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I am submitting herewith a dissertation written by Ashley Dawn Owens entitled "Influence of the Sampling Procedure on Extracted Jet Engine Exhaust Gas Emission Samples." I have examined the final electronic copy of this thesis for form and content and recommend that it be accepted in partial fulfillment of the requirements for the degree of Master of Science, with a major in Mechanical Engineering.

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(Original signatures are on file with official student records.)

INFLUENCE OF THE SAMPLING PROCEDURE ON EXTRACTED JET ENGINE EXHAUST GAS EMISSION SAMPLES

A Thesis
Presented for the
Master of Science
Degree
The University of Tennessee, Knoxville

Ashley Dawn Owens
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For my family

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ABSTRACT

The purpose of this thesis is to analyze the effects of an intrusive sample extraction process on the thermo-chemistry of extracted gas samples taken from exhaust of a GE-J85-H turbojet engine. The engine testing took place at University of Tennessee Space Institute in Tullahoma, TN, where the J85 was installed in a test bay of a research facility. The results of the analysis validate that testing methods used had a low probability of disturbing the exhaust chemistry. The tools used to analyze the thermal history of the extracted samples were the NASA CEA and LSENS programs. Several different cases of exhaust chemistry analysis were run using each program to evaluate exhaust species sampling procedures used during the operation of the J85 engine. The LSENS program validated that the flow through the augmenter, for throttle positions from idle to 100% military power (but non-afterburning), was chemically frozen and that the process of extracting and cooling (quenching) of extracted samples was predicted to not affect the sample concentrations or mass fractions.

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CHAPTER 1: INTRODUCTION

J85 OPERATION & EMISSION TESTING AT UTSI

Emissions are defined as the chemical species forming the combustion products of any given chemical reactions (Turns 2000). The combustion processes in both the primary combustor and afterburner are responsible for the emissions created by military jet engines such as the GE J85 turbojet engine installed and operated at the University of Tennessee Space Institute (UTSI). The J85 is a turbojet engine manufactured by General Electric. The engine has been in service since 1960. The J85 can be found on the T-38 Talon and also on the F-5E/F Tiger II (GE Aviation 2006). The J85 afterburning turbojet engine test bed can be found at the University of Tennessee Space Institute in Tullahoma, Tennessee. The engine is capable of running at idle conditions as well as full after-burning power and all throttle positions in between. Depending on the test requirements, the test can take anywhere from 15 minutes to several hours. An engine control console and control room is setup at the test site to allow for testing and data acquisition (Jet Engine Test Bed 2005). A schematic showing the jet engine components and flow paths can be seen in Figure 1 (Mattingly 2006). The first combustion process occurs in the primary combustor (flow path 3-4) and the second combustion process occurs in the augmenter (flow path 6-7), also known as the afterburner, when it is activated. That is, the second process only occurs when the engine is operating at afterburning (AB) conditions. In operation of the J85 jet engine at UTSI, intrusive, gas sample extracting emissions probes have been used to measure major engine exhaust species. The probes were developed at Arnolds Engineering Development Center, Tullahoma, Tennessee (Beitel 2004). The emissions probes were located inside a traversing, water-cooled rake.

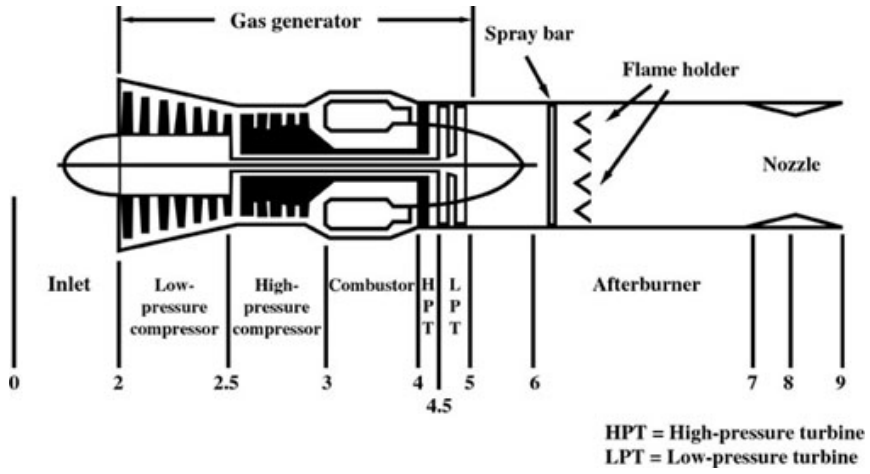
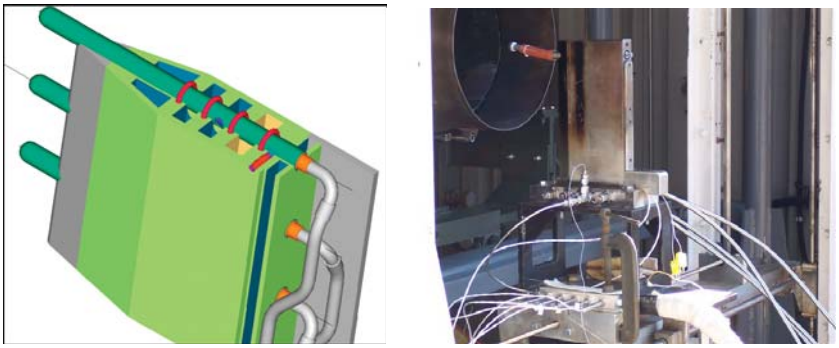


Figure 1. Turbojet engine schematic.

The emissions probes are individually water-cooled to survive the high temperature engine exhaust during testing. The probes are constructed of 304 stainless steel, and encased in an electroformed nickel shell (MacKinnon 2004). Electroforming is defined as a technique in which a metal is electrodeposited onto a conductive substrate (Beitel et al. 2004). The emission probe-rake was constructed from 304 stainless steel as well and a cross sectional view of the rake can be seen in Figure 2 as well as a photo of the actual rake installed near the exhaust exit plane of the J85 afterburner (MacKinnon 2004). In figure 2.(a), passages provide a flow of water used in forced convection cooling of the probes and rake. The silver tubes shown extending from each emissions probe are the gas sample lines that transfer the extracted gas samples to a multi-gas analyzer (MGA) (Jalbert 2004).

THESIS RESEARCH PROBLEM

This thesis was focused on the question of the validity of the gas species measurements made with the MGA. The main issue was whether the emissions



(a) Cross-Section **(b) Installation in exhaust plane**

Figure 2. Cross sectional view and photo of the water-cooled rake.

measured quantitatively by the multi-gas analyzer extracts were changed by continued chemical kinetics as the extracted gas samples traverse the gas sampling line from the emission probe to the analyzer. The extractive sampling system details will be given in a later section, but the problem is that the sample lines are nearly 100 feet long and even though the extracted samples are kept heated to 150ºC (Jalbert 2002) to keep water from condensing from the samples, there was concern that the chemistry of the samples would change. The primary species of concern were CO continuing to oxidize to CO_2, and NO_x thermally decomposing to N_2 and O_2. The purpose of this thesis research was to obtain theoretical estimates of this type of chemical change in the moving samples.

TOOLS OF ANALYSIS

The NASA Chemical Equilibrium with Applications code (CEA), (CEA History 2007), and the NASA Lewis General Chemical Kinetics and Sensitivity Analysis Code (LSENS), (Radhakrishnan 1999), were the two chemistry models used to analyze the potential chemical changes to the extracted gas samples. Vearl N. Huff, Virginia E.

Morrell, and Sanford Gordon are responsible for the groundwork that would later become the CEA code. Their work in developing general chemical equilibrium analysis tools began at the NACA Lewis Flight Propulsion Laboratory in the 1950's. In 1994 the CEA code, used during this experiment, was introduced and the last update came in 2002. (CEA History 2007) D.A. Bittker and V.J. Scullin are responsible for the groundwork that would later become the LSENS code. Bittker and Scullin developed a finite rate chemical analysis tool called the General Chemical Kinetic Program (GCKP), which was one of the first kinetics codes in 1972. Krishnan Radhakrishnan made many modifications to the GCKP code by improving its numerical integration schemes, and the code became known as LSENS. All the work that went into creating the LSENS code was done at the NASA John H. Glenn Research Center at Lewis Field. (Radharkrishnan 2003)

APPROACH OF THE ANALYSIS

During testing, commercial Jet A fuel was the jet fuel used in all cases and it is burned in air in the J85 primary combustor. Jet A is similar in its characteristics to the military fuels, JP-5 and JP-8 (Sturgess 1997). Throughout the remainder of the thesis, the fuel will be referred to as JP-5. Although this thesis is a study of the effects of the sample extraction and transport process on the chemistry of the sample, only emission samples from non-afterburning exhaust conditions were analyzed. LSENS came supplied with a variety of reaction mechanisms but none were the JP-5-air mechanism (Radhakrishnan 1999). A decision had to be made about what kind of reaction mechanism could be used to generate representative emissions species (their molar ratios) as a replacement for JP-5-air. The methane-air reaction mechanism was determined to be the best choice. Some

would argue this was a faulty decision. Methane is not usually preferred since it is a simple hydrocarbon. It has ignition and oxidation characteristics much different from the higher hydrocarbons. It produces more water vapor per kg of fuel than jet-fuel, and less CO_2 (Way 1999). Many would argue that methane should not be used as a reference hydrocarbon because during CH_4 oxidation CH_3 recombination plays a more important role than in usual hydrocarbon fuels. As long as methane is used for experimental and modeling studies, it is a suitable as a reference for hydrocarbon fuel (Westbrook 1984). However, this thesis is not focused on evaluating a reaction mechanism for jet fuel, but rather one that treats the oxidation of CO and the thermal decomposition of NO_x in engine exhaust under rapid quenching (cooling) conditions followed by low, constant temperature thermal and chemical relaxation conditions. For this purpose, the detailed methane-air chemical mechanism initially in LSENS and updated with the Gas Research Institutes (GRI) methane air mechanism seemed ideal because the GRI mechanism has been optimized for study of emissions thermo-chemical behavior. For that reason, the methane air reaction mechanism was utilized and studied.

The remainder of this thesis will give a more in-depth description of the equilibrium codes utilized and the actual steps taken to complete that exhaust analysis. The steps will be broken down into the following categories: 1) simplified air model, 2) methane as jet fuel simulator, 3) reaction mechanism, 4) and the discussion of the results. Also, some recommendations for future research will be given.

CHAPTER 2: TESTING AND MEASUREMENTS

TEST SITE

A GE J85-5-H afterburning turbojet engine is located at the University of Tennessee Space Institute in Tullahoma, TN, and installed in a test bay of a research facility. An engine control console with engine throttle and engine operating instruments is next to the engine at the test site. The control console houses the primary engine control sensor displays, which include compressor discharge pressure, spool speed, nozzle position, oil pressure, and oil temperature. The console also houses the throttle which is used to control the engine and vary the range of operation. Figure 3 shows the control console and the various sensor displays available for viewing during engine testing. During engine operation, from one to three people are inside the console operating the throttle and taking engine operation data, or acting as observers.. The engine is capable of running at idle conditions as well as full- afterburning power and all ranges in between. Adjacent to the research facility is a data acquisition control (DAC) room which houses all the measurement systems. During testing, the data acquisition

Figure 3. Engine control console.

Figure 4. Data acquisition control room.

engineers and research teams are situated inside the DAC room. Also, the engineers and research teams were able to view real time data of the engine operation and exhaust data. A view of the data acquisition control room can be found in Figure 4. The cost of using the test site varies depending on the kind of testing that is to be done, and on the amount of time the engine is operated. Fuel consumption, user's needs, and any special equipment needed can also affect the cost of the testing using the J85. UTSI personnel will quote estimated test cost to interested or potential users.

J85 ENGINE CHARACTERISTICS

The J85 is a military turbojet engine that can be found on the T-38 Talon and the F-5E/F Tiger II (J85 2006). Specifications for the J85 can be seen in Table 1. The J85 at UTSI is the J85-GE- 5H. Although, the J85-GE-5H is not listed in the table, it is similar to the J85-GE-5J (Comparison Chart 2006). The engine is capable of running at afterburning conditions as well as normal idle conditions through full military (dry) power. The engine primary combustion system is an annular combustor, which can be seen in Figure 5 (Seldner 1972). The J85-5H is also equipped with an augmenter to

Table 1. J85 Specifications

Engine	J85-GE-5J	J85-17A/B	J85-21
Physical Dimensions			
Compressor Stages	8	8	8
Turbine Stages	2	2	2
Maximum Diameter (Inches)	21	17.7	26.1
Length (Inches)	104.6	40.5	117
Dry Weight (Lb.)	584	400	684
Power Specifications			
Specific Fuel Consumption at Maximum Power	2.2	0.99	2.13
Max. Power at Sea Level	3,850	2,850	5,000
Overall Pressure Ratio at Maximum Power	6.7	6.9	8.3

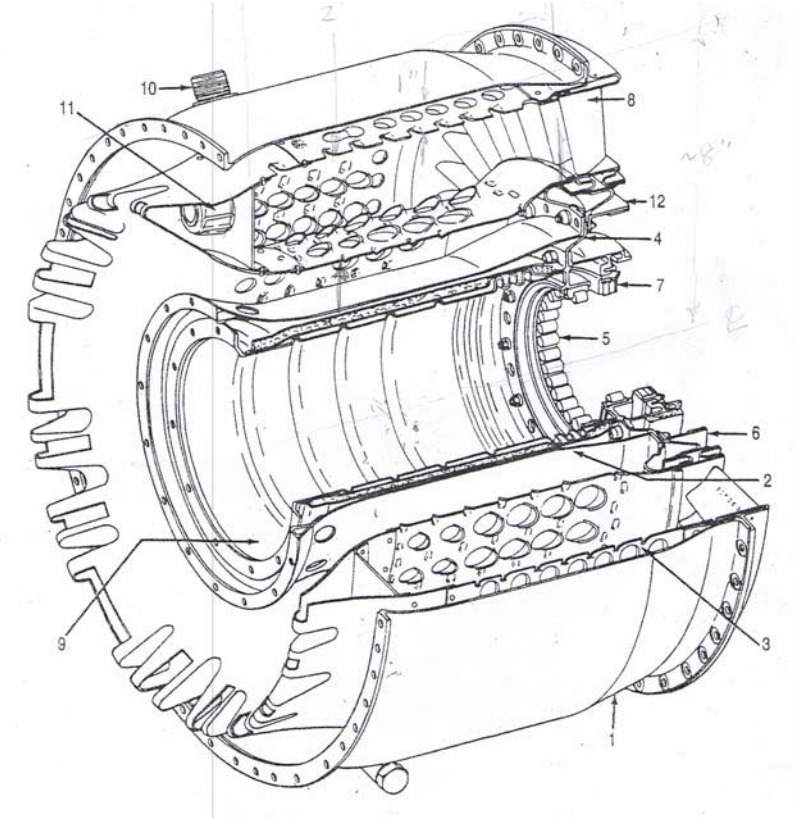


Figure 5. Annular combustor found on a J85.

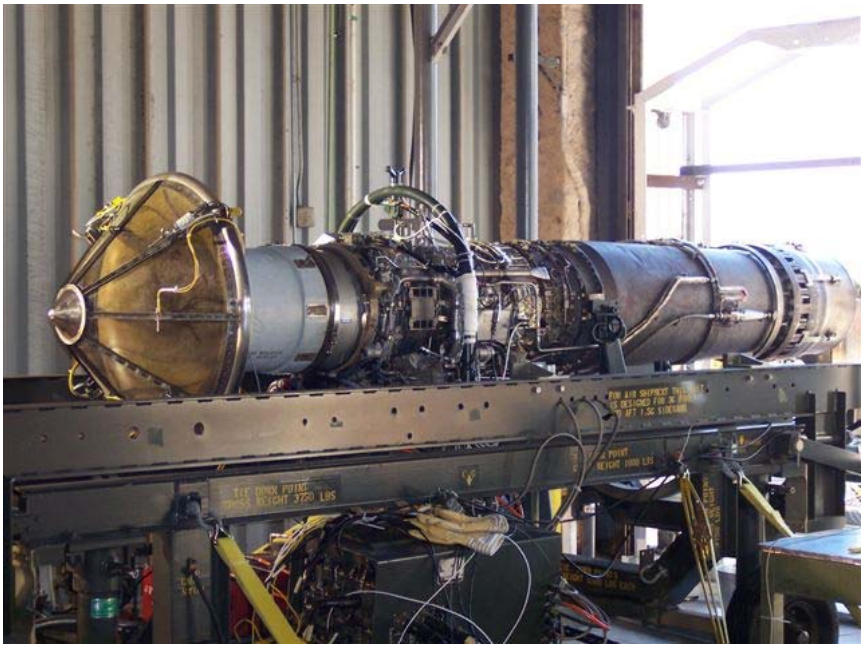


Figure 6. J85-GE-5 used during testing at UTSI.

allow for afterburning operation. The actual engine used for testing at the university can be seen in Figure 6.

MULTI-GAS ANALYZER

Located in the data acquisition control room is an Advanced Fuels Research multi-gas analyzer (MGA). The multi-gas analyzer was developed by Advanced Fuels Research, Inc. It is now offered by On-line Technologies, Inc., part of MKS Instruments (Mksinst). A laptop is interfaced with the MGA to show and record the data being acquired by the MGA. The MGA is typically used to measure the amounts of primary exhaust gas species in the exhaust as the tests were being performed (Jalbert 2002). The major species of interest were defined as CO, CO_2, H_2O, O_2, HC (hydrocarbons) and the

N_2 species NO_2 and N_2. The N_2 was not directly measured by the MGA but it could be determined by difference using the following equation:

$$x_{N_2} = 1 - (x_{CO} + x_{CO_2} + x_{H_2O} + x_{O_2} + x_{HC} + x_{NO_2}) \quad (1)$$

In equation 1, x_i represents the mole fraction of the individual species. To measure the species in the exhaust, the MGA uses advanced infrared and other optical/spectroscopic technologies. For example, based on the amount of infrared absorption, the analyzer can determine certain select species and the quantity of that species which exist in the exhaust stream. The only requirements for the analyzer are 1) the sample must be wet, that is, contain water vapor, and have a volumetric flow rate of one liter/minute and 2) the sample line must be held at a temperature of no less than 150°C. To ensure the minimum volumetric flow rate is obtained, a heated vacuum pump is installed at the inlet of the MGA. The MGA and laptop setup can be seen in Figure 7. The dimensions of the setup are 29" long x 19" wide x 12.5" tall and weighs in at 150 lbs (Jalbert 2002).

Figure 7. MGA and laptop setup.

CHAPTER 3: EQUILIBRIUM (NASA CEA) & FINITE RATE (LSENS) CHEMISTRY CODES

CAPABILITIES

The NASA CEA Equilibrium Code can be used to solve the following problems: 1) chemical equilibrium of multi-phase systems at various thermodynamic states, 2) one-dimensional rocket performance for a finite or infinite-area combustion chamber, 3) Chapman-Jouguet detonations, and 4) shock tube parameters for incident and reflected shock. The various thermodynamic states for the equilibrium calculations can be determined by the following inputs: 1) temperature and pressure, 2) enthalpy and pressure, 3) entropy and pressure, 4) temperature and volume, 5) internal energy and volume, and 6) entropy and volume (Gordon 1994). For the analysis done in the present thesis, the thermodynamic state was specified by the enthalpy and pressure of the reactants.

The NASA Lewis Kinetics and Sensitivity Analysis Code, LSENS, can be used to solve various kinetic problems. The various problem types which can be solved are as follows: 1) constant density and pressure static reactions, 2) assigned pressure static reaction, 3) one-dimensional flow reaction at constant pressure and in constant area duct, 4) one-dimensional flow reaction at assigned pressure and in assigned-area duct, 5) reaction behind incident shock wave, 6) perfectly stirred reactor, 7) sensitivity calculations, and 8) equilibrium calculations (Radhakrishnan 2003). These various kinetic calculations may be adiabatic or non-adiabatic, with specified heat loss or addition to the stream tube or reactor.

The problems of interest for the exhaust analysis are the one-dimensional flow reaction in assigned-area duct, the perfectly stirred reactor, and the equilibrium calculations. The one-dimensional flow reaction was used to demonstrate a plug flow reactor model which is similar to the exhaust flow through the augmenter and nozzle as well as along the sample line flow. The perfectly stirred reactor model was used to gain some insight about the primary combustion process which occurs in the primary combustor during testing.

CHEMICAL EQUILIBRIUM

Chemical equilibrium exists when the minimization of Gibbs free energy is achieved as specified, in the following equation.

$$dG_{T,P} = 0 \tag{2}$$

When chemical equilibrium is achieved there is an equilibrium temperature, pressure, and composition. NASA CEA was used to determine the equilibrium state of the sample data acquired (Turns 2000).

PERFECTLY-STIRRED REACTOR MODEL

The perfectly-stirred reactor model is also known as the well stirred reactor model. The model is based on the assumption that perfect mixing is accomplished inside the combustor or control volume. The model is also assumed to be steady state (Turns 2000). The perfectly-stirred reactor was used as an investigatory tool to study the behavior of the primary combustor. The purpose of the perfectly-stirred reactor model was to see if the emission sample data in CO_2 could be reproduced by the output of a PSR-representation of the primary combustor. The input data for the PSR case came from representative data for the conditions achieved while testing. The actual combustor

of a jet engine is much more complicated in operation than a perfectly stirred reactor (Lefebore 1983). Roughly, about 1/3 to ½ of the total air flow into the actual combustor is sent into the dome of the combustor in a swirling mode. There, all of the fuel is injected into the swirling flow and burned in a swirl-stabilized flame, that incorporates flow recirculation. The remaining 2/3 – 1/2 of the combustor air flow passes around the outside of the primary combustor and then enters the combustor through cooling holes in the combustor walls. This cooling flow mixes with the combusted flow from the dome region and establishes the flow going into the turbines. It is possible to simulate or model a gas turbine combustor as a series of interacting plug flow and perfectly stirred reactors, for example (Sturgess 1997).

A mass flow rate of 0.1389 lb/sec was found by trial-and-error to be an appropriate flow rate for a combustor volume of about 0.39 ft^2. The combustor inlet pressure was set at 1.4 atm to simulate engine idle conditions. The initial temperature used was relatively close to the auto-ignition temperature of methane. The auto ignition temperature was used to allow the methane and air to start reacting since no temperature value was measured during testing. The volume of the combustor was estimated to be proportional to that of a J85 engine sector. The full details of the PSR case can be found in Appendix C and the results are discussed in a later section of the thesis.

PLUG-FLOW REACTOR MODEL

The plug flow reactor was used to simulate the conditions of the emission samples as they traversed both the augmenter duct and nozzle, as well as the sample line. The pressure and temperature were held constant to simulate the conditions either the augmenter duct or in the sample line. Two sample-line cases were run, which were based

on measured emissions data, using LSENS to see if any changes occurred in the sample data as the species traversed the sample line. The first case used the measured data sample set as the initial condition. The second case used for input a prepared sample set which contained more CO and NO_x and less CO_2 than the original sample set. The second case doubled the CO and NO_x and cut the CO_2 in half.

The plug-flow model was also used to simulate the flow path through the augmenter to show if any changes in the flow chemistry occurred in this part of the flow path. The augmenter case used methane-air composition, turbine exit pressure and temperature, and the augmenter length. The turbine exit pressure is estimated as 14.3 psia, the turbine exit temperature was given by test data and is 1437 R, and the augmenter length was measured and found to be 69" or 5.75'. The previous inputs are for the engine operating at idle conditions. All the results for each case mentioned in each section will be discussed in a later section and can be found in Appendix B and C.

CHAPTER 4: SIMPLIFIED "AIR" MODEL

SIMPLIFIED "AIR" MODEL

When using the NASA CEA and LSENS programs, the amounts of air and methane present had to be input to the program. The chemical composition of the air at the test site was not documented, hence not known in detail. Since the composition is not known, a simplified "air" model was needed and determined. The steps to determine the correct simplified "air" model can be found in this section.

TRACE SPECIES

In many cases of chemical analysis, the composition of air can be defined simply as a mixture of N_2 and O_2, where the N_2 accounts for 79% of the mixture and O_2 accounts for the remaining 21% by volume. For this analysis, a more complex composition was used because some small amount of CO_2 is present in atmospheric air. Also, the detailed methane-air reaction mechanism from GRI incorporate argon, as a trace and third-body species. The gases present in the complex composition can be seen in Table 2, along with their molecular weight and volume % (Barry 1998). From table 2, it can be seen that major trace species are present in this composition. The table also assumes there is no water present in this composition. The amount of water vapor present will be accounted for in the next two sections of this chapter. Some of the traces species were ignored and were included in the volume % of N_2. The trace species that were not ignored were Ar and CO_2. Ar was accounted for since it accounts for close to 1% of the air composition and may affect the chemical kinetic process. CO_2 was accounted for so it

Table 2. Composition of Dry Air

Component	Symbol	Volume %	Molecular Weight
Nitrogen	N_2	78.08	28.02
Oxygen	O_2	20.95	32.00
Argon	Ar	0.93	39.88
Carbon Dioxide	CO_2	0.035	44.00
Neon	Ne	0.0018	20.18
Helium	He	0.0005	4.00
Ozone	O_3	0.00006	48.00
Hydrogen	H_2	0.00005	2.02
Krypton	Kr	0.0011	83.80
Xenon	Xe	0.00009	131.3
Methane	CH_4	0.00017	16.05

could be used as a baseline value and once the analysis was complete, the initial value could be subtracted from the final value to show how much CO_2 was produced by the gas turbine. The remaining trace species were not considered significant enough to account for their volume % individually. The ignored species masses were accounted for by lumping them into the N_2 species using equation 3.

$$(x_i * 100)_{N_2} * MW_{N_2} = \left[\sum_i (x_i * 100) * MW_i \right]_{NS} \quad (3)$$

The previous equality states that the adjusted molar percentage of N_2 times the molecular weight of N_2 is equal to the summation of N_2 and each individual trace species molar percentage times the molecular weight of each individual species. The calculations can be found in Appendix A. The adjusted N_2 molar percentage was found to be 78.09.

HUMIDITY ASSUMPTIONS

Since water vapor varies both seasonably and daily in the amount present, some calculations had to be made to estimate the amount present at the time of testing. For chemical calculations, specific humidity must be used, but in terms of environmental conditions, relative humidity is used. For the analysis of this thesis, relative humidity was assumed to be 50% and a standard summer day was assumed to have a temperature of 70ºF. A standard winter day was assumed to have a temperature of 45 ºF. Relative humidity is defined by the following equation.

$$\phi = \frac{P_v}{P_g} \quad (4)$$

The equation above states that the relative humidity is the ratio of the partial pressure of the vapor as it exists in the atmospheric mixture, P_v, to the saturation pressure of the

vapor at the same atmospheric temperature, P_g. Specific humidity is defined by the following equation.

$$\omega = \frac{MW_v}{MW_a} * x_v = \frac{MW_v}{MW_a} * \frac{P_v}{P_a} \quad (5)$$

For water vapor, MW_v=18.02, and for the molecular weight of dry air, MW_a=28.96, which is calculated in Appendix A. P_a is the absolute pressure of the mixture. Thus, specific humidity is given by:

$$\omega = 0.622 * \frac{P_v}{P_a} \quad (6)$$

REFERENCE DAYS

Testing at UTSI occurred all throughout the year. When determining the specific humidity, two reference days were used. One day was assumed to be in the summer and have a temperature of 70ºF. The other reference day was assumed to be in the winter and have a temperature of 45ºF. Both days were assumed to have a relative humidity of 50% as stated earlier. The saturated pressure for these two days was found to be 0.363 psia for the summer day and 0.147 psia for the winter day. Knowing these pressures and using the mean, site-based atmospheric pressure to of 14.3 psia, the specific humidity could be determined using equation 4.3. The specific humidity's for the summer and winter days were calculated to be 0.008 and 0.0032, respectively.

Next, the mass fraction of vapor for each day could be determined by the following equations:

$$m_v = \omega * m_a \quad (7)$$

$$Y_v = \frac{m_v}{m_a + m_v} \tag{8}$$

In the previous equations, m_v denotes the mass of vapor, m_a denotes the mass of air, and Y_v denotes the mass fraction of the vapor. Equation 8 could be simplified to depend only on the specific humidity associated with each day by the following steps:

$$Y_v = \frac{\omega * m_a}{m_a + \omega * m_a} \tag{9}$$

$$Y_v = \frac{\omega * m_a}{m_a (1 + \omega)} \tag{10}$$

$$Y_v = \frac{\omega}{1 + \omega} \tag{11}$$

Finally, the molar fraction could be determined by the following equation, which relates mass fraction to molar fraction.

$$x_v = Y_v * \frac{MW_m}{MW_v} \tag{12}$$

In the previous equation, x_i denotes the vapor molar fraction, Y_i denotes the vapor mass fraction, MW_m denotes the mixture molecular weight, and MW_v denotes the molecular weight of the vapor. The molecular weight of the mixture was determined by the following equation:

$$MW_m = \frac{1}{\frac{Y_a}{MW_a} + \frac{Y_v}{MV_v}} \tag{13}$$

Y_a denotes the mass fraction of air and was determined by the following equation:

$$Y_a = 1 - Y_v \tag{14}$$

In equation 13, MW_a denotes the molecular weight of air. In equation 4.11, Y_a and Y_v depended on the day chosen. The molecular weight of the air mixture for the summer and winter days were calculated to be 28.69 and 28.90, respectively. Once the molecular weight of the mixture was determined for each day, the molar fraction of water vapor could be determined for each day. The molar fractions of water vapor for the summer and winter days were found to be 0.0126 and 0.005, respectively. All the previous calculations can be found in Appendix A.

COMBUSTION AIR

A combustion air model, which would be used in the LSENS program, had to be determined. The first step to determine the composition of the combustion air was to account for the adjusted N_2 value. Table 3 lists the species being considered for the analysis. This composition of air was considered dry combustion air since no water vapor was present. Next, water vapor was added into the mixture. Table 4 list the composition of dry air plus water vapor. In order to normalize the table above, the summer day species were divided by 101.26 and the winter day species were divided by 100.5. Table 5 lists the species and their normalized values for the summer day and the winter day. Once the composition of the air containing water vapor was determined, NASA CEA was used to compare adiabatic flame temperatures for JP-5 and methane. The summer day was chosen as the model day.

One more step was needed to complete the air model. Methane had to be added to the composition and the composition then normalized. The normalized methane-air composition was needed for LSENS input. The first step in determining how much methane was present was to set up a chemical equation which has methane and air as the

Table 3. Species considered for analysis

Component	Symbol	Volume %
Nitrogen	N_2	78.09
Oxygen	O_2	20.95
Argon	Ar	0.93
Carbon Dioxide	CO_2	0.03

Table 4. Composition of Dry Air plus Water Vapor

Component	Symbol	Volume % (Summer)	Volume % (Winter)
Nitrogen	N_2	78.09	78.09
Oxygen	O_2	20.95	20.95
Argon	Ar	0.93	0.93
Carbon Dioxide	CO_2	0.03	0.03
Water Vapor	H_2O	1.26	0.5
Total		101.26	100.5

Table 5. Composition of Dry Air plus Water Vapor (Normalized)

Component	Symbol	Volume % (Summer)	Volume % (Winter)
Nitrogen	N_2	77.12	77.70
Oxygen	O_2	20.69	20.85
Argon	Ar	0.92	0.92
Carbon Dioxide	CO_2	0.03	0.03
Water Vapor	H_2O	1.24	0.5
Mixture Molecular Weight		28.69	28.90

products. The equation can be seen below. The variable *a* could be determined by setting the amount of O_2 present on the reactant side equal to the amount of O_2 present on the product side. The variable *a* was calculated to be 9.667. Once *a* was calculated, the stoichiometric fuel-air ratio, $(f/a)_s$,

$$CH_4 + a*(0.2069O_2 + 0.7712N_2) \rightarrow CO_2 + 2H_2O + a*0.7712N_2 \quad (15)$$

could be calculated and then the equivalence ratio. The stoichiometric condition is achieved when the amount of oxidizer is the amount needed to completely burn a quantity of fuel (Turns 2000). Equations 16 and 17 from (Turns 2000) calculate the fuel-air ratio and the equivalence ratio, *ER*.

$$(f/a)_s = \frac{MW_f}{a*MW_a} \quad (16)$$

$$ER = \frac{(f/a)}{(f/a)_s} \quad (17)$$

To determine the ER, the fuel-air ratio for the engine had to be known. The engine fuel-air ratio remained fairly constant at 0.0175 for the entire engine cycle (Marx 1988). The stoichiometric fuel-air ratio came out to 0.0573 and from this the equivalence ratio was 0.305. The calculations can be found in Appendix A.

The final step in determining how much methane was present was to determine the molar percentage of methane. The first step was to determine the molar stoichiometric fuel air ratio, $\overline{(f/a)_s}$.

$$\overline{(f/a)_s} = \frac{1.0}{a} \quad (18)$$

From (Turns 2000), the molar stoichiometric fuel air ratio was 0.1034 and this value was

used to calculate the operating molar fuel air ratio, $\overline{(f/a)}$.

$$\overline{(f/a)} = ER * \overline{(f/a)_s} \tag{19}$$

The molar fuel air ratio was 0.0310 and this value was used to calculate the moles of methane, x_{CH_4}, in the composition.

$$x_{"air"} = x_{N_2} + x_{O_2} \tag{20}$$

$$x_{CH_4} = x_{"air"} * \overline{(f/a)} \tag{21}$$

The number of moles of methane present were 0.0303. Table 6 shows the composition of air plus methane and the normalized value of each species. The above composition was input into to NASE CEA to show it was thermochemically correct. After proving the composition was thermochemically correct, it was used in LSENS to simulate the primary combustor of the J85. The results from the analysis can be found in Chapter 7.

Table 6. Air composition plus methane

Component	Symbol	Volume % (Summer)	Normalized
Nitrogen	N_2	77.12	74.85
Oxygen	O_2	20.69	20.08
Argon	Ar	0.92	0.90
Carbon Dioxide	CO_2	0.03	0.03
Water Vapor	H_2O	1.24	1.2
Methane	CH_4	3.03	2.94
Total		103.03	100.00

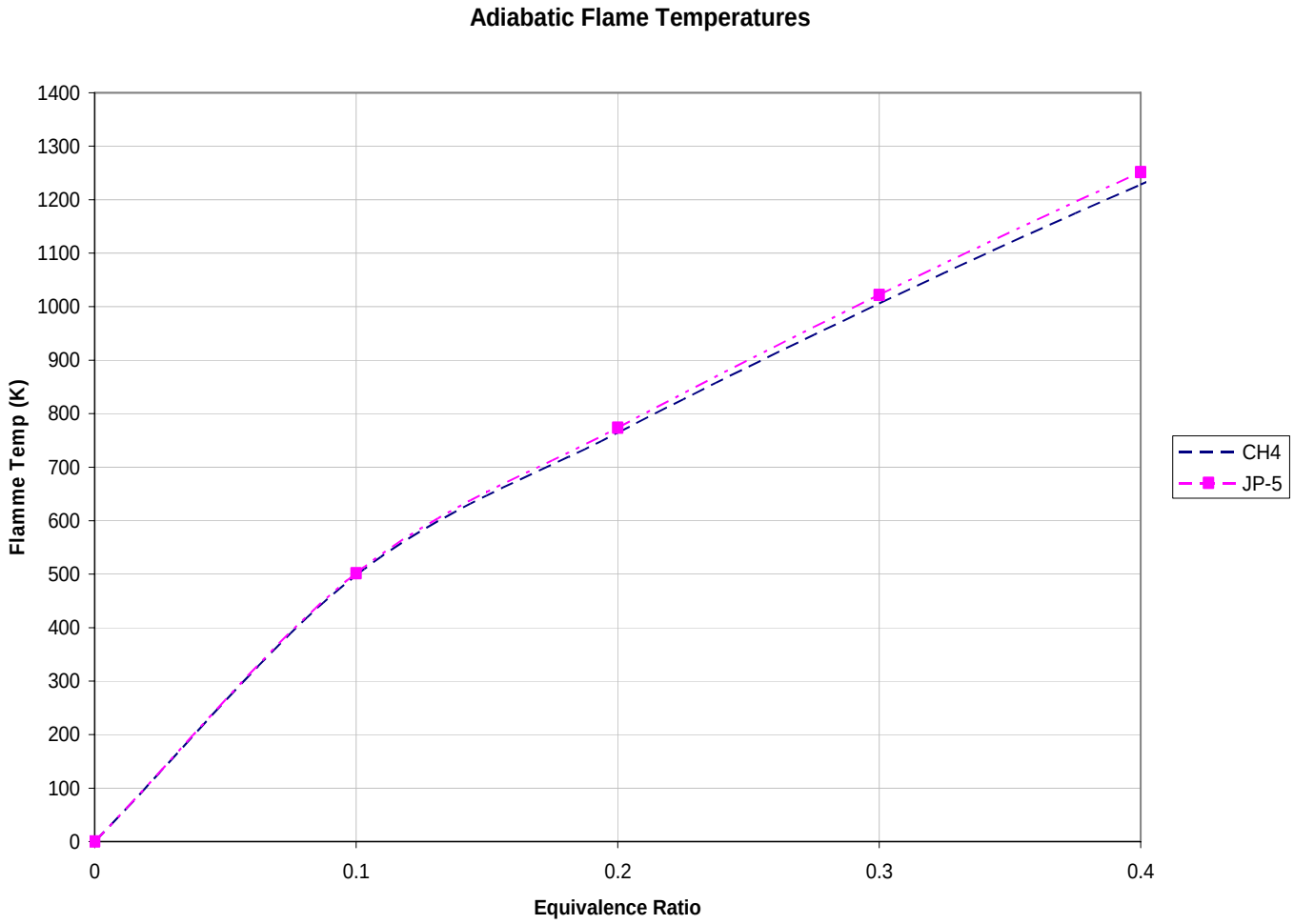
CHAPTER 5: METHANE AS JET FUEL SIMULATOR

ADIABATIC FLAME TEMPERATURE COMPARISON

The reason for selecting the methane-air mechanism for studying the thermochemistry of emissions from JP-5-air combustion will be discussed in more detail. The first comparison dealt with the adiabatic flame temperatures of each fuel. The adiabatic flame temperature is obtained when a fuel-air mixture burns adiabatically at constant pressure such that the absolute enthalpy of the reactants at the initial state equals the absolute enthalpy of the products at the final state (Turns 2000). To compare the adiabatic flame temperatures, the NASA CEA program was used. The composition of the representative air plus water vapor was used for the input to the program. The comparison was done over the equivalence ratio range of 0.1-1.0. Table 7 lists the adiabatic flame temperatures for CH_4 and JP-5 and figure 8 is a graph to show the comparison of adiabatic flame temperatures for each fuel. The graph shows adiabatic flame temperatures over the equivalence range from 0-0.4 since the primary analysis was base on the equivalence ratio of 0.3. As the table and graph show, the adiabatic flame temperatures are relatively close. The % fuel and mole fraction of CO_2 present was also given by the NASA CEA case. The amount of CO_2 for methane and JP-5 were compared and the difference was normalized. Although the amounts of CO_2 vary greatly between the two fuels, the normalized difference was constant over the ER range 0-0.3. The normalized difference can be seen in Figure 9, together with a quadratic polynomial representing the difference which was generated in Excel. The polynomial can be used for an equilibrium correction to the amount of CO_2 predicted for methane to represent the

Table 7. Adiabatic Flame Temperatures

Equivalence Ratio	CH_4 Adiabatic Flame Temp (K)	JP-5 Adiabatic Flame Temp (K)
0.1	497.76	501.41
0.2	764.01	773.59
0.3	1005.92	1022.03
0.4	1228.15	1251.54
0.5	1434.05	1465.5
0.6	1625.58	1665.74
0.7	1803.63	1852.66
0.8	1967.33	2023.51
0.9	2110.79	2167.75
1.0	2207.79	2259.18



Figrure 8. Graph showing adiabatic flame temperatures for JP-5 and methane.

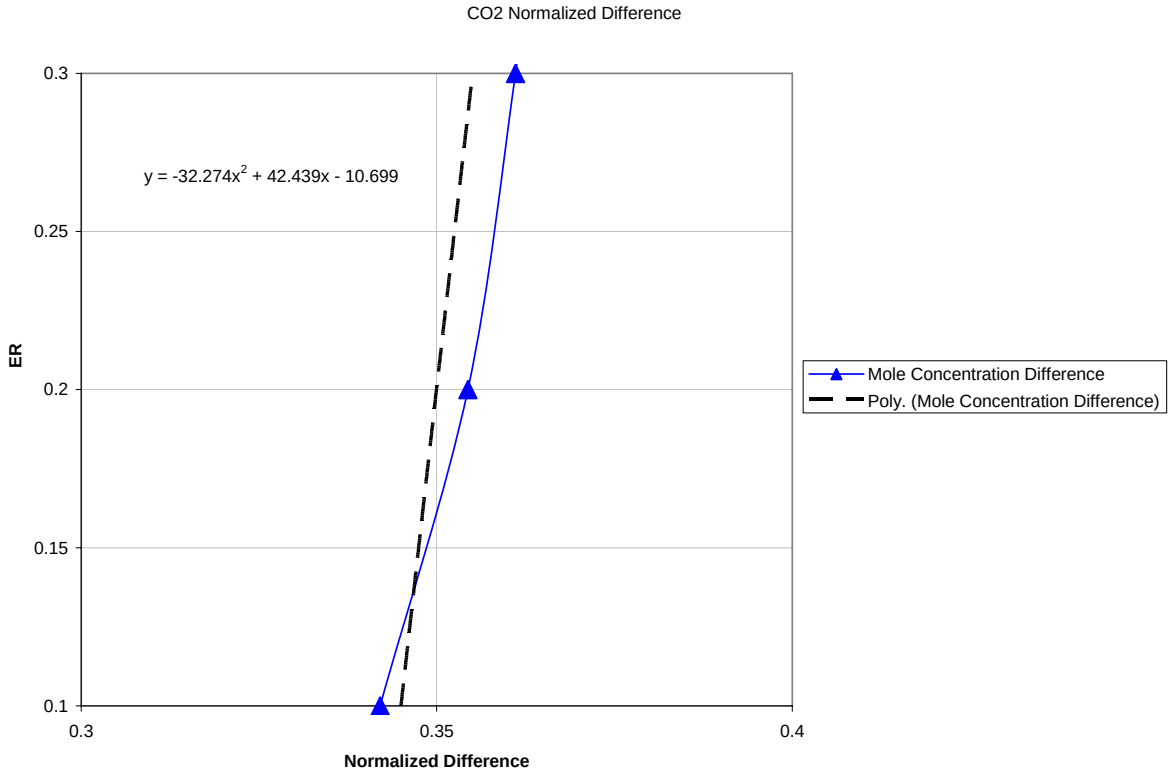


Figure 9. Normalized difference (JP-5 vs. Methane) vs. Equivalence Ratio.

amount of CO_2 produced by JP-5. The full results for the NASA CEA case can be found in Appendix B.

HYDROGEN TO CARBON ATOMS COMPARISON

Three fuels were compared to JP-5 to see how the hydrogen to carbon atoms compared. The three fuels that were of interest were methane, CH_4, propane, C_3H_8, and benzene, C_6H_6. The three fuels were chosen because they each have a reaction mechanism provided with LSENS. The equation used to determine the hydrogen to carbon ratio is shown below.

$$Y_H\% = 100\frac{(H/C)(MW_H)}{MW_C + (H/C)(MW_H)} \tag{22}$$

In the above equation, *(H/C)* represents the moles of H divided by the moles of C, and $Y_H\%$ represents the mass percent ratio of H, which is the mass of H to mass of C in percent. The calculated values for CH_4, C_3H_8, C_6H_6, and JP-5 are 25.15, 18.33, 7.76, and 13.79, respectively. The overall molecular formula for JP-5 is $CH_{1.9}$. As seen from the numbers no fuel is relatively close to JP-5 in hydrogen to carbon atom ratio. It should also be noted that the mass percentage of H in CH_4 is almost twice that of JP-5.

METHANE FORMED IN JET FUEL COMBUSTION

When JP-5 combustion occurs, CH_4 is formed during the process. Figure 10 shows a simple reaction mechanism for JP-5, which shows the formation of CH_4 (Sturgess 1997). The formation of CH_4 occurs in equation 28. Also, equations 4-20 in Figure 10 also occur in the methane oxidation reaction mechanism. Therefore, methane oxidation represent a major part of the combustion process for JP-5.

STEP	REACTION	B_j	N_j	T_j
1.	$C_{12}H_{23} + O_2 \rightarrow 5C_2H_4 + C_2H_3 + O_2$	4.48	1.5	7900
2.	$C_{12}H_{23} + OH \rightarrow 6C_2H_4 + O$	7.3	1.0	4500
3.	$C_2H_4 + H \leftrightarrow C_2H_3 + H_2$	10.48	0.0	9500
4.	$H + H + M \leftrightarrow H_2 + M$	12.3	-1.0	0
5.	$O + O + M \leftrightarrow O_2 + M$	11.0	-1.0	0
6.	$H + OH + M \leftrightarrow H_2O + M$	13.85	-1.0	0
7.	$H + O_2 \leftrightarrow OH + O$	11.35	0.0	8400
8.	$O + H_2 \leftrightarrow OH + H$	10.24	0.0	4730
9.	$CO + OH \leftrightarrow CO_2 + H$	-14.75	7.0	-7000
10.	$H + H_2O \leftrightarrow OH + H_2$	10.92	0.0	10050
11.	$CH_3 + O_2 \leftrightarrow CH_2O + OH$	9.0	0.0	4000
12.	$HO_2 + M \leftrightarrow H + O_2 + M$	12.32	0.0	2300
13.	$HO_2 + H \leftrightarrow 2OH$	9.89	0.0	950
14.	$CH_2O + OH \leftrightarrow H_2O + HCO$	10.90	0.0	2120
15.	$O + H_2O \leftrightarrow 2OH$	10.76	0.0	9000
16.	$N_2 + O \leftrightarrow NO + N$	9.0	0.0	25000
17.	$N + O_2 \leftrightarrow NO + O$	5.0	1.0	2000
18.	$N + OH \leftrightarrow NO + H$	9.0	0.0	0
19.	$HCO + O_2 \leftrightarrow HO_2 + CO$	10.48	0.0	7000
20.	$HCO + OH \leftrightarrow H_2O + CO$	10.30	0.0	0
21.	$C_2H_4 + OH \leftrightarrow C_2H_3 + H_2O$	9.78	0.0	1750
22.	$CH_2O + HO_2 \leftrightarrow HCO + 2OH$	9.0	0.0	4500
23.	$C_2H_2 + HO_2 \leftrightarrow HCO + CH_2O$	9.3	0.0	5500
24.	$C_2H_3 + O_2 \leftrightarrow C_2H_2 + HO_2$	9.23	0.0	5000
25.	$NO + HO_2 \leftrightarrow NO_2 + OH$	3.0	1.0	0
26.	$C_2H_4 + O \leftrightarrow CH_3 + HCO$	9.93	0.0	1500
27.	$C_2H_4 + HO_2 \leftrightarrow CH_3 + HCO + OH$	9.9	0.0	5000
28.	$H_2 + CH_3 \leftrightarrow CH_4 + H$	7.0	-1.5	7140
29.	$C_2H_2 + OH \leftrightarrow CH_3 + CO$	8.2	0.0	2500
30.	$CH_3 + O \leftrightarrow CH_2O + H$	11.11	0.0	1000

Figure 10. JP-5 reaction mechanism showing CH_4 formation (Sturgess 1997).

A study was done by G.J. Sturgess using an abbreviated reaction mechanism for JP-5. Sturgess found that the Kollrack mechanism was a sufficient starting point for an abbreviated reaction mechanism. In the study, Sturgess used a perforated-plate flame holder, and the results of this hybrid modeling showed that this method may be a likely method to estimate the exhaust emissions produced by gas turbine combustion.

SUMMARY

Methane was chosen because the adiabatic flame temperatures are very similar and equilibrium concentrations of CO_2 are almost uniquely relatable over the range of ER anticipated. Also, because methane oxidation steps represents the terminal oxidation steps of JP-5, it was decided to use methane to study the thermochemistry of the emissions from JP-5-air combustion.

CHAPTER 6: RATE MECHANISMS

LSENS

Three sources were used to determine a reasonable rate mechanism for methane-air that could be used to solve the problems at hand. The three sources were 1.) LSENS; 2.) "An Introduction to Combustion" by Steve Turns; and 3.) GRI-Mech 2.1. LSENS came with a methane-air rate mechanism that contained 133 equations and considered 39 species for the problem. This mechanism was the starting point for the methane-oxidation rate mechanism since it was the mechanism that came with the program. The rate mechanism can be seen below in Figure 11. The table below list the reaction number, reaction, and the reaction rate parameters that are given in the LSENS program, circa 1996. This mechanism was studied and the reaction rates were compared to the reaction rates given by GRI-Mech 2.1 (GRI-Mech). GRI-Mech 2.1 will be discussed in a later section. After comparing the reaction rates of each mechanism, the following LSENS reactions and their reaction rates were altered to match those of GRI-Mech 2.1. Figure 12 shows the reactions with the altered reaction rates.

