387285E-06    3
2.29764554E-09-3.69942033E-13-9.17640471E+03 8.53200296E+00                   4
NFO2            121286N  1F  1O  2   0G  300.000  5000.000 1402.000    01
7.87426561E+00 1.96845915E-03-7.17872338E-07 1.16325669E-10-6.95320870E-15    2
-1.61208614E+04-1.54269487E+01 2.24667004E+00 1.67668160E-02-1.55875147E-05    3
6.86560397E-09-1.16944008E-12-1.43754311E+04 1.41382965E+01                   4
NH              31387H  1N  1   0   0G  300.000  5000.000 1372.000    01
2.81165100E+00 1.22460674E-03-3.35793661E-07 4.05930391E-11-1.79431440E-15    2
4.20992331E+04 5.62767540E+00 3.44760661E+00-9.51253674E-05 6.67063814E-07    3
-2.90265714E-10 3.81228377E-14 4.18597637E+04 2.14977565E+00                   4
NH2             121686N  1H  2   0   0G  300.000  5000.000 1394.000    01
2.80244385E+00 3.23587132E-03-1.04228998E-06 1.54908105E-10-8.70197553E-15    2
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 2.19672731E+04 6.63812110E+00 4.01147338E+00-8.54676731E-04 3.83315819E-06    3
-2.32709872E-09 4.52740499E-13 2.17113292E+04 6.55504126E-01                   4
NH3             121386N   1H   3    0    0G   300.000  5000.000 1393.000    01
 2.88401620E+00 5.61845443E-03-1.84299804E-06 2.77697455E-10-1.57630379E-14    2
-6.73754554E+03 4.93609532E+00 3.22106025E+00 3.12440632E-03 2.02973866E-06    3
-1.96738410E-09 4.33304888E-13-6.63436383E+03 3.81307481E+00                   4
NNH             120186N   2H   1    0    0G   300.000  5000.000 1673.000    01
 3.83345954E+00 2.89820985E-03-1.05617909E-06 1.71573121E-10-1.02840840E-14    2
 2.80801005E+04 4.04297348E+00 3.62763978E+00 1.71709968E-03 1.84965500E-06    3
-1.81393008E-09 4.16825495E-13 2.83107768E+04 5.74264700E+00                   4
NO              121286N   1O   1    0    0G   300.000  5000.000 1396.000    01
 3.31829398E+00 1.03282725E-03-3.17366453E-07 4.49838124E-11-2.43402742E-15    2
 9.80114999E+03 6.08542540E+00 3.17431678E+00 1.30123532E-03-4.97570920E-07    3
 9.68205318E-11-7.84724696E-15 9.86054400E+03 6.88704370E+00                   4
NO+             121286N   1O   1E  -1    0G   300.000  5000.000 1000.000    01
 3.72892106E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 1.18012531E+05 2.58400612E+00 3.72892106E+00 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00 1.18012531E+05 2.58400612E+00                   4
NO2             121286N   1O   2    0    0G   300.000  5000.000 1376.000    01
 5.18921030E+00 1.63332102E-03-5.85954270E-07 9.39268692E-11-5.57242103E-15    2
 2.02933492E+03-1.87198794E+00 2.81322111E+00 6.80728201E-03-4.64695332E-06    3
 1.42597021E-09-1.51945923E-13 2.87786077E+03 1.09986609E+01                   4
NO2-            121286N   1O   2E   1    0G   300.000  5000.000 1610.000    01
 5.48778063E-01 8.40841370E-03-2.81868964E-06 4.18153169E-10-2.30446901E-14    2
-2.43208747E+04 2.41646552E+01 4.99260404E+00-1.82821007E-03 5.87419015E-06    3
-2.80835281E-09 4.18906014E-13-2.58373249E+04 3.12055713E-01                   4
NO3             121286N   1O   3    0    0G   300.000  5000.000 1409.000    01
 8.03583058E+00 1.84099258E-03-6.76345091E-07 1.10120919E-10-6.60388373E-15    2
 5.40876480E+03-1.73920709E+01 1.07286714E+00 2.12025782E-02-2.12733090E-05    3
 9.98273496E-09-1.79357527E-12 7.46241506E+03 1.88140853E+01                   4
O               120186O   1    0    0    0G   300.000  5000.000 1000.000    01
 2.55136704E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 2.92191793E+04 4.82418517E+00 2.55136704E+00 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00 2.92191793E+04 4.82418517E+00                   4
O2              121386O   2    0    0    0G   300.000  5000.000 1390.000    01
 3.48109611E+00 9.99067738E-04-3.24728392E-07 4.86062193E-11-2.74625923E-15    2
-1.15525954E+03 4.39116770E+00 2.95105720E+00 2.21573057E-03-1.40755610E-06    3
 4.96079626E-10-7.52714994E-14-9.66849074E+02 7.24909825E+00                   4
O3              121286O   3    0    0    0G   300.000  5000.000 1402.000    01
 5.75832010E+00 1.14061118E-03-4.13926466E-07 6.68593556E-11-3.98766911E-15    2
 1.50688782E+04-5.10369430E+00 2.64921217E+00 9.45221093E-03-8.94343703E-06    3
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 4.03189592E-09-7.04073707E-13 1.60229456E+04 1.11877476E+01              4
OH            121286O  1H  1   0   0G  300.000  5000.000 1373.000   01
 2.92839217E+00 9.87703626E-04-2.63977772E-07 3.07418124E-11-1.28570098E-15   2
 3.86986656E+03 5.30847884E+00 3.50622498E+00-1.80633740E-04 5.89643444E-07   3
-2.34045359E-10 2.75434552E-14 3.64837598E+03 2.13614879E+00              4
S             121286S  1   0   0   0G  300.000  5000.000 1000.000   01
 2.68723866E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00   2
 3.25254231E+04 4.86534294E+00 2.68723866E+00 0.00000000E+00 0.00000000E+00   3
 0.00000000E+00 0.00000000E+00 3.25254231E+04 4.86534294E+00              4
S(L)          120186S  1   0   0   0L  300.000  5000.000 1000.000   01
 3.83963127E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00   2
-9.23346683E+02-1.74629814E+01 3.83963127E+00 0.00000000E+00 0.00000000E+00   3
 0.00000000E+00 0.00000000E+00-9.23346683E+02-1.74629814E+01              4
S(S)          120186S  1   0   0   0S  300.000  5000.000 1000.000   01