TURNS

The next step to investigate the reaction mechanism was to compare it with the reaction mechanism given in An Introduction to Combustion by Steven Turns. The LSENS mechanism had about half the number of equations as the Turns mechanism (Table 5.3, pg. 159-165). Not all equations from the Turns mechanism were added to the LSENS mechanism. Figure 13 shows the equations that were added to the LSENS

	Reaction	Reaction Rate Parameters		
		A_j	n_j	E_j
1	CH4 + M = CH3 + H + M	2.00E+17	0.00	8.80E+04
2	H + CH4 = CH3 + H2	1.26E+14	0.00	1.19E+04
3	CH4 + O2 = CH3 + HO2	7.94E+13	0.00	5.60E+04
4	O + CH4 = CH3 + OH	1.90E+14	0.00	1.17E+04
5	OH + CH4 = CH3 + H2O	2.50E+13	0.00	5.01E+03
6	CH3 + O2 = CH3O + O	2.40E+13	0.00	2.87E+04
7	CH3 + OH = CH3O + H	6.30E+12	0.00	0.00E+00
8	CH3O + M = CH2O + H + M	5.00E+13	0.00	2.10E+04
9	2CH3 = C2H6	2.40E+14	-0.40	0.00E+00
10	H + C2H6 = C2H5 + H2	1.32E+14	0.00	9.70E+03
11	O + C2H6 = C2H5 + OH	1.13E+14	0.00	7.85E+03
12	OH + C2H6 = C2H5 + H2O	8.70E+13	0.00	3.52E+03
13	C2H5 + M = C2H4 + H + M	1.00E+17	0.00	3.10E+04
14	C2H5 + O2 = C2H4 + HO2	2.00E+12	0.00	5.00E+03
15	H + C2H5 = C2H4 + H2	4.80E+13	0.00	0.00E+00
16	CH3 + CH2 = C2H4 + H	2.00E+13	0.00	0.00E+00
17	H + C2H4 = H2 + C2H3	1.50E+14	0.00	1.02E+04
18	C2H4 + M = C2H2 + H2 + M	2.60E+17	0.00	7.93E+04
19	C2H4 + OH = C2H3 + H2O	4.80E+12	0.00	1.23E+03
20	C2H4 + OH = CH3 + CH2O	2.00E+12	0.00	9.60E+02
21	C2H4 + O = CH3 + HCO	3.30E+12	0.00	1.13E+03
22	C2H4 + O = CH2O + CH2	2.50E+13	0.00	5.00E+03
23	C2H3 + M = C2H2 + H + M	3.00E+15	0.00	3.20E+04
24	C2H3 + O2 = CH2O + HCO	3.98E+12	0.00	-2.50E+02
25	C2H3 + H = C2H2 + H2	6.00E+12	0.00	0.00E+00
26	C2H3 + O = C2H2O + H	3.30E+13	0.00	0.00E+00
27	C2H3 + OH = C2H2 + H2O	5.00E+12	0.00	0.00E+00
28	C2H3 + CH2 = C2H2 + CH3	3.00E+13	0.00	0.00E+00
29	C2H3 + C2H = 2C2H2	3.00E+13	0.00	0.00E+00
30	C2H2 + M = C2H + H + M	4.20E+16	0.00	1.07E+05
31	C2H2 + O = CH2 + CO	1.60E+14	0.00	9.89E+03
32	C2H2 + O = C2HO + H	4.00E+14	0.00	1.07E+04
33	C2H2 + OH = C2H + H2O	6.30E+12	0.00	7.00E+03
34	C2H2 + OH = C2H2O + H	3.20E+11	0.00	2.00E+02
35	C2H + O2 = C2HO + O	5.00E+13	0.00	1.50E+03
36	C2H + OH = C2HO + H	2.00E+13	0.00	0.00E+00
37	C2HO + O2 = 2CO + OH	1.46E+12	0.00	2.50E+03
38	C2HO + O = 2CO + H	1.20E+12	0.00	0.00E+00
39	C2HO + OH = 2HCO	1.00E+13	0.00	0.00E+00
40	C2HO + H = CH2 + CO	5.00E+13	0.00	0.00E+00
41	C2HO + CH2 = C2H3 + CO	3.00E+13	0.00	0.00E+00
42	C2HO + CH2 = CH2O + C2H	1.00E+13	0.00	2.00E+03
43	2C2HO = C2H2 + 2CO	1.00E+13	0.00	0.00E+00
44	C2H2O + OH = CH2O + HCO	2.80E+13	0.00	0.00E+00
45	C2H2O + OH = C2HO + H2O	7.50E+12	0.00	3.00E+03
46	C2H2O + H = CH3 + CO	1.13E+13	0.00	3.43E+03
47	C2H2O + H = C2HO + H2	7.50E+13	0.00	8.00E+03
48	C2H2O + O = C2HO + OH	5.00E+13	0.00	8.00E+03
49	C2H2O + O = CH2O + CO	2.00E+13	0.00	0.00E+00
50	C2H2O + M = CH2 + CO + M	2.00E+16	0.00	6.00E+04
51	C2H + O = CO + CH	5.00E+13	0.00	0.00E+00
52	CH3O + O2 = CH2O + HO2	1.00E+13	0.00	7.17E+03
53	CH3O + H = CH2O + H2	2.00E+13	0.00	0.00E+00
54	CH2O + M = HCO + H + M	5.00E+16	0.00	8.10E+04
55	CH2O + OH = HCO + H2O	3.00E+13	0.00	1.20E+03
56	CH2O + H = HCO + H2	2.50E+13	0.00	3.99E+03
57	CH2O + O = HCO + OH	3.50E+13	0.00	3.51E+03
58	CH3 + CH2O = CH4 + HCO	1.00E+10	0.50	6.00E+03
59	CH3 + HCO = CH4 + CO	3.00E+11	0.50	0.00E+00
60	CH3 + HO2 = CH3O + OH	2.00E+13	0.00	0.00E+00
61	CH3 + M = CH2 + H + M	1.95E+16	0.00	9.16E+04
62	H + CH3 = H2 + CH2	2.70E+11	0.67	2.57E+04
63	O + CH3 = OH + CH2	1.90E+11	0.68	2.57E+04

Figure 11. LSENS Rate Mechanism

```
 64 OH + CH3 = H2O + CH2                    2.70E+11  0.67  2.57E+04
 65 CH + CO2 = HCO + CO                     3.70E+12  0.00  0.00E+00
 66 CH + O2 = HCO + O                       1.00E+13  0.00  0.00E+00
 67 CH2 + O2 = CH2O + O                     5.00E+11  0.50  6.96E+03
 68 CH2 + O = CH + OH                       2.00E+11  0.70  2.58E+04
 69 CH2 + OH = CH + H2O                     5.00E+11  0.50  5.90E+03
 70 CH2 + H = CH + H2                       3.20E+11  0.70  4.97E+03
 71 2CH2 = C2H3 + H                         5.00E+12  0.00  0.00E+00
 72 2CH2 = C2H2 + H2                        4.00E+13  0.00  0.00E+00
 73 HCO + O2 = CO + HO2                     3.00E+13  0.00  0.00E+00
 74 HCO + O = CO + OH                       3.00E+13  0.00  0.00E+00
 75 HCO + OH = CO + H2O                     3.00E+13  0.00  0.00E+00
 76 HCO + H = CO + H2                       2.00E+13  0.00  0.00E+00
 77 HCO + M = H + CO + M                    2.90E+14  0.00  1.56E+04
 78 CO + O + M = CO2 + M                    2.40E+15  0.00  4.10E+03
 79 CO + O2 = CO2 + O                       2.50E+12  0.00  4.77E+04
 80 CO + OH = CO2 + H                       4.17E+11  0.00  1.00E+03
 81 CO + HO2 = CO2 + OH                     5.75E+13  0.00  2.29E+04
 82 O + H2O = 2OH                           6.80E+13  0.00  1.84E+04
 83 H + O2 = OH + O                         1.89E+14  0.00  1.64E+04
 84 O + H2 = OH + H                         4.20E+14  0.00  1.38E+04
 85 H + HO2 = H2 + O2                       7.28E+13  0.00  2.13E+03
 86 O + HO2 = OH + O2                       5.00E+13  0.00  1.00E+03
 87 HO2 + OH = H2O + O2                     8.00E+12  0.00  0.00E+00
 88 H + HO2 = 2OH                           1.34E+14  0.00  1.07E+03
 89 H2 + HO2 = H2O2 + H                     7.91E+13  0.00  2.50E+04
 90 OH + H2O2 = H2O + HO2                   6.10E+12  0.00  1.43E+03
 91 2HO2 = H2O2 + O2                        1.80E+12  0.00  0.00E+00
 92 H + H2O2 = OH + H2O                     7.80E+11  0.00  0.00E+00
 93 H2O2 + M = 2OH + M                      1.44E+17  0.00  4.55E+04
 94 H2 + OH = H2O + H                       4.74E+13  0.00  6.10E+03
 95 H + O2 + M = HO2 + M                    1.46E+15  0.00 -1.00E+03
 96 H2O + M = H + OH + M                    1.30E+15  0.00  1.05E+05
 97 H + O + M = OH + M                      7.10E+18 -1.00  0.00E+00
 98 H2 + M = 2H + M                         2.20E+14  0.00  9.60E+04
 99 O2 + M = 2O + M                         1.80E+18 -1.00  1.18E+05
100 CH + N2 = HCN + N                       1.00E+11  0.00  1.90E+04
101 CN + H2 = HCN + H                       6.00E+13  0.00  5.30E+03
102 O + HCN = OH + CN                       1.40E+11  0.68  1.69E+04
103 OH + HCN = HNCO + H                     4.00E+11  0.00  2.80E+03
104 CN + O = CO + N                         1.20E+13  0.00  0.00E+00
105 CN + OH = NCO + H                       2.50E+14  0.00  6.00E+03
106 H2 + NCO = HNCO + H                     1.00E+14  0.00  9.00E+03
107 HNCO + H = NH2 + CO                     1.00E+14  0.00  8.50E+03
108 CN + O2 = NCO + O                       3.20E+13  0.00  1.00E+03
109 CN + CO2 = NCO + CO                     3.70E+12  0.00  0.00E+00
110 O + NCO = NO + CO                       2.00E+13  0.00  0.00E+00
111 N + NCO = N2 + CO                       1.00E+13  0.00  0.00E+00
112 H + NCO = NH + CO                       2.00E+13  0.00  0.00E+00
113 CH + NO = N + HCO                       1.60E+13  0.00  9.94E+03
114 CH + NO = O + HCN                       2.00E+12  0.00  0.00E+00
115 NH + OH = N + H2O                       5.00E+11  0.50  2.00E+03
116 HO2 + NO = NO2 + OH                     2.09E+12  0.00 -4.77E+02
117 O + NO2 = NO + O2                       1.00E+13  0.00  5.96E+02
118 NO + O + M = NO2 + M                    5.62E+15  0.00 -1.16E+03
119 NO2 + H = NO + OH                       3.47E+14  0.00  1.47E+03
120 NO + H = N + OH                         2.63E+14  0.00  5.04E+04
121 NO + O = N + O2                         3.80E+09  1.00  4.14E+04
122 O + N2 = NO + N                         1.80E+14  0.00  7.63E+04
123 N + NO2 = 2NO                           4.00E+12  0.00  0.00E+00
124 N2O + M = N2 + O + M                    6.92E+23 -2.50  6.50E+04
125 O + N2O = N2 + O2                       1.00E+14  0.00  2.80E+04
126 O + N2O = 2NO                           6.92E+13  0.00  2.66E+04
127 N2O + H = N2 + OH                       7.59E+13  0.00  1.51E+04
128 NO2 + H2 = HNO2 + H                     2.40E+13  0.00  2.90E+04
129 OH + NO2 + M = HNO3 + M                 3.00E+15  0.00 -3.80E+03
```

Figure 11. LSENS Rate Mechanism (Cont.)

```
130 OH + NO + M = HNO2 + M                              5.60E+15  0.00 -1.70E+03
131 HNO + H = H2 + NO                                   5.00E+12  0.00  0.00E+00
132 H + NO + M = HNO + M                                5.40E+15  0.00 -6.00E+02
133 HNO + OH = H2O + NO                                 3.60E+13  0.00  0.00E+00
```

Figure 11. LSENS Rate Mechanism (Cont.)

	Reaction	Reaction Rate Parameters		
		A_j	n_j	E_j
2	H + CH4 = CH3 + H2	6.60E+08	1.62	1.08E+04
3	CH4 + O2 = CH3 + HO2	1.00E+12	0.00	0.00E+00
4	O + CH4 = CH3 + OH	1.02E+09	1.50	8.60E+03
5	OH + CH4 = CH3 + H2O	1.00E+08	1.60	3.12E+03
6	CH3 + O2 = CH3O + O	2.68E+13	0.00	2.88E+04
7	CH3 + OH = CH3O + H	3.20E+13	0.00	0.00E+00
10	H + C2H6 = C2H5 + H2	1.15E+08	1.90	7.53E+03
11	O + C2H6 = C2H5 + OH	8.98E+07	1.92	5.69E+03
12	OH + C2H6 = C2H5 + H2O	3.54E+06	2.12	8.70E+02
14	C2H5 + O2 = C2H4 + HO2	8.40E+11	0.00	3.88E+03
15	H + C2H5 = C2H4 + H2	2.00E+12	0.00	0.00E+00
17	H + C2H4 = H2 + C2H3	1.33E+06	2.53	1.22E+04
19	C2H4 + OH = C2H3 + H2O	3.60E+06	2.00	2.50E+03
21	C2H4 + O = CH3 + HCO	1.92E+07	1.83	2.20E+02
24	C2H3 + O2 = CH2O + HCO	3.98E+12	0.00	-2.40E+02
25	C2H3 + H = C2H2 + H2	3.00E+13	0.00	0.00E+00
26	C2H3 + O = C2H2O + H	3.00E+13	0.00	0.00E+00
31	C2H2 + O = CH2 + CO	1.02E+07	2.00	1.90E+03
32	C2H2 + O = C2HO + H	1.02E+07	2.00	1.90E+03
33	C2H2 + OH = C2H + H2O	3.37E+07	2.00	1.40E+04
34	C2H2 + OH = C2H2O + H	5.04E+05	2.30	1.35E+04
37	C2HO + O2 = 2CO + OH	1.60E+12	0.00	8.54E+02
38	C2HO + O = 2CO + H	1.00E+14	0.00	0.00E+00
45	C2H2O + OH = C2HO + H2O	7.50E+12	0.00	2.00E+03
47	C2H2O + H = C2HO + H2	5.00E+13	0.00	8.00E+03
48	C2H2O + O = C2HO + OH	1.00E+13	0.00	8.00E+03
52	CH3O + O2 = CH2O + HO2	4.28E-13	7.60	-3.53E+03
55	CH2O + OH = HCO + H2O	3.43E+09	1.18	-4.47E+02
56	CH2O + H = HCO + H2	2.30E+10	1.05	3.28E+03
57	CH2O + O = HCO + OH	3.90E+13	0.00	3.54E+03
58	CH3 + CH2O = CH4 + HCO	3.32E+03	2.81	5.86E+03
59	CH3 + HCO = CH4 + CO	2.65E+13	0.00	0.00E+00
64	OH + CH3 = H2O + CH2	5.60E+07	1.60	5.42E+03
65	CH + CO2 = HCO + CO	3.40E+12	0.00	6.90E+02
66	CH + O2 = HCO + O	3.30E+13	0.00	0.00E+00
69	CH2 + OH = CH + H2O	1.13E+07	2.00	3.00E+03
72	2CH2 = C2H2 + H2	3.20E+13	0.00	0.00E+00
73	HCO + O2 = CO + HO2	7.60E+12	0.00	4.00E+02
75	HCO + OH = CO + H2O	5.00E+13	0.00	0.00E+00
76	HCO + H = CO + H2	7.34E+13	0.00	0.00E+00
77	HCO + M = H + CO + M	1.87E+17	-1.00	1.70E+04
78	CO + O + M = CO2 + M	6.02E+14	0.00	3.00E+03
79	CO + O2 = CO2 + O	2.50E+12	0.00	4.78E+04
80	CO + OH = CO2 + H	4.76E+07	1.23	7.00E+01
81	CO + HO2 = CO2 + OH	1.50E+14	0.00	2.36E+04
83	H + O2 = OH + O	8.30E+13	0.00	1.44E+04
84	O + H2 = OH + H	5.00E+04	2.67	6.29E+03
85	H + HO2 = H2 + O2	2.80E+13	0.00	1.07E+03
86	O + HO2 = OH + O2	2.00E+13	0.00	0.00E+00
87	HO2 + OH = H2O + O2	2.90E+13	0.00	-5.00E+02
88	H + HO2 = 2OH	1.34E+14	0.00	6.35E+02
89	H2 + HO2 = H2O2 + H	1.21E+07	2.00	5.20E+03
90	OH + H2O2 = H2O + HO2	1.75E+12	0.00	3.20E+02
91	2HO2 = H2O2 + O2	1.30E+11	0.00	-1.63E+03
92	H + H2O2 = OH + H2O	1.00E+13	0.00	3.60E+03

Figure 12. Original LSENS reactions with improved reaction rates.

```
 94 H2 + OH = H2O + H                    2.16E+08  1.51  3.43E+03
 95 H + O2 + M = HO2 + M                 2.80E+18 -0.86  0.00E+00
 97 H + O + M = OH + M                   5.00E+17 -1.00  0.00E+00
101 CN + H2 = HCN + H                    2.10E+13  0.00  4.71E+03
102 O + HCN = OH + CN                    2.13E+09  1.58  2.66E+04
103 OH + HCN = HNCO + H                  4.40E+03  2.26  6.40E+03
104 CN + O = CO + N                      7.70E+13  0.00  0.00E+00
105 CN + OH = NCO + H                    4.00E+13  0.00  0.00E+00
107 HNCO + H = NH2 + CO                  2.25E+07  1.70  3.80E+03
108 CN + O2 = NCO + O                    6.14E+12  0.00 -4.40E+02
110 O + NCO = NO + CO                    2.35E+13  0.00  0.00E+00
111 N + NCO = N2 + CO                    2.00E+13  0.00  0.00E+00
112 H + NCO = NH + CO                    5.40E+13  0.00  0.00E+00
113 CH + NO = N + HCO                    3.00E+13  0.00  0.00E+00
114 CH + NO = O + HCN                    5.00E+13  0.00  0.00E+00
115 NH + OH = N + H2O                    2.00E+09  1.20  0.00E+00
116 HO2 + NO = NO2 + OH                  2.11E+12  0.00 -4.80E+02
117 O + NO2 = NO + O2                    3.90E+12  0.00 -2.40E+02
118 NO + O + M = NO2 + M                 1.06E+20 -1.41  0.00E+00
119 NO2 + H = NO + OH                    1.32E+14  0.00  3.60E+02
125 O + N2O = N2 + O2                    1.40E+12  0.00  1.08E+04
126 O + N2O = 2NO                        2.90E+13  0.00  2.32E+04
127 N2O + H = N2 + OH                    4.40E+14  0.10  1.89E+04
131 HNO + H = H2 + NO                    4.50E+11  0.72  6.60E+02
132 H + NO + M = HNO + M                 8.95E+19 -1.32  7.40E+02
133 HNO + OH = H2O + NO                  1.30E+07  1.90 -9.50E+02
```

Figure 12. Original LSENS reactions with improved reaction rates. (Cont.)

	Reaction	Reaction Rate Parameters		
		A_j	n_j	E_j
1	CH3 + O2 = OH + CH2O	3.60E+10	0.00	8.94E+03
2	2CH3 = H + C2H5	4.99E+12	0.10	1.06E+04
3	C2H2 + O = OH + C2H	4.60E+19	-1.41	2.90E+04
4	C2H2 + OH = CH2CO + H	2.18E-04	4.50	-1.00E+03
5	C2H2 + OH = CH3 + CO	4.83E-04	4.00	-2.00E+03
6	C2H + O2 = HCO + CO	5.00E+13	0.00	1.50E+03
7	C2H2O + O = CH2 + CO2	1.75E+12	0.00	1.35E+03
8	O + CH3 = H + CH2O	8.43E+13	0.00	0.00E+00
9	CH2 + O2 = OH + HCO	1.32E+13	0.00	1.50E+03
10	HCO + O = CO2 + H	3.00E+13	0.00	0.00E+00
11	O + HCN = NCO + H	1.11E+04	2.64	4.98E+03
12	O + HCN = NH + CO	2.77E+03	2.64	4.98E+03
13	CH + NO = H + NCO	2.00E+13	0.00	0.00E+00
14	NH + OH = HNO + H	2.00E+13	0.00	0.00E+00

Figure 13. Turns reactions added to LSENS mechanism.

mechanism from the Turns mechanism. The previous equations were added to improve the CO_2 reaction steps, the CO oxidation steps, and the NO oxidation steps.

GRI-MECH 2.1

GRI stands for Gas Research Institute, which is the sponsor for the GRI-Mech project that was carried out on the campuses of The University of California at Berkeley, Stanford University, The University of Texas at Austin, and SRI International. GRI-Mech is a web based collection of chemical reactions and the rate constants associated with each reaction. Majority of the reactions have been studied in a laboratory so the reaction rates provided by GRI-Mech have been studied and verified. Once the reactions and rate constants are determined, sensitivity runs are compared to experimental data associated with natural gas ignition flame propagation and structures in order to chose those rates which have a significant impact and improve the data comparisons. The next step to improve the reaction rates consists of putting the parameters through an optimization process, and this process is done using a computer to perform the sensitivity studies. The computer program is bounded by precise constraints that are based on uncertainty data, taken during the laboratory testing, and reaction rate theory. The final step in optimizing the rates is to compare the optimized rates to the literature and examine the thermochemistry of free radicals that are found in the mechanism. The mechanism files created once the reactions and the associated rates are determined can be used with either LSENS or by alternate finite-rate chemistry programs (GRI-Mech).

Although there are at present more recent reaction mechanisms for methane oxidation, for example, GRI 3.0 and beyond, it was decided to use the GRI 2.1 mechanism with the modification listed in (Turns 2000), to study the thermochemistry of

the exhaust samples. GRI 2.1 was determined sufficient enough since a thermochemistry analysis was needed. Future studies can implement the more recent versions of the GRI mechanism for methane oxidation.

CHAPTER 7: RESULTS AND DISCUSSION

EQUILIBIUM ANALYSIS OF EXTRACTED SAMPLE

The NASA CEA program was used to determine the equilibrium state of the JP-5 and air reaction. The composition of air including water vapor developed in Chapter 4 was input as the reactant for the problem and JP-5 was input as the fuel. The initial temperature and pressure were 1437 R and 14.3 psia, respectively. Table 8 shows the results obtained from the NASA CEA case and the results obtained from engine testing. From looking at the table, it can be seen that the equilibrium state and the measured state of the engine are not relatively close. The NASA CEA equilibrium state shows that the actual engine exhaust gas is not chemically at equilibrium.

FINITE RATE ANALYSIS OF EXTRACTED SAMPLE

The LSENS program was used to analyze the chemistry of measured, extracted gas emission samples. To simulate the sample line, a constant temperature of 150ºC was used. Also, the transfer tube cross-section area was held constant and the sample line length of 100 ft. was used. The finite rate analysis of the extracted sample verified the assumption that the flow is chemically frozen in the sample line. Since the extracted sample line flow is predicted to be chemically frozen in the sample line, the methods used by AEDC to extract and measure the exhaust samples appears appropriate, and seem to have no major effect on the sample concentrations. The first case to be run using LSENS used a set of original sample data taken during testing. The full set of data for the LSENS case can be seen in Appendix C and is labeled sample line analysis-original data. The second case that was run involved doubling the CO and NO_2 and cutting the CO_2 in

Table 8. NASA CEA equilibrium case vs. measured engine data.

	Mole Fractions	
Species	**NASA CEA**	**Measured**
N_2	0.75708	0.760754
CO_2	0.03845	0.023355
CO	0.00000	0.002340
O_2	0.14664	0.163379
Ar	0.00903	N/A

half in the initial mixtures. After running these cases through LSENS it again predicted that the flow through the sample line is chemically frozen. The amount of CO, CO_2, and NO_2 remained essentially constant as the sample traversed the line running from the rake to the MGA. The full results can be seen in Appendix C and is labeled as sample line analysis – CO & NO_2 doubled, CO_2 cut in half.

FINITE RATE ANALYSIS OF REACTION IN NON-AFTER-BURNING FLOW IN J85 AUGMENTOR

The LSENS program was also used to simulate non-afterburning augmenter flow. The augmenter length was determined to be 5.75 ft. and have an area of 1.507 ft^2. The initial temperature and pressure were 800 K and 14.3 psi, respectively, corresponding to engine idle conditions. The initial temperature is assumed to be the same as the exhaust gas temperature which was obtained from typical J85 test data. The final input requirement was the Mach number and it was estimated to be 0.07. All the previous values are based on the engine operating at idle conditions. The finite rate analysis of the

reactions in the augmenter also predicted that the flow was chemically frozen once it exited the turbine and entered the augmenter. The previous statement applies only for non-afterburning stages of the testing. The flow was determined to be frozen since very high temperatures, in the range of 2200 R, had to be reached before any reactions between the methane and air started to occur. No study was done on the afterburning stage and the effect it would have on the reactions as they traversed down the augmenter. The calculations made with LSENS have verified that sample extraction methods used by AEDC had no significant effect on the chemistry of the samples. The full results can be seen in Appendix C and are labeled as augmenter analysis – methane.

FINITE RATE PERFECTLY STIRRED REACTOR ANALYSIS OF J85 COMBUSTOR

A perfectly stirred reactor analysis was done using a volume proportional to the volume of the J85 engine primary combustor. Once the auto ignition temperature was reached, reactions began to take place in the PSR. The amount of CO_2 produced in the PSR outlet flow had a mole fraction of 0.02762 moles. The mole fraction of the CO_2 measured in the actual engine exhaust was 0.023355. The above results are in poor comparison, since JP-5 produces more CO_2 than methane under expected, similar flame conditions. The case was run several more times to see if a higher or lower temperature would produce less CO_2 than that produced by the actual engine. A higher temperature produced more CO_2 and a lower temperature would not allow for the PSR calculations to take place because no reactions were occurring.

CHAPTER 8: CONCLUSIONS AND RECOMMENDATIONS FOR FUTURE WORK

SUMMARY

Operation of a GE-J85 jet engine takes place in a test bay located on the UTSI campus for a variety of reasons. One reason is the development of an exhaust gas species emissions measuring systems. Typically, during such operation, the engine is constantly monitored and exhaust species are extracted using a designed sample-probe rake. The gas samples are extracted and transported to a MGA which records the amount of certain species present in the exhaust. The research done in this thesis was an investigation to predict whether or not the extracted exhaust gas chemistry changes due to the sample extraction and cooling process that transports the samples to the MGA. To accomplish this, in the present study, extracted gas sample species data were obtained and used as inputs for the NASA CEA and LSENS programs to evaluate any potential sampling effects. The equilibrium and measured state of the samples were not relatively close. LSENS was next used to analyze the chemistry of the gas species as they traversed the sample line. Two separate cases were run to validate the quenching process used by AEDC. After completing the analysis, the conclusion is that testing methods used by AEDC at the UTSI test bed are effectively non-disturbing and the extracted samples are correct. LSENS was also used to analyze the gas samples as they traversed the augmenter under non-after-burning, engine idle operation. The previous case determined the flow in the augmenter to be chemically frozen. The final LSENS case modeled a perfectly stirred reactor to investigate whether the levels of species concentrations

measured were entirely due to chemical kinetics. The PSR output given by the LSENS case did not correlate well with the assumptions mad earlier in the thesis.

RECOMMENDATIONS

For future work, an actual JP-5 reaction mechanism would be useful and allow for a more accurate analysis of the PSR representation of the combustor of the J85 turbojet engine. Another idea for the future would be to model the combustor as a series of interacting plug flows and perfectly stirred reactors. Once the PSR model has been optimized, a case to model the J85 turbine can be introduced to improve results. Also, the chemical kinetics of a fully-afterburning augmenter case must be studied. One final recommendation would be to update the reaction mechanism with GRI-Mech 3.0.

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APPENDIX

APPENDIX A

CALCULATIONS

Amount of N_2 in extracted sample.

$$x_{N_2} = 1 - (x_{CO} + x_{CO_2} + x_{H_2O} + x_{O_2} + x_{HC} + x_{NO_2})$$
$$x_{N_2} = 1 - (0.002340 + 0.023355 + 0.050055 + 0.163379 + 0.000116 + 0.000001)$$
$$x_{N_2} = 0.760754$$

Adjusted N_2 value to account for trace species.

$$(x_i * 100)_{N_2} * MW_{N_2} = \left[\sum_i (x_i * 100) * MW_i \right]_{NS}$$
$$(x_i * 100)_{N_2} * 28.02 = 78.08*28.02+0.0018*20.18+0.0005*4.00+0.00006*48.00+0.00005 * 2.02+0.0011*83.80+0.00009*131.3+0.00017*16.05$$
$$(x_i * 100)_{N_2} * 28.02 = 2187.95$$
$$(x_i * 100)_{N_2} = 78.09 \text{ or}$$
$$x_{i\,N_2} = 0.7809$$

Molecular weight of air.

$$MW_A * 100 = \sum_i (x_i * 100) * MW_i$$
$$MW_A * 100 = 78.09 * 28.02 + 20.9*32.00+0.93*39.88+0.035*44.00$$
$$MW_A * 100 = 2895.51$$
$$MW_A = 28.96$$

Specific humidity for summer day.

$$\omega_s = 0.622 * \frac{P_v}{P_a}$$
$$\omega_s = \frac{0.622 * (0.5 * 0.363)}{(14.30 - 0.50 * 0.363)}$$
$$\omega_s = 0.0080$$

Specific humidity for winter day.

$$\omega_w = 0.622 * \frac{P_v}{P_a}$$
$$\omega_w = \frac{0.622 * (0.5 * 0.147)}{(14.30 - 0.50 * 0.147)}$$

$\omega_w = 0.0032$

Water vapor mass fraction for summer day.

$$Y_{v_s} = \frac{\omega}{1+\omega}$$
$$Y_{v_s} = \frac{0.008}{1+0.008}$$
$$Y_{v_s} = 0.0079$$

Water vapor mass fraction for winter day.

$$Y_{v_w} = \frac{\omega}{1+\omega}$$
$$Y_{v_w} = \frac{0.0032}{1+0.0032}$$
$$Y_{v_w} = 0.0032$$

Air mass fraction for summer day

$$Y_a = 1 - Y_v$$
$$Y_a = 1 - 0.0079$$
$$Y_a = 0.9921$$

Air mass fraction for winter day

$$Y_a = 1 - Y_v$$
$$Y_a = 1 - 0.0032$$
$$Y_a = 0.9968$$

Molecular weight of mixture (air and water vapor) for summer day

$$MW_m = \frac{1}{\frac{Y_a}{MW_a} + \frac{Y_v}{MV_v}}$$
$$MW_m = \frac{1}{\frac{0.9921}{28.96} + \frac{.0079}{18.02}}$$
$$MW_m = 28.82$$

Molecular weight of mixture (air and water vapor) for winter day

$$MW_m = \frac{1}{\frac{Y_a}{MW_a} + \frac{Y_v}{MV_v}}$$

$$MW_m = \frac{1}{\frac{0.9968}{28.96} + \frac{0.0032}{18.02}}$$

$$MW_m = 28.90$$

Water vapor mole fraction for summer day

$$x_v = Y_v * \frac{MW_m}{MW_v}$$

$$x_v = .0079 * \frac{28.69}{18.02}$$

$$x_v = 0.0126$$

Water vapor mole fraction for summer day

$$x_v = Y_v * \frac{MW_m}{MW_v}$$

$$x_v = .0032 * \frac{28.90}{18.02}$$

$$x_v = 0.0051$$

Mass percent ratio of H (Methane)

$$Y_H\,\% = 100\frac{(H/C)(MW_H)}{MW_C + (H/C)(MW_H)}$$

$$Y_H\,\% = 100\frac{(4/1)(1.01)}{12 + (4/1)(1.01)}$$

$$Y_H\,\% = 25.15$$

Mass percent ratio of H (Propane)

$$Y_H\% = 100\frac{(H/C)(MW_H)}{MW_C + (H/C)(MW_H)}$$

$$Y_H\% = 100\frac{(8/3)(1.01)}{12 + (8/3)(1.01)}$$

$$Y_H\% = 18.33$$

Mass percent ratio of H (Benzene)

$$Y_H\% = 100\frac{(H/C)(MW_H)}{MW_C + (H/C)(MW_H)}$$

$$Y_H\% = 100\frac{(6/6)(1.01)}{12 + (6/6)(1.01)}$$

$$Y_H\% = 7.76$$

Mass percent ratio of H (JP-5)

$$Y_H\% = 100\frac{(H/C)(MW_H)}{MW_C + (H/C)(MW_H)}$$

$$Y_H\% = 100\frac{(1.9/1)(1.01)}{12 + (1.9/1)(1.01)}$$

$$Y_H\% = 13.79$$

APPENDIX B

NASA CEA

Adiabatic Flame Temperatures for Methane-Air

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        NASA-GLENN CHEMICAL EQUILIBRIUM PROGRAM CEA, AUGUST 30, 1999
                  BY  BONNIE MCBRIDE AND SANFORD GORDON
     REFS: NASA RP-1311, PART I, 1994 AND NASA RP-1311, PART II, 1996

*******************************************************************************



  problem case=methane hp eq p(psi)=14.4,r,eq.ratio=0.1,0.2,0.3,0.4,0.5,0.6,0.7,
0.8,0.9,1.0
  reactant fuel CH4 moles=100. t,k=298.0
           oxidant O2 moles=20.69 t,k=298.
           oxidant N2 moles=77.12 t,k=298.
           oxidant CO2 moles=0.03 t,k=298.
           oxidant H2O moles=1.24 t,k=298.
           oxidant Ar moles=0.92 t,k=298.
           output si
  end

OPTIONS: TP=F  HP=T  SP=F  TV=F  UV=F  SV=F  DETN=F  SHOCK=F  REFL=F  INCD=F
RKT=F  FROZ=F  EQL=T  IONS=F  SIUNIT=T  DEBUGF=F  SHKDBG=F  DETDBG=F  TRNSPT=F

TRACE= 0.00E+00  S/R= 0.000000E+00  H/R= 0.000000E+00  U/R= 0.000000E+00

P,BAR =     0.992841

   REACTANT           MOLES    (ENERGY/R),K   TEMP,K  DENSITY
       EXPLODED FORMULA
F: CH4            100.000000  -0.897291E+04   298.00  0.0000
         C  1.00000  H  4.00000
O: O2              20.690000  -0.530002E+00   298.00  0.0000
         O  2.00000
O: N2              77.120000  -0.525424E+00   298.00  0.0000
         N  2.00000
O: CO2              0.030000  -0.473288E+05   298.00  0.0000
         C  1.00000  O  2.00000
O: H2O              1.240000  -0.290854E+05   298.00  0.0000
         H  2.00000  O  1.00000
O: Ar               0.920000  -0.375000E+00   298.00  0.0000
         AR 1.00000

 SPECIES BEING CONSIDERED IN THIS SYSTEM
(CONDENSED PHASE MAY HAVE NAME LISTED SEVERAL TIMES)
 LAST thermo.inp UPDATE:   9/16/99

 g 3/98  *Ar              g 7/97  *C               tpis79  *CH
 g 8/99  CH2              g 8/99  CH3              g12/92  CH2OH
 g10/92  CH3O             g 8/99  CH4              g 8/88  CH3OH
 g 8/99  *CN              g12/89  CNN              tpis79  *CO
 g 9/99  *CO2             tpis91  COOH             tpis91  *C2
 g 1/91  C2H              g 6/89  CHCO,ketyl       g12/89  C2H2,vinylidene
 g 1/91  C2H2,acetylene   g 5/90  CH2CO,ketene     g 2/92  C2H3,vinyl
 g12/92  CH3CN            g 6/96  CH3CO,acetyl     g 1/91  C2H4
 g 8/88  C2H4O,ethylen-o  g 8/88  CH3CHO,ethanal   g 8/88  CH3COOH
 g12/92  C2H5             g 8/88  C2H6             g 8/88  CH3N2CH3
 g 8/88  C2H5OH           g12/92  CH3OCH3          g12/92  CCN
 tpis91  CNC              tpis79  C2N2             g12/89  C2O
 tpis79  *C3              x 4/98  C3H3,1-propynl   x 4/98  C3H3,2-propynl
 g12/92  C3H4,allene      g12/92  C3H4,propyne     g 5/90  C3H4,cyclo-
 bur 92  C3H5,allyl       g 2/95  C3H6,propylene   g 1/93  C3H6,cyclo-
 g 6/90  C3H6O            g 6/90  C3H7,n-propyl    g 9/85  C3H7,i-propyl
 g 6/90  C3H8             g 9/88  C3H8O,1propanol  g 9/88  C3H8O,2propanol
 g 7/88  C3O2             g 7/88  C4               g 2/93  C4H2
 g 5/90  C4H4,1,3-cyclo-  x10/92  C4H6,butadiene   x10/93  C4H6,1-butyne
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 x10/93  C4H6,2-butyne    g 5/90  C4H6,cyclo-      x 4/88  C4H8,1-butene
 x 4/88  C4H8,cis2-buten  x 4/88  C4H8,tr2-butene  x 4/88  C4H8,isobutene
 g 5/90  C4H8,cyclo-      g 6/90  (CH3COOH)2       x10/84  C4H9,n-butyl
 x10/84  C4H9,i-butyl     g 1/93  C4H9,s-butyl     g 1/93  C4H9,t-butyl
 g 6/90  C4H10,isobutane  g 6/90  C4H10,n-butane   j 3/61  C4N2
 g 7/88  C5               g 5/90  C5H6,1,3cyclo-   g 1/93  C5H8,cyclo-
 x 4/87  C5H10,1-pentene  g 6/90  C5H10,cyclo-     x10/84  C5H11,pentyl
 g 1/93  C5H11,t-pentyl   x10/85  C5H12,n-pentane  x10/85  C5H12,i-pentane
x10/85  CH3C(CH3)2CH3    g 2/93  C6H2             g 1/91  C6H5,phenyl
 g 6/90  C6H5O,phenoxy    g 1/91  C6H6             g 6/90  C6H5OH,phenol
 g 1/93  C6H10,cyclo-     x 4/87  C6H12,1-hexene   g 6/90  C6H12,cyclo-
x10/83  C6H13,n-hexyl    g 6/96  C6H14,n-hexane   g 1/93  C7H7,benzyl
 g 1/93  C7H8             g 1/93  C7H8O,cresol-mx  x 4/87  C7H14,1-heptene
x10/83  C7H15,n-heptyl   x10/85  C7H16,2-methylh  x10/85  C7H16,n-heptane
 x 4/89  C8H8,styrene     x10/86  C8H10,ethylbenz  x 4/87  C8H16,1-octene
x10/83  C8H17,n-octyl    x 4/85  C8H18,n-octane   x 4/85  C8H18,isooctane
x10/83  C9H19,n-nonyl    g 8/93  C10H8,naphthale  x10/83  C10H21,n-decyl
g12/84  C12H9,o-bipheny  g12/84  C12H10,biphenyl  g 6/97  *H
 g 7/88  HCN              g 9/96  HCO              tpis89  HCCN
g11/92  HNC              g 2/96  HNCO             g 5/99  HNO
tpis89  HNO2             g 5/99  HNO3             g 5/99  HO2
tpis78  *H2              g 8/88  HCHO,formaldehy  g 8/88  HCOOH
 g 8/89  H2O              g 6/99  H2O2             g 8/88  (HCOOH)2
 g 5/97  *N               g 2/96  NCO              g 4/99  *NH
 g 5/99  NH2              tpis89  NH3              tpis89  *NO
 g 4/99  NO2              j12/64  NO3              tpis78  *N2
g12/89  NCN              g 5/99  N2H2             tpis89  NH2NO2
 g 4/99  N2H4             g 4/99  N2O              g 4/99  N2O3
tpis89  N2O4             g 4/99  N2O5             tpis89  N3
 g 4/99  N3H              g 5/97  *O               tpis78  *OH
tpis89  *O2              tpis89  O3               X 4/83  C(gr)
 X 4/83  C(gr)            X 4/83  C(gr)            g 8/89  H2O(s)
 g 8/89  H2O(L)

O/F = 242.186319

                        EFFECTIVE FUEL     EFFECTIVE OXIDANT        MIXTURE
ENTHALPY                    h(2)/R             h(1)/R               h0/R
(KG-MOL)(K)/KG       -0.55932260E+03    -0.13020937E+02    -0.15267370E+02

KG-FORM.WT./KG             bi(2)              bi(1)              b0i
 *C                    0.62334580E-01     0.10406310E-04     0.26668789E-03
 *H                    0.24933832E+00     0.86025500E-03     0.18820150E-02
 *O                    0.00000000E+00     0.14804711E-01     0.14743833E-01
 *N                    0.00000000E+00     0.53502311E-01     0.53282305E-01
 *Ar                   0.00000000E+00     0.31912685E-03     0.31781458E-03

POINT ITN      T            C           H           O           N
                  AR
  1   32     497.756     -99.468     -35.924     -13.369     -11.856
                -23.606
```

THERMODYNAMIC EQUILIBRIUM COMBUSTION PROPERTIES AT ASSIGNED

PRESSURES

```
CASE = methane

            REACTANT                        MOLES         ENERGY      TEMP
                                                          KJ/KG-MOL       K
FUEL        CH4                          100.0000000    -74605.353    298.000
OXIDANT     O2                            20.6900000        -4.407    298.000
OXIDANT     N2                            77.1200000        -4.369    298.000
OXIDANT     CO2                            0.0300000   -393515.570    298.000
OXIDANT     H2O                            1.2400000   -241831.038    298.000
OXIDANT     Ar                             0.9200000        -3.118    298.000
```

```
O/F=  242.18632  %FUEL=  0.411207  R,EQ.RATIO= 0.100000  PHI,EQ.RATIO= 0.071725

THERMODYNAMIC PROPERTIES

P, BAR           0.99284
T, K              497.76
RHO, KG/CU M    6.8934-1
H, KJ/KG         -126.94
U, KJ/KG         -270.97
G, KJ/KG        -3850.71
S, KJ/(KG)(K)     7.4811

M, (1/n)          28.734
(dLV/dLP)t      -1.00000
(dLV/dLT)p        1.0000
Cp, KJ/(KG)(K)    1.0456
GAMMAs            1.3826
SON VEL,M/SEC      446.2

MOLE FRACTIONS

*Ar              0.00913
*CO2             0.00766
H2O              0.02704
*N2              0.76552
*O2              0.19065

 * THERMODYNAMIC PROPERTIES FITTED TO 20000.K

   PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS
   WERE LESS THAN 5.000000E-06 FOR ALL ASSIGNED CONDITIONS

*C              *CH             CH2             CH3             CH2OH
CH3O            CH4             CH3OH           *CN             CNN
*CO             COOH            *C2             C2H             CHCO,ketyl
C2H2,vinylidene C2H2,acetylene  CH2CO,ketene    C2H3,vinyl      CH3CN
CH3CO,acetyl    C2H4            C2H4O,ethylen-o CH3CHO,ethanal  CH3COOH
C2H5            C2H6            CH3N2CH3        C2H5OH          CH3OCH3
CCN             CNC             C2N2            C2O             *C3
C3H3,1-propynl  C3H3,2-propynl  C3H4,allene     C3H4,propyne    C3H4,cyclo-
C3H5,allyl      C3H6,propylene  C3H6,cyclo-     C3H6O           C3H7,n-propyl
C3H7,i-propyl   C3H8            C3H8O,1propanol C3H8O,2propanol C3O2
C4              C4H2            C4H4,1,3-cyclo- C4H6,butadiene  C4H6,1-butyne
C4H6,2-butyne   C4H6,cyclo-     C4H8,1-butene   C4H8,cis2-buten C4H8,tr2-butene
C4H8,isobutene  C4H8,cyclo-     (CH3COOH)2      C4H9,n-butyl    C4H9,i-butyl
C4H9,s-butyl    C4H9,t-butyl    C4H10,isobutane C4H10,n-butane  C4N2
C5              C5H6,1,3cyclo-  C5H8,cyclo-     C5H10,1-pentene C5H10,cyclo-
C5H11,pentyl    C5H11,t-pentyl  C5H12,n-pentane C5H12,i-pentane CH3C(CH3)2CH3
C6H2            C6H5,phenyl     C6H5O,phenoxy   C6H6            C6H5OH,phenol
C6H10,cyclo-    C6H12,1-hexene  C6H12,cyclo-    C6H13,n-hexyl   C6H14,n-hexane
C7H7,benzyl     C7H8            C7H8O,cresol-mx C7H14,1-heptene C7H15,n-heptyl
C7H16,2-methylh C7H16,n-heptane C8H8,styrene    C8H10,ethylbenz C8H16,1-octene
C8H17,n-octyl   C8H18,n-octane  C8H18,isooctane C9H19,n-nonyl   C10H8,naphthale
C10H21,n-decyl  C12H9,o-bipheny C12H10,biphenyl *H              HCN
HCO             HCCN            HNC             HNCO            HNO
HNO2            HNO3            HO2             *H2             HCHO,formaldehy
HCOOH           H2O2            (HCOOH)2        *N              NCO
*NH             NH2             NH3             *NO             NO2
NO3             NCN             N2H2            NH2NO2          N2H4
N2O             N2O3            N2O4            N2O5            N3
N3H             *O              *OH             O3              C(gr)
H2O(s)          H2O(L)
```

O/F = 99.337893

ENTHALPY (KG-MOL)(K)/KG	EFFECTIVE FUEL h(2)/R	EFFECTIVE OXIDANT h(1)/R	MIXTURE h0/R
	-0.55932260E+03	-0.13020937E+02	-0.18465557E+02

KG-FORM.WT./KG	bi(2)	bi(1)	b0i
*C	0.62334580E-01	0.10406310E-04	0.63154924E-03
*H	0.24933832E+00	0.86025500E-03	0.33366680E-02
*O	0.00000000E+00	0.14804711E-01	0.14657162E-01
*N	0.00000000E+00	0.53502311E-01	0.52969089E-01
*Ar	0.00000000E+00	0.31912685E-03	0.31594633E-03

POINT	ITN	T	C	H	O	N	AR
1	5	764.014	-65.673	-25.684	-13.840	-12.251	-24.165

THERMODYNAMIC EQUILIBRIUM COMBUSTION PROPERTIES AT ASSIGNED

PRESSURES

CASE = methane

	REACTANT	MOLES	ENERGY KJ/KG-MOL	TEMP K
FUEL	CH4	100.0000000	-74605.353	298.000
OXIDANT	O2	20.6900000	-4.407	298.000
OXIDANT	N2	77.1200000	-4.369	298.000
OXIDANT	CO2	0.0300000	-393515.570	298.000
OXIDANT	H2O	1.2400000	-241831.038	298.000
OXIDANT	Ar	0.9200000	-3.118	298.000

O/F=   99.33789 %FUEL= 0.996632 R,EQ.RATIO= 0.200000 PHI,EQ.RATIO= 0.174867

THERMODYNAMIC PROPERTIES

P, BAR	0.99284
T, K	764.01
RHO, KG/CU M	4.4702-1
H, KJ/KG	-153.53
U, KJ/KG	-375.63
G, KJ/KG	-6267.28
S, KJ/(KG)(K)	8.0021
M, (1/n)	28.601
(dLV/dLP)t	-1.00000
(dLV/dLT)p	1.0000
Cp, KJ/(KG)(K)	1.1250
GAMMAs	1.3485
SON VEL,M/SEC	547.3

MOLE FRACTIONS

*Ar	0.00904
*CO2	0.01806
H2O	0.04772
*N2	0.75750
*O2	0.16769

 * THERMODYNAMIC PROPERTIES FITTED TO 20000.K

   PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS
   WERE LESS THAN 5.000000E-06 FOR ALL ASSIGNED CONDITIONS

*C	*CH	CH2	CH3	CH2OH

CH3O	CH4	CH3OH	*CN	CNN
*CO	COOH	*C2	C2H	CHCO,ketyl
C2H2,vinylidene	C2H2,acetylene	CH2CO,ketene	C2H3,vinyl	CH3CN
CH3CO,acetyl	C2H4	C2H4O,ethylen-o	CH3CHO,ethanal	CH3COOH
C2H5	C2H6	CH3N2CH3	C2H5OH	CH3OCH3
CCN	CNC	C2N2	C2O	*C3
C3H3,1-propynl	C3H3,2-propynl	C3H4,allene	C3H4,propyne	C3H4,cyclo-
C3H5,allyl	C3H6,propylene	C3H6,cyclo-	C3H6O	C3H7,n-propyl
C3H7,i-propyl	C3H8	C3H8O,1propanol	C3H8O,2propanol	C3O2
C4	C4H2	C4H4,1,3-cyclo-	C4H6,butadiene	C4H6,1-butyne
C4H6,2-butyne	C4H6,cyclo-	C4H8,1-butene	C4H8,cis2-buten	C4H8,tr2-butene
C4H8,isobutene	C4H8,cyclo-	(CH3COOH)2	C4H9,n-butyl	C4H9,i-butyl
C4H9,s-butyl	C4H9,t-butyl	C4H10,isobutane	C4H10,n-butane	C4N2
C5	C5H6,1,3cyclo-	C5H8,cyclo-	C5H10,1-pentene	C5H10,cyclo-
C5H11,pentyl	C5H11,t-pentyl	C5H12,n-pentane	C5H12,i-pentane	CH3C(CH3)2CH3
C6H2	C6H5,phenyl	C6H5O,phenoxy	C6H6	C6H5OH,phenol
C6H10,cyclo-	C6H12,1-hexene	C6H12,cyclo-	C6H13,n-hexyl	C6H14,n-hexane
C7H7,benzyl	C7H8	C7H8O,cresol-mx	C7H14,1-heptene	C7H15,n-heptyl
C7H16,2-methylh	C7H16,n-heptane	C8H8,styrene	C8H10,ethylbenz	C8H16,1-octene
C8H17,n-octyl	C8H18,n-octane	C8H18,isooctane	C9H19,n-nonyl	C10H8,naphthale
C10H21,n-decyl	C12H9,o-bipheny	C12H10,biphenyl	*H	HCN
HCO	HCCN	HNC	HNCO	HNO
HNO2	HNO3	HO2	*H2	HCHO,formaldehy
HCOOH	H2O2	(HCOOH)2	*N	NCO
*NH	NH2	NH3	*NO	NO2
NO3	NCN	N2H2	NH2NO2	N2H4
N2O	N2O3	N2O4	N2O5	N3
N3H	*O	*OH	O3	C(gr)
H2O(s)	H2O(L)			

O/F = 62.483397

ENTHALPY	EFFECTIVE FUEL h(2)/R	EFFECTIVE OXIDANT h(1)/R	MIXTURE h0/R
(KG-MOL)(K)/KG	-0.55932260E+03	-0.13020937E+02	-0.21626363E+02

KG-FORM.WT./KG	bi(2)	bi(1)	b0i
*C	0.62334580E-01	0.10406310E-04	0.99214605E-03
*H	0.24933832E+00	0.86025500E-03	0.47743188E-02
*O	0.00000000E+00	0.14804711E-01	0.14571505E-01
*N	0.00000000E+00	0.53502311E-01	0.52659534E-01
*Ar	0.00000000E+00	0.31912685E-03	0.31409992E-03

POINT	ITN	T	C	H	O	N	AR
1	5	1005.922	-50.500	-21.116	-14.259	-12.586	-24.629

THERMODYNAMIC EQUILIBRIUM COMBUSTION PROPERTIES AT ASSIGNED

PRESSURES

CASE = methane

	REACTANT	MOLES	ENERGY KJ/KG-MOL	TEMP K
FUEL	CH4	100.0000000	-74605.353	298.000
OXIDANT	O2	20.6900000	-4.407	298.000
OXIDANT	N2	77.1200000	-4.369	298.000
OXIDANT	CO2	0.0300000	-393515.570	298.000
OXIDANT	H2O	1.2400000	-241831.038	298.000

```
OXIDANT     Ar                            0.9200000        -3.118    298.000

O/F=   62.48340  %FUEL=  1.575215  R,EQ.RATIO= 0.300000  PHI,EQ.RATIO= 0.278009

THERMODYNAMIC PROPERTIES

P, BAR           0.99284
T, K             1005.92
RHO, KG/CU M    3.3798-1
H, KJ/KG         -179.81
U, KJ/KG         -473.57
G, KJ/KG        -8608.00
S, KJ/(KG)(K)     8.3786

M, (1/n)          28.471
(dLV/dLP)t      -1.00000
(dLV/dLT)p        1.0000
Cp, KJ/(KG)(K)    1.2000
GAMMAs            1.3216
SON VEL,M/SEC      623.1

MOLE FRACTIONS

*Ar              0.00894
*CO2             0.02825
H2O              0.06797
*NO              0.00003
*N2              0.74963
*O2              0.14519

 * THERMODYNAMIC PROPERTIES FITTED TO 20000.K

   PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS
   WERE LESS THAN 5.000000E-06 FOR ALL ASSIGNED CONDITIONS

*C               *CH              CH2              CH3              CH2OH
CH3O             CH4              CH3OH            *CN              CNN
*CO              COOH             *C2              C2H              CHCO,ketyl
C2H2,vinylidene  C2H2,acetylene   CH2CO,ketene     C2H3,vinyl       CH3CN
CH3CO,acetyl     C2H4             C2H4O,ethylen-o  CH3CHO,ethanal   CH3COOH
C2H5             C2H6             CH3N2CH3         C2H5OH           CH3OCH3
CCN              CNC              C2N2             C2O              *C3
C3H3,1-propynl   C3H3,2-propynl   C3H4,allene      C3H4,propyne     C3H4,cyclo-
C3H5,allyl       C3H6,propylene   C3H6,cyclo-      C3H6O            C3H7,n-propyl
C3H7,i-propyl    C3H8             C3H8O,1propanol  C3H8O,2propanol  C3O2
C4               C4H2             C4H4,1,3-cyclo-  C4H6,butadiene   C4H6,1-butyne
C4H6,2-butyne    C4H6,cyclo-      C4H8,1-butene    C4H8,cis2-buten  C4H8,tr2-butene
C4H8,isobutene   C4H8,cyclo-      (CH3COOH)2       C4H9,n-butyl     C4H9,i-butyl
C4H9,s-butyl     C4H9,t-butyl     C4H10,isobutane  C4H10,n-butane   C4N2
C5               C5H6,1,3cyclo-   C5H8,cyclo-      C5H10,1-pentene  C5H10,cyclo-
C5H11,pentyl     C5H11,t-pentyl   C5H12,n-pentane  C5H12,i-pentane  CH3C(CH3)2CH3
C6H2             C6H5,phenyl      C6H5O,phenoxy    C6H6             C6H5OH,phenol
C6H10,cyclo-     C6H12,1-hexene   C6H12,cyclo-     C6H13,n-hexyl    C6H14,n-hexane
C7H7,benzyl      C7H8             C7H8O,cresol-mx  C7H14,1-heptene  C7H15,n-heptyl
C7H16,2-methylh  C7H16,n-heptane  C8H8,styrene     C8H10,ethylbenz  C8H16,1-octene
C8H17,n-octyl    C8H18,n-octane   C8H18,isooctane  C9H19,n-nonyl    C10H8,naphthale
C10H21,n-decyl   C12H9,o-bipheny  C12H10,biphenyl  *H               HCN
HCO              HCCN             HNC              HNCO             HNO
HNO2             HNO3             HO2              *H2              HCHO,formaldehy
HCOOH            H2O2             (HCOOH)2         *N               NCO
*NH              NH2              NH3              NO2              NO3
NCN              N2H2             NH2NO2           N2H4             N2O
N2O3             N2O4             N2O5             N3               N3H
*O               *OH              O3               C(gr)            H2O(s)
H2O(L)
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O/F = 45.575006

ENTHALPY (KG-MOL)(K)/KG	EFFECTIVE FUEL h(2)/R	EFFECTIVE OXIDANT h(1)/R	MIXTURE h0/R
	-0.55932260E+03	-0.13020937E+02	-0.24750440E+02

KG-FORM.WT./KG	bi(2)	bi(1)	b0i
*C	0.62334580E-01	0.10406310E-04	0.13485526E-02
*H	0.24933832E+00	0.86025500E-03	0.61952637E-02
*O	0.00000000E+00	0.14804711E-01	0.14486843E-01
*N	0.00000000E+00	0.53502311E-01	0.52353576E-01
*Ar	0.00000000E+00	0.31912685E-03	0.31227496E-03

POINT	ITN	T	C	H	O	N	AR
1	4	1228.148	-41.798	-18.519	-14.629	-12.863	-25.004

THERMODYNAMIC EQUILIBRIUM COMBUSTION PROPERTIES AT ASSIGNED

PRESSURES

CASE = methane

	REACTANT	MOLES	ENERGY KJ/KG-MOL	TEMP K
FUEL	CH4	100.0000000	-74605.353	298.000
OXIDANT	O2	20.6900000	-4.407	298.000
OXIDANT	N2	77.1200000	-4.369	298.000
OXIDANT	CO2	0.0300000	-393515.570	298.000
OXIDANT	H2O	1.2400000	-241831.038	298.000
OXIDANT	Ar	0.9200000	-3.118	298.000

O/F= 45.57501 %FUEL= 2.147074 R,EQ.RATIO= 0.400000 PHI,EQ.RATIO= 0.381150

THERMODYNAMIC PROPERTIES

P, BAR	0.99284
T, K	1228.15
RHO, KG/CU M	2.7558-1
H, KJ/KG	-205.79
U, KJ/KG	-566.06
G, KJ/KG	-10867.4
S, KJ/(KG)(K)	8.6810
M, (1/n)	28.344
(dLV/dLP)t	-1.00000
(dLV/dLT)p	1.0000
Cp, KJ/(KG)(K)	1.2658
GAMMAs	1.3017
SON VEL,M/SEC	684.8

MOLE FRACTIONS

*Ar	0.00885
*CO2	0.03822
H2O	0.08780
*NO	0.00018
*N2	0.74185
*O2	0.12309

 * THERMODYNAMIC PROPERTIES FITTED TO 20000.K

   PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS

WERE LESS THAN 5.000000E-06 FOR ALL ASSIGNED CONDITIONS

*C	*CH	CH2	CH3	CH2OH
CH3O	CH4	CH3OH	*CN	CNN
*CO	COOH	*C2	C2H	CHCO,ketyl
C2H2,vinylidene	C2H2,acetylene	CH2CO,ketene	C2H3,vinyl	CH3CN
CH3CO,acetyl	C2H4	C2H4O,ethylen-o	CH3CHO,ethanal	CH3COOH
C2H5	C2H6	CH3N2CH3	C2H5OH	CH3OCH3
CCN	CNC	C2N2	C2O	*C3
C3H3,1-propynl	C3H3,2-propynl	C3H4,allene	C3H4,propyne	C3H4,cyclo-
C3H5,allyl	C3H6,propylene	C3H6,cyclo-	C3H6O	C3H7,n-propyl
C3H7,i-propyl	C3H8	C3H8O,1propanol	C3H8O,2propanol	C3O2
C4	C4H2	C4H4,1,3-cyclo-	C4H6,butadiene	C4H6,1-butyne
C4H6,2-butyne	C4H6,cyclo-	C4H8,1-butene	C4H8,cis2-buten	C4H8,tr2-butene
C4H8,isobutene	C4H8,cyclo-	(CH3COOH)2	C4H9,n-butyl	C4H9,i-butyl
C4H9,s-butyl	C4H9,t-butyl	C4H10,isobutane	C4H10,n-butane	C4N2
C5	C5H6,1,3cyclo-	C5H8,cyclo-	C5H10,1-pentene	C5H10,cyclo-
C5H11,pentyl	C5H11,t-pentyl	C5H12,n-pentane	C5H12,i-pentane	CH3C(CH3)2CH3
C6H2	C6H5,phenyl	C6H5O,phenoxy	C6H6	C6H5OH,phenol
C6H10,cyclo-	C6H12,1-hexene	C6H12,cyclo-	C6H13,n-hexyl	C6H14,n-hexane
C7H7,benzyl	C7H8	C7H8O,cresol-mx	C7H14,1-heptene	C7H15,n-heptyl
C7H16,2-methylh	C7H16,n-heptane	C8H8,styrene	C8H10,ethylbenz	C8H16,1-octene
C8H17,n-octyl	C8H18,n-octane	C8H18,isooctane	C9H19,n-nonyl	C10H8,naphthale
C10H21,n-decyl	C12H9,o-bipheny	C12H10,biphenyl	*H	HCN
HCO	HCCN	HNC	HNCO	HNO
HNO2	HNO3	HO2	*H2	HCHO,formaldehy
HCOOH	H2O2	(HCOOH)2	*N	NCO
*NH	NH2	NH3	NO2	NO3
NCN	N2H2	NH2NO2	N2H4	N2O
N2O3	N2O4	N2O5	N3	N3H
*O	*OH	O3	C(gr)	H2O(s)
H2O(L)				

O/F = 35.868712

ENTHALPY (KG-MOL)(K)/KG	EFFECTIVE FUEL h(2)/R	EFFECTIVE OXIDANT h(1)/R	MIXTURE h0/R
	-0.55932260E+03	-0.13020937E+02	-0.27838424E+02

KG-FORM.WT./KG	bi(2)	bi(1)	b0i
*C	0.62334580E-01	0.10406310E-04	0.17008416E-02
*H	0.24933832E+00	0.86025500E-03	0.75997923E-02
*O	0.00000000E+00	0.14804711E-01	0.14403159E-01
*N	0.00000000E+00	0.53502311E-01	0.52051153E-01
*Ar	0.00000000E+00	0.31912685E-03	0.31047109E-03

POINT	ITN	T	C	H	O	N	AR
1	4	1434.047	-36.086	-16.832	-14.968	-13.095	-25.315

THERMODYNAMIC EQUILIBRIUM COMBUSTION PROPERTIES AT ASSIGNED PRESSURES

CASE = methane

	REACTANT	MOLES	ENERGY KJ/KG-MOL	TEMP K
FUEL	CH4	100.0000000	-74605.353	298.000
OXIDANT	O2	20.6900000	-4.407	298.000

```
OXIDANT     N2                          77.1200000        -4.369    298.000
OXIDANT     CO2                          0.0300000   -393515.570    298.000
OXIDANT     H2O                          1.2400000   -241831.038    298.000
OXIDANT     Ar                           0.9200000        -3.118    298.000

O/F=   35.86871  %FUEL=  2.712327  R,EQ.RATIO= 0.500000  PHI,EQ.RATIO= 0.484292

THERMODYNAMIC PROPERTIES

P, BAR           0.99284
T, K             1434.05
RHO, KG/CU M    2.3497-1
H, KJ/KG         -231.46
U, KJ/KG         -654.00
G, KJ/KG        -13048.7
S, KJ/(KG)(K)     8.9378

M, (1/n)          28.218
(dLV/dLP)t      -1.00000
(dLV/dLT)p        1.0001
Cp, KJ/(KG)(K)    1.3269
GAMMAs            1.2855
SON VEL,M/SEC      737.0

MOLE FRACTIONS

*Ar              0.00876
*CO2             0.04799
H2O              0.10721
*NO              0.00059
*N2              0.73411
*OH              0.00004
*O2              0.10130

 * THERMODYNAMIC PROPERTIES FITTED TO 20000.K

   PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS
   WERE LESS THAN 5.000000E-06 FOR ALL ASSIGNED CONDITIONS

*C               *CH              CH2              CH3              CH2OH
CH3O             CH4              CH3OH            *CN              CNN
*CO              COOH             *C2              C2H              CHCO,ketyl
C2H2,vinylidene C2H2,acetylene  CH2CO,ketene     C2H3,vinyl       CH3CN
CH3CO,acetyl     C2H4             C2H4O,ethylen-o CH3CHO,ethanal   CH3COOH
C2H5             C2H6             CH3N2CH3        C2H5OH           CH3OCH3
CCN              CNC              C2N2            C2O              *C3
C3H3,1-propynl   C3H3,2-propynl   C3H4,allene     C3H4,propyne     C3H4,cyclo-
C3H5,allyl       C3H6,propylene   C3H6,cyclo-     C3H6O            C3H7,n-propyl
C3H7,i-propyl    C3H8             C3H8O,1propanol C3H8O,2propanol  C3O2
C4               C4H2             C4H4,1,3-cyclo- C4H6,butadiene   C4H6,1-butyne
C4H6,2-butyne    C4H6,cyclo-      C4H8,1-butene   C4H8,cis2-buten  C4H8,tr2-butene
C4H8,isobutene   C4H8,cyclo-      (CH3COOH)2      C4H9,n-butyl     C4H9,i-butyl
C4H9,s-butyl     C4H9,t-butyl     C4H10,isobutane C4H10,n-butane   C4N2
C5               C5H6,1,3cyclo-   C5H8,cyclo-     C5H10,1-pentene  C5H10,cyclo-
C5H11,pentyl     C5H11,t-pentyl   C5H12,n-pentane C5H12,i-pentane  CH3C(CH3)2CH3
C6H2             C6H5,phenyl      C6H5O,phenoxy   C6H6             C6H5OH,phenol
C6H10,cyclo-     C6H12,1-hexene   C6H12,cyclo-    C6H13,n-hexyl    C6H14,n-hexane
C7H7,benzyl      C7H8             C7H8O,cresol-mx C7H14,1-heptene  C7H15,n-heptyl
C7H16,2-methylh  C7H16,n-heptane  C8H8,styrene    C8H10,ethylbenz  C8H16,1-octene
C8H17,n-octyl    C8H18,n-octane   C8H18,isooctane C9H19,n-nonyl    C10H8,naphthale
C10H21,n-decyl   C12H9,o-bipheny C12H10,biphenyl *H               HCN
HCO              HCCN             HNC             HNCO             HNO
HNO2             HNO3             HO2             *H2              HCHO,formaldehy
HCOOH            H2O2             (HCOOH)2        *N               NCO
*NH              NH2              NH3             NO2              NO3
NCN              N2H2             NH2NO2          N2H4             N2O
N2O3             N2O4             N2O5            N3               N3H
*O               O3               C(gr)           H2O(s)           H2O(L)
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O/F = 29.570882

ENTHALPY (KG-MOL)(K)/KG	EFFECTIVE FUEL h(2)/R	EFFECTIVE OXIDANT h(1)/R	MIXTURE h0/R
	-0.55932260E+03	-0.13020937E+02	-0.30890937E+02

KG-FORM.WT./KG	bi(2)	bi(1)	b0i
*C	0.62334580E-01	0.10406310E-04	0.20490840E-02
*H	0.24933832E+00	0.86025500E-03	0.89881875E-02
*O	0.00000000E+00	0.14804711E-01	0.14320436E-01
*N	0.00000000E+00	0.53502311E-01	0.51752204E-01
*Ar	0.00000000E+00	0.31912685E-03	0.30868794E-03

POINT	ITN	T	C	H	O	N	AR
1	4	1625.581	-31.991	-15.638	-15.293	-13.295	-25.577

THERMODYNAMIC EQUILIBRIUM COMBUSTION PROPERTIES AT ASSIGNED

PRESSURES

CASE = methane

	REACTANT	MOLES	ENERGY KJ/KG-MOL	TEMP K
FUEL	CH4	100.0000000	-74605.353	298.000
OXIDANT	O2	20.6900000	-4.407	298.000
OXIDANT	N2	77.1200000	-4.369	298.000
OXIDANT	CO2	0.0300000	-393515.570	298.000
OXIDANT	H2O	1.2400000	-241831.038	298.000
OXIDANT	Ar	0.9200000	-3.118	298.000

O/F=   29.57088 %FUEL= 3.271087 R,EQ.RATIO= 0.600000 PHI,EQ.RATIO= 0.587434

THERMODYNAMIC PROPERTIES

P, BAR	0.99284
T, K	1625.58
RHO, KG/CU M	2.0638-1
H, KJ/KG	-256.84
U, KJ/KG	-737.93
G, KJ/KG	-15152.0
S, KJ/(KG)(K)	9.1629
M, (1/n)	28.095
(dLV/dLP)t	-1.00002
(dLV/dLT)p	1.0007
Cp, KJ/(KG)(K)	1.3891
GAMMAs	1.2712
SON VEL,M/SEC	782.0

MOLE FRACTIONS

*Ar	0.00867
*CO	0.00001
*CO2	0.05756
H2O	0.12616
*NO	0.00128
*N2	0.72634
*O	0.00001

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*OH              0.00019
*O2              0.07978

 * THERMODYNAMIC PROPERTIES FITTED TO 20000.K

   PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS
   WERE LESS THAN 5.000000E-06 FOR ALL ASSIGNED CONDITIONS

*C              *CH             CH2             CH3             CH2OH
CH3O            CH4             CH3OH           *CN             CNN
COOH            *C2             C2H             CHCO,ketyl      C2H2,vinylidene
C2H2,acetylene  CH2CO,ketene    C2H3,vinyl      CH3CN           CH3CO,acetyl
C2H4            C2H4O,ethylen-o CH3CHO,ethanal  CH3COOH         C2H5
C2H6            CH3N2CH3        C2H5OH          CH3OCH3         CCN
CNC             C2N2            C2O             *C3             C3H3,1-propynl
C3H3,2-propynl  C3H4,allene     C3H4,propyne    C3H4,cyclo-     C3H5,allyl
C3H6,propylene  C3H6,cyclo-     C3H6O           C3H7,n-propyl   C3H7,i-propyl
C3H8            C3H8O,1propanol C3H8O,2propanol C3O2            C4
C4H2            C4H4,1,3-cyclo- C4H6,butadiene  C4H6,1-butyne   C4H6,2-butyne
C4H6,cyclo-     C4H8,1-butene   C4H8,cis2-buten C4H8,tr2-butene C4H8,isobutene
C4H8,cyclo-     (CH3COOH)2      C4H9,n-butyl    C4H9,i-butyl    C4H9,s-butyl
C4H9,t-butyl    C4H10,isobutane C4H10,n-butane  C4N2            C5
C5H6,1,3cyclo-  C5H8,cyclo-     C5H10,1-pentene C5H10,cyclo-    C5H11,pentyl
C5H11,t-pentyl  C5H12,n-pentane C5H12,i-pentane CH3C(CH3)2CH3   C6H2
C6H5,phenyl     C6H5O,phenoxy   C6H6            C6H5OH,phenol   C6H10,cyclo-
C6H12,1-hexene  C6H12,cyclo-    C6H13,n-hexyl   C6H14,n-hexane  C7H7,benzyl
C7H8            C7H8O,cresol-mx C7H14,1-heptene C7H15,n-heptyl  C7H16,2-methylh
C7H16,n-heptane C8H8,styrene    C8H10,ethylbenz C8H16,1-octene  C8H17,n-octyl
C8H18,n-octane  C8H18,isooctane C9H19,n-nonyl   C10H8,naphthale C10H21,n-decyl
C12H9,o-bipheny C12H10,biphenyl *H              HCN             HCO
HCCN            HNC             HNCO            HNO             HNO2
HNO3            HO2             *H2             HCHO,formaldehy HCOOH
H2O2            (HCOOH)2        *N              NCO             *NH
NH2             NH3             NO2             NO3             NCN
N2H2            NH2NO2          N2H4            N2O             N2O3
N2O4            N2O5            N3              N3H             O3
C(gr)           H2O(s)          H2O(L)




O/F =  25.154290

                      EFFECTIVE FUEL     EFFECTIVE OXIDANT        MIXTURE
ENTHALPY                  h(2)/R             h(1)/R              h0/R
(KG-MOL)(K)/KG       -0.55932260E+03    -0.13020937E+02    -0.33908587E+02

KG-FORM.WT./KG             bi(2)              bi(1)              b0i
 *C                    0.62334580E-01     0.10406310E-04     0.23933490E-02
 *H                    0.24933832E+00     0.86025500E-03     0.10360726E-01
 *O                    0.00000000E+00     0.14804711E-01     0.14238658E-01
 *N                    0.00000000E+00     0.53502311E-01     0.51456669E-01
 *Ar                   0.00000000E+00     0.31912685E-03     0.30692515E-03

POINT ITN      T            C           H           O           N
                  AR
  1    4    1803.635     -28.846     -14.734     -15.624     -13.468
                -25.802



        THERMODYNAMIC EQUILIBRIUM COMBUSTION PROPERTIES AT ASSIGNED

                                PRESSURES

CASE = methane
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	REACTANT	MOLES	ENERGY KJ/KG-MOL	TEMP K
FUEL	CH4	100.0000000	-74605.353	298.000
OXIDANT	O2	20.6900000	-4.407	298.000
OXIDANT	N2	77.1200000	-4.369	298.000
OXIDANT	CO2	0.0300000	-393515.570	298.000
OXIDANT	H2O	1.2400000	-241831.038	298.000
OXIDANT	Ar	0.9200000	-3.118	298.000

O/F= 25.15429 %FUEL= 3.823464 R,EQ.RATIO= 0.700000 PHI,EQ.RATIO= 0.690575

THERMODYNAMIC PROPERTIES

P, BAR	0.99284
T, K	1803.63
RHO, KG/CU M	1.8518-1
H, KJ/KG	-281.93
U, KJ/KG	-818.09
G, KJ/KG	-17172.1
S, KJ/(KG)(K)	9.3645
M, (1/n)	27.970
(dLV/dLP)t	-1.00007
(dLV/dLT)p	1.0028
Cp, KJ/(KG)(K)	1.4617
GAMMAs	1.2570
SON VEL,M/SEC	820.9

MOLE FRACTIONS

*Ar	0.00858
*CO	0.00006
*CO2	0.06688
*H2	0.00003
H2O	0.14455
*NO	0.00212
*N2	0.71856
*O	0.00003
*OH	0.00062
*O2	0.05855

* THERMODYNAMIC PROPERTIES FITTED TO 20000.K

PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 5.000000E-06 FOR ALL ASSIGNED CONDITIONS

*C	*CH	CH2	CH3	CH2OH
CH3O	CH4	CH3OH	*CN	CNN
COOH	*C2	C2H	CHCO,ketyl	C2H2,vinylidene
C2H2,acetylene	CH2CO,ketene	C2H3,vinyl	CH3CN	CH3CO,acetyl
C2H4	C2H4O,ethylen-o	CH3CHO,ethanal	CH3COOH	C2H5
C2H6	CH3N2CH3	C2H5OH	CH3OCH3	CCN
CNC	C2N2	C2O	*C3	C3H3,1-propynl
C3H3,2-propynl	C3H4,allene	C3H4,propyne	C3H4,cyclo-	C3H5,allyl
C3H6,propylene	C3H6,cyclo-	C3H6O	C3H7,n-propyl	C3H7,i-propyl
C3H8	C3H8O,1propanol	C3H8O,2propanol	C3O2	C4
C4H2	C4H4,1,3-cyclo-	C4H6,butadiene	C4H6,1-butyne	C4H6,2-butyne
C4H6,cyclo-	C4H8,1-butene	C4H8,cis2-buten	C4H8,tr2-butene	C4H8,isobutene
C4H8,cyclo-	(CH3COOH)2	C4H9,n-butyl	C4H9,i-butyl	C4H9,s-butyl
C4H9,t-butyl	C4H10,isobutane	C4H10,n-butane	C4N2	C5
C5H6,1,3cyclo-	C5H8,cyclo-	C5H10,1-pentene	C5H10,cyclo-	C5H11,pentyl
C5H11,t-pentyl	C5H12,n-pentane	C5H12,i-pentane	CH3C(CH3)2CH3	C6H2
C6H5,phenyl	C6H5O,phenoxy	C6H6	C6H5OH,phenol	C6H10,cyclo-
C6H12,1-hexene	C6H12,cyclo-	C6H13,n-hexyl	C6H14,n-hexane	C7H7,benzyl
C7H8	C7H8O,cresol-mx	C7H14,1-heptene	C7H15,n-heptyl	C7H16,2-methylh
C7H16,n-heptane	C8H8,styrene	C8H10,ethylbenz	C8H16,1-octene	C8H17,n-octyl
C8H18,n-octane	C8H18,isooctane	C9H19,n-nonyl	C10H8,naphthale	C10H21,n-decyl
C12H9,o-bipheny	C12H10,biphenyl	*H	HCN	HCO

HCCN	HNC	HNCO	HNO	HNO2
HNO3	HO2	HCHO,formaldehy	HCOOH	H2O2
(HCOOH)2	*N	NCO	*NH	NH2
NH3	NO2	NO3	NCN	N2H2
NH2NO2	N2H4	N2O	N2O3	N2O4
N2O5	N3	N3H	O3	C(gr)
H2O(s)	H2O(L)			

O/F = 21.885550

ENTHALPY (KG-MOL)(K)/KG	EFFECTIVE FUEL h(2)/R	EFFECTIVE OXIDANT h(1)/R	MIXTURE h0/R
	-0.55932260E+03	-0.13020937E+02	-0.36891968E+02

KG-FORM.WT./KG	bi(2)	bi(1)	b0i
*C	0.62334580E-01	0.10406310E-04	0.27337044E-02
*H	0.24933832E+00	0.86025500E-03	0.11717677E-01
*O	0.00000000E+00	0.14804711E-01	0.14157809E-01
*N	0.00000000E+00	0.53502311E-01	0.51164490E-01
*Ar	0.00000000E+00	0.31912685E-03	0.30518238E-03

POINT	ITN	T	C	H	O	N	AR
1	4	1967.327	-26.267	-14.007	-15.994	-13.617	-25.995

THERMODYNAMIC EQUILIBRIUM COMBUSTION PROPERTIES AT ASSIGNED

PRESSURES

CASE = methane

	REACTANT	MOLES	ENERGY KJ/KG-MOL	TEMP K
FUEL	CH4	100.0000000	-74605.353	298.000
OXIDANT	O2	20.6900000	-4.407	298.000
OXIDANT	N2	77.1200000	-4.369	298.000
OXIDANT	CO2	0.0300000	-393515.570	298.000
OXIDANT	H2O	1.2400000	-241831.038	298.000
OXIDANT	Ar	0.9200000	-3.118	298.000

O/F= 21.88555 %FUEL= 4.369569 R,EQ.RATIO= 0.800000 PHI,EQ.RATIO= 0.793717

THERMODYNAMIC PROPERTIES

P, BAR	0.99284
T, K	1967.33
RHO, KG/CU M	1.6897-1
H, KJ/KG	-306.74
U, KJ/KG	-894.32
G, KJ/KG	-19089.6
S, KJ/(KG)(K)	9.5474
M, (1/n)	27.839
(dLV/dLP)t	-1.00027
(dLV/dLT)p	1.0094
Cp, KJ/(KG)(K)	1.5700
GAMMAs	1.2400
SON VEL,M/SEC	853.6

MOLE FRACTIONS

*Ar	0.00850
*CO	0.00039
*CO2	0.07571
*H	0.00002
*H2	0.00019
H2O	0.16218
*NO	0.00282
*N2	0.71076
*O	0.00010
*OH	0.00145
*O2	0.03788

* THERMODYNAMIC PROPERTIES FITTED TO 20000.K

PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS
WERE LESS THAN 5.000000E-06 FOR ALL ASSIGNED CONDITIONS

*C	*CH	CH2	CH3	CH2OH
CH3O	CH4	CH3OH	*CN	CNN
COOH	*C2	C2H	CHCO,ketyl	C2H2,vinylidene
C2H2,acetylene	CH2CO,ketene	C2H3,vinyl	CH3CN	CH3CO,acetyl
C2H4	C2H4O,ethylen-o	CH3CHO,ethanal	CH3COOH	C2H5
C2H6	CH3N2CH3	C2H5OH	CH3OCH3	CCN
CNC	C2N2	C2O	*C3	C3H3,1-propynl
C3H3,2-propynl	C3H4,allene	C3H4,propyne	C3H4,cyclo-	C3H5,allyl
C3H6,propylene	C3H6,cyclo-	C3H6O	C3H7,n-propyl	C3H7,i-propyl
C3H8	C3H8O,1propanol	C3H8O,2propanol	C3O2	C4
C4H2	C4H4,1,3-cyclo-	C4H6,butadiene	C4H6,1-butyne	C4H6,2-butyne
C4H6,cyclo-	C4H8,1-butene	C4H8,cis2-buten	C4H8,tr2-butene	C4H8,isobutene
C4H8,cyclo-	(CH3COOH)2	C4H9,n-butyl	C4H9,i-butyl	C4H9,s-butyl
C4H9,t-butyl	C4H10,isobutane	C4H10,n-butane	C4N2	C5
C5H6,1,3cyclo-	C5H8,cyclo-	C5H10,1-pentene	C5H10,cyclo-	C5H11,pentyl
C5H11,t-pentyl	C5H12,n-pentane	C5H12,i-pentane	CH3C(CH3)2CH3	C6H2
C6H5,phenyl	C6H5O,phenoxy	C6H6	C6H5OH,phenol	C6H10,cyclo-
C6H12,1-hexene	C6H12,cyclo-	C6H13,n-hexyl	C6H14,n-hexane	C7H7,benzyl
C7H8	C7H8O,cresol-mx	C7H14,1-heptene	C7H15,n-heptyl	C7H16,2-methylh
C7H16,n-heptane	C8H8,styrene	C8H10,ethylbenz	C8H16,1-octene	C8H17,n-octyl
C8H18,n-octane	C8H18,isooctane	C9H19,n-nonyl	C10H8,naphthale	C10H21,n-decyl
C12H9,o-bipheny	C12H10,biphenyl	HCN	HCO	HCCN
HNC	HNCO	HNO	HNO2	HNO3
HO2	HCHO,formaldehy	HCOOH	H2O2	(HCOOH)2
*N	NCO	*NH	NH2	NH3
NO2	NO3	NCN	N2H2	NH2NO2
N2H4	N2O	N2O3	N2O4	N2O5
N3	N3H	O3	C(gr)	H2O(s)
H2O(L)				

O/F = 19.368641

ENTHALPY (KG-MOL)(K)/KG	EFFECTIVE FUEL h(2)/R	EFFECTIVE OXIDANT h(1)/R	MIXTURE h0/R
	-0.55932260E+03	-0.13020937E+02	-0.39841660E+02

KG-FORM.WT./KG	bi(2)	bi(1)	b0i
*C	0.62334580E-01	0.10406310E-04	0.30702164E-02
*H	0.24933832E+00	0.86025500E-03	0.13059305E-01
*O	0.00000000E+00	0.14804711E-01	0.14077873E-01
*N	0.00000000E+00	0.53502311E-01	0.50875611E-01
*Ar	0.00000000E+00	0.31912685E-03	0.30345930E-03

POINT	ITN	T	C	H	O	N	AR
1	4	2110.792	-23.972	-13.373	-16.472	-13.742	

-26.156

THERMODYNAMIC EQUILIBRIUM COMBUSTION PROPERTIES AT ASSIGNED

PRESSURES

CASE = methane

	REACTANT	MOLES	ENERGY KJ/KG-MOL	TEMP K
FUEL	CH4	100.0000000	-74605.353	298.000
OXIDANT	O2	20.6900000	-4.407	298.000
OXIDANT	N2	77.1200000	-4.369	298.000
OXIDANT	CO2	0.0300000	-393515.570	298.000
OXIDANT	H2O	1.2400000	-241831.038	298.000
OXIDANT	Ar	0.9200000	-3.118	298.000

O/F= 19.36864 %FUEL= 4.909508 R,EQ.RATIO= 0.900000 PHI,EQ.RATIO= 0.896858

THERMODYNAMIC PROPERTIES

P, BAR	0.99284
T, K	2110.79
RHO, KG/CU M	1.5660-1
H, KJ/KG	-331.26
U, KJ/KG	-965.25
G, KJ/KG	-20836.1
S, KJ/(KG)(K)	9.7143
M, (1/n)	27.683
(dLV/dLP)t	-1.00093
(dLV/dLT)p	1.0294
Cp, KJ/(KG)(K)	1.7858
GAMMAs	1.2155
SON VEL,M/SEC	877.8

MOLE FRACTIONS

*Ar	0.00840
*CO	0.00193
*CO2	0.08306
*H	0.00010
*H2	0.00083
H2O	0.17862
*NO	0.00288
*N2	0.70274
*O	0.00021
*OH	0.00250
*O2	0.01872

* THERMODYNAMIC PROPERTIES FITTED TO 20000.K

PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS
WERE LESS THAN 5.000000E-06 FOR ALL ASSIGNED CONDITIONS

*C	*CH	CH2	CH3	CH2OH
CH3O	CH4	CH3OH	*CN	CNN
COOH	*C2	C2H	CHCO,ketyl	C2H2,vinylidene
C2H2,acetylene	CH2CO,ketene	C2H3,vinyl	CH3CN	CH3CO,acetyl
C2H4	C2H4O,ethylen-o	CH3CHO,ethanal	CH3COOH	C2H5
C2H6	CH3N2CH3	C2H5OH	CH3OCH3	CCN
CNC	C2N2	C2O	*C3	C3H3,1-propynl
C3H3,2-propynl	C3H4,allene	C3H4,propyne	C3H4,cyclo-	C3H5,allyl
C3H6,propylene	C3H6,cyclo-	C3H6O	C3H7,n-propyl	C3H7,i-propyl
C3H8	C3H8O,1propanol	C3H8O,2propanol	C3O2	C4
C4H2	C4H4,1,3-cyclo-	C4H6,butadiene	C4H6,1-butyne	C4H6,2-butyne

C4H6,cyclo-	C4H8,1-butene	C4H8,cis2-buten	C4H8,tr2-butene	C4H8,isobutene
C4H8,cyclo-	(CH3COOH)2	C4H9,n-butyl	C4H9,i-butyl	C4H9,s-butyl
C4H9,t-butyl	C4H10,isobutane	C4H10,n-butane	C4N2	C5
C5H6,1,3cyclo-	C5H8,cyclo-	C5H10,1-pentene	C5H10,cyclo-	C5H11,pentyl
C5H11,t-pentyl	C5H12,n-pentane	C5H12,i-pentane	CH3C(CH3)2CH3	C6H2
C6H5,phenyl	C6H5O,phenoxy	C6H6	C6H5OH,phenol	C6H10,cyclo-
C6H12,1-hexene	C6H12,cyclo-	C6H13,n-hexyl	C6H14,n-hexane	C7H7,benzyl
C7H8	C7H8O,cresol-mx	C7H14,1-heptene	C7H15,n-heptyl	C7H16,2-methylh
C7H16,n-heptane	C8H8,styrene	C8H10,ethylbenz	C8H16,1-octene	C8H17,n-octyl
C8H18,n-octane	C8H18,isooctane	C9H19,n-nonyl	C10H8,naphthale	C10H21,n-decyl
C12H9,o-bipheny	C12H10,biphenyl	HCN	HCO	HCCN
HNC	HNCO	HNO	HNO2	HNO3
HO2	HCHO,formaldehy	HCOOH	H2O2	(HCOOH)2
*N	NCO	*NH	NH2	NH3
NO2	NO3	NCN	N2H2	NH2NO2
N2H4	N2O	N2O3	N2O4	N2O5
N3	N3H	O3	C(gr)	H2O(s)
H2O(L)				

O/F = 17.370928

ENTHALPY (KG-MOL)(K)/KG	EFFECTIVE FUEL h(2)/R	EFFECTIVE OXIDANT h(1)/R	MIXTURE h0/R
	-0.55932260E+03	-0.13020937E+02	-0.42758230E+02

KG-FORM.WT./KG	bi(2)	bi(1)	b0i
*C	0.62334580E-01	0.10406310E-04	0.34029499E-02
*H	0.24933832E+00	0.86025500E-03	0.14385868E-01
*O	0.00000000E+00	0.14804711E-01	0.13998834E-01
*N	0.00000000E+00	0.53502311E-01	0.50589975E-01
*Ar	0.00000000E+00	0.31912685E-03	0.30175556E-03

POINT	ITN	T	C	H	O	N	AR
1	5	2207.790	-21.587	-12.728	-17.286	-13.827	-26.268

THERMODYNAMIC EQUILIBRIUM COMBUSTION PROPERTIES AT ASSIGNED

PRESSURES

CASE = methane

	REACTANT	MOLES	ENERGY KJ/KG-MOL	TEMP K
FUEL	CH4	100.0000000	-74605.353	298.000
OXIDANT	O2	20.6900000	-4.407	298.000
OXIDANT	N2	77.1200000	-4.369	298.000
OXIDANT	CO2	0.0300000	-393515.570	298.000
OXIDANT	H2O	1.2400000	-241831.038	298.000
OXIDANT	Ar	0.9200000	-3.118	298.000

O/F= 17.37093 %FUEL= 5.443383 R,EQ.RATIO= 1.000000 PHI,EQ.RATIO= 1.000000

THERMODYNAMIC PROPERTIES

P, BAR	0.99284
T, K	2207.79
RHO, KG/CU M	1.4841-1
H, KJ/KG	-355.51
U, KJ/KG	-1024.51

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G, KJ/KG        -22137.6
S, KJ/(KG)(K)     9.8660

M, (1/n)          27.439
(dLV/dLP)t      -1.00228
(dLV/dLT)p        1.0690
Cp, KJ/(KG)(K)    2.1587
GAMMAs            1.1878
SON VEL,M/SEC      891.4

MOLE FRACTIONS

*Ar              0.00828
*CO              0.00824
*CO2             0.08513
*H               0.00035
*H2              0.00351
H2O              0.19233
*NO              0.00173
*N2              0.69321
*O               0.00019
*OH              0.00270
*O2              0.00433

 * THERMODYNAMIC PROPERTIES FITTED TO 20000.K

   PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS
   WERE LESS THAN 5.000000E-06 FOR ALL ASSIGNED CONDITIONS

*C              *CH             CH2             CH3             CH2OH
CH3O            CH4             CH3OH           *CN             CNN
COOH            *C2             C2H             CHCO,ketyl      C2H2,vinylidene
C2H2,acetylene  CH2CO,ketene    C2H3,vinyl      CH3CN           CH3CO,acetyl
C2H4            C2H4O,ethylen-o CH3CHO,ethanal  CH3COOH         C2H5
C2H6            CH3N2CH3        C2H5OH          CH3OCH3         CCN
CNC             C2N2            C2O             *C3             C3H3,1-propynl
C3H3,2-propynl  C3H4,allene     C3H4,propyne    C3H4,cyclo-     C3H5,allyl
C3H6,propylene  C3H6,cyclo-     C3H6O           C3H7,n-propyl   C3H7,i-propyl
C3H8            C3H8O,1propanol C3H8O,2propanol C3O2            C4
C4H2            C4H4,1,3-cyclo- C4H6,butadiene  C4H6,1-butyne   C4H6,2-butyne
C4H6,cyclo-     C4H8,1-butene   C4H8,cis2-buten C4H8,tr2-butene C4H8,isobutene
C4H8,cyclo-     (CH3COOH)2      C4H9,n-butyl    C4H9,i-butyl    C4H9,s-butyl
C4H9,t-butyl    C4H10,isobutane C4H10,n-butane  C4N2            C5
C5H6,1,3cyclo-  C5H8,cyclo-     C5H10,1-pentene C5H10,cyclo-    C5H11,pentyl
C5H11,t-pentyl  C5H12,n-pentane C5H12,i-pentane CH3C(CH3)2CH3   C6H2
C6H5,phenyl     C6H5O,phenoxy   C6H6            C6H5OH,phenol   C6H10,cyclo-
C6H12,1-hexene  C6H12,cyclo-    C6H13,n-hexyl   C6H14,n-hexane  C7H7,benzyl
C7H8            C7H8O,cresol-mx C7H14,1-heptene C7H15,n-heptyl  C7H16,2-methylh
C7H16,n-heptane C8H8,styrene    C8H10,ethylbenz C8H16,1-octene  C8H17,n-octyl
C8H18,n-octane  C8H18,isooctane C9H19,n-nonyl   C10H8,naphthale C10H21,n-decyl
C12H9,o-bipheny C12H10,biphenyl HCN             HCO             HCCN
HNC             HNCO            HNO             HNO2            HNO3
HO2             HCHO,formaldehy HCOOH           H2O2            (HCOOH)2
*N              NCO             *NH             NH2             NH3
NO2             NO3             NCN             N2H2            NH2NO2
N2H4            N2O             N2O3            N2O4            N2O5
N3              N3H             O3              C(gr)           H2O(s)
H2O(L)
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Adiabatic Flame Temperatures for JP-5-Air

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        NASA-GLENN CHEMICAL EQUILIBRIUM PROGRAM CEA, AUGUST 30, 1999
                    BY  BONNIE MCBRIDE AND SANFORD GORDON
     REFS: NASA RP-1311, PART I, 1994 AND NASA RP-1311, PART II, 1996

 ******************************************************************************



  problem case=jp-5 hp eq p(psi)=14.3,r,eq.ratio=0.1,0.2,0.3,0.4,0.5,0.6,0.7,
0.8,0.9,1.0
  reactant fuel JP-5 moles=100. t,k=298.0
           oxidant O2 moles=20.72 t,k=298.
           oxidant N2 moles=77.24 t,k=298.
           oxidant CO2 moles=0.03 t,k=298.
           oxidant H2O moles=1.1 t,k=298.
           oxidant Ar moles=0.92 t,k=298.
           output si
  end

OPTIONS: TP=F  HP=T  SP=F  TV=F  UV=F  SV=F  DETN=F  SHOCK=F  REFL=F  INCD=F
RKT=F  FROZ=F  EQL=T  IONS=F  SIUNIT=T  DEBUGF=F  SHKDBG=F  DETDBG=F  TRNSPT=F

TRACE= 0.00E+00  S/R= 0.000000E+00  H/R= 0.000000E+00  U/R= 0.000000E+00

P,BAR =     0.985946

WARNING!! T=   298.00K DIFFERS FROM   298.15K FOR JP-5            (REACT)

   REACTANT           MOLES    (ENERGY/R),K   TEMP,K  DENSITY
       EXPLODED FORMULA
F: JP-5           100.000000  -0.266799E+04   298.15  0.0000
         C  1.00000  H  1.92000
O: O2              20.720000  -0.530002E+00   298.00  0.0000
         O  2.00000
O: N2              77.240000  -0.525424E+00   298.00  0.0000
         N  2.00000
O: CO2              0.030000  -0.473288E+05   298.00  0.0000
         C  1.00000  O  2.00000
O: H2O              1.100000  -0.290854E+05   298.00  0.0000
         H  2.00000  O  1.00000
O: Ar               0.920000  -0.375000E+00   298.00  0.0000
         AR 1.00000

 SPECIES BEING CONSIDERED IN THIS SYSTEM
(CONDENSED PHASE MAY HAVE NAME LISTED SEVERAL TIMES)
 LAST thermo.inp UPDATE:   9/16/99

 g 3/98  *Ar              g 7/97  *C               tpis79  *CH
 g 8/99  CH2              g 8/99  CH3              g12/92  CH2OH
 g10/92  CH3O             g 8/99  CH4              g 8/88  CH3OH
 g 8/99  *CN              g12/89  CNN              tpis79  *CO
 g 9/99  *CO2             tpis91  COOH             tpis91  *C2
 g 1/91  C2H              g 6/89  CHCO,ketyl       g12/89  C2H2,vinylidene
 g 1/91  C2H2,acetylene   g 5/90  CH2CO,ketene     g 2/92  C2H3,vinyl
 g12/92  CH3CN            g 6/96  CH3CO,acetyl     g 1/91  C2H4
 g 8/88  C2H4O,ethylen-o  g 8/88  CH3CHO,ethanal   g 8/88  CH3COOH
 g12/92  C2H5             g 8/88  C2H6             g 8/88  CH3N2CH3
 g 8/88  C2H5OH           g12/92  CH3OCH3          g12/92  CCN
 tpis91  CNC              tpis79  C2N2             g12/89  C2O
 tpis79  *C3              x 4/98  C3H3,1-propynl   x 4/98  C3H3,2-propynl
 g12/92  C3H4,allene      g12/92  C3H4,propyne     g 5/90  C3H4,cyclo-
 bur 92  C3H5,allyl       g 2/95  C3H6,propylene   g 1/93  C3H6,cyclo-
 g 6/90  C3H6O            g 6/90  C3H7,n-propyl    g 9/85  C3H7,i-propyl
 g 6/90  C3H8             g 9/88  C3H8O,1propanol  g 9/88  C3H8O,2propanol
```

```
 g 7/88  C3O2             g 7/88  C4               g 2/93  C4H2
 g 5/90  C4H4,1,3-cyclo-  x10/92  C4H6,butadiene   x10/93  C4H6,1-butyne
x10/93  C4H6,2-butyne    g 5/90  C4H6,cyclo-      x 4/88  C4H8,1-butene
 x 4/88  C4H8,cis2-buten  x 4/88  C4H8,tr2-butene  x 4/88  C4H8,isobutene
 g 5/90  C4H8,cyclo-      g 6/90  (CH3COOH)2       x10/84  C4H9,n-butyl
x10/84  C4H9,i-butyl     g 1/93  C4H9,s-butyl     g 1/93  C4H9,t-butyl
 g 6/90  C4H10,isobutane  g 6/90  C4H10,n-butane   j 3/61  C4N2
 g 7/88  C5               g 5/90  C5H6,1,3cyclo-   g 1/93  C5H8,cyclo-
 x 4/87  C5H10,1-pentene  g 6/90  C5H10,cyclo-     x10/84  C5H11,pentyl
 g 1/93  C5H11,t-pentyl   x10/85  C5H12,n-pentane  x10/85  C5H12,i-pentane
x10/85  CH3C(CH3)2CH3    g 2/93  C6H2             g 1/91  C6H5,phenyl
 g 6/90  C6H5O,phenoxy    g 1/91  C6H6             g 6/90  C6H5OH,phenol
 g 1/93  C6H10,cyclo-     x 4/87  C6H12,1-hexene   g 6/90  C6H12,cyclo-
x10/83  C6H13,n-hexyl    g 6/96  C6H14,n-hexane   g 1/93  C7H7,benzyl
 g 1/93  C7H8             g 1/93  C7H8O,cresol-mx  x 4/87  C7H14,1-heptene
x10/83  C7H15,n-heptyl   x10/85  C7H16,2-methylh  x10/85  C7H16,n-heptane
 x 4/89  C8H8,styrene     x10/86  C8H10,ethylbenz  x 4/87  C8H16,1-octene
x10/83  C8H17,n-octyl    x 4/85  C8H18,n-octane   x 4/85  C8H18,isooctane
x10/83  C9H19,n-nonyl    g 8/93  C10H8,naphthale  x10/83  C10H21,n-decyl
g12/84  C12H9,o-bipheny  g12/84  C12H10,biphenyl  g 6/97  *H
 g 7/88  HCN              g 9/96  HCO              tpis89  HCCN
g11/92  HNC              g 2/96  HNCO             g 5/99  HNO
tpis89  HNO2             g 5/99  HNO3             g 5/99  HO2
tpis78  *H2              g 8/88  HCHO,formaldehy  g 8/88  HCOOH
 g 8/89  H2O              g 6/99  H2O2             g 8/88  (HCOOH)2
 g 5/97  *N               g 2/96  NCO              g 4/99  *NH
 g 5/99  NH2              tpis89  NH3              tpis89  *NO
 g 4/99  NO2              j12/64  NO3              tpis78  *N2
g12/89  NCN              g 5/99  N2H2             tpis89  NH2NO2
 g 4/99  N2H4             g 4/99  N2O              g 4/99  N2O3
tpis89  N2O4             g 4/99  N2O5             tpis89  N3
 g 4/99  N3H              g 5/97  *O              tpis78  *OH
tpis89  *O2              tpis89  O3               X 4/83  C(gr)
 X 4/83  C(gr)            X 4/83  C(gr)            g 8/89  H2O(s)
 g 8/89  H2O(L)

O/F = 197.504751

                        EFFECTIVE FUEL     EFFECTIVE OXIDANT        MIXTURE
ENTHALPY                    h(2)/R             h(1)/R               h0/R
(KG-MOL)(K)/KG       -0.19130912E+03    -0.11601254E+02    -0.12506562E+02

KG-FORM.WT./KG             bi(2)              bi(1)              b0i
 *C                   0.71705432E-01     0.10399819E-04     0.37157522E-03
 *H                   0.13767443E+00     0.76265339E-03     0.14523687E-02
 *O                   0.00000000E+00     0.14767743E-01     0.14693348E-01
 *N                   0.00000000E+00     0.53552135E-01     0.53282357E-01
 *Ar                  0.00000000E+00     0.31892778E-03     0.31732113E-03

POINT ITN      T            C           H           O           N
                    AR
  1   31     510.243     -96.819     -35.350     -13.391     -11.875
                -23.636
```

THERMODYNAMIC EQUILIBRIUM COMBUSTION PROPERTIES AT ASSIGNED

PRESSURES

CASE = methane

REACTANT		MOLES	ENERGY KJ/KG-MOL	TEMP K
FUEL	JP-5	100.0000000	-22183.000	298.150
OXIDANT	O2	20.7200000	-4.407	298.000
OXIDANT	N2	77.2400000	-4.369	298.000
OXIDANT	CO2	0.0300000	-393515.570	298.000

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OXIDANT     H2O                          1.1000000   -241831.038    298.000
OXIDANT     Ar                           0.9200000        -3.118    298.000

O/F=  197.50475  %FUEL=  0.503766  R,EQ.RATIO= 0.100000  PHI,EQ.RATIO= 0.074807

THERMODYNAMIC PROPERTIES

P, BAR           0.98595
T, K              510.24
RHO, KG/CU M    6.7036-1
H, KJ/KG         -103.99
U, KJ/KG         -251.06
G, KJ/KG        -3921.25
S, KJ/(KG)(K)     7.4813

M, (1/n)          28.845
(dLV/dLP)t      -1.00000
(dLV/dLT)p        1.0000
Cp, KJ/(KG)(K)    1.0445
GAMMAs            1.3811
SON VEL,M/SEC      450.7

MOLE FRACTIONS

*Ar              0.00915
*CO2             0.01072
H2O              0.02095
*N2              0.76846
*O2              0.19072

 * THERMODYNAMIC PROPERTIES FITTED TO 20000.K

   PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS
   WERE LESS THAN 5.000000E-06 FOR ALL ASSIGNED CONDITIONS

*C               *CH              CH2              CH3              CH2OH
CH3O             CH4              CH3OH            *CN              CNN
*CO              COOH             *C2              C2H              CHCO,ketyl
C2H2,vinylidene  C2H2,acetylene   CH2CO,ketene     C2H3,vinyl       CH3CN
CH3CO,acetyl     C2H4             C2H4O,ethylen-o  CH3CHO,ethanal   CH3COOH
C2H5             C2H6             CH3N2CH3         C2H5OH           CH3OCH3
CCN              CNC              C2N2             C2O              *C3
C3H3,1-propynl   C3H3,2-propynl   C3H4,allene      C3H4,propyne     C3H4,cyclo-
C3H5,allyl       C3H6,propylene   C3H6,cyclo-      C3H6O            C3H7,n-propyl
C3H7,i-propyl    C3H8             C3H8O,1propanol  C3H8O,2propanol  C3O2
C4               C4H2             C4H4,1,3-cyclo-  C4H6,butadiene   C4H6,1-butyne
C4H6,2-butyne    C4H6,cyclo-      C4H8,1-butene    C4H8,cis2-buten  C4H8,tr2-butene
C4H8,isobutene   C4H8,cyclo-      (CH3COOH)2       C4H9,n-butyl     C4H9,i-butyl
C4H9,s-butyl     C4H9,t-butyl     C4H10,isobutane  C4H10,n-butane   C4N2
C5               C5H6,1,3cyclo-   C5H8,cyclo-      C5H10,1-pentene  C5H10,cyclo-
C5H11,pentyl     C5H11,t-pentyl   C5H12,n-pentane  C5H12,i-pentane  CH3C(CH3)2CH3
C6H2             C6H5,phenyl      C6H5O,phenoxy    C6H6             C6H5OH,phenol
C6H10,cyclo-     C6H12,1-hexene   C6H12,cyclo-     C6H13,n-hexyl    C6H14,n-hexane
C7H7,benzyl      C7H8             C7H8O,cresol-mx  C7H14,1-heptene  C7H15,n-heptyl
C7H16,2-methylh  C7H16,n-heptane  C8H8,styrene     C8H10,ethylbenz  C8H16,1-octene
C8H17,n-octyl    C8H18,n-octane   C8H18,isooctane  C9H19,n-nonyl    C10H8,naphthale
C10H21,n-decyl   C12H9,o-bipheny  C12H10,biphenyl  *H               HCN
HCO              HCCN             HNC              HNCO             HNO
HNO2             HNO3             HO2              *H2              HCHO,formaldehy
HCOOH            H2O2             (HCOOH)2         *N               NCO
*NH              NH2              NH3              *NO              NO2
NO3              NCN              N2H2             NH2NO2           N2H4
N2O              N2O3             N2O4             N2O5             N3
N3H              *O               *OH              O3               C(gr)
H2O(s)           H2O(L)
```

O/F = 83.188142

ENTHALPY (KG-MOL)(K)/KG	EFFECTIVE FUEL h(2)/R	EFFECTIVE OXIDANT h(1)/R	MIXTURE h0/R
	-0.19130912E+03	-0.11601254E+02	-0.13735853E+02

KG-FORM.WT./KG	bi(2)	bi(1)	b0i
*C	0.71705432E-01	0.10399819E-04	0.86200470E-03
*H	0.13767443E+00	0.76265339E-03	0.23889130E-02
*O	0.00000000E+00	0.14767743E-01	0.14592329E-01
*N	0.00000000E+00	0.53552135E-01	0.52916034E-01
*Ar	0.00000000E+00	0.31892778E-03	0.31513951E-03

POINT	ITN	T	C	H	O	N	AR
1	5	781.185	-64.019	-25.448	-13.867	-12.276	-24.201

THERMODYNAMIC EQUILIBRIUM COMBUSTION PROPERTIES AT ASSIGNED

PRESSURES

CASE = methane

	REACTANT	MOLES	ENERGY KJ/KG-MOL	TEMP K
FUEL	JP-5	100.0000000	-22183.000	298.150
OXIDANT	O2	20.7200000	-4.407	298.000
OXIDANT	N2	77.2400000	-4.369	298.000
OXIDANT	CO2	0.0300000	-393515.570	298.000
OXIDANT	H2O	1.1000000	-241831.038	298.000
OXIDANT	Ar	0.9200000	-3.118	298.000

O/F= 83.18814 %FUEL= 1.187816 R,EQ.RATIO= 0.200000 PHI,EQ.RATIO= 0.177606

THERMODYNAMIC PROPERTIES

P, BAR	0.98595
T, K	781.19
RHO, KG/CU M	4.3788-1
H, KJ/KG	-114.21
U, KJ/KG	-339.37
G, KJ/KG	-6336.22
S, KJ/(KG)(K)	7.9648
M, (1/n)	28.846
(dLV/dLP)t	-1.00000
(dLV/dLT)p	1.0000
Cp, KJ/(KG)(K)	1.1212
GAMMAs	1.3460
SON VEL,M/SEC	550.5

MOLE FRACTIONS

*Ar	0.00909
*CO2	0.02487
H2O	0.03446
*N2	0.76321
*O2	0.16837

 * THERMODYNAMIC PROPERTIES FITTED TO 20000.K

   PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS
   WERE LESS THAN 5.000000E-06 FOR ALL ASSIGNED CONDITIONS

*C	*CH	CH2	CH3	CH2OH
CH3O	CH4	CH3OH	*CN	CNN
*CO	COOH	*C2	C2H	CHCO,ketyl
C2H2,vinylidene	C2H2,acetylene	CH2CO,ketene	C2H3,vinyl	CH3CN
CH3CO,acetyl	C2H4	C2H4O,ethylen-o	CH3CHO,ethanal	CH3COOH
C2H5	C2H6	CH3N2CH3	C2H5OH	CH3OCH3
CCN	CNC	C2N2	C2O	*C3
C3H3,1-propynl	C3H3,2-propynl	C3H4,allene	C3H4,propyne	C3H4,cyclo-
C3H5,allyl	C3H6,propylene	C3H6,cyclo-	C3H6O	C3H7,n-propyl
C3H7,i-propyl	C3H8	C3H8O,1propanol	C3H8O,2propanol	C3O2
C4	C4H2	C4H4,1,3-cyclo-	C4H6,butadiene	C4H6,1-butyne
C4H6,2-butyne	C4H6,cyclo-	C4H8,1-butene	C4H8,cis2-buten	C4H8,tr2-butene
C4H8,isobutene	C4H8,cyclo-	(CH3COOH)2	C4H9,n-butyl	C4H9,i-butyl
C4H9,s-butyl	C4H9,t-butyl	C4H10,isobutane	C4H10,n-butane	C4N2
C5	C5H6,1,3cyclo-	C5H8,cyclo-	C5H10,1-pentene	C5H10,cyclo-
C5H11,pentyl	C5H11,t-pentyl	C5H12,n-pentane	C5H12,i-pentane	CH3C(CH3)2CH3
C6H2	C6H5,phenyl	C6H5O,phenoxy	C6H6	C6H5OH,phenol
C6H10,cyclo-	C6H12,1-hexene	C6H12,cyclo-	C6H13,n-hexyl	C6H14,n-hexane
C7H7,benzyl	C7H8	C7H8O,cresol-mx	C7H14,1-heptene	C7H15,n-heptyl
C7H16,2-methylh	C7H16,n-heptane	C8H8,styrene	C8H10,ethylbenz	C8H16,1-octene
C8H17,n-octyl	C8H18,n-octane	C8H18,isooctane	C9H19,n-nonyl	C10H8,naphthale
C10H21,n-decyl	C12H9,o-bipheny	C12H10,biphenyl	*H	HCN
HCO	HCCN	HNC	HNCO	HNO
HNO2	HNO3	HO2	*H2	HCHO,formaldehy
HCOOH	H2O2	(HCOOH)2	*N	NCO
*NH	NH2	NH3	*NO	NO2
NO3	NCN	N2H2	NH2NO2	N2H4
N2O	N2O3	N2O4	N2O5	N3
N3H	*O	*OH	O3	C(gr)
H2O(s)	H2O(L)			

O/F = 52.690596

ENTHALPY (KG-MOL)(K)/KG	EFFECTIVE FUEL h(2)/R	EFFECTIVE OXIDANT h(1)/R	MIXTURE h0/R
	-0.19130912E+03	-0.11601254E+02	-0.14948356E+02

KG-FORM.WT./KG	bi(2)	bi(1)	b0i
*C	0.71705432E-01	0.10399819E-04	0.13457367E-02
*H	0.13767443E+00	0.76265339E-03	0.33126674E-02
*O	0.00000000E+00	0.14767743E-01	0.14492690E-01
*N	0.00000000E+00	0.53552135E-01	0.52554714E-01
*Ar	0.00000000E+00	0.31892778E-03	0.31298768E-03

POINT	ITN	T	C	H	O	N	AR
1	5	1028.613	-49.181	-20.997	-14.290	-12.613	-24.666

THERMODYNAMIC EQUILIBRIUM COMBUSTION PROPERTIES AT ASSIGNED

PRESSURES

CASE = methane

	REACTANT	MOLES	ENERGY KJ/KG-MOL	TEMP K
FUEL	JP-5	100.0000000	-22183.000	298.150
OXIDANT	O2	20.7200000	-4.407	298.000
OXIDANT	N2	77.2400000	-4.369	298.000

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OXIDANT     CO2                          0.0300000   -393515.570    298.000
OXIDANT     H2O                          1.1000000   -241831.038    298.000
OXIDANT     Ar                           0.9200000        -3.118    298.000

O/F=   52.69060  %FUEL=  1.862524  R,EQ.RATIO= 0.300000  PHI,EQ.RATIO= 0.280405

THERMODYNAMIC PROPERTIES

P, BAR           0.98595
T, K             1028.61
RHO, KG/CU M    3.3256-1
H, KJ/KG         -124.29
U, KJ/KG         -420.76
G, KJ/KG        -8667.22
S, KJ/(KG)(K)     8.3053

M, (1/n)          28.848
(dLV/dLP)t      -1.00000
(dLV/dLT)p        1.0000
Cp, KJ/(KG)(K)    1.1913
GAMMAs            1.3191
SON VEL,M/SEC      625.4

MOLE FRACTIONS

*Ar              0.00903
*CO2             0.03882
H2O              0.04778
*NO              0.00003
*N2              0.75802
*O2              0.14631

 * THERMODYNAMIC PROPERTIES FITTED TO 20000.K

   PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS
   WERE LESS THAN 5.000000E-06 FOR ALL ASSIGNED CONDITIONS

*C              *CH             CH2             CH3             CH2OH
CH3O            CH4             CH3OH           *CN             CNN
*CO             COOH            *C2             C2H             CHCO,ketyl
C2H2,vinylidene C2H2,acetylene  CH2CO,ketene    C2H3,vinyl      CH3CN
CH3CO,acetyl    C2H4            C2H4O,ethylen-o CH3CHO,ethanal  CH3COOH
C2H5            C2H6            CH3N2CH3        C2H5OH          CH3OCH3
CCN             CNC             C2N2            C2O             *C3
C3H3,1-propynl  C3H3,2-propynl  C3H4,allene     C3H4,propyne    C3H4,cyclo-
C3H5,allyl      C3H6,propylene  C3H6,cyclo-     C3H6O           C3H7,n-propyl
C3H7,i-propyl   C3H8            C3H8O,1propanol C3H8O,2propanol C3O2
C4              C4H2            C4H4,1,3-cyclo- C4H6,butadiene  C4H6,1-butyne
C4H6,2-butyne   C4H6,cyclo-     C4H8,1-butene   C4H8,cis2-buten C4H8,tr2-butene
C4H8,isobutene  C4H8,cyclo-     (CH3COOH)2      C4H9,n-butyl    C4H9,i-butyl
C4H9,s-butyl    C4H9,t-butyl    C4H10,isobutane C4H10,n-butane  C4N2
C5              C5H6,1,3cyclo-  C5H8,cyclo-     C5H10,1-pentene C5H10,cyclo-
C5H11,pentyl    C5H11,t-pentyl  C5H12,n-pentane C5H12,i-pentane CH3C(CH3)2CH3
C6H2            C6H5,phenyl     C6H5O,phenoxy   C6H6            C6H5OH,phenol
C6H10,cyclo-    C6H12,1-hexene  C6H12,cyclo-    C6H13,n-hexyl   C6H14,n-hexane
C7H7,benzyl     C7H8            C7H8O,cresol-mx C7H14,1-heptene C7H15,n-heptyl
C7H16,2-methylh C7H16,n-heptane C8H8,styrene    C8H10,ethylbenz C8H16,1-octene
C8H17,n-octyl   C8H18,n-octane  C8H18,isooctane C9H19,n-nonyl   C10H8,naphthale
C10H21,n-decyl  C12H9,o-bipheny C12H10,biphenyl *H              HCN
HCO             HCCN            HNC             HNCO            HNO
HNO2            HNO3            HO2             *H2             HCHO,formaldehy
HCOOH           H2O2            (HCOOH)2        *N              NCO
*NH             NH2             NH3             NO2             NO3
NCN             N2H2            NH2NO2          N2H4            N2O
N2O3            N2O4            N2O5            N3              N3H
*O              *OH             O3              C(gr)           H2O(s)
H2O(L)
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O/F = 38.555713

ENTHALPY (KG-MOL)(K)/KG	EFFECTIVE FUEL h(2)/R	EFFECTIVE OXIDANT h(1)/R	MIXTURE h0/R
	-0.19130912E+03	-0.11601254E+02	-0.16144412E+02

KG-FORM.WT./KG	bi(2)	bi(1)	b0i
*C	0.71705432E-01	0.10399819E-04	0.18229075E-02
*H	0.13767443E+00	0.76265339E-03	0.42238923E-02
*O	0.00000000E+00	0.14767743E-01	0.14394403E-01
*N	0.00000000E+00	0.53552135E-01	0.52198294E-01
*Ar	0.00000000E+00	0.31892778E-03	0.31086503E-03

POINT	ITN	T	C	H	O	N	AR
1	4	1257.303	-40.632	-18.455	-14.663	-12.892	-25.043

THERMODYNAMIC EQUILIBRIUM COMBUSTION PROPERTIES AT ASSIGNED

PRESSURES

CASE = methane

REACTANT		MOLES	ENERGY KJ/KG-MOL	TEMP K
FUEL	JP-5	100.0000000	-22183.000	298.150
OXIDANT	O2	20.7200000	-4.407	298.000
OXIDANT	N2	77.2400000	-4.369	298.000
OXIDANT	CO2	0.0300000	-393515.570	298.000
OXIDANT	H2O	1.1000000	-241831.038	298.000
OXIDANT	Ar	0.9200000	-3.118	298.000

O/F= 38.55571 %FUEL= 2.528080 R,EQ.RATIO= 0.400000 PHI,EQ.RATIO= 0.383205

THERMODYNAMIC PROPERTIES

P, BAR	0.98595
T, K	1257.30
RHO, KG/CU M	2.7209-1
H, KJ/KG	-134.23
U, KJ/KG	-496.60
G, KJ/KG	-10911.9
S, KJ/(KG)(K)	8.5721
M, (1/n)	28.849
(dLV/dLP)t	-1.00000
(dLV/dLT)p	1.0000
Cp, KJ/(KG)(K)	1.2510
GAMMAs	1.2994
SON VEL,M/SEC	686.2

MOLE FRACTIONS

*Ar	0.00897
*CO2	0.05259
H2O	0.06093
*NO	0.00022
*N2	0.75282
*O2	0.12446

 * THERMODYNAMIC PROPERTIES FITTED TO 20000.K

PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS
WERE LESS THAN 5.000000E-06 FOR ALL ASSIGNED CONDITIONS

*C	*CH	CH2	CH3	CH2OH
CH3O	CH4	CH3OH	*CN	CNN
*CO	COOH	*C2	C2H	CHCO,ketyl
C2H2,vinylidene	C2H2,acetylene	CH2CO,ketene	C2H3,vinyl	CH3CN
CH3CO,acetyl	C2H4	C2H4O,ethylen-o	CH3CHO,ethanal	CH3COOH
C2H5	C2H6	CH3N2CH3	C2H5OH	CH3OCH3
CCN	CNC	C2N2	C2O	*C3
C3H3,1-propynl	C3H3,2-propynl	C3H4,allene	C3H4,propyne	C3H4,cyclo-
C3H5,allyl	C3H6,propylene	C3H6,cyclo-	C3H6O	C3H7,n-propyl
C3H7,i-propyl	C3H8	C3H8O,1propanol	C3H8O,2propanol	C3O2
C4	C4H2	C4H4,1,3-cyclo-	C4H6,butadiene	C4H6,1-butyne
C4H6,2-butyne	C4H6,cyclo-	C4H8,1-butene	C4H8,cis2-buten	C4H8,tr2-butene
C4H8,isobutene	C4H8,cyclo-	(CH3COOH)2	C4H9,n-butyl	C4H9,i-butyl
C4H9,s-butyl	C4H9,t-butyl	C4H10,isobutane	C4H10,n-butane	C4N2
C5	C5H6,1,3cyclo-	C5H8,cyclo-	C5H10,1-pentene	C5H10,cyclo-
C5H11,pentyl	C5H11,t-pentyl	C5H12,n-pentane	C5H12,i-pentane	CH3C(CH3)2CH3
C6H2	C6H5,phenyl	C6H5O,phenoxy	C6H6	C6H5OH,phenol
C6H10,cyclo-	C6H12,1-hexene	C6H12,cyclo-	C6H13,n-hexyl	C6H14,n-hexane
C7H7,benzyl	C7H8	C7H8O,cresol-mx	C7H14,1-heptene	C7H15,n-heptyl
C7H16,2-methylh	C7H16,n-heptane	C8H8,styrene	C8H10,ethylbenz	C8H16,1-octene
C8H17,n-octyl	C8H18,n-octane	C8H18,isooctane	C9H19,n-nonyl	C10H8,naphthale
C10H21,n-decyl	C12H9,o-bipheny	C12H10,biphenyl	*H	HCN
HCO	HCCN	HNC	HNCO	HNO
HNO2	HNO3	HO2	*H2	HCHO,formaldehy
HCOOH	H2O2	(HCOOH)2	*N	NCO
*NH	NH2	NH3	NO2	NO3
NCN	N2H2	NH2NO2	N2H4	N2O
N2O3	N2O4	N2O5	N3	N3H
*O	*OH	O3	C(gr)	H2O(s)
H2O(L)				

O/F = 30.400433

ENTHALPY (KG-MOL)(K)/KG	EFFECTIVE FUEL h(2)/R -0.19130912E+03	EFFECTIVE OXIDANT h(1)/R -0.11601254E+02	MIXTURE h0/R -0.17324356E+02
KG-FORM.WT./KG	bi(2)	bi(1)	b0i
*C	0.71705432E-01	0.10399819E-04	0.22936496E-02
*H	0.13767443E+00	0.76265339E-03	0.51228408E-02
*O	0.00000000E+00	0.14767743E-01	0.14297439E-01
*N	0.00000000E+00	0.53552135E-01	0.51846676E-01
*Ar	0.00000000E+00	0.31892778E-03	0.30877099E-03

POINT	ITN	T	C	H	O	N	AR
1	4	1470.566	-35.002	-16.799	-15.005	-13.128	-25.355

THERMODYNAMIC EQUILIBRIUM COMBUSTION PROPERTIES AT ASSIGNED

PRESSURES

CASE = methane

REACTANT	MOLES	ENERGY KJ/KG-MOL	TEMP K