 2.72246464E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00   2
-8.11702815E+02-1.16715458E+01 2.72246464E+00 0.00000000E+00 0.00000000E+00   3
 0.00000000E+00 0.00000000E+00-8.11702815E+02-1.16715458E+01              4
S2            121386S  1   0   0   0G  300.000  5000.000 1000.000   01
 4.29756895E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00   2
 1.41741404E+04 2.94750209E+00 4.29756895E+00 0.00000000E+00 0.00000000E+00   3
 0.00000000E+00 0.00000000E+00 1.41741404E+04 2.94750209E+00              4
SH            121286S  1H  1   0   0G  300.000  5000.000 1401.000   01
 3.25746777E+00 9.49222158E-04-2.84408332E-07 3.94121834E-11-2.09336961E-15   2
 1.57343324E+04 4.66089227E+00 3.20037150E+00 1.02848004E-03-3.07528792E-07   3
 3.13617006E-11 1.42965730E-15 1.57616841E+04 4.99018760E+00              4
SICL          121986SI 1CL 1   0   0G  300.000  5000.000 1396.000   01
 4.63084425E+00-2.79737560E-04 1.76437091E-07-4.05752026E-11 3.06069863E-15   2
 1.75932399E+04 2.05737220E+00 3.75363739E+00 1.97603270E-03-2.14975159E-06   3
 1.08601704E-09-2.08502601E-13 1.78839507E+04 6.70637408E+00              4
SICL2         121986SI 1CL 2   0   0G  300.000  5000.000 1402.000   01
 6.77027737E+00 2.17484839E-04-8.04053338E-08 1.31464694E-11-7.90698739E-16   2
-2.24332721E+04-5.09106461E+00 4.58113497E+00 7.78501466E-03-9.82854322E-06   3
 5.49344366E-09-1.12980978E-12-2.19172052E+04 5.79787939E+00              4
SICL2H2       121986SI 1H  2CL 2   0G  300.000  5000.000 1403.000   01
 9.21075505E+00 3.29810809E-03-1.15737752E-06 1.82875539E-10-1.07432540E-14   2
-4.10339292E+04-2.03745474E+01 2.78431434E+00 2.11938706E-02-2.04623858E-05   3
 9.64524890E-09-1.76913777E-12-3.91133611E+04 1.30787369E+01              4
SICL3         121986SI 1CL 3   0   0G  300.000  5000.000 1403.000   01
 9.57123790E+00 4.05644556E-04-1.49906284E-07 2.45033359E-11-1.47348287E-15   2
-4.16004308E+04-1.71561933E+01 5.72937839E+00 1.35538084E-02-1.69583296E-05   3
 9.42124651E-09-1.92938124E-12-4.06838048E+04 1.99661199E+00              4
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SICL3H        121986SI 1H  1CL 3   0G  300.000 5000.000 1407.000   01
 1.13439464E+01 1.54274453E-03-5.64745917E-07 9.17423488E-11-5.49335660E-15   2
-6.37030238E+04-2.85906846E+01 5.21048589E+00 1.92106596E-02-2.00727321E-05   3
 9.78484168E-09-1.81848962E-12-6.19465347E+04 3.09949291E+00                 4
SICL4         121986SI 1CL 4   0   0G  300.000 5000.000 1403.000   01
 1.23717384E+01 5.94124918E-04-2.19499743E-07 3.58725447E-11-2.15689389E-15   2
-8.37645766E+04-3.15779863E+01 6.97082108E+00 1.89461519E-02-2.35515155E-05   3
 1.30262364E-08-2.65926544E-12-8.24650923E+04-4.60993947E+00                 4
SICLH3        121986SI 1H  3CL 1   0G  300.000 5000.000 1390.000   01
 7.71806931E+00 4.63674248E-03-1.63520476E-06 2.59165320E-10-1.52553023E-14   2
-1.94691807E+04-1.68009517E+01 1.61857228E+00 1.96175133E-02-1.58768554E-05   3
 6.48317140E-09-1.06607917E-12-1.74318868E+04 1.56852579E+01                 4
SIH           121986SI 1H  1   0   0G  300.000 5000.000 1396.000   01
 3.24539314E+00 1.05662736E-03-3.24672487E-07 4.60186038E-11-2.48960566E-15   2
 4.51203808E+04 3.39694332E+00 3.09552390E+00 1.33740168E-03-5.14752770E-07   3
 1.01484343E-10-8.42865557E-15 4.51820181E+04 4.23079604E+00                 4
SIH2          121386SI 1H  2   0   0G  300.000 5000.000 1482.000   01
 4.40997134E+00 2.30252771E-03-8.18278043E-07 1.30332833E-10-7.69756100E-15   2
 3.26564378E+04-1.48569301E+00 3.50947271E+00 1.78509270E-03 2.77260682E-06   3
-2.88401975E-09 7.36969491E-13 3.32336249E+04 4.28493197E+00                 4
SIH2CL        121986SI 1H  2CL 1   0G  300.000 5000.000 1392.000   01
 6.68870392E+00 2.89910899E-03-1.02073510E-06 1.61605748E-10-9.50575820E-15   2
 1.32414095E+03-8.59396116E+00 2.67611483E+00 1.30177545E-02-1.09315408E-05   3
 4.62550413E-09-7.84285824E-13 2.63684269E+03 1.26817551E+01                 4
SIH3          121386SI 1H  3   0   0G  300.000 5000.000 2016.000   01
 4.91614504E+00 4.70744744E-03-1.72912148E-06 2.82440238E-10-1.69965414E-14   2
 2.17378707E+04-4.06657447E+00 2.56538744E+00 8.83918626E-03-3.66665779E-06   3
 2.39433612E-10 1.19113611E-13 2.26436230E+04 8.98315827E+00                 4
SIH3NH2       121386SI 1H  5N  1   0G  300.000 5000.000 1393.000   01
 8.85288883E+00 8.03423438E-03-2.91814981E-06 4.93621750E-10-3.06888156E-14   2
-1.13982422E+04-2.16291690E+01 9.46890136E-01 2.81638387E-02-2.29156654E-05   3
 9.65502643E-09-1.64912767E-12-8.82353108E+03 2.02345255E+01                 4
SIH4          121386SI 1H  4   0   0G  300.000 5000.000 2026.000   01
 5.73008982E+00 6.77249413E-03-2.49806517E-06 4.09241007E-10-2.46793586E-14   2
 1.45759727E+03-1.13248618E+01 1.20261327E+00 1.58890483E-02-8.50862557E-06   3
 1.77524339E-09-6.21346674E-14 3.08341413E+03 1.33832596E+01                 4
SIHCL2        121986SI 1H  1CL 2   0G  300.000 5000.000 1399.000   01
 7.65363370E+00 2.05043477E-03-7.21191278E-07 1.14113377E-10-6.70976943E-15   2
-2.00114154E+04-9.61760347E+00 3.93566274E+00 1.23717510E-02-1.18754903E-05   3
 5.61142155E-09-1.03595577E-12-1.88911888E+04 9.75787768E+00                 4
SN            121286S  1N  1   0   0G  300.000 5000.000 1390.000   01
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 3.89798242E+00 6.31279451E-04-2.16999939E-07 3.37708997E-11-1.94972616E-15    2