```
FUEL        JP-5                      100.0000000    -22183.000    298.150
OXIDANT     O2                         20.7200000        -4.407    298.000
OXIDANT     N2                         77.2400000        -4.369    298.000
OXIDANT     CO2                         0.0300000   -393515.570    298.000
OXIDANT     H2O                         1.1000000   -241831.038    298.000
OXIDANT     Ar                          0.9200000        -3.118    298.000

O/F=   30.40043  %FUEL=  3.184669  R,EQ.RATIO= 0.500000  PHI,EQ.RATIO= 0.486004

THERMODYNAMIC PROPERTIES

P, BAR           0.98595
T, K             1470.57
RHO, KG/CU M    2.3264-1
H, KJ/KG         -144.04
U, KJ/KG         -567.86
G, KJ/KG        -13075.0
S, KJ/(KG)(K)     8.7932

M, (1/n)          28.850
(dLV/dLP)t      -1.00000
(dLV/dLT)p        1.0002
Cp, KJ/(KG)(K)    1.3056
GAMMAs            1.2834
SON VEL,M/SEC      737.5

MOLE FRACTIONS

*Ar              0.00891
*CO2             0.06617
H2O              0.07388
*NO              0.00072
*N2              0.74753
*OH              0.00004
*O2              0.10275

 * THERMODYNAMIC PROPERTIES FITTED TO 20000.K

   PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS
   WERE LESS THAN 5.000000E-06 FOR ALL ASSIGNED CONDITIONS

*C              *CH             CH2             CH3             CH2OH
CH3O            CH4             CH3OH           *CN             CNN
*CO             COOH            *C2             C2H             CHCO,ketyl
C2H2,vinylidene C2H2,acetylene  CH2CO,ketene    C2H3,vinyl      CH3CN
CH3CO,acetyl    C2H4            C2H4O,ethylen-o CH3CHO,ethanal  CH3COOH
C2H5            C2H6            CH3N2CH3        C2H5OH          CH3OCH3
CCN             CNC             C2N2            C2O             *C3
C3H3,1-propynl  C3H3,2-propynl  C3H4,allene     C3H4,propyne    C3H4,cyclo-
C3H5,allyl      C3H6,propylene  C3H6,cyclo-     C3H6O           C3H7,n-propyl
C3H7,i-propyl   C3H8            C3H8O,1propanol C3H8O,2propanol C3O2
C4              C4H2            C4H4,1,3-cyclo- C4H6,butadiene  C4H6,1-butyne
C4H6,2-butyne   C4H6,cyclo-     C4H8,1-butene   C4H8,cis2-buten C4H8,tr2-butene
C4H8,isobutene  C4H8,cyclo-     (CH3COOH)2      C4H9,n-butyl    C4H9,i-butyl
C4H9,s-butyl    C4H9,t-butyl    C4H10,isobutane C4H10,n-butane  C4N2
C5              C5H6,1,3cyclo-  C5H8,cyclo-     C5H10,1-pentene C5H10,cyclo-
C5H11,pentyl    C5H11,t-pentyl  C5H12,n-pentane C5H12,i-pentane CH3C(CH3)2CH3
C6H2            C6H5,phenyl     C6H5O,phenoxy   C6H6            C6H5OH,phenol
C6H10,cyclo-    C6H12,1-hexene  C6H12,cyclo-    C6H13,n-hexyl   C6H14,n-hexane
C7H7,benzyl     C7H8            C7H8O,cresol-mx C7H14,1-heptene C7H15,n-heptyl
C7H16,2-methylh C7H16,n-heptane C8H8,styrene    C8H10,ethylbenz C8H16,1-octene
C8H17,n-octyl   C8H18,n-octane  C8H18,isooctane C9H19,n-nonyl   C10H8,naphthale
C10H21,n-decyl  C12H9,o-bipheny C12H10,biphenyl *H              HCN
HCO             HCCN            HNC             HNCO            HNO
HNO2            HNO3            HO2             *H2             HCHO,formaldehy
HCOOH           H2O2            (HCOOH)2        *N              NCO
*NH             NH2             NH3             NO2             NO3
NCN             N2H2            NH2NO2          N2H4            N2O
N2O3            N2O4            N2O5            N3              N3H
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*O              O3              C(gr)           H2O(s)          H2O(L)



O/F =  25.092817

                        EFFECTIVE FUEL     EFFECTIVE OXIDANT        MIXTURE
ENTHALPY                    h(2)/R             h(1)/R               h0/R
(KG-MOL)(K)/KG       -0.19130912E+03    -0.11601254E+02    -0.18488509E+02

KG-FORM.WT./KG             bi(2)              bi(1)              b0i
 *C                    0.71705432E-01     0.10399819E-04     0.27580922E-02
 *H                    0.13767443E+00     0.76265339E-03     0.60097593E-02
 *O                    0.00000000E+00     0.14767743E-01     0.14201773E-01
 *N                    0.00000000E+00     0.53552135E-01     0.51499764E-01
 *Ar                   0.00000000E+00     0.31892778E-03     0.30670496E-03

POINT ITN      T            C           H           O           N
                    AR
  1    4    1670.196     -30.955     -15.625     -15.333     -13.331
                -25.619



        THERMODYNAMIC EQUILIBRIUM COMBUSTION PROPERTIES AT ASSIGNED

                                    PRESSURES

CASE = methane

            REACTANT                        MOLES         ENERGY      TEMP
                                                         KJ/KG-MOL       K
FUEL        JP-5                       100.0000000    -22183.000    298.150
OXIDANT     O2                          20.7200000        -4.407    298.000
OXIDANT     N2                          77.2400000        -4.369    298.000
OXIDANT     CO2                          0.0300000   -393515.570    298.000
OXIDANT     H2O                          1.1000000   -241831.038    298.000
OXIDANT     Ar                           0.9200000        -3.118    298.000

O/F=   25.09282  %FUEL=  3.832472  R,EQ.RATIO= 0.600000  PHI,EQ.RATIO= 0.588803

THERMODYNAMIC PROPERTIES

P, BAR           0.98595
T, K             1670.20
RHO, KG/CU M    2.0483-1
H, KJ/KG         -153.72
U, KJ/KG         -635.07
G, KJ/KG        -15156.5
S, KJ/(KG)(K)     8.9827

M, (1/n)          28.850
(dLV/dLP)t      -1.00002
(dLV/dLT)p        1.0009
Cp, KJ/(KG)(K)    1.3620
GAMMAs            1.2690
SON VEL,M/SEC      781.5

MOLE FRACTIONS

*Ar              0.00885
*CO              0.00001
*CO2             0.07956
H2O              0.08658
*NO              0.00156
```

*N2	0.74210
*O	0.00001
*OH	0.00022
*O2	0.08111

* THERMODYNAMIC PROPERTIES FITTED TO 20000.K

PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS
WERE LESS THAN 5.000000E-06 FOR ALL ASSIGNED CONDITIONS

*C	*CH	CH2	CH3	CH2OH
CH3O	CH4	CH3OH	*CN	CNN
COOH	*C2	C2H	CHCO,ketyl	C2H2,vinylidene
C2H2,acetylene	CH2CO,ketene	C2H3,vinyl	CH3CN	CH3CO,acetyl
C2H4	C2H4O,ethylen-o	CH3CHO,ethanal	CH3COOH	C2H5
C2H6	CH3N2CH3	C2H5OH	CH3OCH3	CCN
CNC	C2N2	C2O	*C3	C3H3,1-propynl
C3H3,2-propynl	C3H4,allene	C3H4,propyne	C3H4,cyclo-	C3H5,allyl
C3H6,propylene	C3H6,cyclo-	C3H6O	C3H7,n-propyl	C3H7,i-propyl
C3H8	C3H8O,1propanol	C3H8O,2propanol	C3O2	C4
C4H2	C4H4,1,3-cyclo-	C4H6,butadiene	C4H6,1-butyne	C4H6,2-butyne
C4H6,cyclo-	C4H8,1-butene	C4H8,cis2-buten	C4H8,tr2-butene	C4H8,isobutene
C4H8,cyclo-	(CH3COOH)2	C4H9,n-butyl	C4H9,i-butyl	C4H9,s-butyl
C4H9,t-butyl	C4H10,isobutane	C4H10,n-butane	C4N2	C5
C5H6,1,3cyclo-	C5H8,cyclo-	C5H10,1-pentene	C5H10,cyclo-	C5H11,pentyl
C5H11,t-pentyl	C5H12,n-pentane	C5H12,i-pentane	CH3C(CH3)2CH3	C6H2
C6H5,phenyl	C6H5O,phenoxy	C6H6	C6H5OH,phenol	C6H10,cyclo-
C6H12,1-hexene	C6H12,cyclo-	C6H13,n-hexyl	C6H14,n-hexane	C7H7,benzyl
C7H8	C7H8O,cresol-mx	C7H14,1-heptene	C7H15,n-heptyl	C7H16,2-methylh
C7H16,n-heptane	C8H8,styrene	C8H10,ethylbenz	C8H16,1-octene	C8H17,n-octyl
C8H18,n-octane	C8H18,isooctane	C9H19,n-nonyl	C10H8,naphthale	C10H21,n-decyl
C12H9,o-bipheny	C12H10,biphenyl	*H	HCN	HCO
HCCN	HNC	HNCO	HNO	HNO2
HNO3	HO2	*H2	HCHO,formaldehy	HCOOH
H2O2	(HCOOH)2	*N	NCO	*NH
NH2	NH3	NO2	NO3	NCN
N2H2	NH2NO2	N2H4	N2O	N2O3
N2O4	N2O5	N3	N3H	O3
C(gr)	H2O(s)	H2O(L)		

O/F = 21.363040

ENTHALPY (KG-MOL)(K)/KG	EFFECTIVE FUEL h(2)/R	EFFECTIVE OXIDANT h(1)/R	MIXTURE h0/R
	-0.19130912E+03	-0.11601254E+02	-0.19637186E+02

KG-FORM.WT./KG	bi(2)	bi(1)	b0i
*C	0.71705432E-01	0.10399819E-04	0.32163607E-02
*H	0.13767443E+00	0.76265339E-03	0.68848878E-02
*O	0.00000000E+00	0.14767743E-01	0.14107379E-01
*N	0.00000000E+00	0.53552135E-01	0.51157463E-01
*Ar	0.00000000E+00	0.31892778E-03	0.30466640E-03

POINT	ITN	T	C	H	O	N	AR
1	4	1856.533	-27.845	-14.737	-15.668	-13.507	-25.846

THERMODYNAMIC EQUILIBRIUM COMBUSTION PROPERTIES AT ASSIGNED

PRESSURES

CASE = methane

	REACTANT	MOLES	ENERGY KJ/KG-MOL	TEMP K
FUEL	JP-5	100.0000000	-22183.000	298.150
OXIDANT	O2	20.7200000	-4.407	298.000
OXIDANT	N2	77.2400000	-4.369	298.000
OXIDANT	CO2	0.0300000	-393515.570	298.000
OXIDANT	H2O	1.1000000	-241831.038	298.000
OXIDANT	Ar	0.9200000	-3.118	298.000

O/F= 21.36304 %FUEL= 4.471664 R,EQ.RATIO= 0.700000 PHI,EQ.RATIO= 0.691602

THERMODYNAMIC PROPERTIES

P, BAR	0.98595
T, K	1856.53
RHO, KG/CU M	1.8424-1
H, KJ/KG	-163.27
U, KJ/KG	-698.42
G, KJ/KG	-17147.9
S, KJ/(KG)(K)	9.1486
M, (1/n)	28.845
(dLV/dLP)t	-1.00010
(dLV/dLT)p	1.0039
Cp, KJ/(KG)(K)	1.4344
GAMMAs	1.2538
SON VEL,M/SEC	819.1

MOLE FRACTIONS

*Ar	0.00879
*CO	0.00014
*CO2	0.09264
*H2	0.00004
H2O	0.09891
*NO	0.00258
*N2	0.73652
*O	0.00005
*OH	0.00070
*O2	0.05963

* THERMODYNAMIC PROPERTIES FITTED TO 20000.K

PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS
WERE LESS THAN 5.000000E-06 FOR ALL ASSIGNED CONDITIONS

*C	*CH	CH2	CH3	CH2OH
CH3O	CH4	CH3OH	*CN	CNN
COOH	*C2	C2H	CHCO,ketyl	C2H2,vinylidene
C2H2,acetylene	CH2CO,ketene	C2H3,vinyl	CH3CN	CH3CO,acetyl
C2H4	C2H4O,ethylen-o	CH3CHO,ethanal	CH3COOH	C2H5
C2H6	CH3N2CH3	C2H5OH	CH3OCH3	CCN
CNC	C2N2	C2O	*C3	C3H3,1-propynl
C3H3,2-propynl	C3H4,allene	C3H4,propyne	C3H4,cyclo-	C3H5,allyl
C3H6,propylene	C3H6,cyclo-	C3H6O	C3H7,n-propyl	C3H7,i-propyl
C3H8	C3H8O,1propanol	C3H8O,2propanol	C3O2	C4
C4H2	C4H4,1,3-cyclo-	C4H6,butadiene	C4H6,1-butyne	C4H6,2-butyne
C4H6,cyclo-	C4H8,1-butene	C4H8,cis2-buten	C4H8,tr2-butene	C4H8,isobutene
C4H8,cyclo-	(CH3COOH)2	C4H9,n-butyl	C4H9,i-butyl	C4H9,s-butyl
C4H9,t-butyl	C4H10,isobutane	C4H10,n-butane	C4N2	C5
C5H6,1,3cyclo-	C5H8,cyclo-	C5H10,1-pentene	C5H10,cyclo-	C5H11,pentyl
C5H11,t-pentyl	C5H12,n-pentane	C5H12,i-pentane	CH3C(CH3)2CH3	C6H2
C6H5,phenyl	C6H5O,phenoxy	C6H6	C6H5OH,phenol	C6H10,cyclo-
C6H12,1-hexene	C6H12,cyclo-	C6H13,n-hexyl	C6H14,n-hexane	C7H7,benzyl
C7H8	C7H8O,cresol-mx	C7H14,1-heptene	C7H15,n-heptyl	C7H16,2-methylh
C7H16,n-heptane	C8H8,styrene	C8H10,ethylbenz	C8H16,1-octene	C8H17,n-octyl

C8H18,n-octane	C8H18,isooctane	C9H19,n-nonyl	C10H8,naphthale	C10H21,n-decyl
C12H9,o-bipheny	C12H10,biphenyl	*H	HCN	HCO
HCCN	HNC	HNCO	HNO	HNO2
HNO3	HO2	HCHO,formaldehy	HCOOH	H2O2
(HCOOH)2	*N	NCO	*NH	NH2
NH3	NO2	NO3	NCN	N2H2
NH2NO2	N2H4	N2O	N2O3	N2O4
N2O5	N3	N3H	O3	C(gr)
H2O(s)	H2O(L)			

O/F = 18.598564

ENTHALPY (KG-MOL)(K)/KG	EFFECTIVE FUEL h(2)/R	EFFECTIVE OXIDANT h(1)/R	MIXTURE h0/R
	-0.19130912E+03	-0.11601254E+02	-0.20770695E+02

KG-FORM.WT./KG	bi(2)	bi(1)	b0i
*C	0.71705432E-01	0.10399819E-04	0.36685777E-02
*H	0.13767443E+00	0.76265339E-03	0.77484598E-02
*O	0.00000000E+00	0.14767743E-01	0.14014232E-01
*N	0.00000000E+00	0.53552135E-01	0.50819683E-01
*Ar	0.00000000E+00	0.31892778E-03	0.30265477E-03

POINT	ITN	T	C	H	O	N	AR
1	4	2026.760	-25.317	-14.028	-16.039	-13.657	-26.039

THERMODYNAMIC EQUILIBRIUM COMBUSTION PROPERTIES AT ASSIGNED

PRESSURES

CASE = methane

	REACTANT	MOLES	ENERGY KJ/KG-MOL	TEMP K
FUEL	JP-5	100.0000000	-22183.000	298.150
OXIDANT	O2	20.7200000	-4.407	298.000
OXIDANT	N2	77.2400000	-4.369	298.000
OXIDANT	CO2	0.0300000	-393515.570	298.000
OXIDANT	H2O	1.1000000	-241831.038	298.000
OXIDANT	Ar	0.9200000	-3.118	298.000

O/F= 18.59856 %FUEL= 5.102415 R,EQ.RATIO= 0.800000 PHI,EQ.RATIO= 0.794402

THERMODYNAMIC PROPERTIES

P, BAR	0.98595
T, K	2026.76
RHO, KG/CU M	1.6864-1
H, KJ/KG	-172.70
U, KJ/KG	-757.33
G, KJ/KG	-19013.2
S, KJ/(KG)(K)	9.2959
M, (1/n)	28.824
(dLV/dLP)t	-1.00043
(dLV/dLT)p	1.0142
Cp, KJ/(KG)(K)	1.5645
GAMMAs	1.2334
SON VEL,M/SEC	849.2

MOLE FRACTIONS

*Ar	0.00872
*CO	0.00088
*CO2	0.10486
*H	0.00003
*H2	0.00020
H2O	0.11065
*NO	0.00341
*N2	0.73072
*O	0.00016
*OH	0.00161
*O2	0.03875

* THERMODYNAMIC PROPERTIES FITTED TO 20000.K

PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS
WERE LESS THAN 5.000000E-06 FOR ALL ASSIGNED CONDITIONS

*C	*CH	CH2	CH3	CH2OH
CH3O	CH4	CH3OH	*CN	CNN
COOH	*C2	C2H	CHCO,ketyl	C2H2,vinylidene
C2H2,acetylene	CH2CO,ketene	C2H3,vinyl	CH3CN	CH3CO,acetyl
C2H4	C2H4O,ethylen-o	CH3CHO,ethanal	CH3COOH	C2H5
C2H6	CH3N2CH3	C2H5OH	CH3OCH3	CCN
CNC	C2N2	C2O	*C3	C3H3,1-propynl
C3H3,2-propynl	C3H4,allene	C3H4,propyne	C3H4,cyclo-	C3H5,allyl
C3H6,propylene	C3H6,cyclo-	C3H6O	C3H7,n-propyl	C3H7,i-propyl
C3H8	C3H8O,1propanol	C3H8O,2propanol	C3O2	C4
C4H2	C4H4,1,3-cyclo-	C4H6,butadiene	C4H6,1-butyne	C4H6,2-butyne
C4H6,cyclo-	C4H8,1-butene	C4H8,cis2-buten	C4H8,tr2-butene	C4H8,isobutene
C4H8,cyclo-	(CH3COOH)2	C4H9,n-butyl	C4H9,i-butyl	C4H9,s-butyl
C4H9,t-butyl	C4H10,isobutane	C4H10,n-butane	C4N2	C5
C5H6,1,3cyclo-	C5H8,cyclo-	C5H10,1-pentene	C5H10,cyclo-	C5H11,pentyl
C5H11,t-pentyl	C5H12,n-pentane	C5H12,i-pentane	CH3C(CH3)2CH3	C6H2
C6H5,phenyl	C6H5O,phenoxy	C6H6	C6H5OH,phenol	C6H10,cyclo-
C6H12,1-hexene	C6H12,cyclo-	C6H13,n-hexyl	C6H14,n-hexane	C7H7,benzyl
C7H8	C7H8O,cresol-mx	C7H14,1-heptene	C7H15,n-heptyl	C7H16,2-methylh
C7H16,n-heptane	C8H8,styrene	C8H10,ethylbenz	C8H16,1-octene	C8H17,n-octyl
C8H18,n-octane	C8H18,isooctane	C9H19,n-nonyl	C10H8,naphthale	C10H21,n-decyl
C12H9,o-bipheny	C12H10,biphenyl	HCN	HCO	HCCN
HNC	HNCO	HNO	HNO2	HNO3
HO2	HCHO,formaldehy	HCOOH	H2O2	(HCOOH)2
*N	NCO	*NH	NH2	NH3
NO2	NO3	NCN	N2H2	NH2NO2
N2H4	N2O	N2O3	N2O4	N2O5
N3	N3H	O3	C(gr)	H2O(s)
H2O(L)				

O/F = 16.467583

	EFFECTIVE FUEL	EFFECTIVE OXIDANT	MIXTURE
ENTHALPY	h(2)/R	h(1)/R	h0/R
(KG-MOL)(K)/KG	-0.19130912E+03	-0.11601254E+02	-0.21889333E+02

KG-FORM.WT./KG	bi(2)	bi(1)	b0i
*C	0.71705432E-01	0.10399819E-04	0.41148620E-02
*H	0.13767443E+00	0.76265339E-03	0.86007026E-02
*O	0.00000000E+00	0.14767743E-01	0.13922306E-01
*N	0.00000000E+00	0.53552135E-01	0.50486334E-01
*Ar	0.00000000E+00	0.31892778E-03	0.30066952E-03

POINT	ITN	T	C	H	O	N

```
                    AR
  1     4     2170.243      -23.154      -13.431      -16.496      -13.779
                  -26.194
```

THERMODYNAMIC EQUILIBRIUM COMBUSTION PROPERTIES AT ASSIGNED

PRESSURES

CASE = methane

REACTANT		MOLES	ENERGY KJ/KG-MOL	TEMP K
FUEL	JP-5	100.0000000	-22183.000	298.150
OXIDANT	O2	20.7200000	-4.407	298.000
OXIDANT	N2	77.2400000	-4.369	298.000
OXIDANT	CO2	0.0300000	-393515.570	298.000
OXIDANT	H2O	1.1000000	-241831.038	298.000
OXIDANT	Ar	0.9200000	-3.118	298.000

O/F= 16.46758 %FUEL= 5.724891 R,EQ.RATIO= 0.900000 PHI,EQ.RATIO= 0.897201

THERMODYNAMIC PROPERTIES

P, BAR	0.98595
T, K	2170.24
RHO, KG/CU M	1.5714-1
H, KJ/KG	-182.00
U, KJ/KG	-809.43
G, KJ/KG	-20642.3
S, KJ/(KG)(K)	9.4276
M, (1/n)	28.759
(dLV/dLP)t	-1.00145
(dLV/dLT)p	1.0447
Cp, KJ/(KG)(K)	1.8502
GAMMAs	1.2035
SON VEL,M/SEC	869.0

MOLE FRACTIONS

*Ar	0.00865
*CO	0.00399
*CO2	0.11435
*H	0.00014
*H2	0.00082
H2O	0.12144
*NO	0.00348
*N2	0.72424
*O	0.00032
*OH	0.00270
*O2	0.01988

* THERMODYNAMIC PROPERTIES FITTED TO 20000.K

PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS
WERE LESS THAN 5.000000E-06 FOR ALL ASSIGNED CONDITIONS

*C	*CH	CH2	CH3	CH2OH
CH3O	CH4	CH3OH	*CN	CNN
COOH	*C2	C2H	CHCO,ketyl	C2H2,vinylidene
C2H2,acetylene	CH2CO,ketene	C2H3,vinyl	CH3CN	CH3CO,acetyl
C2H4	C2H4O,ethylen-o	CH3CHO,ethanal	CH3COOH	C2H5
C2H6	CH3N2CH3	C2H5OH	CH3OCH3	CCN
CNC	C2N2	C2O	*C3	C3H3,1-propynl
C3H3,2-propynl	C3H4,allene	C3H4,propyne	C3H4,cyclo-	C3H5,allyl
C3H6,propylene	C3H6,cyclo-	C3H6O	C3H7,n-propyl	C3H7,i-propyl

C3H8	C3H8O,1propanol	C3H8O,2propanol	C3O2	C4
C4H2	C4H4,1,3-cyclo-	C4H6,butadiene	C4H6,1-butyne	C4H6,2-butyne
C4H6,cyclo-	C4H8,1-butene	C4H8,cis2-buten	C4H8,tr2-butene	C4H8,isobutene
C4H8,cyclo-	(CH3COOH)2	C4H9,n-butyl	C4H9,i-butyl	C4H9,s-butyl
C4H9,t-butyl	C4H10,isobutane	C4H10,n-butane	C4N2	C5
C5H6,1,3cyclo-	C5H8,cyclo-	C5H10,1-pentene	C5H10,cyclo-	C5H11,pentyl
C5H11,t-pentyl	C5H12,n-pentane	C5H12,i-pentane	CH3C(CH3)2CH3	C6H2
C6H5,phenyl	C6H5O,phenoxy	C6H6	C6H5OH,phenol	C6H10,cyclo-
C6H12,1-hexene	C6H12,cyclo-	C6H13,n-hexyl	C6H14,n-hexane	C7H7,benzyl
C7H8	C7H8O,cresol-mx	C7H14,1-heptene	C7H15,n-heptyl	C7H16,2-methylh
C7H16,n-heptane	C8H8,styrene	C8H10,ethylbenz	C8H16,1-octene	C8H17,n-octyl
C8H18,n-octane	C8H18,isooctane	C9H19,n-nonyl	C10H8,naphthale	C10H21,n-decyl
C12H9,o-bipheny	C12H10,biphenyl	HCN	HCO	HCCN
HNC	HNCO	HNO	HNO2	HNO3
HO2	HCHO,formaldehy	HCOOH	H2O2	(HCOOH)2
*N	NCO	*NH	NH2	NH3
NO2	NO3	NCN	N2H2	NH2NO2
N2H4	N2O	N2O3	N2O4	N2O5
N3	N3H	O3	C(gr)	H2O(s)
H2O(L)				

O/F = 14.774728

ENTHALPY	EFFECTIVE FUEL h(2)/R	EFFECTIVE OXIDANT h(1)/R	MIXTURE h0/R
(KG-MOL)(K)/KG	-0.19130912E+03	-0.11601254E+02	-0.22993392E+02

KG-FORM.WT./KG	bi(2)	bi(1)	b0i
*C	0.71705432E-01	0.10399819E-04	0.45553297E-02
*H	0.13767443E+00	0.76265339E-03	0.94418378E-02
*O	0.00000000E+00	0.14767743E-01	0.13831578E-01
*N	0.00000000E+00	0.53552135E-01	0.50157329E-01
*Ar	0.00000000E+00	0.31892778E-03	0.29871014E-03

POINT	ITN	T	C	H	O	N	AR
1	4	2261.050	-21.170	-12.890	-17.156	-13.856	-26.296

THERMODYNAMIC EQUILIBRIUM COMBUSTION PROPERTIES AT ASSIGNED

PRESSURES

CASE = methane

	REACTANT	MOLES	ENERGY KJ/KG-MOL	TEMP K
FUEL	JP-5	100.0000000	-22183.000	298.150
OXIDANT	O2	20.7200000	-4.407	298.000
OXIDANT	N2	77.2400000	-4.369	298.000
OXIDANT	CO2	0.0300000	-393515.570	298.000
OXIDANT	H2O	1.1000000	-241831.038	298.000
OXIDANT	Ar	0.9200000	-3.118	298.000

O/F= 14.77473 %FUEL= 6.339254 R,EQ.RATIO= 1.000000 PHI,EQ.RATIO= 1.000000

THERMODYNAMIC PROPERTIES

P, BAR	0.98595
T, K	2261.05
RHO, KG/CU M	1.4992-1

```
H, KJ/KG         -191.18
U, KJ/KG         -848.81
G, KJ/KG        -21774.7
S, KJ/(KG)(K)     9.5458

M, (1/n)          28.587
(dLV/dLP)t      -1.00305
(dLV/dLT)p        1.0907
Cp, KJ/(KG)(K)    2.2469
GAMMAs            1.1778
SON VEL,M/SEC      880.1

MOLE FRACTIONS

*Ar              0.00854
*CO              0.01354
*CO2             0.11669
*H               0.00042
*H2              0.00276
H2O              0.13048
*NO              0.00236
*N2              0.71573
*O               0.00031
*OH              0.00300
*O2              0.00617

 * THERMODYNAMIC PROPERTIES FITTED TO 20000.K

   PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS
   WERE LESS THAN 5.000000E-06 FOR ALL ASSIGNED CONDITIONS

*C               *CH              CH2              CH3              CH2OH
CH3O             CH4              CH3OH            *CN              CNN
COOH             *C2              C2H              CHCO,ketyl       C2H2,vinylidene
C2H2,acetylene   CH2CO,ketene     C2H3,vinyl       CH3CN            CH3CO,acetyl
C2H4             C2H4O,ethylen-o  CH3CHO,ethanal   CH3COOH          C2H5
C2H6             CH3N2CH3         C2H5OH           CH3OCH3          CCN
CNC              C2N2             C2O              *C3              C3H3,1-propynl
C3H3,2-propynl   C3H4,allene      C3H4,propyne     C3H4,cyclo-      C3H5,allyl
C3H6,propylene   C3H6,cyclo-      C3H6O            C3H7,n-propyl    C3H7,i-propyl
C3H8             C3H8O,1propanol  C3H8O,2propanol  C3O2             C4
C4H2             C4H4,1,3-cyclo-  C4H6,butadiene   C4H6,1-butyne    C4H6,2-butyne
C4H6,cyclo-      C4H8,1-butene    C4H8,cis2-buten  C4H8,tr2-butene  C4H8,isobutene
C4H8,cyclo-      (CH3COOH)2       C4H9,n-butyl     C4H9,i-butyl     C4H9,s-butyl
C4H9,t-butyl     C4H10,isobutane  C4H10,n-butane   C4N2             C5
C5H6,1,3cyclo-   C5H8,cyclo-      C5H10,1-pentene  C5H10,cyclo-     C5H11,pentyl
C5H11,t-pentyl   C5H12,n-pentane  C5H12,i-pentane  CH3C(CH3)2CH3    C6H2
C6H5,phenyl      C6H5O,phenoxy    C6H6             C6H5OH,phenol    C6H10,cyclo-
C6H12,1-hexene   C6H12,cyclo-     C6H13,n-hexyl    C6H14,n-hexane   C7H7,benzyl
C7H8             C7H8O,cresol-mx  C7H14,1-heptene  C7H15,n-heptyl   C7H16,2-methylh
C7H16,n-heptane  C8H8,styrene     C8H10,ethylbenz  C8H16,1-octene   C8H17,n-octyl
C8H18,n-octane   C8H18,isooctane  C9H19,n-nonyl    C10H8,naphthale  C10H21,n-decyl
C12H9,o-bipheny  C12H10,biphenyl  HCN              HCO              HCCN
HNC              HNCO             HNO              HNO2             HNO3
HO2              HCHO,formaldehy  HCOOH            H2O2             (HCOOH)2
*N               NCO              *NH              NH2              NH3
NO2              NO3              NCN              N2H2             NH2NO2
N2H4             N2O              N2O3             N2O4             N2O5
N3               N3H              O3               C(gr)            H2O(s)
H2O(L)
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Methane-Air Composition Check

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*******************************************************************************

        NASA-GLENN CHEMICAL EQUILIBRIUM PROGRAM CEA, AUGUST 30, 1999
                  BY  BONNIE MCBRIDE AND SANFORD GORDON
     REFS: NASA RP-1311, PART I, 1994 AND NASA RP-1311, PART II, 1996

*******************************************************************************



  problem case=check hp eq p(psi)=14.4,r,eq.ratio=0.3
  reactant fuel CH4 moles=2.94 t,k=298.0
           oxidant O2 moles=20.08 t,k=298.
           oxidant N2 moles=74.85 t,k=298.
           oxidant CO2 moles=0.03 t,k=298.
           oxidant H2O moles=1.2 t,k=298.
           oxidant Ar moles=0.90 t,k=298.
           output si
  end

OPTIONS: TP=F  HP=T  SP=F  TV=F  UV=F  SV=F  DETN=F  SHOCK=F  REFL=F  INCD=F
RKT=F  FROZ=F  EQL=T  IONS=F  SIUNIT=T  DEBUGF=F  SHKDBG=F  DETDBG=F  TRNSPT=F

TRACE= 0.00E+00  S/R= 0.000000E+00  H/R= 0.000000E+00  U/R= 0.000000E+00

P,BAR =     0.992841

   REACTANT           MOLES    (ENERGY/R),K   TEMP,K  DENSITY
       EXPLODED FORMULA
F: CH4              2.940000  -0.897291E+04   298.00  0.0000
         C  1.00000  H  4.00000
O: O2              20.080000  -0.530002E+00   298.00  0.0000
         O  2.00000
O: N2              74.850000  -0.525424E+00   298.00  0.0000
         N  2.00000
O: CO2              0.030000  -0.473288E+05   298.00  0.0000
         C  1.00000  O  2.00000
O: H2O              1.200000  -0.290854E+05   298.00  0.0000
         H  2.00000  O  1.00000
O: Ar               0.900000  -0.375000E+00   298.00  0.0000
         AR 1.00000

 SPECIES BEING CONSIDERED IN THIS SYSTEM
(CONDENSED PHASE MAY HAVE NAME LISTED SEVERAL TIMES)
 LAST thermo.inp UPDATE:   9/16/99

 g 3/98  *Ar              g 7/97  *C               tpis79  *CH
 g 8/99  CH2              g 8/99  CH3              g12/92  CH2OH
 g10/92  CH3O             g 8/99  CH4              g 8/88  CH3OH
 g 8/99  *CN              g12/89  CNN              tpis79  *CO
 g 9/99  *CO2             tpis91  COOH             tpis91  *C2
 g 1/91  C2H              g 6/89  CHCO,ketyl       g12/89  C2H2,vinylidene
 g 1/91  C2H2,acetylene   g 5/90  CH2CO,ketene     g 2/92  C2H3,vinyl
 g12/92  CH3CN            g 6/96  CH3CO,acetyl     g 1/91  C2H4
 g 8/88  C2H4O,ethylen-o  g 8/88  CH3CHO,ethanal   g 8/88  CH3COOH
 g12/92  C2H5             g 8/88  C2H6             g 8/88  CH3N2CH3
 g 8/88  C2H5OH           g12/92  CH3OCH3          g12/92  CCN
 tpis91  CNC              tpis79  C2N2             g12/89  C2O
 tpis79  *C3              x 4/98  C3H3,1-propynl   x 4/98  C3H3,2-propynl
 g12/92  C3H4,allene      g12/92  C3H4,propyne     g 5/90  C3H4,cyclo-
 bur 92  C3H5,allyl       g 2/95  C3H6,propylene   g 1/93  C3H6,cyclo-
 g 6/90  C3H6O            g 6/90  C3H7,n-propyl    g 9/85  C3H7,i-propyl
 g 6/90  C3H8             g 9/88  C3H8O,1propanol  g 9/88  C3H8O,2propanol
 g 7/88  C3O2             g 7/88  C4               g 2/93  C4H2
 g 5/90  C4H4,1,3-cyclo-  x10/92  C4H6,butadiene   x10/93  C4H6,1-butyne
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 x10/93  C4H6,2-butyne    g 5/90  C4H6,cyclo-      x 4/88  C4H8,1-butene
 x 4/88  C4H8,cis2-buten  x 4/88  C4H8,tr2-butene  x 4/88  C4H8,isobutene
 g 5/90  C4H8,cyclo-      g 6/90  (CH3COOH)2       x10/84  C4H9,n-butyl
 x10/84  C4H9,i-butyl     g 1/93  C4H9,s-butyl     g 1/93  C4H9,t-butyl
 g 6/90  C4H10,isobutane  g 6/90  C4H10,n-butane   j 3/61  C4N2
 g 7/88  C5               g 5/90  C5H6,1,3cyclo-   g 1/93  C5H8,cyclo-
 x 4/87  C5H10,1-pentene  g 6/90  C5H10,cyclo-     x10/84  C5H11,pentyl
 g 1/93  C5H11,t-pentyl   x10/85  C5H12,n-pentane  x10/85  C5H12,i-pentane
x10/85  CH3C(CH3)2CH3    g 2/93  C6H2             g 1/91  C6H5,phenyl
 g 6/90  C6H5O,phenoxy    g 1/91  C6H6             g 6/90  C6H5OH,phenol
 g 1/93  C6H10,cyclo-     x 4/87  C6H12,1-hexene   g 6/90  C6H12,cyclo-
x10/83  C6H13,n-hexyl    g 6/96  C6H14,n-hexane   g 1/93  C7H7,benzyl
 g 1/93  C7H8             g 1/93  C7H8O,cresol-mx  x 4/87  C7H14,1-heptene
x10/83  C7H15,n-heptyl   x10/85  C7H16,2-methylh  x10/85  C7H16,n-heptane
 x 4/89  C8H8,styrene     x10/86  C8H10,ethylbenz  x 4/87  C8H16,1-octene
x10/83  C8H17,n-octyl    x 4/85  C8H18,n-octane   x 4/85  C8H18,isooctane
x10/83  C9H19,n-nonyl    g 8/93  C10H8,naphthale  x10/83  C10H21,n-decyl
g12/84  C12H9,o-bipheny  g12/84  C12H10,biphenyl  g 6/97  *H
 g 7/88  HCN              g 9/96  HCO              tpis89  HCCN
g11/92  HNC              g 2/96  HNCO             g 5/99  HNO
tpis89  HNO2             g 5/99  HNO3             g 5/99  HO2
tpis78  *H2              g 8/88  HCHO,formaldehy  g 8/88  HCOOH
 g 8/89  H2O              g 6/99  H2O2             g 8/88  (HCOOH)2
 g 5/97  *N               g 2/96  NCO              g 4/99  *NH
 g 5/99  NH2              tpis89  NH3              tpis89  *NO
 g 4/99  NO2              j12/64  NO3              tpis78  *N2
g12/89  NCN              g 5/99  N2H2             tpis89  NH2NO2
 g 4/99  N2H4             g 4/99  N2O              g 4/99  N2O3
tpis89  N2O4             g 4/99  N2O5             tpis89  N3
 g 4/99  N3H              g 5/97  *O              tpis78  *OH
tpis89  *O2              tpis89  O3               X 4/83  C(gr)
 X 4/83  C(gr)            X 4/83  C(gr)            g 8/89  H2O(s)
 g 8/89  H2O(L)

O/F =  62.485011

                        EFFECTIVE FUEL     EFFECTIVE OXIDANT        MIXTURE
ENTHALPY                    h(2)/R             h(1)/R               h0/R
(KG-MOL)(K)/KG       -0.55932260E+03    -0.12998428E+02    -0.21603990E+02

KG-FORM.WT./KG             bi(2)              bi(1)              b0i
 *C                    0.62334580E-01     0.10721037E-04     0.99243085E-03
 *H                    0.24933832E+00     0.85768298E-03     0.47716877E-02
 *O                    0.00000000E+00     0.14802179E-01     0.14569019E-01
 *N                    0.00000000E+00     0.53497976E-01     0.52655289E-01
 *Ar                   0.00000000E+00     0.32163112E-03     0.31656487E-03

POINT ITN      T            C           H           O           N
                  AR
  1   30    1005.951     -50.498     -21.116     -14.259     -12.586
                -24.621
```

THERMODYNAMIC EQUILIBRIUM COMBUSTION PROPERTIES AT ASSIGNED

PRESSURES

CASE = check

REACTANT		MOLES	ENERGY KJ/KG-MOL	TEMP K
FUEL	CH4	2.9400000	-74605.353	298.000
OXIDANT	O2	20.0800000	-4.407	298.000
OXIDANT	N2	74.8500000	-4.369	298.000
OXIDANT	CO2	0.0300000	-393515.570	298.000
OXIDANT	H2O	1.2000000	-241831.038	298.000
OXIDANT	Ar	0.9000000	-3.118	298.000

```
O/F=   62.48501  %FUEL=  1.575175  R,EQ.RATIO= 0.300000  PHI,EQ.RATIO= 0.278038

THERMODYNAMIC PROPERTIES

P, BAR           0.99284
T, K             1005.95
RHO, KG/CU M    3.3798-1
H, KJ/KG         -179.63
U, KJ/KG         -473.38
G, KJ/KG        -8607.66
S, KJ/(KG)(K)     8.3782

M, (1/n)          28.472
(dLV/dLP)t      -1.00000
(dLV/dLT)p        1.0000
Cp, KJ/(KG)(K)    1.2000
GAMMAs            1.3216
SON VEL,M/SEC      623.1

MOLE FRACTIONS

*Ar              0.00901
*CO2             0.02826
H2O              0.06793
*NO              0.00003
*N2              0.74960
*O2              0.14517

 * THERMODYNAMIC PROPERTIES FITTED TO 20000.K

   PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS
   WERE LESS THAN 5.000000E-06 FOR ALL ASSIGNED CONDITIONS

*C               *CH              CH2              CH3              CH2OH
CH3O             CH4              CH3OH            *CN              CNN
*CO              COOH             *C2              C2H              CHCO,ketyl
C2H2,vinylidene  C2H2,acetylene   CH2CO,ketene     C2H3,vinyl       CH3CN
CH3CO,acetyl     C2H4             C2H4O,ethylen-o  CH3CHO,ethanal   CH3COOH
C2H5             C2H6             CH3N2CH3         C2H5OH           CH3OCH3
CCN              CNC              C2N2             C2O              *C3
C3H3,1-propynl   C3H3,2-propynl   C3H4,allene      C3H4,propyne     C3H4,cyclo-
C3H5,allyl       C3H6,propylene   C3H6,cyclo-      C3H6O            C3H7,n-propyl
C3H7,i-propyl    C3H8             C3H8O,1propanol  C3H8O,2propanol  C3O2
C4               C4H2             C4H4,1,3-cyclo-  C4H6,butadiene   C4H6,1-butyne
C4H6,2-butyne    C4H6,cyclo-      C4H8,1-butene    C4H8,cis2-buten  C4H8,tr2-butene
C4H8,isobutene   C4H8,cyclo-      (CH3COOH)2       C4H9,n-butyl     C4H9,i-butyl
C4H9,s-butyl     C4H9,t-butyl     C4H10,isobutane  C4H10,n-butane   C4N2
C5               C5H6,1,3cyclo-   C5H8,cyclo-      C5H10,1-pentene  C5H10,cyclo-
C5H11,pentyl     C5H11,t-pentyl   C5H12,n-pentane  C5H12,i-pentane  CH3C(CH3)2CH3
C6H2             C6H5,phenyl      C6H5O,phenoxy    C6H6             C6H5OH,phenol
C6H10,cyclo-     C6H12,1-hexene   C6H12,cyclo-     C6H13,n-hexyl    C6H14,n-hexane
C7H7,benzyl      C7H8             C7H8O,cresol-mx  C7H14,1-heptene  C7H15,n-heptyl
C7H16,2-methylh  C7H16,n-heptane  C8H8,styrene     C8H10,ethylbenz  C8H16,1-octene
C8H17,n-octyl    C8H18,n-octane   C8H18,isooctane  C9H19,n-nonyl    C10H8,naphthale
C10H21,n-decyl   C12H9,o-bipheny  C12H10,biphenyl  *H               HCN
HCO              HCCN             HNC              HNCO             HNO
HNO2             HNO3             HO2              *H2              HCHO,formaldehy
HCOOH            H2O2             (HCOOH)2         *N               NCO
*NH              NH2              NH3              NO2              NO3
NCN              N2H2             NH2NO2           N2H4             N2O
N2O3             N2O4             N2O5             N3               N3H
*O               *OH              O3               C(gr)            H2O(s)
H2O(L)
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Equilibrium Analysis of Extracted Sample

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        NASA-GLENN CHEMICAL EQUILIBRIUM PROGRAM CEA, AUGUST 30, 1999
                    BY  BONNIE MCBRIDE AND SANFORD GORDON
     REFS: NASA RP-1311, PART I, 1994 AND NASA RP-1311, PART II, 1996

 ******************************************************************************



problem case=extracted eq tp p(psi)=14.3, r,eq.ratio=0.3, t(k)=798.33
  reactant fuel JP-5 moles=100
           oxidant N2 moles=77.12
           oxidant CO2 moles=0.03
           oxidant H2O moles=1.24
            oxidant Ar moles=0.92
            oxidant O2 moles=20.69
           output si
  end

OPTIONS: TP=T  HP=F  SP=F  TV=F  UV=F  SV=F  DETN=F  SHOCK=F  REFL=F  INCD=F
RKT=F  FROZ=F  EQL=T  IONS=F  SIUNIT=T  DEBUGF=F  SHKDBG=F  DETDBG=F  TRNSPT=F

T,K =   798.3300

TRACE= 0.00E+00  S/R= 0.000000E+00  H/R= 0.000000E+00  U/R= 0.000000E+00

P,BAR =     0.985946

   REACTANT           MOLES    (ENERGY/R),K   TEMP,K  DENSITY
       EXPLODED FORMULA
F: JP-5           100.000000  -0.266799E+04   298.15  0.0000
         C  1.00000  H  1.92000
O: N2              77.120000   0.000000E+00     0.00  0.0000
         N  2.00000
O: CO2              0.030000   0.000000E+00     0.00  0.0000
         C  1.00000  O  2.00000
O: H2O              1.240000   0.000000E+00     0.00  0.0000
         H  2.00000  O  1.00000
O: Ar               0.920000   0.000000E+00     0.00  0.0000
         AR 1.00000
O: O2              20.690000   0.000000E+00     0.00  0.0000
         O  2.00000

 SPECIES BEING CONSIDERED IN THIS SYSTEM
(CONDENSED PHASE MAY HAVE NAME LISTED SEVERAL TIMES)
 LAST thermo.inp UPDATE:   9/16/99

 g 3/98  *Ar              g 7/97  *C               tpis79  *CH
 g 8/99  CH2              g 8/99  CH3              g12/92  CH2OH
 g10/92  CH3O             g 8/99  CH4              g 8/88  CH3OH
 g 8/99  *CN              g12/89  CNN              tpis79  *CO
 g 9/99  *CO2             tpis91  COOH             tpis91  *C2
 g 1/91  C2H              g 6/89  CHCO,ketyl       g12/89  C2H2,vinylidene
 g 1/91  C2H2,acetylene   g 5/90  CH2CO,ketene     g 2/92  C2H3,vinyl
 g12/92  CH3CN            g 6/96  CH3CO,acetyl     g 1/91  C2H4
 g 8/88  C2H4O,ethylen-o  g 8/88  CH3CHO,ethanal   g 8/88  CH3COOH
 g12/92  C2H5             g 8/88  C2H6             g 8/88  CH3N2CH3
 g 8/88  C2H5OH           g12/92  CH3OCH3          g12/92  CCN
 tpis91  CNC              tpis79  C2N2             g12/89  C2O
 tpis79  *C3              x 4/98  C3H3,1-propynl   x 4/98  C3H3,2-propynl
 g12/92  C3H4,allene      g12/92  C3H4,propyne     g 5/90  C3H4,cyclo-
 bur 92  C3H5,allyl       g 2/95  C3H6,propylene   g 1/93  C3H6,cyclo-
 g 6/90  C3H6O            g 6/90  C3H7,n-propyl    g 9/85  C3H7,i-propyl
 g 6/90  C3H8             g 9/88  C3H8O,1propanol  g 9/88  C3H8O,2propanol
 g 7/88  C3O2             g 7/88  C4               g 2/93  C4H2
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 g 5/90  C4H4,1,3-cyclo-  x10/92  C4H6,butadiene   x10/93  C4H6,1-butyne
 x10/93  C4H6,2-butyne    g 5/90  C4H6,cyclo-      x 4/88  C4H8,1-butene
 x 4/88  C4H8,cis2-buten  x 4/88  C4H8,tr2-butene  x 4/88  C4H8,isobutene
 g 5/90  C4H8,cyclo-      g 6/90  (CH3COOH)2       x10/84  C4H9,n-butyl
 x10/84  C4H9,i-butyl     g 1/93  C4H9,s-butyl     g 1/93  C4H9,t-butyl
 g 6/90  C4H10,isobutane  g 6/90  C4H10,n-butane   j 3/61  C4N2
 g 7/88  C5               g 5/90  C5H6,1,3cyclo-   g 1/93  C5H8,cyclo-
 x 4/87  C5H10,1-pentene  g 6/90  C5H10,cyclo-     x10/84  C5H11,pentyl
 g 1/93  C5H11,t-pentyl   x10/85  C5H12,n-pentane  x10/85  C5H12,i-pentane
 x10/85  CH3C(CH3)2CH3    g 2/93  C6H2             g 1/91  C6H5,phenyl
 g 6/90  C6H5O,phenoxy    g 1/91  C6H6             g 6/90  C6H5OH,phenol
 g 1/93  C6H10,cyclo-     x 4/87  C6H12,1-hexene   g 6/90  C6H12,cyclo-
 x10/83  C6H13,n-hexyl    g 6/96  C6H14,n-hexane   g 1/93  C7H7,benzyl
 g 1/93  C7H8             g 1/93  C7H8O,cresol-mx  x 4/87  C7H14,1-heptene
 x10/83  C7H15,n-heptyl   x10/85  C7H16,2-methylh  x10/85  C7H16,n-heptane
 x 4/89  C8H8,styrene     x10/86  C8H10,ethylbenz  x 4/87  C8H16,1-octene
 x10/83  C8H17,n-octyl    x 4/85  C8H18,n-octane   x 4/85  C8H18,isooctane
 x10/83  C9H19,n-nonyl    g 8/93  C10H8,naphthale  x10/83  C10H21,n-decyl
 g12/84  C12H9,o-bipheny  g12/84  C12H10,biphenyl  g 6/97  *H
 g 7/88  HCN              g 9/96  HCO              tpis89  HCCN
 g11/92  HNC              g 2/96  HNCO             g 5/99  HNO
 tpis89  HNO2             g 5/99  HNO3             g 5/99  HO2
 tpis78  *H2              g 8/88  HCHO,formaldehy  g 8/88  HCOOH
 g 8/89  H2O              g 6/99  H2O2             g 8/88  (HCOOH)2
 g 5/97  *N               g 2/96  NCO              g 4/99  *NH
 g 5/99  NH2              tpis89  NH3              tpis89  *NO
 g 4/99  NO2              j12/64  NO3              tpis78  *N2
 g12/89  NCN              g 5/99  N2H2             tpis89  NH2NO2
 g 4/99  N2H4             g 4/99  N2O              g 4/99  N2O3
 tpis89  N2O4             g 4/99  N2O5             tpis89  N3
 g 4/99  N3H              g 5/97  *O              tpis78  *OH
 tpis89  *O2              tpis89  O3               X 4/83  C(gr)
 X 4/83  C(gr)            X 4/83  C(gr)           g 8/89  H2O(s)
 g 8/89  H2O(L)

O/F =  53.188700

                       EFFECTIVE FUEL     EFFECTIVE OXIDANT        MIXTURE
ENTHALPY                   h(2)/R             h(1)/R               h0/R
(KG-MOL)(K)/KG       -0.19130912E+03     0.00000000E+00     -0.35304247E+01

KG-FORM.WT./KG             bi(2)              bi(1)              b0i
 *C                    0.71705432E-01     0.10406310E-04     0.13334686E-02
 *H                    0.13767443E+00     0.86025500E-03     0.33850281E-02
 *N                    0.00000000E+00     0.53502311E-01     0.52514977E-01
 *O                    0.00000000E+00     0.14804711E-01     0.14531504E-01
 *Ar                   0.00000000E+00     0.31912685E-03     0.31323768E-03

POINT ITN      T            C           H           N           O
                  AR
  1   27     798.330     -62.166     -24.856     -12.304     -13.962
                -24.241



              THERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED

                          TEMPERATURE AND PRESSURE

CASE = methane

            REACTANT                        MOLES         ENERGY      TEMP
                                                         KJ/KG-MOL       K
FUEL        JP-5                        100.0000000    -22183.000    298.150
OXIDANT     N2                           77.1200000         0.000      0.000
OXIDANT     CO2                           0.0300000         0.000      0.000
OXIDANT     H2O                           1.2400000         0.000      0.000
OXIDANT     Ar                            0.9200000         0.000      0.000
```

```
OXIDANT     O2                          20.6900000         0.000      0.000

O/F=   53.18870  %FUEL=  1.845403  R,EQ.RATIO= 0.300000  PHI,EQ.RATIO= 0.278009

THERMODYNAMIC PROPERTIES

P, BAR           0.98595
T, K              798.33
RHO, KG/CU M    4.2827-1
H, KJ/KG         -396.15
U, KJ/KG         -626.36
G, KJ/KG        -6794.71
S, KJ/(KG)(K)     8.0149

M, (1/n)          28.833
(dLV/dLP)t      -1.00000
(dLV/dLT)p        1.0000
Cp, KJ/(KG)(K)    1.1373
GAMMAs            1.3397
SON VEL,M/SEC      555.3

MOLE FRACTIONS

*Ar              0.00903
*CO2             0.03845
H2O              0.04880
*N2              0.75708
*O2              0.14664

 * THERMODYNAMIC PROPERTIES FITTED TO 20000.K

   PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS
   WERE LESS THAN 5.000000E-06 FOR ALL ASSIGNED CONDITIONS

*C              *CH             CH2             CH3             CH2OH
CH3O            CH4             CH3OH           *CN             CNN
*CO             COOH            *C2             C2H             CHCO,ketyl
C2H2,vinylidene C2H2,acetylene  CH2CO,ketene    C2H3,vinyl      CH3CN
CH3CO,acetyl    C2H4            C2H4O,ethylen-o CH3CHO,ethanal  CH3COOH
C2H5            C2H6            CH3N2CH3        C2H5OH          CH3OCH3
CCN             CNC             C2N2            C2O             *C3
C3H3,1-propynl  C3H3,2-propynl  C3H4,allene     C3H4,propyne    C3H4,cyclo-
C3H5,allyl      C3H6,propylene  C3H6,cyclo-     C3H6O           C3H7,n-propyl
C3H7,i-propyl   C3H8            C3H8O,1propanol C3H8O,2propanol C3O2
C4              C4H2            C4H4,1,3-cyclo- C4H6,butadiene  C4H6,1-butyne
C4H6,2-butyne   C4H6,cyclo-     C4H8,1-butene   C4H8,cis2-buten C4H8,tr2-butene
C4H8,isobutene  C4H8,cyclo-     (CH3COOH)2      C4H9,n-butyl    C4H9,i-butyl
C4H9,s-butyl    C4H9,t-butyl    C4H10,isobutane C4H10,n-butane  C4N2
C5              C5H6,1,3cyclo-  C5H8,cyclo-     C5H10,1-pentene C5H10,cyclo-
C5H11,pentyl    C5H11,t-pentyl  C5H12,n-pentane C5H12,i-pentane CH3C(CH3)2CH3
C6H2            C6H5,phenyl     C6H5O,phenoxy   C6H6            C6H5OH,phenol
C6H10,cyclo-    C6H12,1-hexene  C6H12,cyclo-    C6H13,n-hexyl   C6H14,n-hexane
C7H7,benzyl     C7H8            C7H8O,cresol-mx C7H14,1-heptene C7H15,n-heptyl
C7H16,2-methylh C7H16,n-heptane C8H8,styrene    C8H10,ethylbenz C8H16,1-octene
C8H17,n-octyl   C8H18,n-octane  C8H18,isooctane C9H19,n-nonyl   C10H8,naphthale
C10H21,n-decyl  C12H9,o-bipheny C12H10,biphenyl *H              HCN
HCO             HCCN            HNC             HNCO            HNO
HNO2            HNO3            HO2             *H2             HCHO,formaldehy
HCOOH           H2O2            (HCOOH)2        *N              NCO
*NH             NH2             NH3             *NO             NO2
NO3             NCN             N2H2            NH2NO2          N2H4
N2O             N2O3            N2O4            N2O5            N3
N3H             *O              *OH             O3              C(gr)
H2O(s)          H2O(L)
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APPENDIX C

LSENS

Sample Line Analysis – Original Data

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                          ** Problem Data **

         1         2         3         4         5         6         7         8
 2345678901234567890123456789012345678901234567890123456789012345678901234567890

LSENS SAMPLE DATA-AIR SAMPLE LINE
   M       +   CH4      =   CH3     +   H         2.0E+17   0.        88000.
   H       +   CH4      =   CH3     +   H2        6.6E+8    1.62      10840.
   CH4     +   O2       =   CH3     +   HO2       1.0E+12   0.        0.
   O       +   CH4      =   CH3     +   OH        1.02E+9   1.5       8600.
   OH      +   CH4      =   CH3     +   H2O       1.0E+8    1.6       3120.
   CH3     +   O2       =   CH3O    +   O         2.68E+13  0.        28800.
   CH3     +   O2       =   OH      +   CH2O      3.6E+10   0.        8940.
   CH3     +   OH       =   CH3O    +   H         3.2E+12   0.        0.
   M       +   CH3O     =   CH2O    +   H         5.0E+13   0.        21000.
   CH3     +   CH3      =   C2H6                  2.4E+14   -.4       0.
   CH3     +   CH3      =   H       +   C2H5      4.99E+12  0.1       10600.
   H       +   C2H6     =   C2H5    +   H2        1.15E+8   1.9       7530.
   O       +   C2H6     =   C2H5    +   OH        8.98E+7   1.92      5690.
   OH      +   C2H6     =   C2H5    +   H2O       3.54E+6   2.12      870.
   M       +   C2H5     =   C2H4    +   H         1.0E+17   0.        31000.
   C2H5    +   O2       =   C2H4    +   HO2       8.4E+11   0.        3875.
   H       +   C2H5     =   C2H4    +   H2        2.0E+12   0.        0.
   CH3     +   CH2      =   C2H4    +   H         2.0E+13   0.        0.
   H       +   C2H4     =   H2      +   C2H3      1.325E+6  2.53      12240.
   M       +   C2H4     =   C2H2    +   H2        2.6E+17   0.        79300.
   C2H4    +   OH       =   C2H3    +   H2O       3.6E+6    2.        2500.
   C2H4    +   OH       =   CH3     +   CH2O      2.0E+12   0.        960.
   C2H4    +   O        =   CH3     +   HCO       1.92E+7   1.83      220.
   C2H4    +   O        =   CH2O    +   CH2       2.5E+13   0.        5000.
   M       +   C2H3     =   C2H2    +   H         3.0E+15   0.        32000.
   C2H3    +   O2       =   CH2O    +   HCO       3.98E+12  0.        -240.
   C2H3    +   H        =   C2H2    +   H2        3.0E+13   0.        0.
   C2H3    +   O        =   C2H2O   +   H         3.0E+13   0.        0.
   C2H3    +   OH       =   C2H2    +   H2O       5.0E+12   0.        0.
   C2H3    +   CH2      =   C2H2    +   CH3       3.0E+13   0.        0.
   C2H3    +   C2H      =2.0C2H2                  3.0E+13   0.        0.
   M       +   C2H2     =   C2H     +   H         4.2E+16   0.        107000.
   C2H2    +   O        =   CH2     +   CO        1.02E+7   2.0       1900.
   C2H2    +   O        =   C2HO    +   H         1.02E+7   2.        1900.
   C2H2    +   O        =   OH      +   C2H       4.6E+19   -1.41     28950.
   C2H2    +   OH       =   C2H     +   H2O       3.37E+7   2.        14000.
   C2H2    +   OH       =   C2H2O   +   H         5.04E+5   2.3       13500.
   C2H2    +   OH       =   CH2CO   +   H         2.18E-4   4.5       -1000.
   C2H2    +   OH       =   CH3     +   CO        4.83E-4   4.        -2000.
   C2H     +   O2       =   C2HO    +   O         5.00E+13  0.0       1500.
   C2H     +   O2       =   HCO     +   CO        5.0E+13   0.0       1500.
   C2H     +   OH       =   C2HO    +   H         2.0E+13   0.0       0.
   C2HO    +   O2       =2.0CO      +   OH        1.6E+12   0.        854.
   C2HO    +   O        =2.0CO      +   H         1.0E+14   0.        0.
   C2HO    +   OH       =2.0HCO                   1.0E+13   0.        0.
   C2HO    +   H        =   CH2     +   CO        1.0E+14   0.        0.
   C2HO    +   CH2      =   C2H3    +   CO        3.0E+13   0.        0.
   C2HO    +   CH2      =   CH2O    +   C2H       1.0E+13   0.        2000.
            2.0C2HO     =   C2H2    +2.0CO        1.0E+13   0.        0.
   C2H2O   +   OH       =   CH2O    +   HCO       2.8E+13   0.        0.
   C2H2O   +   OH       =   C2HO    +   H2O       7.5E+12   0.        2000.
   C2H2O   +   H        =   CH3     +   CO        1.13E+13  0.        3428.
   C2H2O   +   H        =   C2HO    +   H2        5.0E+13   0.        8000.
   C2H2O   +   O        =   C2HO    +   OH        1.0E+13   0.        8000.
   C2H2O   +   O        =   CH2O    +   CO        2.0E+13   0.        0.
   C2H2O   +   O        =   CH2     +   CO2       1.75E+12  0.        1350.
   M       +   C2H2O    =   CH2     +   CO        2.0E+16   0.        60000.
   C2H     +   O        =   CO      +   CH        5.0E+13   0.        0.
   CH3O    +   O2       =   CH2O    +   HO2       4.28E-13  7.6       -3530.
   CH3O    +   H        =   CH2O    +   H2        2.0E+13   0.        0.
   M       +   CH2O     =   HCO     +   H         5.0E+16   0.        81000.
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   CH2O     +   OH       =   HCO      +   H2O       3.43E+9   1.18      -447.
   CH2O     +   H        =   HCO      +   H2        2.3E+10   1.05      3275.
   CH2O     +   O        =   HCO      +   OH        3.9E+13   0.        3540.
   CH3      +   CH2O     =   CH4      +   HCO       3.32E+03  2.81      5860.
   CH3      +   HCO      =   CH4      +   CO        2.65E+13  0.        0.
   CH3      +   HO2      =   CH3O     +   OH        2.0E+13   0.        0.
   M        +   CH3      =   CH2      +   H         1.95E+16  0.        91600.
   H        +   CH3      =   H2       +   CH2       2.7E+11   0.67      25700.
   O        +   CH3      =   OH       +   CH2       1.9E+11   0.68      25700.
   O        +   CH3      =   H        +   CH2O      8.43E+13  0.        0.
   OH       +   CH3      =   H2O      +   CH2       5.6E+7    1.6       5420.
   CH       +   CO2      =   HCO      +   CO        3.4E+12   0.        690.
   CH       +   O2       =   HCO      +   O         3.3E+13   0.        0.
   CH2      +   O2       =   CH2O     +   O         5.0E+11   0.5       6960.
   CH2      +   O2       =   OH       +   HCO       1.32E+13  0.        1500.
   CH2      +   O        =   CH       +   OH        2.0E+11   0.7       25800.
   CH2      +   OH       =   CH       +   H2O       1.13E+7   2.0       3000.
   CH2      +   H        =   CH       +   H2        3.2E+11   0.7       4970.
   CH2      +   CH2      =   C2H3     +   H         5.0E+12   0.        0.
   CH2      +   CH2      =   C2H2     +   H2        3.2E+13   0.        0.
   HCO      +   O2       =   CO       +   HO2       7.6E+12   0.        400.
   HCO      +   O        =   CO       +   OH        3.0E+13   0.        0.
   HCO      +   O        =   CO2      +   H         3.0E+13   0.        0.
   HCO      +   OH       =   CO       +   H2O       5.0E+13   0.        0.
   HCO      +   H        =   CO       +   H2        7.34E+13  0.        0.
   M        +   HCO      =   H        +   CO        1.87E+17  -1.       17000.
   CO       +   O        =   CO2      +   M         6.02E+14  0.        3000.
   CO       +   O2       =   CO2      +   O         2.5E+12   0.        47800.
   CO       +   OH       =   CO2      +   H         4.76E+7   1.23      70.
   CO       +   HO2      =   CO2      +   OH        1.5E+14   0.        23600.
   O        +   H2O      =   OH       +   OH        6.8E+13   0.        18365.
   H        +   O2       =   OH       +   O         8.3E+13   0.        14413.
   O        +   H2       =   OH       +   H         5.00E+04  2.67      6290.
   H        +   HO2      =   H2       +   O2        2.8E+13   0.        1068.
   O        +   HO2      =   OH       +   O2        2.0E+13   0.        0.
   HO2      +   OH       =   H2O      +   O2        2.9E+13   0.        -500.
   H        +   HO2      =2.0OH                     1.34E+14  0.        635.
   H2       +   HO2      =   H2O2     +   H         1.21E+7   2.        5200.
   OH       +   H2O2     =   H2O      +   HO2       1.75E+12  0.        320.
   HO2      +   HO2      =   H2O2     +   O2        1.3E+11   0.        -1630.
   H        +   H2O2     =   OH       +   H2O       1.0E+13   0.        3600.
   M        +   H2O2     =2.0OH                     1.44E+17  0.        45510.
   THIRDBODY
H2         2.30       O2         0.78       H2O        6.0
H2O2       6.6
END
   H2       +   OH       =   H2O      +   H         2.16E+8   1.51      3430.
   H        +   O2       =   HO2      +   M         2.8E+18   -0.86     0.
   THIRDBODY
O2         1.30       N2         1.3
H2O        21.3       CO2        7.0
END
   M        +   H2O      =   H        +   OH        1.30E+15  0.        105140.
   THIRDBODY
H2         4.00       O2         1.5
H2O        20.0       N2         1.5
CO2        4.0
END
   H        +   O        =   OH       +   M         5.00E+17  -1.       0.
   M        +   H2       =   H        +   H         2.2E+14   0.        96000.
   THIRDBODY
H2         4.10       O2         2.0
H2O        15.0       N2         2.0
END
   M        +   O2       =   O        +   O         1.80E+18  -1.       118020.
   CH       +   N2       =   HCN      +   N         1.0E+11   0.        19000.
   CN       +   H2       =   HCN      +   H         2.1E+13   0.        4710.
   O        +   HCN      =   OH       +   CN        2.13E+9   1.58      26600.
   O        +   HCN      =   NCO      +   H         1.11E+4   2.64      4980.
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   O       +   HCN      =   NH      +   CO        2.77E+3   2.64      4980.
   OH      +   HCN      =   HNCO    +   H         4.4E+3    2.26      6400.
   CN      +   O        =   CO      +   N         7.7E+13   0.        0.
   CN      +   OH       =   NCO     +   H         4.0E+13   0.        0.
   H2      +   NCO      =   HNCO    +   H         1.0E+14   0.        9000.
   HNCO    +   H        =   NH2     +   CO        2.25E+7   1.7       3800.
   CN      +   O2       =   NCO     +   O         6.14E+12  0.        -440.
   CN      +   CO2      =   NCO     +   CO        3.7E+12   0.        0.
   O       +   NCO      =   NO      +   CO        2.35E+13  0.        0.
   N       +   NCO      =   N2      +   CO        2.0E+13   0.        0.
   H       +   NCO      =   NH      +   CO        5.4E+13   0.        0.
   CH      +   NO       =   N       +   HCO       3.0E+13   0.        0.
   CH      +   NO       =   O       +   HCN       5.0E+13   0.        0.
   CH      +   NO       =   H       +   NCO       2.0E+13   0.        0.
   NH      +   OH       =   N       +   H2O       2.0E+9    1.2       0.
   NH      +   OH       =   HNO     +   H         2.0E+13   0.        0.
   HO2     +   NO       =   NO2     +   OH        2.11E+12  0.        -480.
   O       +   NO2      =   NO      +   O2        3.9E+12   0.        -240.
   NO      +   O        =   NO2     +   M         1.06E+20  -1.41     0.
   NO2     +   H        =   NO      +   OH        1.32E+14  0.        360.
   NO      +   H        =   N       +   OH        2.63E+14  0.        50410.
   NO      +   O        =   N       +   O2        3.8E+9    1.        41370.
   O       +   N2       =   NO      +   N         1.80E+14  0.        76250.
   N       +   NO2      =2.0NO                    4.0E+12   0.        0.
   M       +   N2O      =   N2      +   O         6.92E+23  -2.5      65000.
   O       +   N2O      =   N2      +   O2        1.4E+12   0.        10810.
   O       +   N2O      =2.0NO                    2.9E+13   0.        23150.
   N2O     +   H        =   N2      +   OH        4.4E+14   0.        18880.
   NO2     +   H2       =   HNO2    +   H         2.4E+13   0.        29000.
   OH      +   NO2      =   HNO3    +   M         3.0E+15   0.        -3800.
   THIRDBODY
O2        0.70      H2        1.4
END
   OH      +   NO       =   HNO2    +   M         5.6E+15   0.        -1700.
   HNO     +   H        =   H2      +   NO        4.5E+11   0.72      660.
   H       +   NO       =   HNO     +   M         8.95E+19  -1.32     740.
   HNO     +   OH       =   H2O     +   NO        1.3E+7    1.9       -950.
                                  Blank Line
END
DISTANCE  AREA      SI        SI
 &PROB  ACON=.TRUE.,CX0=3.167E-05,EXCHR=.TRUE.,CONC=.FALSE.,PRINT=30.48, &END
 $START T=423.15,P=101325.0,v=2.63,&END
CH4        0.0000
O2         0.163379
N2         0.760754
CO2        0.023355
H2O        0.050055
CO         0.002340
NO2        0.000001
                                  Blank Line
                                  Blank Line
&SOLVER  EMAX=1.0E-4, ATOLSP=1.0E-10,  &END
FINIS1
```

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          LSENS: Multipurpose Kinetics and Sensitivity Analysis Program

LSENS CH4-AIR SAMPLE LINE CASE 6

 Reac        Reaction                                    Reaction Rate Parameters
 No.j                                                       Aj     nj      Ej
               kj = Aj * T**nj * exp(-Ej/RT) (cgs units)

    1 CH4 + M = CH3 + H + M                             2.00E+17  0.00  8.80E+04
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2	H + CH4 = CH3 + H2	6.60E+08	1.62	1.08E+04
3	CH4 + O2 = CH3 + HO2	1.00E+12	0.00	0.00E+00
4	O + CH4 = CH3 + OH	1.02E+09	1.50	8.60E+03
5	OH + CH4 = CH3 + H2O	1.00E+08	1.60	3.12E+03
6	CH3 + O2 = CH3O + O	2.68E+13	0.00	2.88E+04
7	CH3 + O2 = OH + CH2O	3.60E+10	0.00	8.94E+03
8	CH3 + OH = CH3O + H	3.20E+12	0.00	0.00E+00
9	CH3O + M = CH2O + H + M	5.00E+13	0.00	2.10E+04
10	2CH3 = C2H6	2.40E+14	-0.40	0.00E+00
11	2CH3 = H + C2H5	4.99E+12	0.10	1.06E+04
12	H + C2H6 = C2H5 + H2	1.15E+08	1.90	7.53E+03
13	O + C2H6 = C2H5 + OH	8.98E+07	1.92	5.69E+03
14	OH + C2H6 = C2H5 + H2O	3.54E+06	2.12	8.70E+02
15	C2H5 + M = C2H4 + H + M	1.00E+17	0.00	3.10E+04
16	C2H5 + O2 = C2H4 + HO2	8.40E+11	0.00	3.88E+03
17	H + C2H5 = C2H4 + H2	2.00E+12	0.00	0.00E+00
18	CH3 + CH2 = C2H4 + H	2.00E+13	0.00	0.00E+00
19	H + C2H4 = H2 + C2H3	1.33E+06	2.53	1.22E+04
20	C2H4 + M = C2H2 + H2 + M	2.60E+17	0.00	7.93E+04
21	C2H4 + OH = C2H3 + H2O	3.60E+06	2.00	2.50E+03
22	C2H4 + OH = CH3 + CH2O	2.00E+12	0.00	9.60E+02
23	C2H4 + O = CH3 + HCO	1.92E+07	1.83	2.20E+02
24	C2H4 + O = CH2O + CH2	2.50E+13	0.00	5.00E+03
25	C2H3 + M = C2H2 + H + M	3.00E+15	0.00	3.20E+04
26	C2H3 + O2 = CH2O + HCO	3.98E+12	0.00	-2.40E+02
27	C2H3 + H = C2H2 + H2	3.00E+13	0.00	0.00E+00
28	C2H3 + O = C2H2O + H	3.00E+13	0.00	0.00E+00
29	C2H3 + OH = C2H2 + H2O	5.00E+12	0.00	0.00E+00
30	C2H3 + CH2 = C2H2 + CH3	3.00E+13	0.00	0.00E+00
31	C2H3 + C2H = 2C2H2	3.00E+13	0.00	0.00E+00
32	C2H2 + M = C2H + H + M	4.20E+16	0.00	1.07E+05
33	C2H2 + O = CH2 + CO	1.02E+07	2.00	1.90E+03
34	C2H2 + O = C2HO + H	1.02E+07	2.00	1.90E+03
35	C2H2 + O = OH + C2H	4.60E+19	-1.41	2.90E+04
36	C2H2 + OH = C2H + H2O	3.37E+07	2.00	1.40E+04
37	C2H2 + OH = C2H2O + H	5.04E+05	2.30	1.35E+04
38	C2H2 + OH = CH2CO + H	2.18E-04	4.50	-1.00E+03
39	C2H2 + OH = CH3 + CO	4.83E-04	4.00	-2.00E+03
40	C2H + O2 = C2HO + O	5.00E+13	0.00	1.50E+03
41	C2H + O2 = HCO + CO	5.00E+13	0.00	1.50E+03
42	C2H + OH = C2HO + H	2.00E+13	0.00	0.00E+00
43	C2HO + O2 = 2CO + OH	1.60E+12	0.00	8.54E+02
44	C2HO + O = 2CO + H	1.00E+14	0.00	0.00E+00
45	C2HO + OH = 2HCO	1.00E+13	0.00	0.00E+00
46	C2HO + H = CH2 + CO	1.00E+14	0.00	0.00E+00
47	C2HO + CH2 = C2H3 + CO	3.00E+13	0.00	0.00E+00
48	C2HO + CH2 = CH2O + C2H	1.00E+13	0.00	2.00E+03
49	2C2HO = C2H2 + 2CO	1.00E+13	0.00	0.00E+00
50	C2H2O + OH = CH2O + HCO	2.80E+13	0.00	0.00E+00
51	C2H2O + OH = C2HO + H2O	7.50E+12	0.00	2.00E+03
52	C2H2O + H = CH3 + CO	1.13E+13	0.00	3.43E+03
53	C2H2O + H = C2HO + H2	5.00E+13	0.00	8.00E+03
54	C2H2O + O = C2HO + OH	1.00E+13	0.00	8.00E+03
55	C2H2O + O = CH2O + CO	2.00E+13	0.00	0.00E+00
56	C2H2O + O = CH2 + CO2	1.75E+12	0.00	1.35E+03
57	C2H2O + M = CH2 + CO + M	2.00E+16	0.00	6.00E+04
58	C2H + O = CO + CH	5.00E+13	0.00	0.00E+00
59	CH3O + O2 = CH2O + HO2	4.28E-13	7.60	-3.53E+03
60	CH3O + H = CH2O + H2	2.00E+13	0.00	0.00E+00
61	CH2O + M = HCO + H + M	5.00E+16	0.00	8.10E+04
62	CH2O + OH = HCO + H2O	3.43E+09	1.18	-4.47E+02
63	CH2O + H = HCO + H2	2.30E+10	1.05	3.28E+03
64	CH2O + O = HCO + OH	3.90E+13	0.00	3.54E+03
65	CH3 + CH2O = CH4 + HCO	3.32E+03	2.81	5.86E+03
66	CH3 + HCO = CH4 + CO	2.65E+13	0.00	0.00E+00
67	CH3 + HO2 = CH3O + OH	2.00E+13	0.00	0.00E+00
68	CH3 + M = CH2 + H + M	1.95E+16	0.00	9.16E+04
69	H + CH3 = H2 + CH2	2.70E+11	0.67	2.57E+04
70	O + CH3 = OH + CH2	1.90E+11	0.68	2.57E+04

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 71 O + CH3 = H + CH2O                                 8.43E+13  0.00  0.00E+00
 72 OH + CH3 = H2O + CH2                               5.60E+07  1.60  5.42E+03
 73 CH + CO2 = HCO + CO                                3.40E+12  0.00  6.90E+02
 74 CH + O2 = HCO + O                                  3.30E+13  0.00  0.00E+00
 75 CH2 + O2 = CH2O + O                                5.00E+11  0.50  6.96E+03
 76 CH2 + O2 = OH + HCO                                1.32E+13  0.00  1.50E+03
 77 CH2 + O = CH + OH                                  2.00E+11  0.70  2.58E+04
 78 CH2 + OH = CH + H2O                                1.13E+07  2.00  3.00E+03
 79 CH2 + H = CH + H2                                  3.20E+11  0.70  4.97E+03
 80 2CH2 = C2H3 + H                                    5.00E+12  0.00  0.00E+00
 81 2CH2 = C2H2 + H2                                   3.20E+13  0.00  0.00E+00
 82 HCO + O2 = CO + HO2                                7.60E+12  0.00  4.00E+02
 83 HCO + O = CO + OH                                  3.00E+13  0.00  0.00E+00
 84 HCO + O = CO2 + H                                  3.00E+13  0.00  0.00E+00
 85 HCO + OH = CO + H2O                                5.00E+13  0.00  0.00E+00
 86 HCO + H = CO + H2                                  7.34E+13  0.00  0.00E+00
 87 HCO + M = H + CO + M                               1.87E+17 -1.00  1.70E+04
 88 CO + O + M = CO2 + M                               6.02E+14  0.00  3.00E+03
 89 CO + O2 = CO2 + O                                  2.50E+12  0.00  4.78E+04
 90 CO + OH = CO2 + H                                  4.76E+07  1.23  7.00E+01
 91 CO + HO2 = CO2 + OH                                1.50E+14  0.00  2.36E+04
 92 O + H2O = 2OH                                      6.80E+13  0.00  1.84E+04
 93 H + O2 = OH + O                                    8.30E+13  0.00  1.44E+04
 94 O + H2 = OH + H                                    5.00E+04  2.67  6.29E+03
 95 H + HO2 = H2 + O2                                  2.80E+13  0.00  1.07E+03
 96 O + HO2 = OH + O2                                  2.00E+13  0.00  0.00E+00
 97 HO2 + OH = H2O + O2                                2.90E+13  0.00 -5.00E+02
 98 H + HO2 = 2OH                                      1.34E+14  0.00  6.35E+02
 99 H2 + HO2 = H2O2 + H                                1.21E+07  2.00  5.20E+03
100 OH + H2O2 = H2O + HO2                              1.75E+12  0.00  3.20E+02
101 2HO2 = H2O2 + O2                                   1.30E+11  0.00 -1.63E+03
102 H + H2O2 = OH + H2O                                1.00E+13  0.00  3.60E+03
103 H2O2 + M = 2OH + M                                 1.44E+17  0.00  4.55E+04
   3body efficiencies
     H2   2.30  O2   0.78  H2O   6.00  H2O2   6.60
104 H2 + OH = H2O + H                                  2.16E+08  1.51  3.43E+03
105 H + O2 + M = HO2 + M                               2.80E+18 -0.86  0.00E+00
   3body efficiencies
     O2   1.30  N2   1.30  H2O  21.30  CO2   7.00
106 H2O + M = H + OH + M                               1.30E+15  0.00  1.05E+05
   3body efficiencies
     H2   4.00  O2   1.50  H2O  20.00  N2   1.50  CO2   4.00
107 H + O + M = OH + M                                 5.00E+17 -1.00  0.00E+00
108 H2 + M = 2H + M                                    2.20E+14  0.00  9.60E+04
   3body efficiencies
     H2   4.10  O2   2.00  H2O  15.00  N2   2.00
109 O2 + M = 2O + M                                    1.80E+18 -1.00  1.18E+05
110 CH + N2 = HCN + N                                  1.00E+11  0.00  1.90E+04
111 CN + H2 = HCN + H                                  2.10E+13  0.00  4.71E+03
112 O + HCN = OH + CN                                  2.13E+09  1.58  2.66E+04
113 O + HCN = NCO + H                                  1.11E+04  2.64  4.98E+03
114 O + HCN = NH + CO                                  2.77E+03  2.64  4.98E+03
115 OH + HCN = HNCO + H                                4.40E+03  2.26  6.40E+03
116 CN + O = CO + N                                    7.70E+13  0.00  0.00E+00
117 CN + OH = NCO + H                                  4.00E+13  0.00  0.00E+00
118 H2 + NCO = HNCO + H                                1.00E+14  0.00  9.00E+03
119 HNCO + H = NH2 + CO                                2.25E+07  1.70  3.80E+03
120 CN + O2 = NCO + O                                  6.14E+12  0.00 -4.40E+02
121 CN + CO2 = NCO + CO                                3.70E+12  0.00  0.00E+00
122 O + NCO = NO + CO                                  2.35E+13  0.00  0.00E+00
123 N + NCO = N2 + CO                                  2.00E+13  0.00  0.00E+00
124 H + NCO = NH + CO                                  5.40E+13  0.00  0.00E+00
125 CH + NO = N + HCO                                  3.00E+13  0.00  0.00E+00
126 CH + NO = O + HCN                                  5.00E+13  0.00  0.00E+00
127 CH + NO = H + NCO                                  2.00E+13  0.00  0.00E+00
128 NH + OH = N + H2O                                  2.00E+09  1.20  0.00E+00
129 NH + OH = HNO + H                                  2.00E+13  0.00  0.00E+00
130 HO2 + NO = NO2 + OH                                2.11E+12  0.00 -4.80E+02
131 O + NO2 = NO + O2                                  3.90E+12  0.00 -2.40E+02
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 132 NO + O + M = NO2 + M                                1.06E+20 -1.41  0.00E+00
 133 NO2 + H = NO + OH                                   1.32E+14  0.00  3.60E+02
 134 NO + H = N + OH                                     2.63E+14  0.00  5.04E+04
 135 NO + O = N + O2                                     3.80E+09  1.00  4.14E+04
 136 O + N2 = NO + N                                     1.80E+14  0.00  7.63E+04
 137 N + NO2 = 2NO                                       4.00E+12  0.00  0.00E+00
 138 N2O + M = N2 + O + M                                6.92E+23 -2.50  6.50E+04
 139 O + N2O = N2 + O2                                   1.40E+12  0.00  1.08E+04
 140 O + N2O = 2NO                                       2.90E+13  0.00  2.32E+04
 141 N2O + H = N2 + OH                                   4.40E+14  0.00  1.89E+04
 142 NO2 + H2 = HNO2 + H                                 2.40E+13  0.00  2.90E+04
 143 OH + NO2 + M = HNO3 + M                             3.00E+15  0.00 -3.80E+03
    3body efficiencies
      O2   0.70  H2   1.40
 144 OH + NO + M = HNO2 + M                              5.60E+15  0.00 -1.70E+03
 145 HNO + H = H2 + NO                                   4.50E+11  0.72  6.60E+02
 146 H + NO + M = HNO + M                                8.95E+19 -1.32  7.40E+02
 147 HNO + OH = H2O + NO                                 1.30E+07  1.90 -9.50E+02


    ** The following  4 elements considered for this problem **
    C  H  O  N

    ** The following  40 reacting species considered for this problem **
CH4 CH3 H H2 O2 HO2 O OH H2O CH3O CH2O C2H6 C2H5 C2H4 CH2 C2H3 C2H2 HCO C2H2O
C2H CO C2HO CH2CO CO2 CH H2O2 N2 HCN N CN NCO NH HNCO NH2 NO HNO NO2 N2O HNO2
HNO3

    ** No inert species considered for this problem **


** New input data given in SI   units **   ** Output required in SI   units **

                      ** Assigned variable profile **

                       ** Constant-area problem **

         Number of species ODE's:   40  Total number of ODE's:   43

                             Integration Controls
Method Flag (MF): 21  Rel. Error: 1.000E-04  Species Abs. Error: 1.000E-10

    Maximum number of steps allowed for the complete problem:  2000

             ** Output required at following   1 axial distances (m) **
  3.048E+01


                       ** Initial Conditions **


         Time 0.00E+00 s  Axial Position 0.00E+00 m  Area 3.17E-05sq m

  Thermodynamic Properties               Integration Indicators

    Pressure (N/m**2)        1.013E+05     Steps from last print      0
    Velocity (m/s)                2.63     Average step size   0.00E+00
    Density (kg/m**3)        8.219E-01     Method Order               0
    Temperature (K)             423.15     Incr. CPU Time          0.00 s
    Mass Flow Rate (kg/s)    6.846E-05
    Entropy (J/kg/K)         7.387E+03     Total number of steps      0
    Mach Number              6.370E-03     Funct evaluations          0
    Gamma (Frozen)               1.383     Jacobian evaluations       0
    Enthalpy (J/kg)         -6.249E+05     Total CPU Time          0.00 s
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Sp. heat, cp (J/kg/K) 1.052E+03

Chemical Properties

Wi = Net molar production rate per unit volume of species i (kmol/m**3/s)
kj = Forward rate const for reaction j (cgs units)
XH,j = Net energy exch rate for reaction j (J-m**3/kg**2/s)
Eq,j = Equilibration factor for reaction j (= Net rate/Positive dir rate)

Species i	Mass Fr.	Mole Fr.	Wi
CH4	0.00E+00	0.00E+00	0.00E+00
CH3	0.00E+00	0.00E+00	0.00E+00
H	0.00E+00	0.00E+00	0.00E+00
H2	0.00E+00	0.00E+00	0.00E+00
O2	1.83E-01	1.63E-01	-1.63E-22
HO2	0.00E+00	0.00E+00	4.18E-29
O	0.00E+00	0.00E+00	1.63E-22
OH	0.00E+00	0.00E+00	4.18E-29
H2O	3.16E-02	5.01E-02	-4.18E-29
CH3O	0.00E+00	0.00E+00	0.00E+00
CH2O	0.00E+00	0.00E+00	0.00E+00
C2H6	0.00E+00	0.00E+00	0.00E+00
C2H5	0.00E+00	0.00E+00	0.00E+00
C2H4	0.00E+00	0.00E+00	0.00E+00
CH2	0.00E+00	0.00E+00	0.00E+00
C2H3	0.00E+00	0.00E+00	0.00E+00
C2H2	0.00E+00	0.00E+00	0.00E+00
HCO	0.00E+00	0.00E+00	0.00E+00
C2H2O	0.00E+00	0.00E+00	0.00E+00
C2H	0.00E+00	0.00E+00	0.00E+00
CO	2.30E-03	2.34E-03	-1.63E-22
C2HO	0.00E+00	0.00E+00	0.00E+00
CH2CO	0.00E+00	0.00E+00	0.00E+00
CO2	3.60E-02	2.34E-02	1.63E-22
CH	0.00E+00	0.00E+00	0.00E+00
H2O2	0.00E+00	0.00E+00	0.00E+00
N2	7.47E-01	7.61E-01	-1.40E-42
HCN	0.00E+00	0.00E+00	0.00E+00
N	0.00E+00	0.00E+00	0.00E+00
CN	0.00E+00	0.00E+00	0.00E+00
NCO	0.00E+00	0.00E+00	0.00E+00
NH	0.00E+00	0.00E+00	0.00E+00
HNCO	0.00E+00	0.00E+00	0.00E+00
NH2	0.00E+00	0.00E+00	0.00E+00
NO	0.00E+00	0.00E+00	6.37E-32
HNO	0.00E+00	0.00E+00	0.00E+00
NO2	1.61E-06	1.00E-06	-6.37E-32
N2O	0.00E+00	0.00E+00	1.40E-42
HNO2	0.00E+00	0.00E+00	0.00E+00
HNO3	0.00E+00	0.00E+00	0.00E+00

Reac No,j	kj	XH,j	Eq,j
1	7.09E-29	0.00E+00	0.00E+00
2	2.99E+07	0.00E+00	0.00E+00
3	1.00E+12	0.00E+00	0.00E+00
4	3.21E+08	0.00E+00	0.00E+00
5	3.90E+10	0.00E+00	0.00E+00
6	3.58E-02	0.00E+00	0.00E+00
7	8.69E+05	0.00E+00	0.00E+00
8	3.20E+12	0.00E+00	0.00E+00
9	7.13E+02	0.00E+00	0.00E+00
10	2.14E+13	0.00E+00	0.00E+00
11	3.06E+07	0.00E+00	0.00E+00
12	1.45E+09	0.00E+00	0.00E+00
13	1.14E+10	0.00E+00	0.00E+00
14	4.65E+11	0.00E+00	0.00E+00
15	9.75E+00	0.00E+00	0.00E+00
16	8.37E+09	0.00E+00	0.00E+00
17	2.00E+12	0.00E+00	0.00E+00
18	2.00E+13	0.00E+00	0.00E+00
19	2.79E+06	0.00E+00	0.00E+00
20	2.87E-24	0.00E+00	0.00E+00
21	3.30E+10	0.00E+00	0.00E+00
22	6.39E+11	0.00E+00	0.00E+00
23	9.47E+11	0.00E+00	0.00E+00
24	6.54E+10	0.00E+00	0.00E+00
25	8.91E-02	0.00E+00	0.00E+00
26	5.29E+12	0.00E+00	0.00E+00
27	3.00E+13	0.00E+00	0.00E+00
28	3.00E+13	0.00E+00	0.00E+00
29	5.00E+12	0.00E+00	0.00E+00
30	3.00E+13	0.00E+00	0.00E+00
31	3.00E+13	0.00E+00	0.00E+00
32	2.29E-39	0.00E+00	0.00E+00
33	1.91E+11	0.00E+00	0.00E+00
34	1.91E+11	0.00E+00	0.00E+00
35	1.02E+01	0.00E+00	0.00E+00
36	3.55E+05	0.00E+00	0.00E+00
37	5.90E+04	0.00E+00	0.00E+00
38	4.72E+08	0.00E+00	0.00E+00
39	1.67E+08	0.00E+00	0.00E+00
40	8.40E+12	0.00E+00	0.00E+00
41	8.40E+12	0.00E+00	0.00E+00
42	2.00E+13	0.00E+00	0.00E+00
43	5.79E+11	0.00E+00	0.00E+00
44	1.00E+14	0.00E+00	0.00E+00
45	1.00E+13	0.00E+00	0.00E+00
46	1.00E+14	0.00E+00	0.00E+00
47	3.00E+13	0.00E+00	0.00E+00
48	9.27E+11	0.00E+00	0.00E+00
49	1.00E+13	0.00E+00	0.00E+00
50	2.80E+13	0.00E+00	0.00E+00
51	6.95E+11	0.00E+00	0.00E+00
52	1.92E+11	0.00E+00	0.00E+00
53	3.69E+09	0.00E+00	0.00E+00
54	7.38E+08	0.00E+00	0.00E+00
55	2.00E+13	0.00E+00	0.00E+00
56	3.51E+11	0.00E+00	0.00E+00
57	2.05E-15	0.00E+00	0.00E+00

58	5.00E+13	0.00E+00	0.00E+00
59	2.61E+09	0.00E+00	0.00E+00
60	2.00E+13	0.00E+00	0.00E+00
61	7.31E-26	0.00E+00	0.00E+00
62	7.34E+12	0.00E+00	0.00E+00
63	2.68E+11	0.00E+00	0.00E+00
64	5.79E+11	0.00E+00	0.00E+00
65	7.50E+07	0.00E+00	0.00E+00
66	2.65E+13	0.00E+00	0.00E+00
67	2.00E+13	0.00E+00	0.00E+00
68	9.55E-32	0.00E+00	0.00E+00
69	8.27E-01	0.00E+00	0.00E+00
70	6.18E-01	0.00E+00	0.00E+00
71	8.43E+13	0.00E+00	0.00E+00
72	1.42E+09	0.00E+00	0.00E+00
73	1.50E+12	0.00E+00	0.00E+00
74	3.30E+13	0.00E+00	0.00E+00
75	2.62E+09	0.00E+00	0.00E+00
76	2.22E+12	0.00E+00	0.00E+00
77	6.52E-01	0.00E+00	0.00E+00
78	5.71E+10	0.00E+00	0.00E+00
79	5.98E+10	0.00E+00	0.00E+00
80	5.00E+12	0.00E+00	0.00E+00
81	3.20E+13	0.00E+00	0.00E+00
82	4.72E+12	0.00E+00	0.00E+00
83	3.00E+13	0.00E+00	0.00E+00
84	3.00E+13	0.00E+00	0.00E+00
85	5.00E+13	9.26E-41	1.00E+00
86	7.34E+13	0.00E+00	0.00E+00
87	7.33E+05	0.00E+00	0.00E+00
88	1.70E+13	0.00E+00	1.00E+00
89	5.13E-13	-8.14E-15	1.00E+00
90	7.45E+10	0.00E+00	0.00E+00
91	9.71E+01	0.00E+00	0.00E+00
92	2.22E+04	0.00E+00	0.00E+00
93	2.99E+06	0.00E+00	0.00E+00
94	2.90E+08	0.00E+00	0.00E+00
95	7.86E+12	0.00E+00	0.00E+00
96	2.00E+13	0.00E+00	0.00E+00
97	5.26E+13	1.75E-20	1.00E+00
98	6.30E+13	0.00E+00	0.00E+00
99	4.47E+09	0.00E+00	0.00E+00
100	1.20E+12	0.00E+00	0.00E+00
101	9.03E+11	0.00E+00	0.00E+00
102	1.38E+11	0.00E+00	0.00E+00
103	4.50E-07	0.00E+00	0.00E+00
104	3.38E+10	0.00E+00	0.00E+00
105	1.54E+16	0.00E+00	0.00E+00
106	6.47E-40	4.93E-38	1.00E+00
107	1.18E+15	0.00E+00	0.00E+00
108	5.76E-36	0.00E+00	0.00E+00
109	4.71E-46	4.62E-44	1.00E+00
110	1.54E+01	0.00E+00	0.00E+00
111	7.76E+10	0.00E+00	0.00E+00
112	5.49E-01	0.00E+00	0.00E+00
113	2.55E+08	0.00E+00	0.00E+00
114	6.37E+07	0.00E+00	0.00E+00
115	1.88E+06	0.00E+00	0.00E+00
116	7.70E+13	0.00E+00	0.00E+00
117	4.00E+13	0.00E+00	0.00E+00
118	2.25E+09	0.00E+00	0.00E+00
119	7.15E+09	0.00E+00	0.00E+00
120	1.04E+13	0.00E+00	0.00E+00
121	3.70E+12	0.00E+00	0.00E+00
122	2.35E+13	0.00E+00	0.00E+00
123	2.00E+13	0.00E+00	1.00E+00
124	5.40E+13	0.00E+00	0.00E+00
125	3.00E+13	0.00E+00	0.00E+00
126	5.00E+13	0.00E+00	0.00E+00

127	2.00E+13	0.00E+00	0.00E+00
128	2.84E+12	0.00E+00	0.00E+00
129	2.00E+13	0.00E+00	0.00E+00
130	3.73E+12	0.00E+00	0.00E+00
131	5.19E+12	0.00E+00	0.00E+00
132	2.10E+16	2.89E-23	1.00E+00
133	8.60E+13	0.00E+00	0.00E+00
134	2.42E-12	0.00E+00	0.00E+00
135	6.91E-10	0.00E+00	0.00E+00
136	7.47E-26	0.00E+00	0.00E+00
137	4.00E+12	0.00E+00	0.00E+00
138	5.04E-17	0.00E+00	0.00E+00
139	3.66E+06	4.21E-34	1.00E+00
140	3.20E+01	0.00E+00	0.00E+00
141	7.80E+04	0.00E+00	0.00E+00
142	2.52E-02	0.00E+00	0.00E+00
143	2.75E+17	0.00E+00	0.00E+00
144	4.23E+16	0.00E+00	0.00E+00
145	1.60E+13	0.00E+00	0.00E+00
146	1.27E+16	0.00E+00	0.00E+00
147	3.93E+12	0.00E+00	0.00E+00

Derivs (SI units): T 2.40E-18 RHO -4.66E-21 V 1.49E-20

Mix Mol Wt. 28.538 Total Energy Exch Rate -8.14E-15 Mass Fr. Sum 1.00000
(J-m**3/kg**2/s)

CPU Time for initialization of LSENS = 0.00 s

Negative concentration for species CH4

Negative concentration for species CH3

Negative concentration for species CH3O

Negative concentration for species C2H6

Negative concentration for species C2H5

Negative concentration for species C2H4

Negative concentration for species C2H2

Negative concentration for species C2H

Negative concentration for species C2HO

Negative concentration for species HNCO

Negative concentration for species NH2

Time 1.16E+01 s Axial Position 3.05E+01 m Area 3.17E-05sq m

Thermodynamic Properties		Integration Indicators	
Pressure (N/m**2)	1.013E+05	Steps from last print	3
Velocity (m/s)	2.63	Average step size	1.02E+05
Density (kg/m**3)	8.219E-01	Method Order	1
Temperature (K)	423.15	Incr. CPU Time	0.00 s
Mass Flow Rate (kg/s)	6.846E-05		
Entropy (J/kg/K)	7.387E+03	Total number of steps	3
Mach Number	6.370E-03	Funct evaluations	4
Gamma (Frozen)	1.383	Jacobian evaluations	2
Enthalpy (J/kg)	-6.249E+05	Total CPU Time	0.00 s

Sp. heat, cp (J/kg/K) 1.052E+03

Chemical Properties

Wi = Net molar production rate per unit volume of species i (kmol/m**3/s)
kj = Forward rate const for reaction j (cgs units)
XH,j = Net energy exch rate for reaction j (J-m**3/kg**2/s)
Eq,j = Equilibration factor for reaction j (= Net rate/Positive dir rate)

Species i	Mass Fr.	Mole Fr.	Wi
CH4	-4.19E-31	-7.46E-31	-4.99E-25
CH3	-2.73E-34	-5.18E-34	4.99E-25
H	1.32E-32	3.73E-31	4.11E-33
H2	1.01E-33	1.42E-32	3.51E-35
O2	1.83E-01	1.63E-01	-3.03E-23
HO2	2.55E-23	2.21E-23	5.54E-25
O	1.73E-23	3.09E-23	3.29E-25
OH	2.26E-28	3.79E-28	4.16E-30
H2O	3.16E-02	5.01E-02	-2.86E-26
CH3O	-7.72E-45	-7.01E-45	0.00E+00
CH2O	5.57E-31	5.29E-31	-6.09E-35
C2H6	-3.01E-49	0.00E+00	0.00E+00
C2H5	-9.14E-63	0.00E+00	0.00E+00
C2H4	-3.10E-50	0.00E+00	0.00E+00
CH2	1.21E-62	0.00E+00	0.00E+00
C2H3	1.13E-45	1.40E-45	-8.55E-40
C2H2	-2.26E-42	-2.47E-42	0.00E+00
HCO	1.60E-36	1.57E-36	-1.96E-39
C2H2O	7.62E-46	0.00E+00	0.00E+00
C2H	-1.77E-45	-1.40E-45	4.60E-39
CO	2.30E-03	2.34E-03	-1.92E-22
C2HO	-3.80E-46	0.00E+00	-2.28E-39
CH2CO	1.01E-58	0.00E+00	0.00E+00
CO2	3.60E-02	2.34E-02	1.92E-22
CH	6.85E-63	0.00E+00	0.00E+00
H2O2	1.46E-31	1.22E-31	3.06E-36
N2	7.47E-01	7.61E-01	-5.30E-32
HCN	1.19E-59	0.00E+00	0.00E+00
N	1.05E-41	2.14E-41	-2.83E-40
CN	1.44E-43	1.58E-43	0.00E+00
NCO	3.12E-41	2.12E-41	0.00E+00
NH	4.47E-51	0.00E+00	0.00E+00
HNCO	-7.84E-65	0.00E+00	0.00E+00
NH2	-1.03E-84	0.00E+00	0.00E+00
NO	5.64E-20	5.36E-20	1.33E-22
HNO	4.99E-40	4.59E-40	0.00E+00
NO2	1.61E-06	1.00E-06	-1.33E-22
N2O	3.30E-29	2.14E-29	5.30E-32
HNO2	2.56E-36	1.55E-36	2.10E-41
HNO3	2.12E-24	9.62E-25	2.37E-27

Reac No,j	kj	XH,j	Eq,j
1	7.09E-29	3.51E-42	1.00E+00
2	2.99E+07	0.00E+00	1.00E+00
3	1.00E+12	1.64E-16	8.31E-01
4	3.21E+08	-9.39E-44	1.00E+00
5	3.90E+10	-5.54E-31	1.00E+00
6	3.58E-02	-4.45E-34	1.00E+00
7	8.69E+05	2.01E-26	1.00E+00
8	3.20E+12	0.00E+00	1.00E+00
9	7.13E+02	-5.33E-40	1.00E+00
10	2.14E+13	0.00E+00	1.00E+00
11	3.06E+07	0.00E+00	1.00E+00
12	1.45E+09	0.00E+00	1.00E+00
13	1.14E+10	0.00E+00	1.00E+00
14	4.65E+11	0.00E+00	6.95E-01
15	9.75E+00	0.00E+00	9.97E-01
16	8.37E+09	0.00E+00	1.00E+00
17	2.00E+12	0.00E+00	1.00E+00
18	2.00E+13	0.00E+00	1.00E+00
19	2.79E+06	0.00E+00	5.99E-01
20	2.87E-24	0.00E+00	1.00E+00
21	3.30E+10	1.82E-44	1.00E+00
22	6.39E+11	0.00E+00	1.00E+00
23	9.47E+11	0.00E+00	1.00E+00
24	6.54E+10	0.00E+00	1.00E+00
25	8.91E-02	2.38E-44	1.00E+00
26	5.29E+12	-4.21E-31	1.00E+00
27	3.00E+13	0.00E+00	1.00E+00
28	3.00E+13	0.00E+00	1.00E+00
29	5.00E+12	0.00E+00	1.00E+00
30	3.00E+13	0.00E+00	7.57E-01
31	3.00E+13	0.00E+00	1.00E+00
32	2.29E-39	0.00E+00	1.00E+00
33	1.91E+11	0.00E+00	1.00E+00
34	1.91E+11	0.00E+00	1.00E+00
35	1.02E+01	0.00E+00	9.99E-01
36	3.55E+05	3.57E-36	1.00E+00
37	5.90E+04	0.00E+00	1.00E+00
38	4.72E+08	0.00E+00	1.00E+00
39	1.67E+08	0.00E+00	1.00E+00
40	8.40E+12	4.44E-31	1.00E+00
41	8.40E+12	2.07E-30	1.00E+00
42	2.00E+13	0.00E+00	1.00E+00
43	5.79E+11	1.05E-32	1.00E+00
44	1.00E+14	0.00E+00	1.00E+00
45	1.00E+13	0.00E+00	1.00E+00
46	1.00E+14	0.00E+00	9.97E-01
47	3.00E+13	0.00E+00	1.00E+00
48	9.27E+11	0.00E+00	1.00E+00
49	1.00E+13	0.00E+00	3.25E-01
50	2.80E+13	0.00E+00	9.92E-01
51	6.95E+11	-3.28E-43	1.00E+00
52	1.92E+11	-1.23E-41	1.00E+00
53	3.69E+09	0.00E+00	1.00E+00
54	7.38E+08	0.00E+00	1.00E+00
55	2.00E+13	0.00E+00	1.00E+00
56	3.51E+11	0.00E+00	1.00E+00
57	2.05E-15	-5.61E-45	1.00E+00

58	5.00E+13	0.00E+00	1.00E+00
59	2.61E+09	4.83E-34	1.00E+00
60	2.00E+13	0.00E+00	1.00E+00
61	7.31E-26	0.00E+00	1.00E+00
62	7.34E+12	2.33E-38	1.00E+00
63	2.68E+11	0.00E+00	1.00E+00
64	5.79E+11	-5.90E-40	1.00E+00
65	7.50E+07	0.00E+00	1.00E+00
66	2.65E+13	0.00E+00	1.00E+00
67	2.00E+13	2.60E-41	1.00E+00
68	9.55E-32	0.00E+00	1.00E+00
69	8.27E-01	0.00E+00	1.00E+00
70	6.18E-01	0.00E+00	1.00E+00
71	8.43E+13	4.85E-40	1.00E+00
72	1.42E+09	0.00E+00	1.00E+00
73	1.50E+12	0.00E+00	1.00E+00
74	3.30E+13	0.00E+00	1.00E+00
75	2.62E+09	0.00E+00	1.00E+00
76	2.22E+12	0.00E+00	1.00E+00
77	6.52E-01	0.00E+00	1.00E+00
78	5.71E+10	0.00E+00	1.00E+00
79	5.98E+10	0.00E+00	9.99E-01
80	5.00E+12	0.00E+00	1.00E+00
81	3.20E+13	0.00E+00	1.00E+00
82	4.72E+12	-2.27E-22	1.00E+00
83	3.00E+13	-6.50E-43	1.00E+00
84	3.00E+13	-8.38E-43	1.00E+00
85	5.00E+13	9.26E-41	1.00E+00
86	7.34E+13	0.00E+00	1.00E+00
87	7.33E+05	-9.54E-23	1.00E+00
88	1.70E+13	-2.31E-14	1.00E+00
89	5.13E-13	-8.14E-15	1.00E+00
90	7.45E+10	-8.43E-18	1.00E+00
91	9.71E+01	-1.52E-21	1.00E+00
92	2.22E+04	2.98E-18	1.00E+00
93	2.99E+06	1.57E-23	1.00E+00
94	2.90E+08	0.00E+00	9.99E-01
95	7.86E+12	-1.75E-38	1.00E+00
96	2.00E+13	-3.56E-30	1.00E+00
97	5.26E+13	1.75E-20	1.00E+00
98	6.30E+13	-9.06E-38	1.00E+00
99	4.47E+09	-4.78E-40	1.00E+00
100	1.20E+12	6.46E-28	1.00E+00
101	9.03E+11	-7.58E-32	9.98E-01
102	1.38E+11	0.00E+00	1.00E+00
103	4.50E-07	1.76E-35	1.00E+00
104	3.38E+10	3.26E-27	1.00E+00
105	1.54E+16	-1.75E-17	1.00E+00
106	6.47E-40	4.04E-38	8.19E-01
107	1.18E+15	-2.06E-40	1.00E+00
108	5.76E-36	-5.61E-45	1.00E+00
109	4.71E-46	-6.51E-33	1.00E+00
110	1.54E+01	0.00E+00	1.00E+00
111	7.76E+10	0.00E+00	1.00E+00
112	5.49E-01	0.00E+00	1.00E+00
113	2.55E+08	0.00E+00	1.00E+00
114	6.37E+07	0.00E+00	1.00E+00
115	1.88E+06	0.00E+00	1.00E+00
116	7.70E+13	0.00E+00	1.00E+00
117	4.00E+13	0.00E+00	1.00E+00
118	2.25E+09	0.00E+00	1.00E+00
119	7.15E+09	0.00E+00	9.82E-01
120	1.04E+13	-8.72E-30	1.00E+00
121	3.70E+12	-2.38E-30	9.51E-01
122	2.35E+13	0.00E+00	1.00E+00
123	2.00E+13	0.00E+00	1.00E+00
124	5.40E+13	0.00E+00	9.78E-01
125	3.00E+13	0.00E+00	1.00E+00
126	5.00E+13	0.00E+00	1.00E+00

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                                    127  2.00E+13  0.00E+00  1.00E+00
                                    128  2.84E+12  5.61E-45  1.00E+00
                                    129  2.00E+13  0.00E+00  9.93E-01
                                    130  3.73E+12  7.60E-22  1.00E+00
                                    131  5.19E+12 -3.78E-14  1.00E+00
                                    132  2.10E+16  2.89E-23  1.00E+00
                                    133  8.60E+13 -4.81E-21  1.00E+00
                                    134  2.42E-12  0.00E+00  1.00E+00
                                    135  6.91E-10 -4.16E-32  1.00E+00
                                    136  7.47E-26 -5.61E-45  8.88E-01
                                    137  4.00E+12 -3.40E-32  1.00E+00
                                    138  5.04E-17 -1.32E-23  1.00E+00
                                    139  3.66E+06  4.21E-34  1.00E+00
                                    140  3.20E+01  0.00E+00  1.00E+00
                                    141  7.80E+04  0.00E+00  9.98E-01
                                    142  2.52E-02  4.65E-38  1.00E+00
                                    143  2.75E+17 -7.26E-19  1.00E+00
                                    144  4.23E+16 -6.34E-33  1.00E+00
                                    145  1.60E+13  0.00E+00  1.00E+00
                                    146  1.27E+16 -1.86E-36  1.00E+00
                                    147  3.93E+12  7.09E-42  1.00E+00

Derivs (SI units):  T         2.05E-17  RHO      -3.95E-20  V         1.26E-19

Mix Mol Wt.   28.538  Total Energy Exch Rate -6.89E-14  Mass Fr. Sum   1.00000
                        (J-m**3/kg**2/s)


(LSENS)  End of this case


            Summary of computational work required for problem:
              Total no. of steps -                       3
              Total no. of derivative evaluations -      4
              Total no. of Jacobian evaluations -        2
              Total CPU Time -                        0.00 s

              Total CPU time (including I/O) =        0.00 s

(LSENS)     Read data for next case



                             ** Problem Data **

        1         2         3         4         5         6         7         8
2345678901234567890123456789012345678901234567890123456789012345678901234567890

                                  Blank Line
                                  Blank Line
                                  Blank Line
                                  Blank Line
                                  Blank Line
                                  Blank Line
 (CIMAGE) ** Warning: End of problem data, but no
    end of file indicator or incomplete data




(KINP)  ** Error: The ACTION switch (= "    " is illegal **
  Legal values are ADD, NEW, CHANGE, and REPEAT


(LSENS)     A fatal error has occurred - Case terminated
```