 3.04461123E+04 4.15001810E+00 3.29541748E+00 2.11848642E-03-1.64837344E-06    3
 6.71128268E-10-1.11995649E-13 3.06477236E+04 7.35851114E+00                   4
SO            121286S  1O  1   0   0G  300.000  5000.000 1390.000    01
 3.75878573E+00 8.50694004E-04-2.89265332E-07 4.48229083E-11-2.58804080E-15    2
-6.47076349E+02 4.82778708E+00 3.02820510E+00 2.63044758E-03-1.97919206E-06    3
 7.88054392E-10-1.29619928E-13-3.99859065E+02 8.72694577E+00                   4
SO2           121286S  1O  2   0   0G  300.000  5000.000 1401.000    01
 5.86421731E+00 1.04258812E-03-3.78185254E-07 6.10682966E-11-3.64153312E-15    2
-3.78031051E+04-4.50481781E+00 2.95891547E+00 8.94704098E-03-8.65823042E-06    3
 3.99420119E-09-7.12875654E-13-3.69230595E+04 1.06737028E+01                   4
SO3           121286S  1O  3   0   0G  300.000  5000.000 1405.000    01
 7.95068457E+00 1.89875954E-03-6.92700907E-07 1.12273628E-10-6.71212482E-15    2
-5.06582593E+04-1.62412490E+01 2.40564312E+00 1.64934130E-02-1.53516672E-05    3
 6.75464382E-09-1.14763548E-12-4.89419933E+04 1.28817538E+01                   4
NH2OH        B/JB189 N  1H  3O  1   0G  300.000  2000.000 1000.000    01
 4.70580719E+00-2.26531112E-03 2.21933248E-05-2.23621560E-08 6.84881804E-12    2
-5.98691011E+03 3.33801919E+00 4.70580719E+00-2.26531112E-03 2.21933248E-05    3
-2.23621560E-08 6.84881804E-12-5.98691011E+03 3.33801919E+00                   4
NH2O       M/JB86    N  1H  2O  1   0G  300.000  2000.000 1000.000    01
 2.87075695E+00 3.98444067E-03 3.23180309E-06-3.34730599E-09 7.44482418E-13    2
 6.94671208E+03 1.08302682E+01 2.87075695E+00 3.98444067E-03 3.23180309E-06    3
-3.34730599E-09 7.44482418E-13 6.94671208E+03 1.08302682E+01                   4
HNNOHC     JB5-86    N  2H  2O  1   0G  300.000  2000.000 1000.000    01
 2.26720691E-01 2.54796682E-02-2.58417386E-05 1.50031100E-08-3.72624531E-12    2
 1.13304783E+04 2.22053283E+01 2.26720691E-01 2.54796682E-02-2.58417386E-05    3
 1.50031100E-08-3.72624531E-12 1.13304783E+04 2.22053283E+01                   4
HNNOHT     JB5-86    N  2H  2O  1   0G  300.000  2000.000 1000.000    01
-1.80487731E+00 3.61312975E-02-4.18245008E-05 2.43906600E-08-5.63396598E-12    2
 1.04791264E+04 3.11252668E+01-1.80487731E+00 3.61312975E-02-4.18245008E-05    3
 2.43906600E-08-5.63396598E-12 1.04791264E+04 3.11252668E+01                   4
HNNOH      JB5-86    N  2H  2O  1   0G  300.000  2000.000 1000.000    01
-1.57378102E-01 2.81911406E-02-3.01947602E-05 1.76488514E-08-4.28094788E-12    2
 1.08043745E+04 2.44409912E+01-1.57378102E-01 2.81911406E-02-3.01947602E-05    3
 1.76488514E-08-4.28094788E-12 1.08043745E+04 2.44409912E+01                   4
CH3O2         121686C  1H  3O  2   0G  300.000  2000.000 1000.000    01
 5.33796421E+00-1.76044643E-03 2.85973381E-05-2.82899040E-08 8.32514182E-12    2
 4.75018059E+01 1.40387985E+00 5.33796421E+00-1.76044643E-03 2.85973381E-05    3
-2.82899040E-08 8.32514182E-12 4.75018059E+01 1.40387985E+00                   4
NH2NO      M/JB189 N  2H  2O  1   0G  300.000  2000.000 1000.000    01
 1.07826681E+00 2.20375076E-02-2.10921999E-05 1.23738567E-08-3.22969585E-12    2
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 7.87099242E+03 1.89257641E+01 1.07826681E+00 2.20375076E-02-2.10921999E-05    3
 1.23738567E-08-3.22969585E-12 7.87099242E+03 1.89257641E+01                   4
C2H5OH    5/18/90 THERMC  2H  6O  1   0G  300.000  5000.000 1375.000   01
 8.37039899E+00 1.35074846E-02-4.53599690E-06 6.96181476E-10-4.00872039E-14    2
-3.27080102E+04-2.05450485E+01 1.97328240E-01 2.93248516E-02-1.49681169E-05    3
 3.19689404E-09-1.38940752E-13-2.95200856E+04 2.45493813E+01                   4
C2H5O     5/18/90 THERMC  2H  5O  1   0G  300.000  5000.000 1376.000   01
 7.87619733E+00 1.15189494E-02-3.87916875E-06 5.96552017E-10-3.43992098E-14    2
-6.20061110E+03-1.82237108E+01 1.71469722E-01 2.69508994E-02-1.46965861E-05    3
 3.56930070E-09-2.55633385E-13-3.25996605E+03 2.40808731E+01                   4
CH2N      Sch3o-1CPch2oC  1H  2N  1   0G  300.000  5000.000 1681.000   01
 3.33593366E+00 5.91890317E-03-2.11566694E-06 3.39266108E-10-2.01530700E-14    2
 2.82250021E+04 5.79640396E+00 2.80503095E+00 4.58949789E-03 1.95605764E-06    3
-2.57411553E-09 6.18397800E-13 2.86502750E+04 9.55962511E+00                   4
CL                CL 1   0   0   0G  300.000  5000.000 1000.000   01
 2.66710953E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00    2
 1.37493409E+04 4.68310055E+00 2.66710953E+00 0.00000000E+00 0.00000000E+00    3
 0.00000000E+00 0.00000000E+00 1.37493409E+04 4.68310055E+00                   4
HCL                  0H  1CL 1   0G  300.000  5000.000 1353.000   01
 2.88267596E+00 1.15483695E-03-3.11781543E-07 3.67661128E-11-1.55941326E-15    2
-1.19172528E+04 5.82197313E+00 3.32303253E+00 1.79985358E-04 4.91728701E-07    3
-2.57409343E-10 3.91190799E-14-1.20745838E+04 3.43927774E+00                   4
CL2               CL 2   0   0   0G  300.000  5000.000 1390.000   01
 4.16121067E+00 4.91269585E-04-1.65113435E-07 2.52394058E-11-1.44417423E-15    2
-1.31106455E+03 2.87209029E+00 3.78856058E+00 1.38207012E-03-9.94173684E-07    3
 3.83086387E-10-6.16574535E-14-1.18293247E+03 4.86752923E+00                   4