Sample Line Analysis – CO & NO_2 doubled, CO_2 cut in half

```
                          ** Problem Data **

         1         2         3         4         5         6         7         8
 2345678901234567890123456789012345678901234567890123456789012345678901234567890

LSENS SAMPLE DATA-AIR SAMPLE LINE
   M       +   CH4      =   CH3     +   H         2.0E+17   0.        88000.
   H       +   CH4      =   CH3     +   H2        6.6E+8    1.62      10840.
   CH4     +   O2       =   CH3     +   HO2       1.0E+12   0.        0.
   O       +   CH4      =   CH3     +   OH        1.02E+9   1.5       8600.
   OH      +   CH4      =   CH3     +   H2O       1.0E+8    1.6       3120.
   CH3     +   O2       =   CH3O    +   O         2.68E+13  0.        28800.
   CH3     +   O2       =   OH      +   CH2O      3.6E+10   0.        8940.
   CH3     +   OH       =   CH3O    +   H         3.2E+12   0.        0.
   M       +   CH3O     =   CH2O    +   H         5.0E+13   0.        21000.
   CH3     +   CH3      =   C2H6                  2.4E+14   -.4       0.
   CH3     +   CH3      =   H       +   C2H5      4.99E+12  0.1       10600.
   H       +   C2H6     =   C2H5    +   H2        1.15E+8   1.9       7530.
   O       +   C2H6     =   C2H5    +   OH        8.98E+7   1.92      5690.
   OH      +   C2H6     =   C2H5    +   H2O       3.54E+6   2.12      870.
   M       +   C2H5     =   C2H4    +   H         1.0E+17   0.        31000.
   C2H5    +   O2       =   C2H4    +   HO2       8.4E+11   0.        3875.
   H       +   C2H5     =   C2H4    +   H2        2.0E+12   0.        0.
   CH3     +   CH2      =   C2H4    +   H         2.0E+13   0.        0.
   H       +   C2H4     =   H2      +   C2H3      1.325E+6  2.53      12240.
   M       +   C2H4     =   C2H2    +   H2        2.6E+17   0.        79300.
   C2H4    +   OH       =   C2H3    +   H2O       3.6E+6    2.        2500.
   C2H4    +   OH       =   CH3     +   CH2O      2.0E+12   0.        960.
   C2H4    +   O        =   CH3     +   HCO       1.92E+7   1.83      220.
   C2H4    +   O        =   CH2O    +   CH2       2.5E+13   0.        5000.
   M       +   C2H3     =   C2H2    +   H         3.0E+15   0.        32000.
   C2H3    +   O2       =   CH2O    +   HCO       3.98E+12  0.        -240.
   C2H3    +   H        =   C2H2    +   H2        3.0E+13   0.        0.
   C2H3    +   O        =   C2H2O   +   H         3.0E+13   0.        0.
   C2H3    +   OH       =   C2H2    +   H2O       5.0E+12   0.        0.
   C2H3    +   CH2      =   C2H2    +   CH3       3.0E+13   0.        0.
   C2H3    +   C2H      =2.0C2H2                  3.0E+13   0.        0.
   M       +   C2H2     =   C2H     +   H         4.2E+16   0.        107000.
   C2H2    +   O        =   CH2     +   CO        1.02E+7   2.0       1900.
   C2H2    +   O        =   C2HO    +   H         1.02E+7   2.        1900.
   C2H2    +   O        =   OH      +   C2H       4.6E+19   -1.41     28950.
   C2H2    +   OH       =   C2H     +   H2O       3.37E+7   2.        14000.
   C2H2    +   OH       =   C2H2O   +   H         5.04E+5   2.3       13500.
   C2H2    +   OH       =   CH2CO   +   H         2.18E-4   4.5       -1000.
   C2H2    +   OH       =   CH3     +   CO        4.83E-4   4.        -2000.
   C2H     +   O2       =   C2HO    +   O         5.00E+13  0.0       1500.
   C2H     +   O2       =   HCO     +   CO        5.0E+13   0.0       1500.
   C2H     +   OH       =   C2HO    +   H         2.0E+13   0.0       0.
   C2HO    +   O2       =2.0CO      +   OH        1.6E+12   0.        854.
   C2HO    +   O        =2.0CO      +   H         1.0E+14   0.        0.
   C2HO    +   OH       =2.0HCO                   1.0E+13   0.        0.
   C2HO    +   H        =   CH2     +   CO        1.0E+14   0.        0.
   C2HO    +   CH2      =   C2H3    +   CO        3.0E+13   0.        0.
   C2HO    +   CH2      =   CH2O    +   C2H       1.0E+13   0.        2000.
            2.0C2HO     =   C2H2    +2.0CO        1.0E+13   0.        0.
   C2H2O   +   OH       =   CH2O    +   HCO       2.8E+13   0.        0.
   C2H2O   +   OH       =   C2HO    +   H2O       7.5E+12   0.        2000.
   C2H2O   +   H        =   CH3     +   CO        1.13E+13  0.        3428.
   C2H2O   +   H        =   C2HO    +   H2        5.0E+13   0.        8000.
   C2H2O   +   O        =   C2HO    +   OH        1.0E+13   0.        8000.
   C2H2O   +   O        =   CH2O    +   CO        2.0E+13   0.        0.
   C2H2O   +   O        =   CH2     +   CO2       1.75E+12  0.        1350.
   M       +   C2H2O    =   CH2     +   CO        2.0E+16   0.        60000.
   C2H     +   O        =   CO      +   CH        5.0E+13   0.        0.
   CH3O    +   O2       =   CH2O    +   HO2       4.28E-13  7.6       -3530.
   CH3O    +   H        =   CH2O    +   H2        2.0E+13   0.        0.
   M       +   CH2O     =   HCO     +   H         5.0E+16   0.        81000.
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   CH2O    +   OH      =   HCO     +   H2O       3.43E+9   1.18      -447.
   CH2O    +   H       =   HCO     +   H2        2.3E+10   1.05      3275.
   CH2O    +   O       =   HCO     +   OH        3.9E+13   0.        3540.
   CH3     +   CH2O    =   CH4     +   HCO       3.32E+03  2.81      5860.
   CH3     +   HCO     =   CH4     +   CO        2.65E+13  0.        0.
   CH3     +   HO2     =   CH3O    +   OH        2.0E+13   0.        0.
   M       +   CH3     =   CH2     +   H         1.95E+16  0.        91600.
   H       +   CH3     =   H2      +   CH2       2.7E+11   0.67      25700.
   O       +   CH3     =   OH      +   CH2       1.9E+11   0.68      25700.
   O       +   CH3     =   H       +   CH2O      8.43E+13  0.        0.
   OH      +   CH3     =   H2O     +   CH2       5.6E+7    1.6       5420.
   CH      +   CO2     =   HCO     +   CO        3.4E+12   0.        690.
   CH      +   O2      =   HCO     +   O         3.3E+13   0.        0.
   CH2     +   O2      =   CH2O    +   O         5.0E+11   0.5       6960.
   CH2     +   O2      =   OH      +   HCO       1.32E+13  0.        1500.
   CH2     +   O       =   CH      +   OH        2.0E+11   0.7       25800.
   CH2     +   OH      =   CH      +   H2O       1.13E+7   2.0       3000.
   CH2     +   H       =   CH      +   H2        3.2E+11   0.7       4970.
   CH2     +   CH2     =   C2H3    +   H         5.0E+12   0.        0.
   CH2     +   CH2     =   C2H2    +   H2        3.2E+13   0.        0.
   HCO     +   O2      =   CO      +   HO2       7.6E+12   0.        400.
   HCO     +   O       =   CO      +   OH        3.0E+13   0.        0.
   HCO     +   O       =   CO2     +   H         3.0E+13   0.        0.
   HCO     +   OH      =   CO      +   H2O       5.0E+13   0.        0.
   HCO     +   H       =   CO      +   H2        7.34E+13  0.        0.
   M       +   HCO     =   H       +   CO        1.87E+17  -1.       17000.
   CO      +   O       =   CO2     +   M         6.02E+14  0.        3000.
   CO      +   O2      =   CO2     +   O         2.5E+12   0.        47800.
   CO      +   OH      =   CO2     +   H         4.76E+7   1.23      70.
   CO      +   HO2     =   CO2     +   OH        1.5E+14   0.        23600.
   O       +   H2O     =   OH      +   OH        6.8E+13   0.        18365.
   H       +   O2      =   OH      +   O         8.3E+13   0.        14413.
   O       +   H2      =   OH      +   H         5.00E+04  2.67      6290.
   H       +   HO2     =   H2      +   O2        2.8E+13   0.        1068.
   O       +   HO2     =   OH      +   O2        2.0E+13   0.        0.
   HO2     +   OH      =   H2O     +   O2        2.9E+13   0.        -500.
   H       +   HO2     =2.0OH                    1.34E+14  0.        635.
   H2      +   HO2     =   H2O2    +   H         1.21E+7   2.        5200.
   OH      +   H2O2    =   H2O     +   HO2       1.75E+12  0.        320.
   HO2     +   HO2     =   H2O2    +   O2        1.3E+11   0.        -1630.
   H       +   H2O2    =   OH      +   H2O       1.0E+13   0.        3600.
   M       +   H2O2    =2.0OH                    1.44E+17  0.        45510.
   THIRDBODY
H2        2.30      O2        0.78      H2O       6.0
H2O2      6.6
END
   H2      +   OH      =   H2O     +   H         2.16E+8   1.51      3430.
   H       +   O2      =   HO2     +   M         2.8E+18   -0.86     0.
   THIRDBODY
O2        1.30      N2        1.3
H2O       21.3      CO2       7.0
END
   M       +   H2O     =   H       +   OH        1.30E+15  0.        105140.
   THIRDBODY
H2        4.00      O2        1.5
H2O       20.0      N2        1.5
CO2       4.0
END
   H       +   O       =   OH      +   M         5.00E+17  -1.       0.
   M       +   H2      =   H       +   H         2.2E+14   0.        96000.
   THIRDBODY
H2        4.10      O2        2.0
H2O       15.0      N2        2.0
END
   M       +   O2      =   O       +   O         1.80E+18  -1.       118020.
   CH      +   N2      =   HCN     +   N         1.0E+11   0.        19000.
   CN      +   H2      =   HCN     +   H         2.1E+13   0.        4710.
   O       +   HCN     =   OH      +   CN        2.13E+9   1.58      26600.
   O       +   HCN     =   NCO     +   H         1.11E+4   2.64      4980.
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   O       +   HCN      =   NH      +   CO        2.77E+3   2.64      4980.
   OH      +   HCN      =   HNCO    +   H         4.4E+3    2.26      6400.
   CN      +   O        =   CO      +   N         7.7E+13   0.        0.
   CN      +   OH       =   NCO     +   H         4.0E+13   0.        0.
   H2      +   NCO      =   HNCO    +   H         1.0E+14   0.        9000.
   HNCO    +   H        =   NH2     +   CO        2.25E+7   1.7       3800.
   CN      +   O2       =   NCO     +   O         6.14E+12  0.        -440.
   CN      +   CO2      =   NCO     +   CO        3.7E+12   0.        0.
   O       +   NCO      =   NO      +   CO        2.35E+13  0.        0.
   N       +   NCO      =   N2      +   CO        2.0E+13   0.        0.
   H       +   NCO      =   NH      +   CO        5.4E+13   0.        0.
   CH      +   NO       =   N       +   HCO       3.0E+13   0.        0.
   CH      +   NO       =   O       +   HCN       5.0E+13   0.        0.
   CH      +   NO       =   H       +   NCO       2.0E+13   0.        0.
   NH      +   OH       =   N       +   H2O       2.0E+9    1.2       0.
   NH      +   OH       =   HNO     +   H         2.0E+13   0.        0.
   HO2     +   NO       =   NO2     +   OH        2.11E+12  0.        -480.
   O       +   NO2      =   NO      +   O2        3.9E+12   0.        -240.
   NO      +   O        =   NO2     +   M         1.06E+20  -1.41     0.
   NO2     +   H        =   NO      +   OH        1.32E+14  0.        360.
   NO      +   H        =   N       +   OH        2.63E+14  0.        50410.
   NO      +   O        =   N       +   O2        3.8E+9    1.        41370.
   O       +   N2       =   NO      +   N         1.80E+14  0.        76250.
   N       +   NO2      =2.0NO                    4.0E+12   0.        0.
   M       +   N2O      =   N2      +   O         6.92E+23  -2.5      65000.
   O       +   N2O      =   N2      +   O2        1.4E+12   0.        10810.
   O       +   N2O      =2.0NO                    2.9E+13   0.        23150.
   N2O     +   H        =   N2      +   OH        4.4E+14   0.        18880.
   NO2     +   H2       =   HNO2    +   H         2.4E+13   0.        29000.
   OH      +   NO2      =   HNO3    +   M         3.0E+15   0.        -3800.
   THIRDBODY
O2        0.70      H2        1.4
END
   OH      +   NO       =   HNO2    +   M         5.6E+15   0.        -1700.
   HNO     +   H        =   H2      +   NO        4.5E+11   0.72      660.
   H       +   NO       =   HNO     +   M         8.95E+19  -1.32     740.
   HNO     +   OH       =   H2O     +   NO        1.3E+7    1.9       -950.
                                  Blank Line
END
DISTANCE  AREA      SI        SI
 &PROB  ACON=.TRUE.,CX0=3.167E-05,EXCHR=.TRUE.,CONC=.FALSE.,PRINT=30.48, &END
 $START T=423.15,P=101325.0,v=2.63,&END
CH4        0.0000
O2         0.163379
N2         0.770206
CO2        0.011678
H2O        0.050055
CO         0.004680
NO2        0.000002
                                  Blank Line
                                  Blank Line
&SOLVER  EMAX=1.0E-4, ATOLSP=1.0E-10,  &END
FINIS1
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          LSENS: Multipurpose Kinetics and Sensitivity Analysis Program

LSENS CH4-AIR SAMPLE LINE CASE 6

 Reac        Reaction                                    Reaction Rate Parameters
 No.j                                                       Aj     nj      Ej
               kj = Aj * T**nj * exp(-Ej/RT) (cgs units)

    1 CH4 + M = CH3 + H + M                              2.00E+17  0.00  8.80E+04
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2	H + CH4 = CH3 + H2	6.60E+08	1.62	1.08E+04
3	CH4 + O2 = CH3 + HO2	1.00E+12	0.00	0.00E+00
4	O + CH4 = CH3 + OH	1.02E+09	1.50	8.60E+03
5	OH + CH4 = CH3 + H2O	1.00E+08	1.60	3.12E+03
6	CH3 + O2 = CH3O + O	2.68E+13	0.00	2.88E+04
7	CH3 + O2 = OH + CH2O	3.60E+10	0.00	8.94E+03
8	CH3 + OH = CH3O + H	3.20E+12	0.00	0.00E+00
9	CH3O + M = CH2O + H + M	5.00E+13	0.00	2.10E+04
10	2CH3 = C2H6	2.40E+14	-0.40	0.00E+00
11	2CH3 = H + C2H5	4.99E+12	0.10	1.06E+04
12	H + C2H6 = C2H5 + H2	1.15E+08	1.90	7.53E+03
13	O + C2H6 = C2H5 + OH	8.98E+07	1.92	5.69E+03
14	OH + C2H6 = C2H5 + H2O	3.54E+06	2.12	8.70E+02
15	C2H5 + M = C2H4 + H + M	1.00E+17	0.00	3.10E+04
16	C2H5 + O2 = C2H4 + HO2	8.40E+11	0.00	3.88E+03
17	H + C2H5 = C2H4 + H2	2.00E+12	0.00	0.00E+00
18	CH3 + CH2 = C2H4 + H	2.00E+13	0.00	0.00E+00
19	H + C2H4 = H2 + C2H3	1.33E+06	2.53	1.22E+04
20	C2H4 + M = C2H2 + H2 + M	2.60E+17	0.00	7.93E+04
21	C2H4 + OH = C2H3 + H2O	3.60E+06	2.00	2.50E+03
22	C2H4 + OH = CH3 + CH2O	2.00E+12	0.00	9.60E+02
23	C2H4 + O = CH3 + HCO	1.92E+07	1.83	2.20E+02
24	C2H4 + O = CH2O + CH2	2.50E+13	0.00	5.00E+03
25	C2H3 + M = C2H2 + H + M	3.00E+15	0.00	3.20E+04
26	C2H3 + O2 = CH2O + HCO	3.98E+12	0.00	-2.40E+02
27	C2H3 + H = C2H2 + H2	3.00E+13	0.00	0.00E+00
28	C2H3 + O = C2H2O + H	3.00E+13	0.00	0.00E+00
29	C2H3 + OH = C2H2 + H2O	5.00E+12	0.00	0.00E+00
30	C2H3 + CH2 = C2H2 + CH3	3.00E+13	0.00	0.00E+00
31	C2H3 + C2H = 2C2H2	3.00E+13	0.00	0.00E+00
32	C2H2 + M = C2H + H + M	4.20E+16	0.00	1.07E+05
33	C2H2 + O = CH2 + CO	1.02E+07	2.00	1.90E+03
34	C2H2 + O = C2HO + H	1.02E+07	2.00	1.90E+03
35	C2H2 + O = OH + C2H	4.60E+19	-1.41	2.90E+04
36	C2H2 + OH = C2H + H2O	3.37E+07	2.00	1.40E+04
37	C2H2 + OH = C2H2O + H	5.04E+05	2.30	1.35E+04
38	C2H2 + OH = CH2CO + H	2.18E-04	4.50	-1.00E+03
39	C2H2 + OH = CH3 + CO	4.83E-04	4.00	-2.00E+03
40	C2H + O2 = C2HO + O	5.00E+13	0.00	1.50E+03
41	C2H + O2 = HCO + CO	5.00E+13	0.00	1.50E+03
42	C2H + OH = C2HO + H	2.00E+13	0.00	0.00E+00
43	C2HO + O2 = 2CO + OH	1.60E+12	0.00	8.54E+02
44	C2HO + O = 2CO + H	1.00E+14	0.00	0.00E+00
45	C2HO + OH = 2HCO	1.00E+13	0.00	0.00E+00
46	C2HO + H = CH2 + CO	1.00E+14	0.00	0.00E+00
47	C2HO + CH2 = C2H3 + CO	3.00E+13	0.00	0.00E+00
48	C2HO + CH2 = CH2O + C2H	1.00E+13	0.00	2.00E+03
49	2C2HO = C2H2 + 2CO	1.00E+13	0.00	0.00E+00
50	C2H2O + OH = CH2O + HCO	2.80E+13	0.00	0.00E+00
51	C2H2O + OH = C2HO + H2O	7.50E+12	0.00	2.00E+03
52	C2H2O + H = CH3 + CO	1.13E+13	0.00	3.43E+03
53	C2H2O + H = C2HO + H2	5.00E+13	0.00	8.00E+03
54	C2H2O + O = C2HO + OH	1.00E+13	0.00	8.00E+03
55	C2H2O + O = CH2O + CO	2.00E+13	0.00	0.00E+00
56	C2H2O + O = CH2 + CO2	1.75E+12	0.00	1.35E+03
57	C2H2O + M = CH2 + CO + M	2.00E+16	0.00	6.00E+04
58	C2H + O = CO + CH	5.00E+13	0.00	0.00E+00
59	CH3O + O2 = CH2O + HO2	4.28E-13	7.60	-3.53E+03
60	CH3O + H = CH2O + H2	2.00E+13	0.00	0.00E+00
61	CH2O + M = HCO + H + M	5.00E+16	0.00	8.10E+04
62	CH2O + OH = HCO + H2O	3.43E+09	1.18	-4.47E+02
63	CH2O + H = HCO + H2	2.30E+10	1.05	3.28E+03
64	CH2O + O = HCO + OH	3.90E+13	0.00	3.54E+03
65	CH3 + CH2O = CH4 + HCO	3.32E+03	2.81	5.86E+03
66	CH3 + HCO = CH4 + CO	2.65E+13	0.00	0.00E+00
67	CH3 + HO2 = CH3O + OH	2.00E+13	0.00	0.00E+00
68	CH3 + M = CH2 + H + M	1.95E+16	0.00	9.16E+04
69	H + CH3 = H2 + CH2	2.70E+11	0.67	2.57E+04
70	O + CH3 = OH + CH2	1.90E+11	0.68	2.57E+04

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 71 O + CH3 = H + CH2O                                 8.43E+13  0.00  0.00E+00
 72 OH + CH3 = H2O + CH2                               5.60E+07  1.60  5.42E+03
 73 CH + CO2 = HCO + CO                                3.40E+12  0.00  6.90E+02
 74 CH + O2 = HCO + O                                  3.30E+13  0.00  0.00E+00
 75 CH2 + O2 = CH2O + O                                5.00E+11  0.50  6.96E+03
 76 CH2 + O2 = OH + HCO                                1.32E+13  0.00  1.50E+03
 77 CH2 + O = CH + OH                                  2.00E+11  0.70  2.58E+04
 78 CH2 + OH = CH + H2O                                1.13E+07  2.00  3.00E+03
 79 CH2 + H = CH + H2                                  3.20E+11  0.70  4.97E+03
 80 2CH2 = C2H3 + H                                    5.00E+12  0.00  0.00E+00
 81 2CH2 = C2H2 + H2                                   3.20E+13  0.00  0.00E+00
 82 HCO + O2 = CO + HO2                                7.60E+12  0.00  4.00E+02
 83 HCO + O = CO + OH                                  3.00E+13  0.00  0.00E+00
 84 HCO + O = CO2 + H                                  3.00E+13  0.00  0.00E+00
 85 HCO + OH = CO + H2O                                5.00E+13  0.00  0.00E+00
 86 HCO + H = CO + H2                                  7.34E+13  0.00  0.00E+00
 87 HCO + M = H + CO + M                               1.87E+17 -1.00  1.70E+04
 88 CO + O + M = CO2 + M                               6.02E+14  0.00  3.00E+03
 89 CO + O2 = CO2 + O                                  2.50E+12  0.00  4.78E+04
 90 CO + OH = CO2 + H                                  4.76E+07  1.23  7.00E+01
 91 CO + HO2 = CO2 + OH                                1.50E+14  0.00  2.36E+04
 92 O + H2O = 2OH                                      6.80E+13  0.00  1.84E+04
 93 H + O2 = OH + O                                    8.30E+13  0.00  1.44E+04
 94 O + H2 = OH + H                                    5.00E+04  2.67  6.29E+03
 95 H + HO2 = H2 + O2                                  2.80E+13  0.00  1.07E+03
 96 O + HO2 = OH + O2                                  2.00E+13  0.00  0.00E+00
 97 HO2 + OH = H2O + O2                                2.90E+13  0.00 -5.00E+02
 98 H + HO2 = 2OH                                      1.34E+14  0.00  6.35E+02
 99 H2 + HO2 = H2O2 + H                                1.21E+07  2.00  5.20E+03
100 OH + H2O2 = H2O + HO2                              1.75E+12  0.00  3.20E+02
101 2HO2 = H2O2 + O2                                   1.30E+11  0.00 -1.63E+03
102 H + H2O2 = OH + H2O                                1.00E+13  0.00  3.60E+03
103 H2O2 + M = 2OH + M                                 1.44E+17  0.00  4.55E+04
   3body efficiencies
     H2   2.30  O2   0.78  H2O   6.00  H2O2   6.60
104 H2 + OH = H2O + H                                  2.16E+08  1.51  3.43E+03
105 H + O2 + M = HO2 + M                               2.80E+18 -0.86  0.00E+00
   3body efficiencies
     O2   1.30  N2   1.30  H2O  21.30  CO2   7.00
106 H2O + M = H + OH + M                               1.30E+15  0.00  1.05E+05
   3body efficiencies
     H2   4.00  O2   1.50  H2O  20.00  N2   1.50  CO2   4.00
107 H + O + M = OH + M                                 5.00E+17 -1.00  0.00E+00
108 H2 + M = 2H + M                                    2.20E+14  0.00  9.60E+04
   3body efficiencies
     H2   4.10  O2   2.00  H2O  15.00  N2   2.00
109 O2 + M = 2O + M                                    1.80E+18 -1.00  1.18E+05
110 CH + N2 = HCN + N                                  1.00E+11  0.00  1.90E+04
111 CN + H2 = HCN + H                                  2.10E+13  0.00  4.71E+03
112 O + HCN = OH + CN                                  2.13E+09  1.58  2.66E+04
113 O + HCN = NCO + H                                  1.11E+04  2.64  4.98E+03
114 O + HCN = NH + CO                                  2.77E+03  2.64  4.98E+03
115 OH + HCN = HNCO + H                                4.40E+03  2.26  6.40E+03
116 CN + O = CO + N                                    7.70E+13  0.00  0.00E+00
117 CN + OH = NCO + H                                  4.00E+13  0.00  0.00E+00
118 H2 + NCO = HNCO + H                                1.00E+14  0.00  9.00E+03
119 HNCO + H = NH2 + CO                                2.25E+07  1.70  3.80E+03
120 CN + O2 = NCO + O                                  6.14E+12  0.00 -4.40E+02
121 CN + CO2 = NCO + CO                                3.70E+12  0.00  0.00E+00
122 O + NCO = NO + CO                                  2.35E+13  0.00  0.00E+00
123 N + NCO = N2 + CO                                  2.00E+13  0.00  0.00E+00
124 H + NCO = NH + CO                                  5.40E+13  0.00  0.00E+00
125 CH + NO = N + HCO                                  3.00E+13  0.00  0.00E+00
126 CH + NO = O + HCN                                  5.00E+13  0.00  0.00E+00
127 CH + NO = H + NCO                                  2.00E+13  0.00  0.00E+00
128 NH + OH = N + H2O                                  2.00E+09  1.20  0.00E+00
129 NH + OH = HNO + H                                  2.00E+13  0.00  0.00E+00
130 HO2 + NO = NO2 + OH                                2.11E+12  0.00 -4.80E+02
131 O + NO2 = NO + O2                                  3.90E+12  0.00 -2.40E+02
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 132 NO + O + M = NO2 + M                                1.06E+20 -1.41  0.00E+00
 133 NO2 + H = NO + OH                                   1.32E+14  0.00  3.60E+02
 134 NO + H = N + OH                                     2.63E+14  0.00  5.04E+04
 135 NO + O = N + O2                                     3.80E+09  1.00  4.14E+04
 136 O + N2 = NO + N                                     1.80E+14  0.00  7.63E+04
 137 N + NO2 = 2NO                                       4.00E+12  0.00  0.00E+00
 138 N2O + M = N2 + O + M                                6.92E+23 -2.50  6.50E+04
 139 O + N2O = N2 + O2                                   1.40E+12  0.00  1.08E+04
 140 O + N2O = 2NO                                       2.90E+13  0.00  2.32E+04
 141 N2O + H = N2 + OH                                   4.40E+14  0.00  1.89E+04
 142 NO2 + H2 = HNO2 + H                                 2.40E+13  0.00  2.90E+04
 143 OH + NO2 + M = HNO3 + M                             3.00E+15  0.00 -3.80E+03
    3body efficiencies
      O2   0.70  H2   1.40
 144 OH + NO + M = HNO2 + M                              5.60E+15  0.00 -1.70E+03
 145 HNO + H = H2 + NO                                   4.50E+11  0.72  6.60E+02
 146 H + NO + M = HNO + M                                8.95E+19 -1.32  7.40E+02
 147 HNO + OH = H2O + NO                                 1.30E+07  1.90 -9.50E+02


    ** The following  4 elements considered for this problem **
    C  H  O  N

    ** The following  40 reacting species considered for this problem **
CH4 CH3 H H2 O2 HO2 O OH H2O CH3O CH2O C2H6 C2H5 C2H4 CH2 C2H3 C2H2 HCO C2H2O
C2H CO C2HO CH2CO CO2 CH H2O2 N2 HCN N CN NCO NH HNCO NH2 NO HNO NO2 N2O HNO2
HNO3

    ** No inert species considered for this problem **


** New input data given in SI   units **   ** Output required in SI   units **

                      ** Assigned variable profile **

                       ** Constant-area problem **

         Number of species ODE's:   40  Total number of ODE's:   43

                             Integration Controls
Method Flag (MF): 21  Rel. Error: 1.000E-04  Species Abs. Error: 1.000E-10

    Maximum number of steps allowed for the complete problem:  2000

             ** Output required at following   1 axial distances (m) **
  3.048E+01


                       ** Initial Conditions **


         Time 0.00E+00 s  Axial Position 0.00E+00 m  Area 3.17E-05sq m

  Thermodynamic Properties               Integration Indicators

    Pressure (N/m**2)        1.013E+05     Steps from last print      0
    Velocity (m/s)                2.63     Average step size   0.00E+00
    Density (kg/m**3)        8.165E-01     Method Order               0
    Temperature (K)             423.15     Incr. CPU Time          0.00 s
    Mass Flow Rate (kg/s)    6.801E-05
    Entropy (J/kg/K)         7.416E+03     Total number of steps      0
    Mach Number              6.343E-03     Funct evaluations          0
    Gamma (Frozen)               1.386     Jacobian evaluations       0
    Enthalpy (J/kg)         -4.765E+05     Total CPU Time          0.00 s
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Sp. heat, cp (J/kg/K) 1.054E+03

Chemical Properties

Wi = Net molar production rate per unit volume of species i (kmol/m**3/s)
kj = Forward rate const for reaction j (cgs units)
XH,j = Net energy exch rate for reaction j (J-m**3/kg**2/s)
Eq,j = Equilibration factor for reaction j (= Net rate/Positive dir rate)

Species i	Mass Fr.	Mole Fr.	Wi
CH4	0.00E+00	0.00E+00	0.00E+00
CH3	0.00E+00	0.00E+00	0.00E+00
H	0.00E+00	0.00E+00	0.00E+00
H2	0.00E+00	0.00E+00	0.00E+00
O2	1.84E-01	1.63E-01	-3.25E-22
HO2	0.00E+00	0.00E+00	4.18E-29
O	0.00E+00	0.00E+00	3.25E-22
OH	0.00E+00	0.00E+00	4.18E-29
H2O	3.18E-02	5.01E-02	-4.18E-29
CH3O	0.00E+00	0.00E+00	0.00E+00
CH2O	0.00E+00	0.00E+00	0.00E+00
C2H6	0.00E+00	0.00E+00	0.00E+00
C2H5	0.00E+00	0.00E+00	0.00E+00
C2H4	0.00E+00	0.00E+00	0.00E+00
CH2	0.00E+00	0.00E+00	0.00E+00
C2H3	0.00E+00	0.00E+00	0.00E+00
C2H2	0.00E+00	0.00E+00	0.00E+00
HCO	0.00E+00	0.00E+00	0.00E+00
C2H2O	0.00E+00	0.00E+00	0.00E+00
C2H	0.00E+00	0.00E+00	0.00E+00
CO	4.62E-03	4.68E-03	-3.25E-22
C2HO	0.00E+00	0.00E+00	0.00E+00
CH2CO	0.00E+00	0.00E+00	0.00E+00
CO2	1.81E-02	1.17E-02	3.25E-22
CH	0.00E+00	0.00E+00	0.00E+00
H2O2	0.00E+00	0.00E+00	0.00E+00
N2	7.61E-01	7.70E-01	-1.40E-42
HCN	0.00E+00	0.00E+00	0.00E+00
N	0.00E+00	0.00E+00	0.00E+00
CN	0.00E+00	0.00E+00	0.00E+00
NCO	0.00E+00	0.00E+00	0.00E+00
NH	0.00E+00	0.00E+00	0.00E+00
HNCO	0.00E+00	0.00E+00	0.00E+00
NH2	0.00E+00	0.00E+00	0.00E+00
NO	0.00E+00	0.00E+00	1.27E-31
HNO	0.00E+00	0.00E+00	0.00E+00
NO2	3.25E-06	2.00E-06	-1.27E-31
N2O	0.00E+00	0.00E+00	1.40E-42
HNO2	0.00E+00	0.00E+00	0.00E+00
HNO3	0.00E+00	0.00E+00	0.00E+00

Reac No,j	kj	XH,j	Eq,j
1	7.09E-29	0.00E+00	0.00E+00
2	2.99E+07	0.00E+00	0.00E+00
3	1.00E+12	0.00E+00	0.00E+00
4	3.21E+08	0.00E+00	0.00E+00
5	3.90E+10	0.00E+00	0.00E+00
6	3.58E-02	0.00E+00	0.00E+00
7	8.69E+05	0.00E+00	0.00E+00
8	3.20E+12	0.00E+00	0.00E+00
9	7.13E+02	0.00E+00	0.00E+00
10	2.14E+13	0.00E+00	0.00E+00
11	3.06E+07	0.00E+00	0.00E+00
12	1.45E+09	0.00E+00	0.00E+00
13	1.14E+10	0.00E+00	0.00E+00
14	4.65E+11	0.00E+00	0.00E+00
15	9.75E+00	0.00E+00	0.00E+00
16	8.37E+09	0.00E+00	0.00E+00
17	2.00E+12	0.00E+00	0.00E+00
18	2.00E+13	0.00E+00	0.00E+00
19	2.79E+06	0.00E+00	0.00E+00
20	2.87E-24	0.00E+00	0.00E+00
21	3.30E+10	0.00E+00	0.00E+00
22	6.39E+11	0.00E+00	0.00E+00
23	9.47E+11	0.00E+00	0.00E+00
24	6.54E+10	0.00E+00	0.00E+00
25	8.91E-02	0.00E+00	0.00E+00
26	5.29E+12	0.00E+00	0.00E+00
27	3.00E+13	0.00E+00	0.00E+00
28	3.00E+13	0.00E+00	0.00E+00
29	5.00E+12	0.00E+00	0.00E+00
30	3.00E+13	0.00E+00	0.00E+00
31	3.00E+13	0.00E+00	0.00E+00
32	2.29E-39	0.00E+00	0.00E+00
33	1.91E+11	0.00E+00	0.00E+00
34	1.91E+11	0.00E+00	0.00E+00
35	1.02E+01	0.00E+00	0.00E+00
36	3.55E+05	0.00E+00	0.00E+00
37	5.90E+04	0.00E+00	0.00E+00
38	4.72E+08	0.00E+00	0.00E+00
39	1.67E+08	0.00E+00	0.00E+00
40	8.40E+12	0.00E+00	0.00E+00
41	8.40E+12	0.00E+00	0.00E+00
42	2.00E+13	0.00E+00	0.00E+00
43	5.79E+11	0.00E+00	0.00E+00
44	1.00E+14	0.00E+00	0.00E+00
45	1.00E+13	0.00E+00	0.00E+00
46	1.00E+14	0.00E+00	0.00E+00
47	3.00E+13	0.00E+00	0.00E+00
48	9.27E+11	0.00E+00	0.00E+00
49	1.00E+13	0.00E+00	0.00E+00
50	2.80E+13	0.00E+00	0.00E+00
51	6.95E+11	0.00E+00	0.00E+00
52	1.92E+11	0.00E+00	0.00E+00
53	3.69E+09	0.00E+00	0.00E+00
54	7.38E+08	0.00E+00	0.00E+00
55	2.00E+13	0.00E+00	0.00E+00
56	3.51E+11	0.00E+00	0.00E+00
57	2.05E-15	0.00E+00	0.00E+00

58	5.00E+13	0.00E+00	0.00E+00
59	2.61E+09	0.00E+00	0.00E+00
60	2.00E+13	0.00E+00	0.00E+00
61	7.31E-26	0.00E+00	0.00E+00
62	7.34E+12	0.00E+00	0.00E+00
63	2.68E+11	0.00E+00	0.00E+00
64	5.79E+11	0.00E+00	0.00E+00
65	7.50E+07	0.00E+00	0.00E+00
66	2.65E+13	0.00E+00	0.00E+00
67	2.00E+13	0.00E+00	0.00E+00
68	9.55E-32	0.00E+00	0.00E+00
69	8.27E-01	0.00E+00	0.00E+00
70	6.18E-01	0.00E+00	0.00E+00
71	8.43E+13	0.00E+00	0.00E+00
72	1.42E+09	0.00E+00	0.00E+00
73	1.50E+12	0.00E+00	0.00E+00
74	3.30E+13	0.00E+00	0.00E+00
75	2.62E+09	0.00E+00	0.00E+00
76	2.22E+12	0.00E+00	0.00E+00
77	6.52E-01	0.00E+00	0.00E+00
78	5.71E+10	0.00E+00	0.00E+00
79	5.98E+10	0.00E+00	0.00E+00
80	5.00E+12	0.00E+00	0.00E+00
81	3.20E+13	0.00E+00	0.00E+00
82	4.72E+12	0.00E+00	0.00E+00
83	3.00E+13	0.00E+00	0.00E+00
84	3.00E+13	0.00E+00	0.00E+00
85	5.00E+13	1.88E-40	1.00E+00
86	7.34E+13	0.00E+00	0.00E+00
87	7.33E+05	0.00E+00	0.00E+00
88	1.70E+13	0.00E+00	1.00E+00
89	5.13E-13	-1.65E-14	1.00E+00
90	7.45E+10	0.00E+00	0.00E+00
91	9.71E+01	0.00E+00	0.00E+00
92	2.22E+04	0.00E+00	0.00E+00
93	2.99E+06	0.00E+00	0.00E+00
94	2.90E+08	0.00E+00	0.00E+00
95	7.86E+12	0.00E+00	0.00E+00
96	2.00E+13	0.00E+00	0.00E+00
97	5.26E+13	1.77E-20	1.00E+00
98	6.30E+13	0.00E+00	0.00E+00
99	4.47E+09	0.00E+00	0.00E+00
100	1.20E+12	0.00E+00	0.00E+00
101	9.03E+11	0.00E+00	0.00E+00
102	1.38E+11	0.00E+00	0.00E+00
103	4.50E-07	0.00E+00	0.00E+00
104	3.38E+10	0.00E+00	0.00E+00
105	1.54E+16	0.00E+00	0.00E+00
106	6.47E-40	4.93E-38	1.00E+00
107	1.18E+15	0.00E+00	0.00E+00
108	5.76E-36	0.00E+00	0.00E+00
109	4.71E-46	4.62E-44	1.00E+00
110	1.54E+01	0.00E+00	0.00E+00
111	7.76E+10	0.00E+00	0.00E+00
112	5.49E-01	0.00E+00	0.00E+00
113	2.55E+08	0.00E+00	0.00E+00
114	6.37E+07	0.00E+00	0.00E+00
115	1.88E+06	0.00E+00	0.00E+00
116	7.70E+13	0.00E+00	0.00E+00
117	4.00E+13	0.00E+00	0.00E+00
118	2.25E+09	0.00E+00	0.00E+00
119	7.15E+09	0.00E+00	0.00E+00
120	1.04E+13	0.00E+00	0.00E+00
121	3.70E+12	0.00E+00	0.00E+00
122	2.35E+13	0.00E+00	0.00E+00
123	2.00E+13	0.00E+00	1.00E+00
124	5.40E+13	0.00E+00	0.00E+00
125	3.00E+13	0.00E+00	0.00E+00
126	5.00E+13	0.00E+00	0.00E+00

127	2.00E+13	0.00E+00	0.00E+00
128	2.84E+12	0.00E+00	0.00E+00
129	2.00E+13	0.00E+00	0.00E+00
130	3.73E+12	0.00E+00	0.00E+00
131	5.19E+12	0.00E+00	0.00E+00
132	2.10E+16	5.85E-23	1.00E+00
133	8.60E+13	0.00E+00	0.00E+00
134	2.42E-12	0.00E+00	0.00E+00
135	6.91E-10	0.00E+00	0.00E+00
136	7.47E-26	0.00E+00	0.00E+00
137	4.00E+12	0.00E+00	0.00E+00
138	5.04E-17	0.00E+00	0.00E+00
139	3.66E+06	4.32E-34	1.00E+00
140	3.20E+01	0.00E+00	0.00E+00
141	7.80E+04	0.00E+00	0.00E+00
142	2.52E-02	0.00E+00	0.00E+00
143	2.75E+17	0.00E+00	0.00E+00
144	4.23E+16	0.00E+00	0.00E+00
145	1.60E+13	0.00E+00	0.00E+00
146	1.27E+16	0.00E+00	0.00E+00
147	3.93E+12	0.00E+00	0.00E+00

Derivs (SI units): T 4.82E-18 RHO -9.29E-21 V 2.99E-20

Mix Mol Wt. 28.351 Total Energy Exch Rate -1.65E-14 Mass Fr. Sum 1.00000
(J-m**3/kg**2/s)

CPU Time for initialization of LSENS = 0.00 s

Negative concentration for species C2H6

Negative concentration for species C2H5

Negative concentration for species C2H4

Negative concentration for species CH2

Negative concentration for species C2H2O

Negative concentration for species C2HO

Negative concentration for species CH2CO

Negative concentration for species HCN

Negative concentration for species N

Time 1.16E+01 s Axial Position 3.05E+01 m Area 3.17E-05sq m

Thermodynamic Properties		Integration Indicators	
Pressure (N/m**2)	1.013E+05	Steps from last print	3
Velocity (m/s)	2.63	Average step size	1.02E+05
Density (kg/m**3)	8.165E-01	Method Order	1
Temperature (K)	423.15	Incr. CPU Time	0.00 s
Mass Flow Rate (kg/s)	6.801E-05		
Entropy (J/kg/K)	7.416E+03	Total number of steps	3
Mach Number	6.343E-03	Funct evaluations	4
Gamma (Frozen)	1.386	Jacobian evaluations	2
Enthalpy (J/kg)	-4.765E+05	Total CPU Time	0.00 s
Sp. heat, cp (J/kg/K)	1.054E+03		

Chemical Properties

Wi = Net molar production rate per unit volume of species i (kmol/m**3/s)
kj = Forward rate const for reaction j (cgs units)
XH,j = Net energy exch rate for reaction j (J-m**3/kg**2/s)
Eq,j = Equilibration factor for reaction j (= Net rate/Positive dir rate)

Species i	Mass Fr.	Mole Fr.	Wi
CH4	7.60E-33	1.34E-32	4.20E-25
CH3	1.93E-34	3.64E-34	-4.20E-25
H	1.37E-32	3.85E-31	2.21E-33
H2	1.05E-33	1.48E-32	3.62E-35
O2	1.84E-01	1.63E-01	-5.86E-23
HO2	2.57E-23	2.21E-23	-3.65E-25
O	1.75E-23	3.09E-23	1.72E-25
OH	1.14E-28	1.90E-28	1.09E-30
H2O	3.18E-02	5.01E-02	-2.86E-26
CH3O	5.47E-45	5.61E-45	0.00E+00
CH2O	1.42E-32	1.34E-32	4.29E-35
C2H6	-9.96E-50	0.00E+00	0.00E+00
C2H5	-3.02E-63	0.00E+00	0.00E+00
C2H4	-4.25E-49	0.00E+00	0.00E+00
CH2	-9.11E-64	0.00E+00	0.00E+00
C2H3	9.46E-45	9.81E-45	-7.11E-39
C2H2	7.27E-42	7.92E-42	0.00E+00
HCO	3.32E-36	3.24E-36	3.33E-38
C2H2O	-1.36E-47	0.00E+00	0.00E+00
C2H	4.21E-46	0.00E+00	-1.08E-39
CO	4.62E-03	4.68E-03	-3.84E-22
C2HO	-4.62E-44	-3.22E-44	3.05E-39
CH2CO	-5.32E-60	0.00E+00	0.00E+00
CO2	1.81E-02	1.17E-02	3.84E-22
CH	1.29E-61	0.00E+00	0.00E+00
H2O2	1.47E-31	1.22E-31	3.06E-36
N2	7.61E-01	7.70E-01	-5.37E-32
HCN	-8.04E-60	0.00E+00	0.00E+00
N	-6.03E-41	-1.22E-40	2.02E-39
CN	6.82E-43	7.43E-43	0.00E+00
NCO	7.19E-41	4.85E-41	0.00E+00
NH	7.01E-51	0.00E+00	0.00E+00
HNCO	3.17E-64	0.00E+00	0.00E+00
NH2	1.99E-84	0.00E+00	0.00E+00
NO	1.13E-19	1.07E-19	2.66E-22
HNO	6.14E-40	5.61E-40	0.00E+00
NO2	3.25E-06	2.00E-06	-2.66E-22
N2O	3.36E-29	2.16E-29	5.37E-32
HNO2	1.53E-36	9.24E-37	2.10E-41
HNO3	2.15E-24	9.69E-25	2.37E-27

Reac No,j	kj	XH,j	Eq,j
1	7.09E-29	-2.57E-42	1.00E+00
2	2.99E+07	0.00E+00	1.00E+00
3	1.00E+12	-1.40E-16	9.96E-01
4	3.21E+08	0.00E+00	1.00E+00
5	3.90E+10	3.95E-31	1.00E+00
6	3.58E-02	3.17E-34	1.00E+00
7	8.69E+05	-1.43E-26	1.00E+00
8	3.20E+12	0.00E+00	1.00E+00
9	7.13E+02	3.80E-40	1.00E+00
10	2.14E+13	0.00E+00	1.00E+00
11	3.06E+07	0.00E+00	1.00E+00
12	1.45E+09	0.00E+00	1.00E+00
13	1.14E+10	0.00E+00	1.00E+00
14	4.65E+11	0.00E+00	8.47E-01
15	9.75E+00	0.00E+00	8.65E-01
16	8.37E+09	0.00E+00	1.00E+00
17	2.00E+12	0.00E+00	1.00E+00
18	2.00E+13	0.00E+00	1.00E+00
19	2.79E+06	0.00E+00	3.47E-01
20	2.87E-24	0.00E+00	1.00E+00
21	3.30E+10	1.70E-43	1.00E+00
22	6.39E+11	0.00E+00	9.98E-01
23	9.47E+11	0.00E+00	1.00E+00
24	6.54E+10	0.00E+00	1.00E+00
25	8.91E-02	2.05E-43	1.00E+00
26	5.29E+12	-3.55E-30	1.00E+00
27	3.00E+13	0.00E+00	1.00E+00
28	3.00E+13	0.00E+00	1.00E+00
29	5.00E+12	0.00E+00	1.00E+00
30	3.00E+13	0.00E+00	1.23E-01
31	3.00E+13	0.00E+00	1.00E+00
32	2.29E-39	0.00E+00	1.00E+00
33	1.91E+11	0.00E+00	1.00E+00
34	1.91E+11	0.00E+00	1.00E+00
35	1.02E+01	0.00E+00	9.82E-01
36	3.55E+05	-8.54E-37	1.00E+00
37	5.90E+04	0.00E+00	1.00E+00
38	4.72E+08	0.00E+00	1.00E+00
39	1.67E+08	0.00E+00	1.00E+00
40	8.40E+12	-1.06E-31	1.00E+00
41	8.40E+12	-4.95E-31	1.00E+00
42	2.00E+13	0.00E+00	1.00E+00
43	5.79E+11	1.29E-30	1.00E+00
44	1.00E+14	0.00E+00	1.00E+00
45	1.00E+13	0.00E+00	1.00E+00
46	1.00E+14	0.00E+00	1.00E+00
47	3.00E+13	0.00E+00	1.00E+00
48	9.27E+11	0.00E+00	1.00E+00
49	1.00E+13	0.00E+00	9.99E-01
50	2.80E+13	0.00E+00	9.56E-01
51	6.95E+11	-4.00E-41	1.00E+00
52	1.92E+11	1.75E-41	1.00E+00
53	3.69E+09	0.00E+00	2.01E-01
54	7.38E+08	0.00E+00	9.99E-01
55	2.00E+13	0.00E+00	1.00E+00
56	3.51E+11	0.00E+00	1.00E+00
57	2.05E-15	0.00E+00	1.00E+00
58	5.00E+13	0.00E+00	1.00E+00
59	2.61E+09	-3.44E-34	1.00E+00
60	2.00E+13	0.00E+00	1.00E+00
61	7.31E-26	0.00E+00	1.00E+00

62	7.34E+12	4.87E-38	1.00E+00
63	2.68E+11	0.00E+00	1.00E+00
64	5.79E+11	-1.51E-41	1.00E+00
65	7.50E+07	0.00E+00	1.00E+00
66	2.65E+13	0.00E+00	1.00E+00
67	2.00E+13	-1.85E-41	1.00E+00
68	9.55E-32	0.00E+00	1.00E+00
69	8.27E-01	0.00E+00	1.00E+00
70	6.18E-01	0.00E+00	1.00E+00
71	8.43E+13	-3.46E-40	1.00E+00
72	1.42E+09	0.00E+00	1.00E+00
73	1.50E+12	0.00E+00	1.00E+00
74	3.30E+13	0.00E+00	1.00E+00
75	2.62E+09	0.00E+00	1.00E+00
76	2.22E+12	0.00E+00	1.00E+00
77	6.52E-01	0.00E+00	1.00E+00
78	5.71E+10	0.00E+00	1.00E+00
79	5.98E+10	0.00E+00	8.30E-01
80	5.00E+12	0.00E+00	1.00E+00
81	3.20E+13	0.00E+00	1.00E+00
82	4.72E+12	-4.73E-22	1.00E+00
83	3.00E+13	-1.37E-42	1.00E+00
84	3.00E+13	-1.75E-42	1.00E+00
85	5.00E+13	1.88E-40	1.00E+00
86	7.34E+13	0.00E+00	1.00E+00
87	7.33E+05	-1.99E-22	1.00E+00
88	1.70E+13	-4.69E-14	1.00E+00
89	5.13E-13	-1.65E-14	1.00E+00
90	7.45E+10	-8.56E-18	1.00E+00
91	9.71E+01	-3.07E-21	1.00E+00
92	2.22E+04	3.03E-18	1.00E+00
93	2.99E+06	1.64E-23	1.00E+00
94	2.90E+08	0.00E+00	9.99E-01
95	7.86E+12	-1.83E-38	1.00E+00
96	2.00E+13	-3.61E-30	1.00E+00
97	5.26E+13	1.77E-20	1.00E+00
98	6.30E+13	-9.45E-38	1.00E+00
99	4.47E+09	-4.99E-40	1.00E+00
100	1.20E+12	6.54E-28	1.00E+00
101	9.03E+11	-7.68E-32	9.98E-01
102	1.38E+11	0.00E+00	1.00E+00
103	4.50E-07	1.78E-35	1.00E+00
104	3.38E+10	3.41E-27	1.00E+00
105	1.54E+16	-1.78E-17	1.00E+00
106	6.47E-40	4.47E-38	9.07E-01
107	1.18E+15	-2.16E-40	1.00E+00
108	5.76E-36	-5.61E-45	1.00E+00
109	4.71E-46	-6.62E-33	1.00E+00
110	1.54E+01	0.00E+00	1.00E+00
111	7.76E+10	0.00E+00	1.00E+00
112	5.49E-01	0.00E+00	1.00E+00
113	2.55E+08	0.00E+00	1.00E+00
114	6.37E+07	0.00E+00	1.00E+00
115	1.88E+06	0.00E+00	1.00E+00
116	7.70E+13	0.00E+00	1.00E+00
117	4.00E+13	0.00E+00	1.00E+00
118	2.25E+09	0.00E+00	1.00E+00
119	7.15E+09	0.00E+00	9.80E-01
120	1.04E+13	-4.15E-29	1.00E+00
121	3.70E+12	-1.13E-29	9.75E-01
122	2.35E+13	0.00E+00	1.00E+00
123	2.00E+13	0.00E+00	1.00E+00
124	5.40E+13	0.00E+00	9.71E-01
125	3.00E+13	0.00E+00	1.00E+00
126	5.00E+13	0.00E+00	1.00E+00
127	2.00E+13	0.00E+00	1.00E+00
128	2.84E+12	-3.50E-44	1.00E+00
129	2.00E+13	0.00E+00	9.95E-01
130	3.73E+12	7.71E-22	1.00E+00

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                                    131  5.19E+12 -7.67E-14  1.00E+00
                                    132  2.10E+16  5.85E-23  1.00E+00
                                    133  8.60E+13 -1.00E-20  1.00E+00
                                    134  2.42E-12  0.00E+00  1.00E+00
                                    135  6.91E-10  2.41E-31  1.00E+00
                                    136  7.47E-26  7.01E-44  9.90E-01
                                    137  4.00E+12  3.94E-31  1.00E+00
                                    138  5.04E-17 -1.35E-23  1.00E+00
                                    139  3.66E+06  4.32E-34  1.00E+00
                                    140  3.20E+01  0.00E+00  1.00E+00
                                    141  7.80E+04  0.00E+00  9.99E-01
                                    142  2.52E-02  9.77E-38  1.00E+00
                                    143  2.75E+17 -7.37E-19  1.00E+00
                                    144  4.23E+16 -6.43E-33  1.00E+00
                                    145  1.60E+13  0.00E+00  1.00E+00
                                    146  1.27E+16 -3.88E-36  1.00E+00
                                    147  3.93E+12  1.44E-41  1.00E+00

Derivs (SI units):  T         4.13E-17  RHO      -7.91E-20  V         2.55E-19

Mix Mol Wt.   28.351  Total Energy Exch Rate -1.40E-13  Mass Fr. Sum   1.00000
                         (J-m**3/kg**2/s)


(LSENS)  End of this case



            Summary of computational work required for problem:
              Total no. of steps -                        3
              Total no. of derivative evaluations -       4
              Total no. of Jacobian evaluations -         2
              Total CPU Time -                         0.00 s

              Total CPU time (including I/O) =         0.00 s

(LSENS)     Read data for next case



                              ** Problem Data **

        1         2         3         4         5         6         7         8
2345678901234567890123456789012345678901234567890123456789012345678901234567890

                                  Blank Line
                                  Blank Line
                                  Blank Line
                                  Blank Line
                                  Blank Line
                                  Blank Line
 (CIMAGE) ** Warning: End of problem data, but no
    end of file indicator or incomplete data




(KINP)  ** Error: The ACTION switch (= "    " is illegal **
  Legal values are ADD, NEW, CHANGE, and REPEAT


(LSENS)     A fatal error has occurred - Case terminated
```