CHCL              C  1H  1CL 1   0G  300.000  2000.000 1000.000   01
 2.37536795E+00 1.01754596E-02-1.52631760E-05 1.39527921E-08-4.54298319E-12    2
 3.46912633E+04 1.22399880E+01 2.37536795E+00 1.01754596E-02-1.52631760E-05    3
 1.39527921E-08-4.54298319E-12 3.46912633E+04 1.22399880E+01                   4
CH2CL             C  1H  2CL 1   0G  300.000  2000.000 1000.000   01
 3.18383529E+00 5.37444984E-03-2.51703540E-06 3.70727486E-09-1.75691015E-12    2
 1.19629839E+04 1.03450240E+01 3.18383529E+00 5.37444984E-03-2.51703540E-06    3
 3.70727486E-09-1.75691015E-12 1.19629839E+04 1.03450240E+01                   4
CCL2              C  1   0CL 2   0G  300.000  2000.000 1000.000   01
 2.46317229E+00 1.61088661E-02-2.45197559E-05 1.75803583E-08-4.55214607E-12    2
 2.49540872E+04 6.76677259E+00 2.46317229E+00 1.61088661E-02-2.45197559E-05    3
 1.75803583E-08-4.55214607E-12 2.49540872E+04 6.76677259E+00                   4
CHCL2             C  1H  1CL 2   0G  300.000  2000.000 1000.000   01
 3.46911778E+00 1.65978612E-02-2.75878746E-05 2.39707377E-08-7.35694606E-12    2
 1.02546749E+04 1.02452164E+01 3.46911778E+00 1.65978612E-02-2.75878746E-05    3
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2.39707377E-08-7.35694606E-12 1.02546749E+04 1.02452164E+01 4
CCL3 C 1 0CL 3 0G 300.000 2000.000 1000.000 01
2.39672944E+00 2.79857026E-02-4.40850698E-05 3.18165970E-08-8.44662348E-12 2
7.93429344E+03 1.54378287E+01 2.39672944E+00 2.79857026E-02-4.40850698E-05 3
3.18165970E-08-8.44662348E-12 7.93429344E+03 1.54378287E+01 4
CCL4 C 1 0CL 4 0G 300.000 2000.000 1000.000 01
2.80093383E+00 3.86214265E-02-6.12505069E-05 4.40455483E-08-1.16058761E-11 2
-1.36170304E+04 1.22354135E+01 2.80093383E+00 3.86214265E-02-6.12505069E-05 3
4.40455483E-08-1.16058761E-11-1.36170304E+04 1.22354135E+01 4
CH3CL C 1H 3CL 1 0G 300.000 2000.000 1000.000 01
2.18917485E+00 8.26683373E-03 4.93302840E-06-9.14008576E-09 3.18724996E-12 2
-1.08609522E+04 1.31106595E+01 2.18917485E+00 8.26683373E-03 4.93302840E-06 3
-9.14008576E-09 3.18724996E-12-1.08609522E+04 1.31106595E+01 4
CH2CL2 C 1H 2CL 2 0G 300.000 2000.000 1000.000 01
2.12813700E+00 1.65229869E-02-1.14522223E-05 3.62692507E-09-3.67636728E-13 2
-1.27492982E+04 1.58971650E+01 2.12813700E+00 1.65229869E-02-1.14522223E-05 3
3.62692507E-09-3.67636728E-13-1.27492982E+04 1.58971650E+01 4
CHCL3 C 1H 1CL 3 0G 300.000 2000.000 1000.000 01
1.85582211E+00 2.96729961E-02-3.89295985E-05 2.50736353E-08-6.16754518E-12 2
-1.37540476E+04 1.76412503E+01 1.85582211E+00 2.96729961E-02-3.89295985E-05 3
2.50736353E-08-6.16754518E-12-1.37540476E+04 1.76412503E+01 4
C2HCL C 2H 1CL 1 0G 300.000 2000.000 1000.000 01
3.47050220E+00 1.50083393E-02-1.88298455E-05 1.22184989E-08-3.04130427E-12 2
2.20452689E+04 5.73685604E+00 3.47050220E+00 1.50083393E-02-1.88298455E-05 3
1.22184989E-08-3.04130427E-12 2.20452689E+04 5.73685604E+00 4
C2CL2 C 2 0CL 2 0G 300.000 2000.000 1000.000 01
4.26035055E+00 1.91979763E-02-2.99402259E-05 2.24320846E-08-6.19156376E-12 2
2.33134904E+04 3.86986121E+00 4.26035055E+00 1.91979763E-02-2.99402259E-05 3
2.24320846E-08-6.19156376E-12 2.33134904E+04 3.86986121E+00 4
C2H3CL C 2H 3CL 1 0G 300.000 2000.000 1000.000 01
1.54353504E+00 1.55064366E-02 4.65016919E-06-1.59061125E-08 6.30513129E-12 2
3.06543327E+03 1.82198534E+01 1.54353504E+00 1.55064366E-02 4.65016919E-06 3
-1.59061125E-08 6.30513129E-12 3.06543327E+03 1.82198534E+01 4
CH2CCL2 C 2H 2CL 2 0G 300.000 2000.000 1000.000 01
2.84156601E+00 2.04013529E-02-1.09882876E-05-6.80156527E-10 1.53539649E-12 2
-1.35432666E+03 1.30550456E+01 2.84156601E+00 2.04013529E-02-1.09882876E-05 3
-6.80156527E-10 1.53539649E-12-1.35432666E+03 1.30550456E+01 4
CHCLCHCL C 2H 2CL 2 0G 300.000 2000.000 1000.000 01
2.84156601E+00 2.04013529E-02-1.09882876E-05-6.80156527E-10 1.53539649E-12 2
-1.30399954E+03 1.30550456E+01 2.84156601E+00 2.04013529E-02-1.09882876E-05 3
-6.80156527E-10 1.53539649E-12-1.30399954E+03 1.30550456E+01 4

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CH2CCL            C  2H  2CL 1   0G  300.000 2000.000 1000.000   01
-3.20966882E-01 2.57907429E-02-2.23147408E-05 1.07542247E-08-2.16693243E-12   2
 2.95339486E+04 2.74610541E+01-3.20966882E-01 2.57907429E-02-2.23147408E-05   3
 1.07542247E-08-2.16693243E-12 2.95339486E+04 2.74610541E+01              4
C2H2CL            C  2H  2CL 1   0G  300.000 2000.000 1000.000   01
-3.20966882E-01 2.57907429E-02-2.23147408E-05 1.07542247E-08-2.16693243E-12   2
 2.95339486E+04 2.74610541E+01-3.20966882E-01 2.57907429E-02-2.23147408E-05   3
 1.07542247E-08-2.16693243E-12 2.95339486E+04 2.74610541E+01              4
CCL2CH            C  2H  1CL 2   0G  300.000 2000.000 1000.000   01
 7.68917671E-01 3.97793060E-02-5.35819557E-05 3.57479121E-08-9.11589525E-12   2
 2.77101872E+04 2.04776803E+01 7.68917671E-01 3.97793060E-02-5.35819557E-05   3
 3.57479121E-08-9.11589525E-12 2.77101872E+04 2.04776803E+01              4
C2HCL2            C  2H  1CL 2   0G  300.000 2000.000 1000.000   01
 7.68917671E-01 3.97793060E-02-5.35819557E-05 3.57479121E-08-9.11589525E-12   2
 2.77101872E+04 2.04776803E+01 7.68917671E-01 3.97793060E-02-5.35819557E-05   3
 3.57479121E-08-9.11589525E-12 2.77101872E+04 2.04776803E+01              4
C2HCL3            C  2H  1CL 3   0G  300.000 2000.000 1000.000   01
 3.10879666E+00 3.01575684E-02-3.19717629E-05 1.51881701E-08-2.59243777E-12   2
-2.71819968E+03 1.36517480E+01 3.10879666E+00 3.01575684E-02-3.19717629E-05   3
 1.51881701E-08-2.59243777E-12-2.71819968E+03 1.36517480E+01              4
CH2CLCH2          C  2H  4CL 1   0G  300.000 2000.000 1000.000   01
 1.29115977E+00 2.11511827E-02-4.16036228E-06-8.10901766E-09 4.05531201E-12   2
 9.14351887E+03 2.10699570E+01 1.29115977E+00 2.11511827E-02-4.16036228E-06   3
-8.10901766E-09 4.05531201E-12 9.14351887E+03 2.10699570E+01              4
CH2CH2CL          C  2H  4CL 1   0G  300.000 2000.000 1000.000   01
 1.29115977E+00 2.11511827E-02-4.16036228E-06-8.10901766E-09 4.05531201E-12   2
 9.14351887E+03 2.10699570E+01 1.29115977E+00 2.11511827E-02-4.16036228E-06   3
-8.10901766E-09 4.05531201E-12 9.14351887E+03 2.10699570E+01              4
C2H4CL            C  2H  4CL 1   0G  300.000 2000.000 1000.000   01
 3.39618687E+00 8.87937721E-03 1.92054800E-05-2.67453262E-08 9.22648144E-12   2
 7.27883184E+03 1.12471671E+01 3.39618687E+00 8.87937721E-03 1.92054800E-05   3
-2.67453262E-08 9.22648144E-12 7.27883184E+03 1.12471671E+01              4
CH3CHCL           C  2H  4CL 1   0G  300.000 2000.000 1000.000   01
 3.39618687E+00 8.87937721E-03 1.92054800E-05-2.67453262E-08 9.22648144E-12   2
 7.27883184E+03 1.12471671E+01 3.39618687E+00 8.87937721E-03 1.92054800E-05   3
-2.67453262E-08 9.22648144E-12 7.27883184E+03 1.12471671E+01              4
CH3CCL2           C  2H  3CL 2   0G  300.000 2000.000 1000.000   01
 4.31595143E+00 1.29866143E-02 1.11102343E-05-2.09980983E-08 7.64397665E-12   2
 3.36006162E+03 8.26491515E+00 4.31595143E+00 1.29866143E-02 1.11102343E-05   3
-2.09980983E-08 7.64397665E-12 3.36006162E+03 8.26491515E+00              4
CHCL2CH2          C  2H  3CL 2   0G  300.000 2000.000 1000.000   01
```

4.60365931E+00 1.15741881E-02 1.35848637E-05-2.26666867E-08 8.01818572E-12 2
6.28761749E+03 7.30308918E+00 4.60365931E+00 1.15741881E-02 1.35848637E-05 3
-2.26666867E-08 8.01818572E-12 6.28761749E+03 7.30308918E+00 4
CH2CLCHCL C 2H 3CL 2 0G 300.000 2000.000 1000.000 01
3.34221510E+00 1.77067888E-02 1.72931112E-06-1.35989749E-08 5.69413117E-12 2
3.96270673E+03 1.38681842E+01 3.34221510E+00 1.77067888E-02 1.72931112E-06 3
-1.35989749E-08 5.69413117E-12 3.96270673E+03 1.38681842E+01 4
C2H3CL2 C 2H 3CL 2 0G 300.000 2000.000 1000.000 01
4.31595143E+00 1.29866143E-02 1.11102343E-05-2.09980983E-08 7.64397665E-12 2
3.81300576E+03 8.61720503E+00 4.31595143E+00 1.29866143E-02 1.11102343E-05 3
-2.09980983E-08 7.64397665E-12 3.81300576E+03 8.61720503E+00 4
CH2CLCCL2 C 2H 2CL 3 0G 300.000 2000.000 1000.000 01
3.44109008E+00 2.89264767E-02-2.40705856E-05 8.30602404E-09-6.60112752E-13 2
1.40780575E+03 1.46496451E+01 3.44109008E+00 2.89264767E-02-2.40705856E-05 3
8.30602404E-09-6.60112752E-13 1.40780575E+03 1.46496451E+01 4
CCL3CH2 C 2H 2CL 3 0G 300.000 2000.000 1000.000 01
3.44109008E+00 2.89264767E-02-2.40705856E-05 8.30602404E-09-6.60112752E-13 2
3.87383496E+03 1.44986637E+01 3.44109008E+00 2.89264767E-02-2.40705856E-05 3
8.30602404E-09-6.60112752E-13 3.87383496E+03 1.44986637E+01 4
C2H2CL3 C 2H 2CL 3 0G 300.000 2000.000 1000.000 01
3.44109008E+00 2.89264767E-02-2.40705856E-05 8.30602404E-09-6.60112752E-13 2
2.16271265E+03 1.45993180E+01 3.44109008E+00 2.89264767E-02-2.40705856E-05 3
8.30602404E-09-6.60112752E-13 2.16271265E+03 1.45993180E+01 4
C2H5CL C 2H 5CL 1 0G 300.000 2000.000 1000.000 01
6.40153092E+00-1.04706144E-02 6.85348017E-05-7.15756620E-08 2.27017352E-11 2
-1.54056729E+04-2.58421584E+00 6.40153092E+00-1.04706144E-02 6.85348017E-05 3
-7.15756620E-08 2.27017352E-11-1.54056729E+04-2.58421584E+00 4
CH3CHCL2 C 2H 4CL 2 0G 300.000 2000.000 1000.000 01
5.20586614E+00 7.73907827E-03 2.97193832E-05-3.97381393E-08 1.37258618E-11 2
-1.74867274E+04 3.68290491E+00 5.20586614E+00 7.73907827E-03 2.97193832E-05 3
-3.97381393E-08 1.37258618E-11-1.74867274E+04 3.68290491E+00 4
C2H4CL2 C 2H 4CL 2 0G 300.000 2000.000 1000.000 01
5.21168068E+00 1.24331618E-02 1.29969925E-05-2.25127853E-08 8.36985882E-12 2
-1.77821768E+04 3.30483747E+00 5.21168068E+00 1.24331618E-02 1.29969925E-05 3
-2.25127853E-08 8.36985882E-12-1.77821768E+04 3.30483747E+00 4
CH2CLCH2CL C 2H 4CL 2 0G 300.000 2000.000 1000.000 01
5.21168068E+00 1.24331618E-02 1.29969925E-05-2.25127853E-08 8.36985882E-12 2
-1.77821768E+04 3.30483747E+00 5.21168068E+00 1.24331618E-02 1.29969925E-05 3
-2.25127853E-08 8.36985882E-12-1.77821768E+04 3.30483747E+00 4
CH3CCL3 C 2H 3CL 3 0G 300.000 2000.000 1000.000 01
6.84452635E+00 1.29585678E-02 1.37034623E-05-2.46359936E-08 9.01203120E-12 2

-1.82443847E+04-3.70299057E+00 6.84452635E+00 1.29585678E-02 1.37034623E-05 3
-2.46359936E-08 9.01203120E-12-1.82443847E+04-3.70299057E+00 4
C2H3CL3 C 2H 3CL 3 0G 300.000 2000.000 1000.000 01
6.84452635E+00 1.29585678E-02 1.37034623E-05-2.46359936E-08 9.01203120E-12 2
-1.82443847E+04-3.70299057E+00 6.84452635E+00 1.29585678E-02 1.37034623E-05 3
-2.46359936E-08 9.01203120E-12-1.82443847E+04-3.70299057E+00 4
C2H2CL4 C 2H 2CL 4 0G 300.000 2000.000 1000.000 01
5.92851649E+00 2.71037347E-02-1.43506598E-05-2.99378968E-09 3.13066269E-12 2
-2.15627297E+04 2.09022367E+00 5.92851649E+00 2.71037347E-02-1.43506598E-05 3
-2.99378968E-09 3.13066269E-12-2.15627297E+04 2.09022367E+00 4
C2HCL4 C 2H 1CL 4 0G 300.000 2000.000 1000.000 01
3.20984892E+00 4.17296537E-02-5.24624832E-05 3.18342997E-08-7.35754189E-12 2