Perfectly Stirred Reactor Model – Primary Combustor

```
                          ** Problem Data **

         1         2         3         4         5         6         7         8
 2345678901234567890123456789012345678901234567890123456789012345678901234567890

LSENS CH4-AIR
   M       +   CH4      =   CH3     +   H         2.0E+17   0.        88000.
   H       +   CH4      =   CH3     +   H2        6.6E+8    1.62      10840.
   CH4     +   O2       =   CH3     +   HO2       1.0E+12   0.        0.
   O       +   CH4      =   CH3     +   OH        1.02E+9   1.5       8600.
   OH      +   CH4      =   CH3     +   H2O       1.0E+8    1.6       3120.
   CH3     +   O2       =   CH3O    +   O         2.68E+13  0.        28800.
   CH3     +   O2       =   OH      +   CH2O      3.6E+10   0.        8940.
   CH3     +   OH       =   CH3O    +   H         3.2E+12   0.        0.
   M       +   CH3O     =   CH2O    +   H         5.0E+13   0.        21000.
   CH3     +   CH3      =   C2H6                  2.4E+14   -.4       0.
   CH3     +   CH3      =   H       +   C2H5      4.99E+12  0.1       10600.
   H       +   C2H6     =   C2H5    +   H2        1.15E+8   1.9       7530.
   O       +   C2H6     =   C2H5    +   OH        8.98E+7   1.92      5690.
   OH      +   C2H6     =   C2H5    +   H2O       3.54E+6   2.12      870.
   M       +   C2H5     =   C2H4    +   H         1.0E+17   0.        31000.
   C2H5    +   O2       =   C2H4    +   HO2       8.4E+11   0.        3875.
   H       +   C2H5     =   C2H4    +   H2        2.0E+12   0.        0.
   CH3     +   CH2      =   C2H4    +   H         2.0E+13   0.        0.
   H       +   C2H4     =   H2      +   C2H3      1.325E+6  2.53      12240.
   M       +   C2H4     =   C2H2    +   H2        2.6E+17   0.        79300.
   C2H4    +   OH       =   C2H3    +   H2O       3.6E+6    2.        2500.
   C2H4    +   OH       =   CH3     +   CH2O      2.0E+12   0.        960.
   C2H4    +   O        =   CH3     +   HCO       1.92E+7   1.83      220.
   C2H4    +   O        =   CH2O    +   CH2       2.5E+13   0.        5000.
   M       +   C2H3     =   C2H2    +   H         3.0E+15   0.        32000.
   C2H3    +   O2       =   CH2O    +   HCO       3.98E+12  0.        -240.
   C2H3    +   H        =   C2H2    +   H2        3.0E+13   0.        0.
   C2H3    +   O        =   C2H2O   +   H         3.0E+13   0.        0.
   C2H3    +   OH       =   C2H2    +   H2O       5.0E+12   0.        0.
   C2H3    +   CH2      =   C2H2    +   CH3       3.0E+13   0.        0.
   C2H3    +   C2H      =2.0C2H2                  3.0E+13   0.        0.
   M       +   C2H2     =   C2H     +   H         4.2E+16   0.        107000.
   C2H2    +   O        =   CH2     +   CO        1.02E+7   2.0       1900.
   C2H2    +   O        =   C2HO    +   H         1.02E+7   2.        1900.
   C2H2    +   O        =   OH      +   C2H       4.6E+19   -1.41     28950.
   C2H2    +   OH       =   C2H     +   H2O       3.37E+7   2.        14000.
   C2H2    +   OH       =   C2H2O   +   H         5.04E+5   2.3       13500.
   C2H2    +   OH       =   CH2CO   +   H         2.18E-4   4.5       -1000.
   C2H2    +   OH       =   CH3     +   CO        4.83E-4   4.        -2000.
   C2H     +   O2       =   C2HO    +   O         5.00E+13  0.0       1500.
   C2H     +   O2       =   HCO     +   CO        5.0E+13   0.0       1500.
   C2H     +   OH       =   C2HO    +   H         2.0E+13   0.0       0.
   C2HO    +   O2       =2.0CO      +   OH        1.6E+12   0.        854.
   C2HO    +   O        =2.0CO      +   H         1.0E+14   0.        0.
   C2HO    +   OH       =2.0HCO                   1.0E+13   0.        0.
   C2HO    +   H        =   CH2     +   CO        1.0E+14   0.        0.
   C2HO    +   CH2      =   C2H3    +   CO        3.0E+13   0.        0.
   C2HO    +   CH2      =   CH2O    +   C2H       1.0E+13   0.        2000.
            2.0C2HO     =   C2H2    +2.0CO        1.0E+13   0.        0.
   C2H2O   +   OH       =   CH2O    +   HCO       2.8E+13   0.        0.
   C2H2O   +   OH       =   C2HO    +   H2O       7.5E+12   0.        2000.
   C2H2O   +   H        =   CH3     +   CO        1.13E+13  0.        3428.
   C2H2O   +   H        =   C2HO    +   H2        5.0E+13   0.        8000.
   C2H2O   +   O        =   C2HO    +   OH        1.0E+13   0.        8000.
   C2H2O   +   O        =   CH2O    +   CO        2.0E+13   0.        0.
   C2H2O   +   O        =   CH2     +   CO2       1.75E+12  0.        1350.
   M       +   C2H2O    =   CH2     +   CO        2.0E+16   0.        60000.
   C2H     +   O        =   CO      +   CH        5.0E+13   0.        0.
   CH3O    +   O2       =   CH2O    +   HO2       4.28E-13  7.6       -3530.
   CH3O    +   H        =   CH2O    +   H2        2.0E+13   0.        0.
   M       +   CH2O     =   HCO     +   H         5.0E+16   0.        81000.
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   CH2O    +   OH      =   HCO     +   H2O       3.43E+9   1.18      -447.
   CH2O    +   H       =   HCO     +   H2        2.3E+10   1.05      3275.
   CH2O    +   O       =   HCO     +   OH        3.9E+13   0.        3540.
   CH3     +   CH2O    =   CH4     +   HCO       3.32E+03  2.81      5860.
   CH3     +   HCO     =   CH4     +   CO        2.65E+13  0.        0.
   CH3     +   HO2     =   CH3O    +   OH        2.0E+13   0.        0.
   M       +   CH3     =   CH2     +   H         1.95E+16  0.        91600.
   H       +   CH3     =   H2      +   CH2       2.7E+11   0.67      25700.
   O       +   CH3     =   OH      +   CH2       1.9E+11   0.68      25700.
   O       +   CH3     =   H       +   CH2O      8.43E+13  0.        0.
   OH      +   CH3     =   H2O     +   CH2       5.6E+7    1.6       5420.
   CH      +   CO2     =   HCO     +   CO        3.4E+12   0.        690.
   CH      +   O2      =   HCO     +   O         3.3E+13   0.        0.
   CH2     +   O2      =   CH2O    +   O         5.0E+11   0.5       6960.
   CH2     +   O2      =   OH      +   HCO       1.32E+13  0.        1500.
   CH2     +   O       =   CH      +   OH        2.0E+11   0.7       25800.
   CH2     +   OH      =   CH      +   H2O       1.13E+7   2.0       3000.
   CH2     +   H       =   CH      +   H2        3.2E+11   0.7       4970.
   CH2     +   CH2     =   C2H3    +   H         5.0E+12   0.        0.
   CH2     +   CH2     =   C2H2    +   H2        3.2E+13   0.        0.
   HCO     +   O2      =   CO      +   HO2       7.6E+12   0.        400.
   HCO     +   O       =   CO      +   OH        3.0E+13   0.        0.
   HCO     +   O       =   CO2     +   H         3.0E+13   0.        0.
   HCO     +   OH      =   CO      +   H2O       5.0E+13   0.        0.
   HCO     +   H       =   CO      +   H2        7.34E+13  0.        0.
   M       +   HCO     =   H       +   CO        1.87E+17  -1.       17000.
   CO      +   O       =   CO2     +   M         6.02E+14  0.        3000.
   CO      +   O2      =   CO2     +   O         2.5E+12   0.        47800.
   CO      +   OH      =   CO2     +   H         4.76E+7   1.23      70.
   CO      +   HO2     =   CO2     +   OH        1.5E+14   0.        23600.
   O       +   H2O     =   OH      +   OH        6.8E+13   0.        18365.
   H       +   O2      =   OH      +   O         8.3E+13   0.        14413.
   O       +   H2      =   OH      +   H         5.00E+04  2.67      6290.
   H       +   HO2     =   H2      +   O2        2.8E+13   0.        1068.
   O       +   HO2     =   OH      +   O2        2.0E+13   0.        0.
   HO2     +   OH      =   H2O     +   O2        2.9E+13   0.        -500.
   H       +   HO2     =2.0OH                    1.34E+14  0.        635.
   H2      +   HO2     =   H2O2    +   H         1.21E+7   2.        5200.
   OH      +   H2O2    =   H2O     +   HO2       1.75E+12  0.        320.
   HO2     +   HO2     =   H2O2    +   O2        1.3E+11   0.        -1630.
   H       +   H2O2    =   OH      +   H2O       1.0E+13   0.        3600.
   M       +   H2O2    =2.0OH                    1.44E+17  0.        45510.
   THIRDBODY
H2        2.30      O2        0.78      H2O       6.0
H2O2      6.6
END
   H2      +   OH      =   H2O     +   H         2.16E+8   1.51      3430.
   H       +   O2      =   HO2     +   M         2.8E+18   -0.86     0.
   THIRDBODY
O2        1.30      N2        1.3
H2O       21.3      CO2       7.0
END
   M       +   H2O     =   H       +   OH        1.30E+15  0.        105140.
   THIRDBODY
H2        4.00      O2        1.5
H2O       20.0      N2        1.5
CO2       4.0
END
   H       +   O       =   OH      +   M         5.00E+17  -1.       0.
   M       +   H2      =   H       +   H         2.2E+14   0.        96000.
   THIRDBODY
H2        4.10      O2        2.0
H2O       15.0      N2        2.0
END
   M       +   O2      =   O       +   O         1.80E+18  -1.       118020.
   CH      +   N2      =   HCN     +   N         1.0E+11   0.        19000.
   CN      +   H2      =   HCN     +   H         2.1E+13   0.        4710.
   O       +   HCN     =   OH      +   CN        2.13E+9   1.58      26600.
   O       +   HCN     =   NCO     +   H         1.11E+4   2.64      4980.
```

```
   O       +   HCN      =   NH      +   CO        2.77E+3   2.64      4980.
   OH      +   HCN      =   HNCO    +   H         4.4E+3    2.26      6400.
   CN      +   O        =   CO      +   N         7.7E+13   0.        0.
   CN      +   OH       =   NCO     +   H         4.0E+13   0.        0.
   H2      +   NCO      =   HNCO    +   H         1.0E+14   0.        9000.
   HNCO    +   H        =   NH2     +   CO        2.25E+7   1.7       3800.
   CN      +   O2       =   NCO     +   O         6.14E+12  0.        -440.
   CN      +   CO2      =   NCO     +   CO        3.7E+12   0.        0.
   O       +   NCO      =   NO      +   CO        2.35E+13  0.        0.
   N       +   NCO      =   N2      +   CO        2.0E+13   0.        0.
   H       +   NCO      =   NH      +   CO        5.4E+13   0.        0.
   CH      +   NO       =   N       +   HCO       3.0E+13   0.        0.
   CH      +   NO       =   O       +   HCN       5.0E+13   0.        0.
   CH      +   NO       =   H       +   NCO       2.0E+13   0.        0.
   NH      +   OH       =   N       +   H2O       2.0E+9    1.2       0.
   NH      +   OH       =   HNO     +   H         2.0E+13   0.        0.
   HO2     +   NO       =   NO2     +   OH        2.11E+12  0.        -480.
   O       +   NO2      =   NO      +   O2        3.9E+12   0.        -240.
   NO      +   O        =   NO2     +   M         1.06E+20  -1.41     0.
   NO2     +   H        =   NO      +   OH        1.32E+14  0.        360.
   NO      +   H        =   N       +   OH        2.63E+14  0.        50410.
   NO      +   O        =   N       +   O2        3.8E+9    1.        41370.
   O       +   N2       =   NO      +   N         1.80E+14  0.        76250.
   N       +   NO2      =2.0NO                    4.0E+12   0.        0.
   M       +   N2O      =   N2      +   O         6.92E+23  -2.5      65000.
   O       +   N2O      =   N2      +   O2        1.4E+12   0.        10810.
   O       +   N2O      =2.0NO                    2.9E+13   0.        23150.
   N2O     +   H        =   N2      +   OH        4.4E+14   0.        18880.
   NO2     +   H2       =   HNO2    +   H         2.4E+13   0.        29000.
   OH      +   NO2      =   HNO3    +   M         3.0E+15   0.        -3800.
   THIRDBODY
O2        0.70      H2        1.4
END
   OH      +   NO       =   HNO2    +   M         5.6E+15   0.        -1700.
   HNO     +   H        =   H2      +   NO        4.5E+11   0.72      660.
   H       +   NO       =   HNO     +   M         8.95E+19  -1.32     740.
   HNO     +   OH       =   H2O     +   NO        1.3E+7    1.9       -950.
                                  Blank Line
AR
DISTANCE  AREA      FPS       FPS
&prob  welstr=.true.,  COMBUS=.TRUE., conc=.false.,
   ACON=.TRUE., &end
 &wsprob  dotmax=0.1389, delmd=0.06945, mpr=1,  volume=0.393,
   &end
 &start  t=1551, p=2965, mdot=0.034725, x=0.0,ERATIO=0.30,
  AREA=3.41E-04, &end
CH4        0.0296
O2         0.2011
N2         0.7494
CO2        0.0003
H2O        0.0107
AR         0.0089
END
 &SOLVER  EMAX=1.0E-4, ATOLSP=1.0E-13,  &END
FINIS
```

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          LSENS: Multipurpose Kinetics and Sensitivity Analysis Program

LSENS CH4-AIR SAMPLE LINE CASE 6

 Reac        Reaction                                    Reaction Rate Parameters
 No.j                                                       Aj     nj      Ej
                kj = Aj * T**nj * exp(-Ej/RT) (cgs units)
```

1	CH4 + M = CH3 + H + M	2.00E+17	0.00	8.80E+04
2	H + CH4 = CH3 + H2	6.60E+08	1.62	1.08E+04
3	CH4 + O2 = CH3 + HO2	1.00E+12	0.00	0.00E+00
4	O + CH4 = CH3 + OH	1.02E+09	1.50	8.60E+03
5	OH + CH4 = CH3 + H2O	1.00E+08	1.60	3.12E+03
6	CH3 + O2 = CH3O + O	2.68E+13	0.00	2.88E+04
7	CH3 + O2 = OH + CH2O	3.60E+10	0.00	8.94E+03
8	CH3 + OH = CH3O + H	3.20E+12	0.00	0.00E+00
9	CH3O + M = CH2O + H + M	5.00E+13	0.00	2.10E+04
10	2CH3 = C2H6	2.40E+14	-0.40	0.00E+00
11	2CH3 = H + C2H5	4.99E+12	0.10	1.06E+04
12	H + C2H6 = C2H5 + H2	1.15E+08	1.90	7.53E+03
13	O + C2H6 = C2H5 + OH	8.98E+07	1.92	5.69E+03
14	OH + C2H6 = C2H5 + H2O	3.54E+06	2.12	8.70E+02
15	C2H5 + M = C2H4 + H + M	1.00E+17	0.00	3.10E+04
16	C2H5 + O2 = C2H4 + HO2	8.40E+11	0.00	3.88E+03
17	H + C2H5 = C2H4 + H2	2.00E+12	0.00	0.00E+00
18	CH3 + CH2 = C2H4 + H	2.00E+13	0.00	0.00E+00
19	H + C2H4 = H2 + C2H3	1.33E+06	2.53	1.22E+04
20	C2H4 + M = C2H2 + H2 + M	2.60E+17	0.00	7.93E+04
21	C2H4 + OH = C2H3 + H2O	3.60E+06	2.00	2.50E+03
22	C2H4 + OH = CH3 + CH2O	2.00E+12	0.00	9.60E+02
23	C2H4 + O = CH3 + HCO	1.92E+07	1.83	2.20E+02
24	C2H4 + O = CH2O + CH2	2.50E+13	0.00	5.00E+03
25	C2H3 + M = C2H2 + H + M	3.00E+15	0.00	3.20E+04
26	C2H3 + O2 = CH2O + HCO	3.98E+12	0.00	-2.40E+02
27	C2H3 + H = C2H2 + H2	3.00E+13	0.00	0.00E+00
28	C2H3 + O = C2H2O + H	3.00E+13	0.00	0.00E+00
29	C2H3 + OH = C2H2 + H2O	5.00E+12	0.00	0.00E+00
30	C2H3 + CH2 = C2H2 + CH3	3.00E+13	0.00	0.00E+00
31	C2H3 + C2H = 2C2H2	3.00E+13	0.00	0.00E+00
32	C2H2 + M = C2H + H + M	4.20E+16	0.00	1.07E+05
33	C2H2 + O = CH2 + CO	1.02E+07	2.00	1.90E+03
34	C2H2 + O = C2HO + H	1.02E+07	2.00	1.90E+03
35	C2H2 + O = OH + C2H	4.60E+19	-1.41	2.90E+04
36	C2H2 + OH = C2H + H2O	3.37E+07	2.00	1.40E+04
37	C2H2 + OH = C2H2O + H	5.04E+05	2.30	1.35E+04
38	C2H2 + OH = CH2CO + H	2.18E-04	4.50	-1.00E+03
39	C2H2 + OH = CH3 + CO	4.83E-04	4.00	-2.00E+03
40	C2H + O2 = C2HO + O	5.00E+13	0.00	1.50E+03
41	C2H + O2 = HCO + CO	5.00E+13	0.00	1.50E+03
42	C2H + OH = C2HO + H	2.00E+13	0.00	0.00E+00
43	C2HO + O2 = 2CO + OH	1.60E+12	0.00	8.54E+02
44	C2HO + O = 2CO + H	1.00E+14	0.00	0.00E+00
45	C2HO + OH = 2HCO	1.00E+13	0.00	0.00E+00
46	C2HO + H = CH2 + CO	1.00E+14	0.00	0.00E+00
47	C2HO + CH2 = C2H3 + CO	3.00E+13	0.00	0.00E+00
48	C2HO + CH2 = CH2O + C2H	1.00E+13	0.00	2.00E+03
49	2C2HO = C2H2 + 2CO	1.00E+13	0.00	0.00E+00
50	C2H2O + OH = CH2O + HCO	2.80E+13	0.00	0.00E+00
51	C2H2O + OH = C2HO + H2O	7.50E+12	0.00	2.00E+03
52	C2H2O + H = CH3 + CO	1.13E+13	0.00	3.43E+03
53	C2H2O + H = C2HO + H2	5.00E+13	0.00	8.00E+03
54	C2H2O + O = C2HO + OH	1.00E+13	0.00	8.00E+03
55	C2H2O + O = CH2O + CO	2.00E+13	0.00	0.00E+00
56	C2H2O + O = CH2 + CO2	1.75E+12	0.00	1.35E+03
57	C2H2O + M = CH2 + CO + M	2.00E+16	0.00	6.00E+04
58	C2H + O = CO + CH	5.00E+13	0.00	0.00E+00
59	CH3O + O2 = CH2O + HO2	4.28E-13	7.60	-3.53E+03
60	CH3O + H = CH2O + H2	2.00E+13	0.00	0.00E+00
61	CH2O + M = HCO + H + M	5.00E+16	0.00	8.10E+04
62	CH2O + OH = HCO + H2O	3.43E+09	1.18	-4.47E+02
63	CH2O + H = HCO + H2	2.30E+10	1.05	3.28E+03
64	CH2O + O = HCO + OH	3.90E+13	0.00	3.54E+03
65	CH3 + CH2O = CH4 + HCO	3.32E+03	2.81	5.86E+03
66	CH3 + HCO = CH4 + CO	2.65E+13	0.00	0.00E+00
67	CH3 + HO2 = CH3O + OH	2.00E+13	0.00	0.00E+00
68	CH3 + M = CH2 + H + M	1.95E+16	0.00	9.16E+04

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 69 H + CH3 = H2 + CH2                                  2.70E+11  0.67  2.57E+04
 70 O + CH3 = OH + CH2                                  1.90E+11  0.68  2.57E+04
 71 O + CH3 = H + CH2O                                  8.43E+13  0.00  0.00E+00
 72 OH + CH3 = H2O + CH2                                5.60E+07  1.60  5.42E+03
 73 CH + CO2 = HCO + CO                                 3.40E+12  0.00  6.90E+02
 74 CH + O2 = HCO + O                                   3.30E+13  0.00  0.00E+00
 75 CH2 + O2 = CH2O + O                                 5.00E+11  0.50  6.96E+03
 76 CH2 + O2 = OH + HCO                                 1.32E+13  0.00  1.50E+03
 77 CH2 + O = CH + OH                                   2.00E+11  0.70  2.58E+04
 78 CH2 + OH = CH + H2O                                 1.13E+07  2.00  3.00E+03
 79 CH2 + H = CH + H2                                   3.20E+11  0.70  4.97E+03
 80 2CH2 = C2H3 + H                                     5.00E+12  0.00  0.00E+00
 81 2CH2 = C2H2 + H2                                    3.20E+13  0.00  0.00E+00
 82 HCO + O2 = CO + HO2                                 7.60E+12  0.00  4.00E+02
 83 HCO + O = CO + OH                                   3.00E+13  0.00  0.00E+00
 84 HCO + O = CO2 + H                                   3.00E+13  0.00  0.00E+00
 85 HCO + OH = CO + H2O                                 5.00E+13  0.00  0.00E+00
 86 HCO + H = CO + H2                                   7.34E+13  0.00  0.00E+00
 87 HCO + M = H + CO + M                                1.87E+17 -1.00  1.70E+04
 88 CO + O + M = CO2 + M                                6.02E+14  0.00  3.00E+03
 89 CO + O2 = CO2 + O                                   2.50E+12  0.00  4.78E+04
 90 CO + OH = CO2 + H                                   4.76E+07  1.23  7.00E+01
 91 CO + HO2 = CO2 + OH                                 1.50E+14  0.00  2.36E+04
 92 O + H2O = 2OH                                       6.80E+13  0.00  1.84E+04
 93 H + O2 = OH + O                                     8.30E+13  0.00  1.44E+04
 94 O + H2 = OH + H                                     5.00E+04  2.67  6.29E+03
 95 H + HO2 = H2 + O2                                   2.80E+13  0.00  1.07E+03
 96 O + HO2 = OH + O2                                   2.00E+13  0.00  0.00E+00
 97 HO2 + OH = H2O + O2                                 2.90E+13  0.00 -5.00E+02
 98 H + HO2 = 2OH                                       1.34E+14  0.00  6.35E+02
 99 H2 + HO2 = H2O2 + H                                 1.21E+07  2.00  5.20E+03
100 OH + H2O2 = H2O + HO2                               1.75E+12  0.00  3.20E+02
101 2HO2 = H2O2 + O2                                    1.30E+11  0.00 -1.63E+03
102 H + H2O2 = OH + H2O                                 1.00E+13  0.00  3.60E+03
103 H2O2 + M = 2OH + M                                  1.44E+17  0.00  4.55E+04
   3body efficiencies
     H2   2.30  O2   0.78  H2O   6.00  H2O2   6.60
104 H2 + OH = H2O + H                                   2.16E+08  1.51  3.43E+03
105 H + O2 + M = HO2 + M                                2.80E+18 -0.86  0.00E+00
   3body efficiencies
     O2   1.30  N2   1.30  H2O  21.30  CO2   7.00
106 H2O + M = H + OH + M                                1.30E+15  0.00  1.05E+05
   3body efficiencies
     H2   4.00  O2   1.50  H2O  20.00  N2   1.50  CO2   4.00
107 H + O + M = OH + M                                  5.00E+17 -1.00  0.00E+00
108 H2 + M = 2H + M                                     2.20E+14  0.00  9.60E+04
   3body efficiencies
     H2   4.10  O2   2.00  H2O  15.00  N2   2.00
109 O2 + M = 2O + M                                     1.80E+18 -1.00  1.18E+05
110 CH + N2 = HCN + N                                   1.00E+11  0.00  1.90E+04
111 CN + H2 = HCN + H                                   2.10E+13  0.00  4.71E+03
112 O + HCN = OH + CN                                   2.13E+09  1.58  2.66E+04
113 O + HCN = NCO + H                                   1.11E+04  2.64  4.98E+03
114 O + HCN = NH + CO                                   2.77E+03  2.64  4.98E+03
115 OH + HCN = HNCO + H                                 4.40E+03  2.26  6.40E+03
116 CN + O = CO + N                                     7.70E+13  0.00  0.00E+00
117 CN + OH = NCO + H                                   4.00E+13  0.00  0.00E+00
118 H2 + NCO = HNCO + H                                 1.00E+14  0.00  9.00E+03
119 HNCO + H = NH2 + CO                                 2.25E+07  1.70  3.80E+03
120 CN + O2 = NCO + O                                   6.14E+12  0.00 -4.40E+02
121 CN + CO2 = NCO + CO                                 3.70E+12  0.00  0.00E+00
122 O + NCO = NO + CO                                   2.35E+13  0.00  0.00E+00
123 N + NCO = N2 + CO                                   2.00E+13  0.00  0.00E+00
124 H + NCO = NH + CO                                   5.40E+13  0.00  0.00E+00
125 CH + NO = N + HCO                                   3.00E+13  0.00  0.00E+00
126 CH + NO = O + HCN                                   5.00E+13  0.00  0.00E+00
127 CH + NO = H + NCO                                   2.00E+13  0.00  0.00E+00
128 NH + OH = N + H2O                                   2.00E+09  1.20  0.00E+00
129 NH + OH = HNO + H                                   2.00E+13  0.00  0.00E+00
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 130 HO2 + NO = NO2 + OH                                 2.11E+12  0.00 -4.80E+02
 131 O + NO2 = NO + O2                                   3.90E+12  0.00 -2.40E+02
 132 NO + O + M = NO2 + M                                1.06E+20 -1.41  0.00E+00
 133 NO2 + H = NO + OH                                   1.32E+14  0.00  3.60E+02
 134 NO + H = N + OH                                     2.63E+14  0.00  5.04E+04
 135 NO + O = N + O2                                     3.80E+09  1.00  4.14E+04
 136 O + N2 = NO + N                                     1.80E+14  0.00  7.63E+04
 137 N + NO2 = 2NO                                       4.00E+12  0.00  0.00E+00
 138 N2O + M = N2 + O + M                                6.92E+23 -2.50  6.50E+04
 139 O + N2O = N2 + O2                                   1.40E+12  0.00  1.08E+04
 140 O + N2O = 2NO                                       2.90E+13  0.00  2.32E+04
 141 N2O + H = N2 + OH                                   4.40E+14  0.00  1.89E+04
 142 NO2 + H2 = HNO2 + H                                 2.40E+13  0.00  2.90E+04
 143 OH + NO2 + M = HNO3 + M                             3.00E+15  0.00 -3.80E+03
    3body efficiencies
      O2   0.70  H2   1.40
 144 OH + NO + M = HNO2 + M                              5.60E+15  0.00 -1.70E+03
 145 HNO + H = H2 + NO                                   4.50E+11  0.72  6.60E+02
 146 H + NO + M = HNO + M                                8.95E+19 -1.32  7.40E+02
 147 HNO + OH = H2O + NO                                 1.30E+07  1.90 -9.50E+02


    ** The following  5 elements considered for this problem **
    AR C  H  O  N

    ** The following  40 reacting species considered for this problem **
CH4 CH3 H H2 O2 HO2 O OH H2O CH3O CH2O C2H6 C2H5 C2H4 CH2 C2H3 C2H2 HCO C2H2O
C2H CO C2HO CH2CO CO2 CH H2O2 N2 HCN N CN NCO NH HNCO NH2 NO HNO NO2 N2O HNO2
HNO3

    ** The following  1 inert species considered for this problem **
AR


** New input data given in FPS  units **   ** Output required in FPS  units **

                  ** Perfectly Stirred Reactor problem **

                  Reactor volume =  3.930E-01 ft**3
              Mass flow rate to start iteration =  3.472E-02 lbm/s

Assigned mass flow rate problem:  mass flow rate increment =  6.945E-02 lb/s
              Reactor mass flow rate =  1.389E-01 lb/s

    Fuel-air equivalence ratio =  0.3000  Oxygen mole fraction in air =  0.0000


                        ** Initial Conditions **



         Time 0.00E+00 s  Axial Position 0.00E+00 ft  Area 3.41E-04sq ft


  Thermodynamic Properties              Integration Indicators

    Pressure (lbf/ft**2)       2965.000     Steps from last print      0
    Velocity (ft/s)               0.00      Average step size   0.00E+00
    Density (lb/ft**3)        3.521E-02     Method Order               0
    Temperature (R)             1551.00     Incr. CPU Time          0.00 s
    Mass Flow Rate (lb/s)     3.472E-02
    Entropy (Btu/lb/R)        1.928E+00     Total number of steps      0
    Mach Number               0.000E+00     Funct evaluations          0
    Gamma (Frozen)                1.332     Jacobian evaluations       0
    Enthalpy (Btu/lb)         1.905E+02     Total CPU Time          0.00 s
    Sp. heat, cp (Btu/lb/R)   2.798E-01
```

Chemical Properties

Wi = Net molar production rate per unit volume of species i (mole/ft**3/s)
kj = Forward rate const for reaction j (cgs units)
Xj = Net reaction conv rate for reaction j (mole-ft**3/lb**2/s)
Eq,j = Equilibration factor for reaction j (= Net rate/Positive dir rate)

Species i	Mass Fr.	Mole Fr.	Wi	Reac No,j	kj	Xj	Eq,j
CH4	1.67E-02	2.96E-02	-1.46E+02	1	9.57E-06	5.60E-12	1.00E+00
CH3	0.00E+00	0.00E+00	1.46E+02	2	6.69E+10	0.00E+00	0.00E+00
H	0.00E+00	0.00E+00	6.95E-15	3	1.00E+12	1.18E+05	1.00E+00
H2	0.00E+00	0.00E+00	0.00E+00	4	1.70E+11	0.00E+00	0.00E+00
O2	2.26E-01	2.01E-01	-1.46E+02	5	8.04E+11	0.00E+00	0.00E+00
HO2	0.00E+00	0.00E+00	1.46E+02	6	1.33E+06	0.00E+00	0.00E+00
O	0.00E+00	0.00E+00	1.63E-20	7	1.94E+08	0.00E+00	0.00E+00
OH	0.00E+00	0.00E+00	1.59E-13	8	3.20E+12	0.00E+00	0.00E+00
H2O	6.77E-03	1.07E-02	-1.59E-13	9	2.36E+08	0.00E+00	0.00E+00
CH3O	0.00E+00	0.00E+00	0.00E+00	10	1.61E+13	0.00E+00	0.00E+00
CH2O	0.00E+00	0.00E+00	0.00E+00	11	2.01E+10	0.00E+00	0.00E+00
C2H6	0.00E+00	0.00E+00	0.00E+00	12	5.35E+11	0.00E+00	0.00E+00
C2H5	0.00E+00	0.00E+00	0.00E+00	13	1.40E+12	0.00E+00	0.00E+00
C2H4	0.00E+00	0.00E+00	0.00E+00	14	3.56E+12	0.00E+00	0.00E+00
CH2	0.00E+00	0.00E+00	0.00E+00	15	1.37E+09	0.00E+00	0.00E+00
C2H3	0.00E+00	0.00E+00	0.00E+00	16	8.74E+10	0.00E+00	0.00E+00
C2H2	0.00E+00	0.00E+00	0.00E+00	17	2.00E+12	0.00E+00	0.00E+00
HCO	0.00E+00	0.00E+00	0.00E+00	18	2.00E+13	0.00E+00	0.00E+00
C2H2O	0.00E+00	0.00E+00	0.00E+00	19	2.78E+10	0.00E+00	0.00E+00
C2H	0.00E+00	0.00E+00	0.00E+00	20	2.00E-03	0.00E+00	0.00E+00
CO	0.00E+00	0.00E+00	3.31E-27	21	6.21E+11	0.00E+00	0.00E+00
C2HO	0.00E+00	0.00E+00	0.00E+00	22	1.14E+12	0.00E+00	0.00E+00
CH2CO	0.00E+00	0.00E+00	0.00E+00	23	3.97E+12	0.00E+00	0.00E+00
CO2	4.64E-04	3.00E-04	-3.31E-27	24	1.35E+12	0.00E+00	0.00E+00
CH	0.00E+00	0.00E+00	0.00E+00	25	2.29E+07	0.00E+00	0.00E+00
H2O2	0.00E+00	0.00E+00	0.00E+00	26	4.58E+12	0.00E+00	0.00E+00
N2	7.38E-01	7.49E-01	-1.63E-20	27	3.00E+13	0.00E+00	0.00E+00
HCN	0.00E+00	0.00E+00	0.00E+00	28	3.00E+13	0.00E+00	0.00E+00
N	0.00E+00	0.00E+00	0.00E+00	29	5.00E+12	0.00E+00	0.00E+00
CN	0.00E+00	0.00E+00	0.00E+00	30	3.00E+13	0.00E+00	0.00E+00
NCO	0.00E+00	0.00E+00	0.00E+00	31	3.00E+13	0.00E+00	0.00E+00
NH	0.00E+00	0.00E+00	0.00E+00	32	3.05E-11	0.00E+00	0.00E+00
HNCO	0.00E+00	0.00E+00	0.00E+00	33	2.50E+12	0.00E+00	0.00E+00
NH2	0.00E+00	0.00E+00	0.00E+00	34	2.50E+12	0.00E+00	0.00E+00
NO	0.00E+00	0.00E+00	0.00E+00	35	1.52E+08	0.00E+00	0.00E+00
HNO	0.00E+00	0.00E+00	0.00E+00	36	7.04E+09	0.00E+00	0.00E+00
NO2	0.00E+00	0.00E+00	0.00E+00	37	1.07E+09	0.00E+00	0.00E+00
N2O	0.00E+00	0.00E+00	1.63E-20	38	6.33E+09	0.00E+00	0.00E+00
HNO2	0.00E+00	0.00E+00	0.00E+00	39	8.56E+08	0.00E+00	0.00E+00
HNO3	0.00E+00	0.00E+00	0.00E+00	40	2.08E+13	0.00E+00	0.00E+00
AR	1.25E-02	8.90E-03	0.00E+00	41	2.08E+13	0.00E+00	0.00E+00
				42	2.00E+13	0.00E+00	0.00E+00
				43	9.72E+11	0.00E+00	0.00E+00
				44	1.00E+14	0.00E+00	0.00E+00
				45	1.00E+13	0.00E+00	0.00E+00
				46	1.00E+14	0.00E+00	0.00E+00
				47	3.00E+13	0.00E+00	0.00E+00
				48	3.11E+12	0.00E+00	0.00E+00
				49	1.00E+13	0.00E+00	0.00E+00
				50	2.80E+13	0.00E+00	0.00E+00
				51	2.33E+12	0.00E+00	0.00E+00
				52	1.53E+12	0.00E+00	0.00E+00
				53	4.68E+11	0.00E+00	0.00E+00
				54	9.35E+10	0.00E+00	0.00E+00
				55	2.00E+13	0.00E+00	0.00E+00
				56	7.95E+11	0.00E+00	0.00E+00
				57	1.21E+01	0.00E+00	0.00E+00
				58	5.00E+13	0.00E+00	0.00E+00
				59	6.84E+10	0.00E+00	0.00E+00

60	2.00E+13	0.00E+00	0.00E+00
61	1.43E-04	0.00E+00	0.00E+00
62	1.30E+13	0.00E+00	0.00E+00
63	4.10E+12	0.00E+00	0.00E+00
64	4.93E+12	0.00E+00	0.00E+00
65	1.92E+10	0.00E+00	0.00E+00
66	2.65E+13	0.00E+00	0.00E+00
67	2.00E+13	0.00E+00	0.00E+00
68	1.14E-07	0.00E+00	0.00E+00
69	7.58E+06	0.00E+00	0.00E+00
70	5.71E+06	0.00E+00	0.00E+00
71	8.43E+13	0.00E+00	0.00E+00
72	1.17E+11	0.00E+00	0.00E+00
73	2.27E+12	0.00E+00	0.00E+00
74	3.30E+13	0.00E+00	0.00E+00
75	2.52E+11	0.00E+00	0.00E+00
76	5.50E+12	0.00E+00	0.00E+00
77	6.49E+06	0.00E+00	0.00E+00
78	1.45E+12	0.00E+00	0.00E+00
79	1.99E+12	0.00E+00	0.00E+00
80	5.00E+12	0.00E+00	0.00E+00
81	3.20E+13	0.00E+00	0.00E+00
82	6.02E+12	0.00E+00	0.00E+00
83	3.00E+13	0.00E+00	0.00E+00
84	3.00E+13	0.00E+00	0.00E+00
85	5.00E+13	0.00E+00	0.00E+00
86	7.34E+13	0.00E+00	0.00E+00
87	1.06E+10	0.00E+00	0.00E+00
88	1.04E+14	-2.67E-24	1.00E+00
89	1.88E+00	0.00E+00	0.00E+00
90	1.86E+11	0.00E+00	0.00E+00
91	1.55E+08	0.00E+00	0.00E+00
92	1.49E+09	0.00E+00	0.00E+00
93	1.83E+10	0.00E+00	0.00E+00
94	8.73E+10	0.00E+00	0.00E+00
95	1.50E+13	0.00E+00	0.00E+00
96	2.00E+13	0.00E+00	0.00E+00
97	3.88E+13	-1.28E-10	1.00E+00
98	9.25E+13	0.00E+00	0.00E+00
99	4.31E+11	0.00E+00	0.00E+00
100	1.45E+12	0.00E+00	0.00E+00
101	3.37E+11	0.00E+00	0.00E+00
102	1.22E+12	0.00E+00	0.00E+00
103	4.12E+05	0.00E+00	0.00E+00
104	7.89E+11	0.00E+00	0.00E+00
105	8.37E+15	0.00E+00	0.00E+00
106	2.80E-12	9.94E-19	1.00E+00
107	5.80E+14	0.00E+00	0.00E+00
108	9.85E-11	0.00E+00	0.00E+00
109	2.43E-15	9.67E-21	1.00E+00
110	1.52E+06	0.00E+00	0.00E+00
111	1.34E+12	0.00E+00	0.00E+00
112	1.66E+07	0.00E+00	0.00E+00
113	3.40E+10	0.00E+00	0.00E+00
114	8.49E+09	0.00E+00	0.00E+00
115	4.51E+08	0.00E+00	0.00E+00
116	7.70E+13	0.00E+00	0.00E+00
117	4.00E+13	0.00E+00	0.00E+00
118	5.22E+11	0.00E+00	0.00E+00
119	2.39E+11	0.00E+00	0.00E+00
120	7.94E+12	0.00E+00	0.00E+00
121	3.70E+12	0.00E+00	0.00E+00
122	2.35E+13	0.00E+00	0.00E+00
123	2.00E+13	0.00E+00	0.00E+00
124	5.40E+13	0.00E+00	0.00E+00
125	3.00E+13	0.00E+00	0.00E+00
126	5.00E+13	0.00E+00	0.00E+00
127	2.00E+13	0.00E+00	0.00E+00
128	6.66E+12	0.00E+00	0.00E+00

129	2.00E+13	0.00E+00	0.00E+00
130	2.79E+12	0.00E+00	0.00E+00
131	4.49E+12	0.00E+00	0.00E+00
132	7.70E+15	0.00E+00	0.00E+00
133	1.07E+14	0.00E+00	0.00E+00
134	4.31E+01	0.00E+00	0.00E+00
135	1.05E+02	0.00E+00	0.00E+00
136	8.23E-06	0.00E+00	0.00E+00
137	4.00E+12	0.00E+00	0.00E+00
138	1.04E+00	0.00E+00	0.00E+00
139	2.54E+09	-1.31E-17	1.00E+00
140	3.90E+07	0.00E+00	0.00E+00
141	7.16E+09	0.00E+00	0.00E+00
142	1.06E+06	0.00E+00	0.00E+00
143	2.76E+16	0.00E+00	0.00E+00
144	1.51E+16	0.00E+00	0.00E+00
145	3.97E+13	0.00E+00	0.00E+00
146	7.75E+15	0.00E+00	0.00E+00
147	8.55E+12	0.00E+00	0.00E+00

Mix Mol Wt. 28.465 Total Energy Exch Rate (Btu-ft**3/lb**2/s) 1.13E+10 Mass Fr. Sum 1.00000

CPU Time for initialization of LSENS = 0.00 s

** Equilibrium Conditions **

Time 0.00E+00 s Axial Position 0.00E+00 ft Area 3.41E-04sq ft

Thermodynamic Properties

Pressure (lbf/ft**2)	2965.000
Velocity (ft/s)	0.00
Density (lb/ft**3)	1.980E-02
Temperature (R)	2758.99
Mass Flow Rate (lb/s)	3.472E-02
Entropy (Btu/lb/R)	2.104E+00
Mach Number	0.000E+00
Gamma (Frozen)	1.294
Enthalpy (Btu/lb)	1.905E+02
Sp. heat, cp (Btu/lb/R)	3.074E-01

Integration Indicators

Steps from last print	0
Average step size	0.00E+00
Method Order	0
Incr. CPU Time	0.00 s
Total number of steps	0
Funct evaluations	0
Jacobian evaluations	0
Total CPU Time	0.00 s

Chemical Properties

Wi = Net molar production rate per unit volume of species i (mole/ft**3/s)
kj = Forward rate const for reaction j (cgs units)
Xj = Net reaction conv rate for reaction j (mole-ft**3/lb**2/s)
Eq,j = Equilibration factor for reaction j (= Net rate/Positive dir rate)

Species i	Mass Fr.	Mole Fr.	Wi	Reac No,j	kj	Xj	Eq,j
CH4	1.60E-09	2.85E-09	1.04E-06	1	5.67E+04	-1.06E-09	2.50E-01
CH3	1.50E-09	2.85E-09	-9.64E-07	2	2.72E+12	-7.45E-10	2.50E-01
H	5.18E-10	1.46E-08	9.77E-05	3	1.00E+12	-2.65E-03	2.50E-01
H2	3.20E-08	4.52E-07	-4.41E-09	4	3.64E+12	-1.35E-07	2.50E-01
O2	1.59E-01	1.41E-01	-3.95E-04	5	4.49E+12	-6.21E-06	2.50E-01
HO2	4.39E-07	3.79E-07	2.73E-05	6	2.10E+09	5.81E-06	3.48E-01
O	1.11E-06	1.98E-06	2.32E-04	7	1.91E+09	1.52E-05	1.00E+00
OH	4.41E-05	7.38E-05	5.41E-05	8	3.20E+12	4.63E-06	3.48E-01

H2O	4.42E-02	6.99E-02	-4.70E-06
CH3O	3.10E-09	2.85E-09	-8.00E-06
CH2O	3.00E-09	2.85E-09	2.77E-05
C2H6	3.01E-09	2.85E-09	-4.23E-08
C2H5	2.91E-09	2.85E-09	-8.45E-05
C2H4	2.81E-09	2.85E-09	8.45E-05
CH2	1.40E-09	2.85E-09	-3.13E-05
C2H3	2.70E-09	2.85E-09	-1.52E-05
C2H2	2.60E-09	2.85E-09	6.56E-06
HCO	2.90E-09	2.85E-09	2.08E-04
C2H2O	4.20E-09	2.85E-09	-3.88E-08
C2H	2.50E-09	2.85E-09	-1.95E-04
CO	5.17E-07	5.25E-07	1.38E-04
C2HO	4.10E-09	2.85E-09	9.14E-05
CH2CO	4.20E-09	2.85E-09	1.06E-10
CO2	4.62E-02	2.99E-02	-4.23E-06
CH	1.30E-09	2.85E-09	-1.07E-04
H2O2	3.40E-09	2.85E-09	2.44E-06
N2	7.37E-01	7.49E-01	7.86E-07
HCN	2.70E-09	2.85E-09	1.27E-06
N	1.40E-09	2.85E-09	-3.74E-06
CN	2.60E-09	2.85E-09	-2.46E-05
NCO	4.20E-09	2.85E-09	2.51E-05
NH	1.50E-09	2.85E-09	-5.02E-08
HNCO	4.30E-09	2.85E-09	6.51E-11
NH2	1.60E-09	2.85E-09	5.19E-13
NO	1.21E-03	1.15E-03	5.12E-07
HNO	3.10E-09	2.85E-09	-5.64E-08
NO2	8.84E-06	5.47E-06	2.56E-05
N2O	1.25E-07	8.09E-08	7.07E-15
HNO2	8.81E-08	5.34E-08	2.59E-10
HNO3	6.30E-09	2.85E-09	-2.56E-05
AR	1.25E-02	8.90E-03	0.00E+00