5.11270076E+02 1.55825679E+01 3.20984892E+00 4.17296537E-02-5.24624832E-05 3
3.18342997E-08-7.35754189E-12 5.11270076E+02 1.55825679E+01 4
C2HCL5 C 2H 1CL 5 0G 300.000 2000.000 1000.000 01
6.39739265E+00 3.45648161E-02-3.02280816E-05 9.65755457E-09-4.81632878E-13 2
-2.03066989E+04 3.11658059E-01 6.39739265E+00 3.45648161E-02-3.02280816E-05 3
9.65755457E-09-4.81632878E-13-2.03066989E+04 3.11658059E-01 4
C2CL6 C 2 0CL 6 0G 300.000 2000.000 1000.000 01
5.39691283E+00 5.64627025E-02-8.14342569E-05 5.42459942E-08-1.35447044E-11 2
-2.05105880E+04 3.45438063E+00 5.39691283E+00 5.64627025E-02-8.14342569E-05 3
5.42459942E-08-1.35447044E-11-2.05105880E+04 3.45438063E+00 4
C2CL5 C 2 0CL 5 0G 300.000 2000.000 1000.000 01
4.64817530E+00 4.70603746E-02-6.81254866E-05 4.67543384E-08-1.20981946E-11 2
8.12195505E+02 8.53599901E+00 4.64817530E+00 4.70603746E-02-6.81254866E-05 3
4.67543384E-08-1.20981946E-11 8.12195505E+02 8.53599901E+00 4
C2CL3 C 2 0CL 3 0G 300.000 2000.000 1000.000 01
4.42740916E+00 2.78107584E-02-2.84567048E-05 1.25867811E-08-1.90499233E-12 2
2.61161970E+04 7.40849819E+00 4.42740916E+00 2.78107584E-02-2.84567048E-05 3
1.25867811E-08-1.90499233E-12 2.61161970E+04 7.40849819E+00 4
C2CL4 C 2 0CL 4 0G 300.000 2000.000 1000.000 01
4.18662915E+00 3.62229835E-02-4.99242503E-05 3.30118455E-08-8.34899113E-12 2
-4.18958239E+03 8.26655799E+00 4.18662915E+00 3.62229835E-02-4.99242503E-05 3
3.30118455E-08-8.34899113E-12-4.18958239E+03 8.26655799E+00 4
CH2CLCHCL2 C 2H 3CL 3 0G 300.000 2000.000 1000.000 01
4.68683131E+00 2.01901616E-02 3.55626799E-06-1.84519481E-08 7.68373753E-12 2
-2.01091543E+04 8.29307295E+00 4.68683131E+00 2.01901616E-02 3.55626799E-06 3
-1.84519481E-08 7.68373753E-12-2.01091543E+04 8.29307295E+00 4
CLO 0 0CL 1O 1G 300.000 5000.000 1391.000 01
3.97507537E+00 6.56685973E-04-2.27709560E-07 3.56632488E-11-2.06485219E-15 2
1.08827727E+04 4.21626321E+00 3.30207849E+00 2.33584599E-03-1.86174305E-06 3

```
 7.70511312E-10-1.29965089E-13 1.11058160E+04 7.79282954E+00              4
CL2O                0   0CL  2O   1G   300.000  2000.000 1000.000    01
 2.14783739E+00 1.97622828E-02-3.30539297E-05 2.46068117E-08-6.62376080E-12    2
 9.29647629E+03 1.53546250E+01 2.14783739E+00 1.97622828E-02-3.30539297E-05    3
 2.46068117E-08-6.62376080E-12 9.29647629E+03 1.53546250E+01              4
CLO2                0   0CL  1O   2G   300.000  2000.000 1000.000    01
 1.10252923E+00 2.05073882E-02-3.19970509E-05 2.34702785E-08-6.34910951E-12    2
 1.15808813E+04 1.97925613E+01 1.10252923E+00 2.05073882E-02-3.19970509E-05    3
 2.34702785E-08-6.34910951E-12 1.15808813E+04 1.97925613E+01              4
HOCL                0H   1CL  1O   1G   300.000  2000.000 1000.000    01
 2.40050367E+00 1.04291334E-02-1.48656811E-05 1.07554997E-08-2.89596681E-12    2
-1.00260312E+04 1.22297760E+01 2.40050367E+00 1.04291334E-02-1.48656811E-05    3
 1.07554997E-08-2.89596681E-12-1.00260312E+04 1.22297760E+01              4
COCL2             C  1   0CL  2O   1G   300.000  2000.000 1000.000    01
 1.91099887E+00 2.61831771E-02-3.94373912E-05 2.80674646E-08-7.41269586E-12    2
-2.79091331E+04 1.69567858E+01 1.91099887E+00 2.61831771E-02-3.94373912E-05    3
 2.80674646E-08-7.41269586E-12-2.79091331E+04 1.69567858E+01              4
CHCLO             C  1H   1CL  1O   1G   300.000  2000.000 1000.000    01
 1.75590767E+00 1.83627582E-02-2.31403933E-05 1.52262473E-08-3.85646867E-12    2
-2.09420769E+04 1.65345359E+01 1.75590767E+00 1.83627582E-02-2.31403933E-05    3
 1.52262473E-08-3.85646867E-12-2.09420769E+04 1.65345359E+01              4
CLO                 0   0CL  1O   1G   300.000  5000.000 1391.000    01
 3.97507537E+00 6.56685973E-04-2.27709560E-07 3.56632488E-11-2.06485219E-15    2
 1.08827727E+04 4.21626321E+00 3.30207849E+00 2.33584599E-03-1.86174305E-06    3
 7.70511312E-10-1.29965089E-13 1.11058160E+04 7.79282954E+00              4
CL2O                0   0CL  2O   1G   300.000  2000.000 1000.000    01
 2.14783739E+00 1.97622828E-02-3.30539297E-05 2.46068117E-08-6.62376080E-12    2
 9.29647629E+03 1.53546250E+01 2.14783739E+00 1.97622828E-02-3.30539297E-05    3
 2.46068117E-08-6.62376080E-12 9.29647629E+03 1.53546250E+01              4
OCLO                0   0CL  1O   2G   300.000  2000.000 1000.000    01
 1.10252923E+00 2.05073882E-02-3.19970509E-05 2.34702785E-08-6.34910951E-12    2
 1.15808813E+04 1.97925613E+01 1.10252923E+00 2.05073882E-02-3.19970509E-05    3
 2.34702785E-08-6.34910951E-12 1.15808813E+04 1.97925613E+01              4
HOCL                0H   1CL  1O   1G   300.000  2000.000 1000.000    01
 2.40050367E+00 1.04291334E-02-1.48656811E-05 1.07554997E-08-2.89596681E-12    2
-1.00260312E+04 1.22297760E+01 2.40050367E+00 1.04291334E-02-1.48656811E-05    3
 1.07554997E-08-2.89596681E-12-1.00260312E+04 1.22297760E+01              4
COCL2             C  1   0CL  2O   1G   300.000  2000.000 1000.000    01
 1.91099887E+00 2.61831771E-02-3.94373912E-05 2.80674646E-08-7.41269586E-12    2
-2.79091331E+04 1.69567858E+01 1.91099887E+00 2.61831771E-02-3.94373912E-05    3
 2.80674646E-08-7.41269586E-12-2.79091331E+04 1.69567858E+01              4
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CHCLO             C  1H  1CL 1O  1G  300.000 2000.000 1000.000   01
 1.75590767E+00 1.83627582E-02-2.31403933E-05 1.52262473E-08-3.85646867E-12   2
-2.09420769E+04 1.65345359E+01 1.75590767E+00 1.83627582E-02-2.31403933E-05   3
 1.52262473E-08-3.85646867E-12-2.09420769E+04 1.65345359E+01                 4
CCL               C  1   0CL 1   0G  300.000 5000.000 1392.000   01
 4.10858306E+00 4.53019987E-04-1.67983008E-07 2.68052271E-11-1.52213690E-15   2
 5.06180393E+04 3.25404676E+00 3.29470846E+00 2.66642521E-03-2.50517917E-06   3
 1.15326344E-09-2.08419461E-13 5.08667809E+04 7.50999534E+00                 4
C2CL              C  2   0CL 1   0G  300.000 2000.000 1000.000   01
 3.62992504E+00 1.16590191E-02-1.98822931E-05 1.66302512E-08-4.93256681E-12   2
 6.19165723E+04 6.44259262E+00 3.62992504E+00 1.16590191E-02-1.98822931E-05   3
 1.66302512E-08-4.93256681E-12 6.19165723E+04 6.44259262E+00                 4
C2HCL2            C  2H  1CL 2   0G  300.000 2000.000 1000.000   01
 7.68917671E-01 3.97793060E-02-5.35819557E-05 3.57479121E-08-9.11589525E-12   2
 2.79114957E+04 2.13835686E+01 7.68917671E-01 3.97793060E-02-5.35819557E-05   3
 3.57479121E-08-9.11589525E-12 2.79114957E+04 2.13835686E+01                 4
C2H2CL2           C  2H  2CL 2   0G  300.000 2000.000 1000.000   01
 2.84156601E+00 2.04013529E-02-1.09882876E-05-6.80156527E-10 1.53539649E-12   2
-1.10269103E+03 1.30550456E+01 2.84156601E+00 2.04013529E-02-1.09882876E-05   3
-6.80156527E-10 1.53539649E-12-1.10269103E+03 1.30550456E+01                 4
PHCL2             C  6H  4CL 2   0G  300.000 2000.000 1000.000   01
 1.74952492E+01-5.79793150E-02 2.17623482E-04-2.19081615E-07 6.86549615E-11   2
-5.88144805E+02-4.92907898E+01 1.74952492E+01-5.79793150E-02 2.17623482E-04   3
-2.19081615E-07 6.86549615E-11-5.88144805E+02-4.92907898E+01                 4
CC6H5CL           C  6H  5CL 1   0G  300.000 2000.000 1000.000   01
 1.07241814E-01 3.56531141E-02 2.76594694E-05-6.74460612E-08 3.03102632E-11   2
 4.44819879E+03 2.56700359E+01 1.07241814E-01 3.56531141E-02 2.76594694E-05   3
-6.74460612E-08 3.03102632E-11 4.44819879E+03 2.56700359E+01                 4
PHPHCL            C 12H  9CL 1   0G  300.000 2000.000 1000.000   01
 3.22140333E+01-1.50557173E-01 5.17665602E-04-5.29466299E-07 1.75126462E-10   2
 1.27525640E+04-1.00048528E+02 3.22140333E+01-1.50557173E-01 5.17665602E-04   3
-5.29466299E-07 1.75126462E-10 1.27525640E+04-1.00048528E+02                 4
PHCLPHCL          C 12H  8CL 2   0G  300.000 2000.000 1000.000   01
 3.67893175E+01-1.66423001E-01 5.53288467E-04-5.65048687E-07 1.87283104E-10   2
 1.20951166E+04-1.19005357E+02 3.67893175E+01-1.66423001E-01 5.53288467E-04   3
-5.65048687E-07 1.87283104E-10 1.20951166E+04-1.19005357E+02                 4
CH2CLO            C  1H  2CL 1O  1G  300.000 2000.000 1000.000   01
 1.86586922E+00 1.43613373E-02-5.46157433E-06-1.90580996E-09 1.30095706E-12   2
-8.63510766E+01 1.71610224E+01 1.86586922E+00 1.43613373E-02-5.46157433E-06   3
-1.90580996E-09 1.30095706E-12-8.63510766E+01 1.71610224E+01                 4
CH2CLOO           C  1H  2CL 1O  2G  300.000 2000.000 1000.000   01
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 9.56565307E+00-1.71562805E-02 5.06895498E-05-4.21205837E-08 1.14326127E-11    2
-6.98005205E+02-1.44903470E+01 9.56565307E+00-1.71562805E-02 5.06895498E-05    3
-4.21205837E-08 1.14326127E-11-6.98005205E+02-1.44903470E+01                   4
CH2OOCL            C  1H  2CL 1O  2G  300.000 2000.000 1000.000   01
 4.53265386E-01 4.15935707E-02-5.91217198E-05 4.41726349E-08-1.24482007E-11    2
 3.48978859E+03 2.68456540E+01 4.53265386E-01 4.15935707E-02-5.91217198E-05    3
 4.41726349E-08-1.24482007E-11 3.48978859E+03 2.68456540E+01                   4
CCLO               C  1   0CL 1O  1G  300.000 2000.000 1000.000   01
 3.84415675E+00 8.04979988E-03-1.19244158E-05 9.08219582E-09-2.56939741E-12    2
-3.42839223E+03 8.12012827E+00 3.84415675E+00 8.04979988E-03-1.19244158E-05    3
 9.08219582E-09-2.56939741E-12-3.42839223E+03 8.12012827E+00                   4
CH3NH2        SWS   H  5C  1N  1   0G  300.000 5000.000 1398.000   11
 6.47610097E+00 9.19291737E-03-3.59217976E-06 6.61773656E-10-4.39266506E-14    2
-5.97124150E+03-1.22200903E+01-9.74097436E-01 2.82513562E-02-2.26382047E-05    3
 9.43883461E-09-1.60188961E-12-3.55113858E+03 2.72023150E+01                   4
CH2NH2        THERM N  1C  1H  4   0G  300.000 5000.000 1397.000   11
 6.25536362E+00 7.41169902E-03-2.46075625E-06 3.74232445E-10-2.13943637E-14    2
 1.55206038E+04-9.67270914E+00 2.62592095E+00 1.57721009E-02-9.99810392E-06    3
 3.55606246E-09-5.50456849E-13 1.68160464E+04 9.89963553E+00                   4
CH2NH         MELIUS N  1C  1H  3   0G  300.000 5000.000 1539.000   01
 4.48362607E+00 6.86071758E-03-2.28603111E-06 3.48588292E-10-1.99681442E-14    2
 8.78014378E+03-5.23858460E-01 1.23459945E+00 1.24353810E-02-4.67168910E-06    3
-5.43823190E-11 2.98930094E-13 1.00917447E+04 1.76086018E+01                   4
CHNH          MELIUS N  1C  1H  2   0G  300.000 5000.000 1384.000   01
 4.69721735E+00 4.45461026E-03-1.52627715E-06 2.37210150E-10-1.37717587E-14    2
 3.12634196E+04-7.51417111E-01 2.35799584E+00 8.54249139E-03-3.62645315E-06    3
 3.56163933E-10 9.22757498E-14 3.22248649E+04 1.23189312E+01                   4
C3H4               C  3H  4   0   0G  300.000 2000.000 1000.000   01
 5.36526912E+00-1.09768220E-03 3.70038268E-05-4.05209802E-08 1.29995100E-11    2
 2.04910635E+04-1.70020960E+00 5.36526912E+00-1.09768220E-03 3.70038268E-05    3
-4.05209802E-08 1.29995100E-11 2.04910635E+04-1.70020960E+00                   4
CH3NH      THERM92   N  1C  1H  4   0G  300.000 5000.000 1391.000   01
 5.31637547E+00 7.69093789E-03-2.38211364E-06 3.52621065E-10-2.00517988E-14    2
 1.93118655E+04-3.58307099E+00 1.42618660E+00 1.66609066E-02-1.04141549E-05    3
 3.69533627E-09-5.65659465E-13 2.06907454E+04 1.73783225E+01                   4
NH2CL          NJIT N  1H  2   0CL 1G  300.000 5000.000 1466.000   01
 4.98336282E+00 4.49147303E-03-1.60335042E-06 2.56136140E-10-1.51588185E-14    2
 8.67073997E+02-9.11798645E-01 3.57619922E+00 1.64856028E-03 8.27811902E-06    3
-7.41890622E-09 1.82935397E-12 1.97175301E+03 8.82673451E+00                   4
NOCL           NJIT N  1   0CL 1O  1G  300.000 5000.000 1398.000   01
 6.02228882E+00 8.94013303E-04-3.23511170E-07 5.21569899E-11-3.10674611E-15    2
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 4.14379498E+03-3.61900201E+00 3.87336292E+00 6.47798531E-03-5.88588067E-06   3
 2.56416458E-09-4.35022771E-13 4.81977028E+03 7.69903004E+00                 4
NO2CL           NJIT N  1CL 1   0O  2G  300.000  5000.000 1408.000   01
 7.80417255E+00 1.90351086E-03-6.66666568E-07 1.05232323E-10-6.17863550E-15   2
-1.39235356E+03-1.32609949E+01 2.66354051E+00 1.71733903E-02-1.80803618E-05   3
 9.02401349E-09-1.71917657E-12 4.47658333E+01 1.31539579E+01                 4
NHCL            MAO N  1H  1   0CL 1G  300.000  5000.000 1370.000   01
 6.09733712E+00 1.20823607E-03-5.02032262E-07 8.81172587E-11-5.55223630E-15   2
 2.61754343E+04-8.14704150E+00 1.22728558E+00 1.25325449E-02-1.03924669E-05   3
 3.94725373E-09-5.74455577E-13 2.78478019E+04 1.79878951E+01                 4
NCL             MAO N  1   0CL 1   0G  300.000  5000.000 1384.000   01
 4.55799123E+00-2.57429065E-04 2.15057932E-07-5.53858911E-11 4.48519844E-15   2
 3.11669698E+04 9.04484801E-01 2.91399290E+00 3.98807608E-03-4.14030934E-06   3
 2.03077366E-09-3.82447721E-13 3.17043472E+04 9.60201206E+00                 4
CNCL            BENS N  1CL 1C  1   0G  300.000  5000.000 1387.000   01
 6.16791001E+00 1.20973462E-03-4.35827865E-07 7.00556244E-11-4.16413723E-15   2
 1.44431558E+04-7.63101630E+00 3.66241176E+00 7.94671241E-03-7.52410958E-06   3
 3.49777423E-09-6.38763855E-13 1.52226615E+04 5.50838447E+00                 4
N1H             NJIT N  1H  1   0   0G  300.000  5000.000 1628.000   01
 3.27880506E+00 6.23423071E-04-2.04797956E-07 3.03575613E-11-1.67990043E-15   2
 5.98945087E+04 2.94402276E+00 3.32318659E+00 4.80287097E-04-3.85096563E-08   3
-5.29997006E-11 1.36445577E-14 5.98841064E+04 2.72145691E+00                 4
NA              80792NA 1           G 0300.00  5000.00  1000.00     1
 0.02574480E+02-0.16058803E-03 0.12506410E-06-0.04516575E-09 0.06941744E-13   2
 0.12191291E+05 0.03830900E+02 0.02591348E+02-0.05961520E-02 0.13276515E-05   3
-0.12111229E-08 0.03890066E-11 0.12206420E+05 0.03841789E+02                 4
NA+             80792NA 1E -1       G 0300.00  5000.00  1000.00     1
 0.02500251E+02 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00   2
 0.07260903E+06 0.03538490E+02 0.02500251E+02 0.00000000E+00 0.00000000E+00   3
 0.00000000E+00 0.00000000E+00 0.07260904E+06 0.03538490E+02                 4
NACL            81092CL 1NA 1       G 0300.00  5000.00  1000.00     1
 0.04393820E+02 0.02153336E-02-0.06198756E-06 0.12668785E-10-0.09427806E-14   2
-0.02315863E+06 0.02486064E+02 0.03953003E+02 0.15141874E-02-0.09819465E-05   3
-0.02807090E-08 0.03543574E-11-0.02305831E+06 0.04701214E+02                 4
NAO             80792NA 1O  1       G 0300.00  5000.00  1000.00     1
 0.04349803E+02 0.02849959E-02-0.08615992E-06 0.01754054E-09-0.13016768E-14   2
 0.08731694E+05 0.02618339E+02 0.03765727E+02 0.01980030E-01-0.12563033E-05   3
-0.03909831E-08 0.04664039E-11 0.08866889E+05 0.05562273E+02                 4
NAO2     12/10/96    NA 1O  2   0   0G  300.000  5000.000 3000.000   11
 3.97550289E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00   2
-7.72782262E+03 4.92845326E+00 3.97550289E+00 0.00000000E+00 0.00000000E+00   3
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 0.00000000E+00 0.00000000E+00-7.72782262E+03 4.92845326E+00                4
NAOH            80792H   1NA  1O   1    G  0300.00   5000.00  1000.00     1
 0.05527852E+02 0.14206231E-02-0.04439615E-05 0.06635638E-09-0.03866820E-13   2
-0.02545869E+06-0.04374785E+02 0.04727895E+02 0.05001262E-01-0.04534391E-04   3
 0.07051240E-08 0.06671123E-11-0.02537946E+06-0.07649678E+01                4
E               120186E   1   0   0   0G   300.000  5000.000 1000.000    01
 2.50104422E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00   2
-7.45686320E+02-1.17386177E+01 2.50104422E+00 0.00000000E+00 0.00000000E+00   3
 0.00000000E+00 0.00000000E+00-7.45686320E+02-1.17386177E+01                4
HCO+            121286H   1C   1O   1E  -1G   300.000  5000.000 1391.000    01
 4.14002984E+00 2.67478901E-03-8.43649800E-07 1.23153635E-10-6.83155157E-15   2
 9.87257892E+04-1.97043195E-01 3.15265127E+00 4.85291729E-03-2.69482804E-06   3
 8.52706574E-10-1.20118416E-13 9.90879604E+04 5.16203108E+00                4
END
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