9	5.07E+10	2.85E-03	1.00E+00
10	1.28E+13	-4.73E-05	1.00E+00
11	3.20E+11	-7.34E-08	9.99E-01
12	1.10E+13	8.45E-09	9.38E-01
13	1.81E+13	1.89E-06	9.38E-01
14	1.51E+13	5.87E-05	9.38E-01
15	3.80E+12	2.14E-01	1.00E+00
16	2.35E+11	1.87E-03	1.00E+00
17	2.00E+12	1.65E-09	1.00E+00
18	2.00E+13	3.20E-09	1.00E+00
19	2.73E+12	1.13E-09	5.01E-01
20	1.28E+06	7.22E-08	1.00E+00
21	3.72E+12	7.75E-06	5.01E-01
22	1.46E+12	6.06E-06	1.00E+00
23	1.21E+13	1.34E-06	1.00E+00
24	4.84E+12	5.39E-07	1.00E+00
25	8.21E+10	4.62E-03	1.00E+00
26	4.31E+12	3.42E-02	1.00E+00
27	3.00E+13	2.47E-08	1.00E+00
28	3.00E+13	3.34E-06	1.00E+00
29	5.00E+12	2.08E-05	1.00E+00
30	3.00E+13	4.81E-09	1.00E+00
31	3.00E+13	4.81E-09	1.00E+00
32	2.33E+01	-4.76E-09	1.00E+00
33	1.28E+13	1.43E-06	1.00E+00
34	1.28E+13	1.43E-06	1.00E+00
35	1.11E+11	-4.47E-05	1.00E+00
36	7.99E+11	-1.21E-02	1.00E+00
37	1.27E+11	5.28E-07	1.00E+00
38	6.54E+10	2.72E-07	1.00E+00
39	5.14E+09	2.14E-08	1.00E+00
40	3.06E+13	2.43E-01	1.00E+00
41	3.06E+13	2.43E-01	1.00E+00
42	2.00E+13	8.31E-05	1.00E+00
43	1.21E+12	9.61E-03	1.00E+00
44	1.00E+14	1.11E-05	1.00E+00
45	1.00E+13	4.15E-05	1.00E+00
46	1.00E+14	8.22E-08	1.00E+00
47	3.00E+13	4.81E-09	1.00E+00
48	5.19E+12	8.30E-10	1.00E+00
49	1.00E+13	1.60E-09	1.00E+00
50	2.80E+13	1.16E-04	1.00E+00
51	3.89E+12	-1.89E-05	5.39E-01
52	3.67E+12	3.02E-09	1.00E+00
53	3.62E+12	-3.47E-09	5.39E-01
54	7.23E+11	-9.40E-08	5.39E-01
55	2.00E+13	2.23E-06	1.00E+00
56	1.12E+12	1.25E-07	9.99E-01
57	5.57E+07	3.13E-06	9.99E-01
58	5.00E+13	5.57E-06	1.00E+00
59	2.21E+12	1.76E-02	1.00E+00
60	2.00E+13	1.65E-08	1.00E+00
61	1.41E+05	7.80E-09	9.82E-01
62	2.28E+13	9.30E-05	9.82E-01
63	1.74E+13	1.40E-08	9.82E-01
64	1.22E+13	1.33E-06	9.82E-01
65	4.33E+11	6.84E-11	9.86E-01
66	2.65E+13	4.24E-09	1.00E+00
67	2.00E+13	1.49E-07	3.48E-01
68	1.70E+03	-2.51E-09	9.63E-01
69	7.97E+09	-1.72E-10	9.63E-01
70	6.03E+09	-1.77E-08	9.63E-01
71	8.43E+13	9.38E-06	1.00E+00
72	1.18E+12	-1.29E-04	9.63E-01
73	2.71E+12	4.56E-03	1.00E+00
74	3.30E+13	2.62E-01	1.00E+00
75	1.99E+12	1.58E-02	1.00E+00
76	8.07E+12	6.41E-02	1.00E+00
77	7.11E+09	-5.35E-09	8.71E-01

78	9.91E+12	-2.78E-04	8.71E-01
79	1.06E+13	-5.91E-08	8.71E-01
80	5.00E+12	8.01E-10	1.00E+00
81	3.20E+13	5.13E-09	1.00E+00
82	6.66E+12	5.30E-02	1.00E+00
83	3.00E+13	3.34E-06	1.00E+00
84	3.00E+13	3.34E-06	1.00E+00
85	5.00E+13	2.08E-04	1.00E+00
86	7.34E+13	6.04E-08	1.00E+00
87	4.60E+11	2.59E-02	1.00E+00
88	2.25E+14	4.91E-13	9.55E-06
89	3.82E+05	2.63E-13	4.69E-07
90	3.85E+11	4.94E-10	1.67E-06
91	6.47E+10	1.11E-12	4.35E-06
92	1.64E+11	-5.71E-07	1.28E-06
93	7.31E+11	-3.59E-08	1.20E-06
94	2.03E+12	-5.22E-12	1.45E-07
95	1.97E+13	8.69E-12	4.02E-06
96	2.00E+13	1.15E-09	3.88E-06
97	3.42E+13	9.74E-08	5.16E-06
98	1.09E+14	3.19E-11	2.67E-06
99	5.16E+12	1.12E-05	6.41E-01
100	1.58E+12	-1.17E-05	6.41E-01
101	2.22E+11	4.04E-07	6.41E-01
102	3.07E+12	-4.51E-09	6.41E-01
103	4.67E+10	-6.19E-03	6.41E-01
104	4.52E+12	3.38E-09	1.13E-06
105	5.10E+15	2.66E-08	4.00E-06
106	1.33E+00	-4.80E-11	9.15E-06
107	3.26E+14	1.64E-14	7.87E-06
108	4.51E+00	-9.28E-16	8.02E-06
109	1.75E-02	-4.43E-13	9.08E-06
110	1.95E+08	8.23E-06	1.00E+00
111	4.47E+12	1.14E-07	1.00E+00
112	3.70E+10	-1.50E-05	1.00E+00
113	5.56E+11	6.07E-08	9.82E-01
114	1.39E+11	1.54E-08	1.00E+00
115	8.51E+09	3.54E-08	1.00E+00
116	7.70E+13	8.57E-06	1.00E+00
117	4.00E+13	1.66E-04	1.00E+00
118	5.21E+12	1.32E-07	9.96E-01
119	1.68E+12	1.32E-09	9.58E-01
120	7.09E+12	5.64E-02	1.00E+00
121	3.70E+12	6.23E-03	1.00E+00
122	2.35E+13	2.62E-06	1.00E+00
123	2.00E+13	3.20E-09	1.00E+00
124	5.40E+13	4.44E-08	1.00E+00
125	3.00E+13	1.93E-03	1.00E+00
126	5.00E+13	3.22E-03	1.00E+00
127	2.00E+13	1.29E-03	1.00E+00
128	1.33E+13	4.51E-05	8.18E-01
129	2.00E+13	8.31E-05	1.00E+00
130	2.47E+12	6.66E-09	3.15E-07
131	4.22E+12	3.22E-09	3.56E-06
132	3.42E+15	9.40E-09	5.51E-06
133	1.17E+14	4.37E-10	2.36E-06
134	1.71E+07	-1.61E-04	1.00E+00
135	7.35E+06	-9.37E-03	1.00E+00
136	2.42E+03	-2.01E-03	1.00E+00
137	4.00E+12	1.23E-06	1.00E+00
138	4.06E+06	-1.91E-11	2.94E-06
139	4.03E+10	7.82E-13	6.14E-06
140	1.45E+10	1.30E-13	2.84E-06
141	8.94E+11	1.03E-13	4.94E-06
142	1.76E+09	-1.75E-13	2.04E-06
143	1.04E+16	-6.54E-02	9.87E-01
144	9.79E+15	6.60E-07	3.62E-06
145	7.12E+13	5.30E-08	9.04E-01
146	4.38E+15	-1.52E-04	9.04E-01

```
                                    147  2.00E+13  7.52E-05  9.04E-01

 Mix Mol Wt.   28.464  Total Energy Exch Rate -1.14E+05  Mass Fr. Sum   1.00000
                        (Btu-ft**3/lb**2/s)

      Computational work required for equilibrium calculation:
        No. of iterations =    16     CPU Time =  0.00E+00 s


          INITIAL ESTIMATES (SIGMAS) AT TEMPERATURE =   1532.77 K:

                        CH4        1.00000E-10
                        CH3        1.00000E-10
                        H          5.13529E-10
                        H2         1.58962E-08
                        O2         4.96416E-03
                        HO2        1.33111E-08
                        O          6.95022E-08
                        OH         2.59319E-06
                        H2O        2.45436E-03
                        CH3O       1.00000E-10
                        CH2O       1.00000E-10
                        C2H6       1.00000E-10
                        C2H5       1.00000E-10
                        C2H4       1.00000E-10
                        CH2        1.00000E-10
                        C2H3       1.00000E-10
                        C2H2       1.00000E-10
                        HCO        1.00000E-10
                        C2H2O      1.00000E-10
                        C2H        1.00000E-10
                        CO         1.84535E-08
                        C2HO       1.00000E-10
                        CH2CO      1.00000E-10
                        CO2        1.05041E-03
                        CH         1.00000E-10
                        H2O2       1.00000E-10
                        N2         2.63073E-02
                        HCN        1.00000E-10
                        N          1.00000E-10
                        CN         1.00000E-10
                        NCO        1.00000E-10
                        NH         1.00000E-10
                        HNCO       1.00000E-10
                        NH2        1.00000E-10
                        NO         4.02316E-05
                        HNO        1.00000E-10
                        NO2        1.92064E-07
                        N2O        2.84193E-09
                        HNO2       1.87495E-09
                        HNO3       1.00000E-10
                        AR         3.12669E-04


LSENS CH4-AIR SAMPLE LINE CASE 6

                        ** PSR Calculation **

                        Initial state        Final state  Final/initial ratio

 Pressure       lb/ft**2   2.965E+03           2.965E+03       1.000E+00
 Temp.             R       1.551E+03           2.758E+03       1.778E+00
 Entropy        Btu/lb/R   1.928E+00           2.104E+00       1.091E+00
 Density        lb/ft**3   3.521E-02           1.980E-02       5.623E-01
 Enthalpy       Btu/lb     1.905E+02           1.905E+02       1.000E+00
 Sp. heat (cp)  Btu/lb/R   2.798E-01           3.073E-01       1.098E+00
 Mix mol. wt.              2.846E+01           2.846E+01
 Gamma                     1.332E+00           1.294E+00
```

Species	Mole Fr.	Mass Fr.	Mole Fr.	Mass Fr.
CH4	2.960E-02	1.668E-02	4.149E-05	2.339E-05
CH3	0.000E+00	0.000E+00	6.514E-06	3.441E-06
H	0.000E+00	0.000E+00	2.618E-07	9.272E-09
H2	0.000E+00	0.000E+00	4.900E-06	3.471E-07
O2	2.011E-01	2.261E-01	1.420E-01	1.597E-01
HO2	0.000E+00	0.000E+00	1.811E-06	2.100E-06
O	0.000E+00	0.000E+00	6.868E-06	3.861E-06
OH	0.000E+00	0.000E+00	1.232E-04	7.365E-05
H2O	1.070E-02	6.772E-03	6.972E-02	4.414E-02
CH3O	0.000E+00	0.000E+00	1.291E-08	1.407E-08
CH2O	0.000E+00	0.000E+00	3.706E-06	3.911E-06
C2H6	0.000E+00	0.000E+00	1.924E-07	2.033E-07
C2H5	0.000E+00	0.000E+00	2.846E-09	2.906E-09
C2H4	0.000E+00	0.000E+00	5.226E-07	5.152E-07
CH2	0.000E+00	0.000E+00	2.846E-09	1.403E-09
C2H3	0.000E+00	0.000E+00	2.846E-09	2.705E-09
C2H2	0.000E+00	0.000E+00	9.728E-08	8.901E-08
HCO	0.000E+00	0.000E+00	1.974E-08	2.012E-08
C2H2O	0.000E+00	0.000E+00	2.846E-09	4.204E-09
C2H	0.000E+00	0.000E+00	2.846E-09	2.503E-09
CO	0.000E+00	0.000E+00	2.519E-04	2.480E-04
C2HO	0.000E+00	0.000E+00	2.846E-09	4.103E-09
CH2CO	0.000E+00	0.000E+00	1.955E-06	2.887E-06
CO2	3.000E-04	4.638E-04	2.959E-02	4.576E-02
CH	0.000E+00	0.000E+00	2.846E-09	1.302E-09
H2O2	0.000E+00	0.000E+00	2.229E-08	2.665E-08
N2	7.494E-01	7.375E-01	7.492E-01	7.375E-01
HCN	0.000E+00	0.000E+00	2.846E-09	2.703E-09
N	0.000E+00	0.000E+00	2.846E-09	1.401E-09
CN	0.000E+00	0.000E+00	2.846E-09	2.602E-09
NCO	0.000E+00	0.000E+00	2.846E-09	4.202E-09
NH	0.000E+00	0.000E+00	2.846E-09	1.501E-09
HNCO	0.000E+00	0.000E+00	2.846E-09	4.303E-09
NH2	0.000E+00	0.000E+00	2.846E-09	1.602E-09
NO	0.000E+00	0.000E+00	5.344E-05	5.635E-05
HNO	0.000E+00	0.000E+00	2.846E-09	3.101E-09
NO2	0.000E+00	0.000E+00	6.366E-07	1.029E-06
N2O	0.000E+00	0.000E+00	2.274E-07	3.517E-07
HNO2	0.000E+00	0.000E+00	2.846E-09	4.701E-09
HNO3	0.000E+00	0.000E+00	2.846E-09	6.301E-09
AR	8.900E-03	1.249E-02	8.898E-03	1.249E-02

Volume 3.930E-01 ft**3 Mass Flo 3.473E-02 lb/s
mdot/vol = 8.8359E-02 Res time = 2.2408E+02 ms Iterations = 11

LSENS CH4-AIR SAMPLE LINE CASE 6

** PSR Calculation **

		Initial state	Final state	Final/initial ratio
Pressure	lb/ft**2	2.965E+03	2.965E+03	1.000E+00
Temp.	R	1.551E+03	2.743E+03	1.769E+00
Entropy	Btu/lb/R	1.928E+00	2.103E+00	1.091E+00
Density	lb/ft**3	3.521E-02	1.990E-02	5.651E-01
Enthalpy	Btu/lb	1.905E+02	1.905E+02	1.000E+00
Sp. heat (cp)	Btu/lb/R	2.798E-01	3.071E-01	1.097E+00
Mix mol. wt.		2.846E+01	2.845E+01	
Gamma		1.332E+00	1.294E+00	

Species	Mole Fr.	Mass Fr.	Mole Fr.	Mass Fr.
CH4	2.960E-02	1.668E-02	1.651E-04	9.311E-05
CH3	0.000E+00	0.000E+00	1.789E-05	9.452E-06
H	0.000E+00	0.000E+00	6.156E-07	2.181E-08
H2	0.000E+00	0.000E+00	1.374E-05	9.734E-07
O2	2.011E-01	2.261E-01	1.426E-01	1.604E-01
HO2	0.000E+00	0.000E+00	2.399E-06	2.783E-06
O	0.000E+00	0.000E+00	7.727E-06	4.345E-06
OH	0.000E+00	0.000E+00	1.025E-04	6.130E-05
H2O	1.070E-02	6.772E-03	6.941E-02	4.395E-02
CH3O	0.000E+00	0.000E+00	3.277E-08	3.574E-08
CH2O	0.000E+00	0.000E+00	1.265E-05	1.335E-05
C2H6	0.000E+00	0.000E+00	1.719E-06	1.817E-06
C2H5	0.000E+00	0.000E+00	2.845E-09	2.906E-09
C2H4	0.000E+00	0.000E+00	4.512E-06	4.449E-06
CH2	0.000E+00	0.000E+00	2.845E-09	1.403E-09
C2H3	0.000E+00	0.000E+00	2.845E-09	2.705E-09
C2H2	0.000E+00	0.000E+00	6.657E-07	6.093E-07
HCO	0.000E+00	0.000E+00	2.593E-08	2.645E-08
C2H2O	0.000E+00	0.000E+00	2.845E-09	4.204E-09
C2H	0.000E+00	0.000E+00	2.845E-09	2.503E-09
CO	0.000E+00	0.000E+00	8.737E-04	8.602E-04
C2HO	0.000E+00	0.000E+00	2.845E-09	4.103E-09
CH2CO	0.000E+00	0.000E+00	3.672E-06	5.426E-06
CO2	3.000E-04	4.638E-04	2.880E-02	4.454E-02
CH	0.000E+00	0.000E+00	2.845E-09	1.302E-09
H2O2	0.000E+00	0.000E+00	1.835E-08	2.194E-08
N2	7.494E-01	7.375E-01	7.490E-01	7.375E-01
HCN	0.000E+00	0.000E+00	2.845E-09	2.703E-09
N	0.000E+00	0.000E+00	2.845E-09	1.401E-09
CN	0.000E+00	0.000E+00	2.845E-09	2.602E-09
NCO	0.000E+00	0.000E+00	2.845E-09	4.202E-09
NH	0.000E+00	0.000E+00	2.845E-09	1.501E-09
HNCO	0.000E+00	0.000E+00	2.845E-09	4.303E-09
NH2	0.000E+00	0.000E+00	2.845E-09	1.602E-09
NO	0.000E+00	0.000E+00	3.659E-06	3.859E-06
HNO	0.000E+00	0.000E+00	2.845E-09	3.101E-09
NO2	0.000E+00	0.000E+00	6.056E-08	9.792E-08
N2O	0.000E+00	0.000E+00	2.162E-07	3.344E-07
HNO2	0.000E+00	0.000E+00	2.845E-09	4.701E-09
HNO3	0.000E+00	0.000E+00	2.845E-09	6.301E-09
AR	8.900E-03	1.249E-02	8.896E-03	1.249E-02

Volume 3.930E-01 ft**3 Mass Flo 1.042E-01 lb/s
mdot/vol = 2.6508E-01 Res time = 7.5070E+01 ms Iterations = 4

LSENS CH4-AIR SAMPLE LINE CASE 6

** PSR Calculation **

		Initial state	Final state	Final/initial ratio
Pressure	lb/ft**2	2.965E+03	2.965E+03	1.000E+00
Temp.	R	1.551E+03	2.721E+03	1.755E+00
Entropy	Btu/lb/R	1.928E+00	2.102E+00	1.090E+00
Density	lb/ft**3	3.521E-02	2.005E-02	5.694E-01
Enthalpy	Btu/lb	1.905E+02	1.905E+02	1.000E+00
Sp. heat (cp)	Btu/lb/R	2.798E-01	3.067E-01	1.096E+00
Mix mol. wt.		2.846E+01	2.844E+01	
Gamma		1.332E+00	1.295E+00	

Species	Mole Fr.	Mass Fr.	Mole Fr.	Mass Fr.

```
CH4                2.960E-02   1.668E-02      3.566E-04   2.012E-04
CH3                0.000E+00   0.000E+00      2.616E-05   1.383E-05
H                  0.000E+00   0.000E+00      7.313E-07   2.592E-08
H2                 0.000E+00   0.000E+00      2.608E-05   1.849E-06
O2                 2.011E-01   2.261E-01      1.435E-01   1.615E-01
HO2                0.000E+00   0.000E+00      3.090E-06   3.586E-06
O                  0.000E+00   0.000E+00      6.288E-06   3.538E-06
OH                 0.000E+00   0.000E+00      6.288E-05   3.760E-05
H2O                1.070E-02   6.772E-03      6.895E-02   4.368E-02
CH3O               0.000E+00   0.000E+00      3.994E-08   4.359E-08
CH2O               0.000E+00   0.000E+00      2.589E-05   2.734E-05
C2H6               0.000E+00   0.000E+00      5.502E-06   5.818E-06
C2H5               0.000E+00   0.000E+00      2.844E-09   2.906E-09
C2H4               0.000E+00   0.000E+00      1.389E-05   1.370E-05
CH2                0.000E+00   0.000E+00      2.844E-09   1.403E-09
C2H3               0.000E+00   0.000E+00      2.844E-09   2.705E-09
C2H2               0.000E+00   0.000E+00      1.571E-06   1.439E-06
HCO                0.000E+00   0.000E+00      3.234E-08   3.300E-08
C2H2O              0.000E+00   0.000E+00      2.844E-09   4.204E-09
C2H                0.000E+00   0.000E+00      2.844E-09   2.503E-09
CO                 0.000E+00   0.000E+00      1.798E-03   1.771E-03
C2HO               0.000E+00   0.000E+00      2.844E-09   4.103E-09
CH2CO              0.000E+00   0.000E+00      3.910E-06   5.779E-06
CO2                3.000E-04   4.638E-04      2.762E-02   4.274E-02
CH                 0.000E+00   0.000E+00      2.844E-09   1.302E-09
H2O2               0.000E+00   0.000E+00      1.374E-08   1.644E-08
N2                 7.494E-01   7.375E-01      7.487E-01   7.375E-01
HCN                0.000E+00   0.000E+00      2.844E-09   2.703E-09
N                  0.000E+00   0.000E+00      2.844E-09   1.401E-09
CN                 0.000E+00   0.000E+00      2.844E-09   2.602E-09
NCO                0.000E+00   0.000E+00      2.844E-09   4.202E-09
NH                 0.000E+00   0.000E+00      2.844E-09   1.501E-09
HNCO               0.000E+00   0.000E+00      2.844E-09   4.303E-09
NH2                0.000E+00   0.000E+00      2.844E-09   1.602E-09
NO                 0.000E+00   0.000E+00      6.926E-08   7.308E-08
HNO                0.000E+00   0.000E+00      2.844E-09   3.101E-09
NO2                0.000E+00   0.000E+00      2.844E-09   4.601E-09
N2O                0.000E+00   0.000E+00      1.728E-07   2.675E-07
HNO2               0.000E+00   0.000E+00      2.844E-09   4.701E-09
HNO3               0.000E+00   0.000E+00      2.844E-09   6.301E-09
AR                 8.900E-03   1.249E-02      8.892E-03   1.249E-02


      Volume    3.930E-01 ft**3         Mass Flo  1.389E-01 lb/s
    mdot/vol =  3.5344E-01  Res time =  5.6729E+01 ms  Iterations =     5

     Computational work required for PSR problem:
       No. of Iterations =    20  CPU Time =  0.00E+00 s



(LSENS)  End of this case

              Total CPU time (including I/O) =        0.00 s

(LSENS)     Read data for next case



                           ** Problem Data **

        1         2         3         4         5         6         7         8
2345678901234567890123456789012345678901234567890123456789012345678901234567890

                           Blank Line
```

```
                                  Blank Line
 (CIMAGE) ** Warning: End of problem data, but no
    end of file indicator or incomplete data




(KINP)  ** Error: The ACTION switch (= "    " is illegal **
  Legal values are ADD, NEW, CHANGE, and REPEAT


(LSENS)     A fatal error has occurred - Case terminated
```

Plug Flow Model – Methane Analysis

```
                                ** Problem Data **

         1         2         3         4         5         6         7         8
 2345678901234567890123456789012345678901234567890123456789012345678901234567890

LSENS CH4-AIR
   M       +   CH4      =   CH3     +   H         2.0E+17   0.        88000.
   H       +   CH4      =   CH3     +   H2        6.6E+8    1.62      10840.
   CH4     +   O2       =   CH3     +   HO2       1.0E+12   0.        0.
   O       +   CH4      =   CH3     +   OH        1.02E+9   1.5       8600.
   OH      +   CH4      =   CH3     +   H2O       1.0E+8    1.6       3120.
   CH3     +   O2       =   CH3O    +   O         2.68E+13  0.        28800.
   CH3     +   O2       =   OH      +   CH2O      3.6E+10   0.        8940.
   CH3     +   OH       =   CH3O    +   H         3.2E+12   0.        0.
   M       +   CH3O     =   CH2O    +   H         5.0E+13   0.        21000.
   CH3     +   CH3      =   C2H6                  2.4E+14   -.4       0.
   CH3     +   CH3      =   H       +   C2H5      4.99E+12  0.1       10600.
   H       +   C2H6     =   C2H5    +   H2        1.15E+8   1.9       7530.
   O       +   C2H6     =   C2H5    +   OH        8.98E+7   1.92      5690.
   OH      +   C2H6     =   C2H5    +   H2O       3.54E+6   2.12      870.
   M       +   C2H5     =   C2H4    +   H         1.0E+17   0.        31000.
   C2H5    +   O2       =   C2H4    +   HO2       8.4E+11   0.        3875.
   H       +   C2H5     =   C2H4    +   H2        2.0E+12   0.        0.
   CH3     +   CH2      =   C2H4    +   H         2.0E+13   0.        0.
   H       +   C2H4     =   H2      +   C2H3      1.325E+6  2.53      12240.
   M       +   C2H4     =   C2H2    +   H2        2.6E+17   0.        79300.
   C2H4    +   OH       =   C2H3    +   H2O       3.6E+6    2.        2500.
   C2H4    +   OH       =   CH3     +   CH2O      2.0E+12   0.        960.
   C2H4    +   O        =   CH3     +   HCO       1.92E+7   1.83      220.
   C2H4    +   O        =   CH2O    +   CH2       2.5E+13   0.        5000.
   M       +   C2H3     =   C2H2    +   H         3.0E+15   0.        32000.
   C2H3    +   O2       =   CH2O    +   HCO       3.98E+12  0.        -240.
   C2H3    +   H        =   C2H2    +   H2        3.0E+13   0.        0.
   C2H3    +   O        =   C2H2O   +   H         3.0E+13   0.        0.
   C2H3    +   OH       =   C2H2    +   H2O       5.0E+12   0.        0.
   C2H3    +   CH2      =   C2H2    +   CH3       3.0E+13   0.        0.
   C2H3    +   C2H      =2.0C2H2                  3.0E+13   0.        0.
   M       +   C2H2     =   C2H     +   H         4.2E+16   0.        107000.
   C2H2    +   O        =   CH2     +   CO        1.02E+7   2.0       1900.
   C2H2    +   O        =   C2HO    +   H         1.02E+7   2.        1900.
   C2H2    +   O        =   OH      +   C2H       4.6E+19   -1.41     28950.
   C2H2    +   OH       =   C2H     +   H2O       3.37E+7   2.        14000.
   C2H2    +   OH       =   C2H2O   +   H         5.04E+5   2.3       13500.
   C2H2    +   OH       =   CH2CO   +   H         2.18E-4   4.5       -1000.
   C2H2    +   OH       =   CH3     +   CO        4.83E-4   4.        -2000.
   C2H     +   O2       =   C2HO    +   O         5.00E+13  0.0       1500.
   C2H     +   O2       =   HCO     +   CO        5.0E+13   0.0       1500.
   C2H     +   OH       =   C2HO    +   H         2.0E+13   0.0       0.
   C2HO    +   O2       =2.0CO      +   OH        1.6E+12   0.        854.
   C2HO    +   O        =2.0CO      +   H         1.0E+14   0.        0.
   C2HO    +   OH       =2.0HCO                   1.0E+13   0.        0.
   C2HO    +   H        =   CH2     +   CO        1.0E+14   0.        0.
   C2HO    +   CH2      =   C2H3    +   CO        3.0E+13   0.        0.
   C2HO    +   CH2      =   CH2O    +   C2H       1.0E+13   0.        2000.
            2.0C2HO     =   C2H2    +2.0CO        1.0E+13   0.        0.
   C2H2O   +   OH       =   CH2O    +   HCO       2.8E+13   0.        0.
   C2H2O   +   OH       =   C2HO    +   H2O       7.5E+12   0.        2000.
   C2H2O   +   H        =   CH3     +   CO        1.13E+13  0.        3428.
   C2H2O   +   H        =   C2HO    +   H2        5.0E+13   0.        8000.
   C2H2O   +   O        =   C2HO    +   OH        1.0E+13   0.        8000.
   C2H2O   +   O        =   CH2O    +   CO        2.0E+13   0.        0.
   C2H2O   +   O        =   CH2     +   CO2       1.75E+12  0.        1350.
   M       +   C2H2O    =   CH2     +   CO        2.0E+16   0.        60000.
   C2H     +   O        =   CO      +   CH        5.0E+13   0.        0.
   CH3O    +   O2       =   CH2O    +   HO2       4.28E-13  7.6       -3530.
   CH3O    +   H        =   CH2O    +   H2        2.0E+13   0.        0.
   M       +   CH2O     =   HCO     +   H         5.0E+16   0.        81000.
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   CH2O    +   OH      =   HCO     +   H2O       3.43E+9   1.18      -447.
   CH2O    +   H       =   HCO     +   H2        2.3E+10   1.05      3275.
   CH2O    +   O       =   HCO     +   OH        3.9E+13   0.        3540.
   CH3     +   CH2O    =   CH4     +   HCO       3.32E+03  2.81      5860.
   CH3     +   HCO     =   CH4     +   CO        2.65E+13  0.        0.
   CH3     +   HO2     =   CH3O    +   OH        2.0E+13   0.        0.
   M       +   CH3     =   CH2     +   H         1.95E+16  0.        91600.
   H       +   CH3     =   H2      +   CH2       2.7E+11   0.67      25700.
   O       +   CH3     =   OH      +   CH2       1.9E+11   0.68      25700.
   O       +   CH3     =   H       +   CH2O      8.43E+13  0.        0.
   OH      +   CH3     =   H2O     +   CH2       5.6E+7    1.6       5420.
   CH      +   CO2     =   HCO     +   CO        3.4E+12   0.        690.
   CH      +   O2      =   HCO     +   O         3.3E+13   0.        0.
   CH2     +   O2      =   CH2O    +   O         5.0E+11   0.5       6960.
   CH2     +   O2      =   OH      +   HCO       1.32E+13  0.        1500.
   CH2     +   O       =   CH      +   OH        2.0E+11   0.7       25800.
   CH2     +   OH      =   CH      +   H2O       1.13E+7   2.0       3000.
   CH2     +   H       =   CH      +   H2        3.2E+11   0.7       4970.
   CH2     +   CH2     =   C2H3    +   H         5.0E+12   0.        0.
   CH2     +   CH2     =   C2H2    +   H2        3.2E+13   0.        0.
   HCO     +   O2      =   CO      +   HO2       7.6E+12   0.        400.
   HCO     +   O       =   CO      +   OH        3.0E+13   0.        0.
   HCO     +   O       =   CO2     +   H         3.0E+13   0.        0.
   HCO     +   OH      =   CO      +   H2O       5.0E+13   0.        0.
   HCO     +   H       =   CO      +   H2        7.34E+13  0.        0.
   M       +   HCO     =   H       +   CO        1.87E+17  -1.       17000.
   CO      +   O       =   CO2     +   M         6.02E+14  0.        3000.
   CO      +   O2      =   CO2     +   O         2.5E+12   0.        47800.
   CO      +   OH      =   CO2     +   H         4.76E+7   1.23      70.
   CO      +   HO2     =   CO2     +   OH        1.5E+14   0.        23600.
   O       +   H2O     =   OH      +   OH        6.8E+13   0.        18365.
   H       +   O2      =   OH      +   O         8.3E+13   0.        14413.
   O       +   H2      =   OH      +   H         5.00E+04  2.67      6290.
   H       +   HO2     =   H2      +   O2        2.8E+13   0.        1068.
   O       +   HO2     =   OH      +   O2        2.0E+13   0.        0.
   HO2     +   OH      =   H2O     +   O2        2.9E+13   0.        -500.
   H       +   HO2     =2.0OH                    1.34E+14  0.        635.
   H2      +   HO2     =   H2O2    +   H         1.21E+7   2.        5200.
   OH      +   H2O2    =   H2O     +   HO2       1.75E+12  0.        320.
   HO2     +   HO2     =   H2O2    +   O2        1.3E+11   0.        -1630.
   H       +   H2O2    =   OH      +   H2O       1.0E+13   0.        3600.
   M       +   H2O2    =2.0OH                    1.44E+17  0.        45510.
   THIRDBODY
H2        2.30      O2        0.78      H2O       6.0
H2O2      6.6
END
   H2      +   OH      =   H2O     +   H         2.16E+8   1.51      3430.
   H       +   O2      =   HO2     +   M         2.8E+18   -0.86     0.
   THIRDBODY
O2        1.30      N2        1.3
H2O       21.3      CO2       7.0
END
   M       +   H2O     =   H       +   OH        1.30E+15  0.        105140.
   THIRDBODY
H2        4.00      O2        1.5
H2O       20.0      N2        1.5
CO2       4.0
END
   H       +   O       =   OH      +   M         5.00E+17  -1.       0.
   M       +   H2      =   H       +   H         2.2E+14   0.        96000.
   THIRDBODY
H2        4.10      O2        2.0
H2O       15.0      N2        2.0
END
   M       +   O2      =   O       +   O         1.80E+18  -1.       118020.
   CH      +   N2      =   HCN     +   N         1.0E+11   0.        19000.
   CN      +   H2      =   HCN     +   H         2.1E+13   0.        4710.
   O       +   HCN     =   OH      +   CN        2.13E+9   1.58      26600.
   O       +   HCN     =   NCO     +   H         1.11E+4   2.64      4980.
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   O       +   HCN      =   NH      +   CO        2.77E+3   2.64      4980.
   OH      +   HCN      =   HNCO    +   H         4.4E+3    2.26      6400.
   CN      +   O        =   CO      +   N         7.7E+13   0.        0.
   CN      +   OH       =   NCO     +   H         4.0E+13   0.        0.
   H2      +   NCO      =   HNCO    +   H         1.0E+14   0.        9000.
   HNCO    +   H        =   NH2     +   CO        2.25E+7   1.7       3800.
   CN      +   O2       =   NCO     +   O         6.14E+12  0.        -440.
   CN      +   CO2      =   NCO     +   CO        3.7E+12   0.        0.
   O       +   NCO      =   NO      +   CO        2.35E+13  0.        0.
   N       +   NCO      =   N2      +   CO        2.0E+13   0.        0.
   H       +   NCO      =   NH      +   CO        5.4E+13   0.        0.
   CH      +   NO       =   N       +   HCO       3.0E+13   0.        0.
   CH      +   NO       =   O       +   HCN       5.0E+13   0.        0.
   CH      +   NO       =   H       +   NCO       2.0E+13   0.        0.
   NH      +   OH       =   N       +   H2O       2.0E+9    1.2       0.
   NH      +   OH       =   HNO     +   H         2.0E+13   0.        0.
   HO2     +   NO       =   NO2     +   OH        2.11E+12  0.        -480.
   O       +   NO2      =   NO      +   O2        3.9E+12   0.        -240.
   NO      +   O        =   NO2     +   M         1.06E+20  -1.41     0.
   NO2     +   H        =   NO      +   OH        1.32E+14  0.        360.
   NO      +   H        =   N       +   OH        2.63E+14  0.        50410.
   NO      +   O        =   N       +   O2        3.8E+9    1.        41370.
   O       +   N2       =   NO      +   N         1.80E+14  0.        76250.
   N       +   NO2      =2.0NO                    4.0E+12   0.        0.
   M       +   N2O      =   N2      +   O         6.92E+23  -2.5      65000.
   O       +   N2O      =   N2      +   O2        1.4E+12   0.        10810.
   O       +   N2O      =2.0NO                    2.9E+13   0.        23150.
   N2O     +   H        =   N2      +   OH        4.4E+14   0.        18880.
   NO2     +   H2       =   HNO2    +   H         2.4E+13   0.        29000.
   OH      +   NO2      =   HNO3    +   M         3.0E+15   0.        -3800.
   THIRDBODY
O2        0.70      H2        1.4
END
   OH      +   NO       =   HNO2    +   M         5.6E+15   0.        -1700.
   HNO     +   H        =   H2      +   NO        4.5E+11   0.72      660.
   H       +   NO       =   HNO     +   M         8.95E+19  -1.32     740.
   HNO     +   OH       =   H2O     +   NO        1.3E+7    1.9       -950.
                                  Blank Line
AR
DISTANCE  AREA  FPS       FPS
&PROB  CX0=1.507, COMBUS=.FALSE., EXCHR=.TRUE.,CONC=.FALSE.
PRINT=2.875, 5.75, &END
$START T=1150.,MACH=0.1,P=2060,ERATIO=0.30,&END
CH4        0.0294
O2         0.2008
N2         0.7485
CO2        0.0003
H2O        0.0120
AR         0.0090
                                  Blank Line
&SOLVER  EMAX=1.0E-4, ATOLSP=1.0E-10,  &END
FINIS1
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          LSENS: Multipurpose Kinetics and Sensitivity Analysis Program

LSENS CH4-AIR CONST. P CASE 6

 Reac        Reaction                                    Reaction Rate Parameters
 No.j                                                       Aj     nj      Ej
                kj = Aj * T**nj * exp(-Ej/RT) (cgs units)

    1 CH4 + M = CH3 + H + M                            2.00E+17  0.00  8.80E+04
    2 H + CH4 = CH3 + H2                               6.60E+08  1.62  1.08E+04
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 3 CH4 + O2 = CH3 + HO2                    1.00E+12  0.00  0.00E+00
 4 O + CH4 = CH3 + OH                      1.02E+09  1.50  8.60E+03
 5 OH + CH4 = CH3 + H2O                    1.00E+08  1.60  3.12E+03
 6 CH3 + O2 = CH3O + O                     2.68E+13  0.00  2.88E+04
 7 CH3 + O2 = OH + CH2O                    3.60E+10  0.00  8.94E+03
 8 CH3 + OH = CH3O + H                     3.20E+12  0.00  0.00E+00
 9 CH3O + M = CH2O + H + M                 5.00E+13  0.00  2.10E+04
10 2CH3 = C2H6                             2.40E+14 -0.40  0.00E+00
11 2CH3 = H + C2H5                         4.99E+12  0.10  1.06E+04
12 H + C2H6 = C2H5 + H2                    1.15E+08  1.90  7.53E+03
13 O + C2H6 = C2H5 + OH                    8.98E+07  1.92  5.69E+03
14 OH + C2H6 = C2H5 + H2O                  3.54E+06  2.12  8.70E+02
15 C2H5 + M = C2H4 + H + M                 1.00E+17  0.00  3.10E+04
16 C2H5 + O2 = C2H4 + HO2                  8.40E+11  0.00  3.88E+03
17 H + C2H5 = C2H4 + H2                    2.00E+12  0.00  0.00E+00
18 CH3 + CH2 = C2H4 + H                    2.00E+13  0.00  0.00E+00
19 H + C2H4 = H2 + C2H3                    1.33E+06  2.53  1.22E+04
20 C2H4 + M = C2H2 + H2 + M                2.60E+17  0.00  7.93E+04
21 C2H4 + OH = C2H3 + H2O                  3.60E+06  2.00  2.50E+03
22 C2H4 + OH = CH3 + CH2O                  2.00E+12  0.00  9.60E+02
23 C2H4 + O = CH3 + HCO                    1.92E+07  1.83  2.20E+02
24 C2H4 + O = CH2O + CH2                   2.50E+13  0.00  5.00E+03
25 C2H3 + M = C2H2 + H + M                 3.00E+15  0.00  3.20E+04
26 C2H3 + O2 = CH2O + HCO                  3.98E+12  0.00 -2.40E+02
27 C2H3 + H = C2H2 + H2                    3.00E+13  0.00  0.00E+00
28 C2H3 + O = C2H2O + H                    3.00E+13  0.00  0.00E+00
29 C2H3 + OH = C2H2 + H2O                  5.00E+12  0.00  0.00E+00
30 C2H3 + CH2 = C2H2 + CH3                 3.00E+13  0.00  0.00E+00
31 C2H3 + C2H = 2C2H2                      3.00E+13  0.00  0.00E+00
32 C2H2 + M = C2H + H + M                  4.20E+16  0.00  1.07E+05
33 C2H2 + O = CH2 + CO                     1.02E+07  2.00  1.90E+03
34 C2H2 + O = C2HO + H                     1.02E+07  2.00  1.90E+03
35 C2H2 + O = OH + C2H                     4.60E+19 -1.41  2.90E+04
36 C2H2 + OH = C2H + H2O                   3.37E+07  2.00  1.40E+04
37 C2H2 + OH = C2H2O + H                   5.04E+05  2.30  1.35E+04
38 C2H2 + OH = CH2CO + H                   2.18E-04  4.50 -1.00E+03
39 C2H2 + OH = CH3 + CO                    4.83E-04  4.00 -2.00E+03
40 C2H + O2 = C2HO + O                     5.00E+13  0.00  1.50E+03
41 C2H + O2 = HCO + CO                     5.00E+13  0.00  1.50E+03
42 C2H + OH = C2HO + H                     2.00E+13  0.00  0.00E+00
43 C2HO + O2 = 2CO + OH                    1.60E+12  0.00  8.54E+02
44 C2HO + O = 2CO + H                      1.00E+14  0.00  0.00E+00
45 C2HO + OH = 2HCO                        1.00E+13  0.00  0.00E+00
46 C2HO + H = CH2 + CO                     1.00E+14  0.00  0.00E+00
47 C2HO + CH2 = C2H3 + CO                  3.00E+13  0.00  0.00E+00
48 C2HO + CH2 = CH2O + C2H                 1.00E+13  0.00  2.00E+03
49 2C2HO = C2H2 + 2CO                      1.00E+13  0.00  0.00E+00
50 C2H2O + OH = CH2O + HCO                 2.80E+13  0.00  0.00E+00
51 C2H2O + OH = C2HO + H2O                 7.50E+12  0.00  2.00E+03
52 C2H2O + H = CH3 + CO                    1.13E+13  0.00  3.43E+03
53 C2H2O + H = C2HO + H2                   5.00E+13  0.00  8.00E+03
54 C2H2O + O = C2HO + OH                   1.00E+13  0.00  8.00E+03
55 C2H2O + O = CH2O + CO                   2.00E+13  0.00  0.00E+00
56 C2H2O + O = CH2 + CO2                   1.75E+12  0.00  1.35E+03
57 C2H2O + M = CH2 + CO + M                2.00E+16  0.00  6.00E+04
58 C2H + O = CO + CH                       5.00E+13  0.00  0.00E+00
59 CH3O + O2 = CH2O + HO2                  4.28E-13  7.60 -3.53E+03
60 CH3O + H = CH2O + H2                    2.00E+13  0.00  0.00E+00
61 CH2O + M = HCO + H + M                  5.00E+16  0.00  8.10E+04
62 CH2O + OH = HCO + H2O                   3.43E+09  1.18 -4.47E+02
63 CH2O + H = HCO + H2                     2.30E+10  1.05  3.28E+03
64 CH2O + O = HCO + OH                     3.90E+13  0.00  3.54E+03
65 CH3 + CH2O = CH4 + HCO                  3.32E+03  2.81  5.86E+03
66 CH3 + HCO = CH4 + CO                    2.65E+13  0.00  0.00E+00
67 CH3 + HO2 = CH3O + OH                   2.00E+13  0.00  0.00E+00
68 CH3 + M = CH2 + H + M                   1.95E+16  0.00  9.16E+04
69 H + CH3 = H2 + CH2                      2.70E+11  0.67  2.57E+04
70 O + CH3 = OH + CH2                      1.90E+11  0.68  2.57E+04
71 O + CH3 = H + CH2O                      8.43E+13  0.00  0.00E+00
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 72 OH + CH3 = H2O + CH2                                 5.60E+07  1.60  5.42E+03
 73 CH + CO2 = HCO + CO                                  3.40E+12  0.00  6.90E+02
 74 CH + O2 = HCO + O                                    3.30E+13  0.00  0.00E+00
 75 CH2 + O2 = CH2O + O                                  5.00E+11  0.50  6.96E+03
 76 CH2 + O2 = OH + HCO                                  1.32E+13  0.00  1.50E+03
 77 CH2 + O = CH + OH                                    2.00E+11  0.70  2.58E+04
 78 CH2 + OH = CH + H2O                                  1.13E+07  2.00  3.00E+03
 79 CH2 + H = CH + H2                                    3.20E+11  0.70  4.97E+03
 80 2CH2 = C2H3 + H                                      5.00E+12  0.00  0.00E+00
 81 2CH2 = C2H2 + H2                                     3.20E+13  0.00  0.00E+00
 82 HCO + O2 = CO + HO2                                  7.60E+12  0.00  4.00E+02
 83 HCO + O = CO + OH                                    3.00E+13  0.00  0.00E+00
 84 HCO + O = CO2 + H                                    3.00E+13  0.00  0.00E+00
 85 HCO + OH = CO + H2O                                  5.00E+13  0.00  0.00E+00
 86 HCO + H = CO + H2                                    7.34E+13  0.00  0.00E+00
 87 HCO + M = H + CO + M                                 1.87E+17 -1.00  1.70E+04
 88 CO + O + M = CO2 + M                                 6.02E+14  0.00  3.00E+03
 89 CO + O2 = CO2 + O                                    2.50E+12  0.00  4.78E+04
 90 CO + OH = CO2 + H                                    4.76E+07  1.23  7.00E+01
 91 CO + HO2 = CO2 + OH                                  1.50E+14  0.00  2.36E+04
 92 O + H2O = 2OH                                        6.80E+13  0.00  1.84E+04
 93 H + O2 = OH + O                                      8.30E+13  0.00  1.44E+04
 94 O + H2 = OH + H                                      5.00E+04  2.67  6.29E+03
 95 H + HO2 = H2 + O2                                    2.80E+13  0.00  1.07E+03
 96 O + HO2 = OH + O2                                    2.00E+13  0.00  0.00E+00
 97 HO2 + OH = H2O + O2                                  2.90E+13  0.00 -5.00E+02
 98 H + HO2 = 2OH                                        1.34E+14  0.00  6.35E+02
 99 H2 + HO2 = H2O2 + H                                  1.21E+07  2.00  5.20E+03
100 OH + H2O2 = H2O + HO2                                1.75E+12  0.00  3.20E+02
101 2HO2 = H2O2 + O2                                     1.30E+11  0.00 -1.63E+03
102 H + H2O2 = OH + H2O                                  1.00E+13  0.00  3.60E+03
103 H2O2 + M = 2OH + M                                   1.44E+17  0.00  4.55E+04
   3body efficiencies
     H2   2.30  O2   0.78  H2O   6.00  H2O2   6.60
104 H2 + OH = H2O + H                                    2.16E+08  1.51  3.43E+03
105 H + O2 + M = HO2 + M                                 2.80E+18 -0.86  0.00E+00
   3body efficiencies
     O2   1.30  N2   1.30  H2O  21.30  CO2   7.00
106 H2O + M = H + OH + M                                 1.30E+15  0.00  1.05E+05
   3body efficiencies
     H2   4.00  O2   1.50  H2O  20.00  N2   1.50  CO2   4.00
107 H + O + M = OH + M                                   5.00E+17 -1.00  0.00E+00
108 H2 + M = 2H + M                                      2.20E+14  0.00  9.60E+04
   3body efficiencies
     H2   4.10  O2   2.00  H2O  15.00  N2   2.00
109 O2 + M = 2O + M                                      1.80E+18 -1.00  1.18E+05
110 CH + N2 = HCN + N                                    1.00E+11  0.00  1.90E+04
111 CN + H2 = HCN + H                                    2.10E+13  0.00  4.71E+03
112 O + HCN = OH + CN                                    2.13E+09  1.58  2.66E+04
113 O + HCN = NCO + H                                    1.11E+04  2.64  4.98E+03
114 O + HCN = NH + CO                                    2.77E+03  2.64  4.98E+03
115 OH + HCN = HNCO + H                                  4.40E+03  2.26  6.40E+03
116 CN + O = CO + N                                      7.70E+13  0.00  0.00E+00
117 CN + OH = NCO + H                                    4.00E+13  0.00  0.00E+00
118 H2 + NCO = HNCO + H                                  1.00E+14  0.00  9.00E+03
119 HNCO + H = NH2 + CO                                  2.25E+07  1.70  3.80E+03
120 CN + O2 = NCO + O                                    6.14E+12  0.00 -4.40E+02
121 CN + CO2 = NCO + CO                                  3.70E+12  0.00  0.00E+00
122 O + NCO = NO + CO                                    2.35E+13  0.00  0.00E+00
123 N + NCO = N2 + CO                                    2.00E+13  0.00  0.00E+00
124 H + NCO = NH + CO                                    5.40E+13  0.00  0.00E+00
125 CH + NO = N + HCO                                    3.00E+13  0.00  0.00E+00
126 CH + NO = O + HCN                                    5.00E+13  0.00  0.00E+00
127 CH + NO = H + NCO                                    2.00E+13  0.00  0.00E+00
128 NH + OH = N + H2O                                    2.00E+09  1.20  0.00E+00
129 NH + OH = HNO + H                                    2.00E+13  0.00  0.00E+00
130 HO2 + NO = NO2 + OH                                  2.11E+12  0.00 -4.80E+02
131 O + NO2 = NO + O2                                    3.90E+12  0.00 -2.40E+02
132 NO + O + M = NO2 + M                                 1.06E+20 -1.41  0.00E+00
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 133 NO2 + H = NO + OH                                 1.32E+14  0.00  3.60E+02
 134 NO + H = N + OH                                   2.63E+14  0.00  5.04E+04
 135 NO + O = N + O2                                   3.80E+09  1.00  4.14E+04
 136 O + N2 = NO + N                                   1.80E+14  0.00  7.63E+04
 137 N + NO2 = 2NO                                     4.00E+12  0.00  0.00E+00
 138 N2O + M = N2 + O + M                              6.92E+23 -2.50  6.50E+04
 139 O + N2O = N2 + O2                                 1.40E+12  0.00  1.08E+04
 140 O + N2O = 2NO                                     2.90E+13  0.00  2.32E+04
 141 N2O + H = N2 + OH                                 4.40E+14  0.00  1.89E+04
 142 NO2 + H2 = HNO2 + H                               2.40E+13  0.00  2.90E+04
 143 OH + NO2 + M = HNO3 + M                           3.00E+15  0.00 -3.80E+03
    3body efficiencies
      O2   0.70  H2   1.40
 144 OH + NO + M = HNO2 + M                            5.60E+15  0.00 -1.70E+03
 145 HNO + H = H2 + NO                                 4.50E+11  0.72  6.60E+02
 146 H + NO + M = HNO + M                              8.95E+19 -1.32  7.40E+02
 147 HNO + OH = H2O + NO                               1.30E+07  1.90 -9.50E+02


    ** The following  5 elements considered for this problem **
    AR C  H  O  N

    ** The following  40 reacting species considered for this problem **
CH4 CH3 H H2 O2 HO2 O OH H2O CH3O CH2O C2H6 C2H5 C2H4 CH2 C2H3 C2H2 HCO C2H2O
C2H CO C2HO CH2CO CO2 CH H2O2 N2 HCN N CN NCO NH HNCO NH2 NO HNO NO2 N2O HNO2
HNO3

    ** The following  1 inert species considered for this problem **
AR


** New input data given in CGS  units **   ** Output required in CGS  units **

                      ** Assigned variable profile **

              Area is given by the following polynomial
   Area (cm**2) =   0.000E+00x**3 + 0.000E+00x**2 + 0.000E+00x + 1.507E+00

                       ** Constant-area problem **

    Fuel-air equivalence ratio =  0.3000  Oxygen mole fraction in air =  0.0000

         Number of species ODE's:   40  Total number of ODE's:   43

                            Integration Controls
Method Flag (MF): 21  Rel. Error: 1.000E-04  Species Abs. Error: 1.000E-10

    Maximum number of steps allowed for the complete problem:  2000

            ** Output required at following   2 axial distances (cm) **
  2.875E+00  5.750E+00



                       ** Initial Conditions **



         Time 0.00E+00 s  Axial Position 0.00E+00 cm  Area 1.51E+00sq cm


  Thermodynamic Properties              Integration Indicators

    Pressure (atm)            2060.000     Steps from last print      0
    Velocity (cm/s)            6633.70     Average step size   0.00E+00
    Density (g/cm**3)        6.212E-01     Method Order               0
    Temperature (K)            1150.00     Incr. CPU Time          0.00 s
    Mass Flow Rate (g/s)     6.210E+03
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Entropy (cal/g/K)	1.503E+00	Total number of steps	0
Mach Number	1.000E-01	Funct evaluations	0
Gamma (Frozen)	1.310	Jacobian evaluations	0
Enthalpy (cal/g)	1.865E+02	Total CPU Time	0.00 s
Sp. heat, cp (cal/g/K)	2.954E-01		

Chemical Properties

Wi = Net molar production rate per unit volume of species i (mole/cm**3/s)
kj = Forward rate const for reaction j (cgs units)
XH,j = Net energy exch rate for reaction j (cal-cm**3/g**2/s)
Eq,j = Equilibration factor for reaction j (= Net rate/Positive dir rate)

Species i	Mass Fr.	Mole Fr.	Wi	Reac No,j	kj	XH,j	Eq,j
CH4	1.66E-02	2.94E-02	-2.81E+06	1	3.78E+00	1.44E+01	1.00E+00
CH3	0.00E+00	0.00E+00	2.81E+06	2	5.22E+11	0.00E+00	0.00E+00
H	0.00E+00	0.00E+00	5.29E-05	3	1.00E+12	3.88E+11	1.00E+00
H2	0.00E+00	0.00E+00	0.00E+00	4	9.23E+11	0.00E+00	0.00E+00
O2	2.26E-01	2.01E-01	-2.81E+06	5	2.01E+12	0.00E+00	0.00E+00
HO2	0.00E+00	0.00E+00	2.81E+06	6	9.01E+07	0.00E+00	0.00E+00
O	0.00E+00	0.00E+00	2.05E-10	7	7.20E+08	0.00E+00	0.00E+00
OH	0.00E+00	0.00E+00	6.82E-05	8	3.20E+12	0.00E+00	0.00E+00
H2O	7.60E-03	1.20E-02	-6.82E-05	9	5.11E+09	0.00E+00	0.00E+00
CH3O	0.00E+00	0.00E+00	0.00E+00	10	1.43E+13	0.00E+00	0.00E+00
CH2O	0.00E+00	0.00E+00	0.00E+00	11	9.77E+10	0.00E+00	0.00E+00
C2H6	0.00E+00	0.00E+00	0.00E+00	12	2.79E+12	0.00E+00	0.00E+00
C2H5	0.00E+00	0.00E+00	0.00E+00	13	5.60E+12	0.00E+00	0.00E+00
C2H4	0.00E+00	0.00E+00	0.00E+00	14	7.45E+12	0.00E+00	0.00E+00
CH2	0.00E+00	0.00E+00	0.00E+00	15	1.28E+11	0.00E+00	0.00E+00
C2H3	0.00E+00	0.00E+00	0.00E+00	16	1.54E+11	0.00E+00	0.00E+00
C2H2	0.00E+00	0.00E+00	0.00E+00	17	2.00E+12	0.00E+00	0.00E+00
HCO	0.00E+00	0.00E+00	0.00E+00	18	2.00E+13	0.00E+00	0.00E+00
C2H2O	0.00E+00	0.00E+00	0.00E+00	19	3.46E+11	0.00E+00	0.00E+00
C2H	0.00E+00	0.00E+00	0.00E+00	20	2.21E+02	0.00E+00	0.00E+00
CO	0.00E+00	0.00E+00	1.02E-14	21	1.59E+12	0.00E+00	0.00E+00
C2HO	0.00E+00	0.00E+00	0.00E+00	22	1.31E+12	0.00E+00	0.00E+00
CH2CO	0.00E+00	0.00E+00	0.00E+00	23	6.96E+12	0.00E+00	0.00E+00
CO2	4.64E-04	3.00E-04	-1.02E-14	24	2.80E+12	0.00E+00	0.00E+00
CH	0.00E+00	0.00E+00	0.00E+00	25	2.49E+09	0.00E+00	0.00E+00
H2O2	0.00E+00	0.00E+00	0.00E+00	26	4.42E+12	0.00E+00	0.00E+00
N2	7.37E-01	7.48E-01	-1.94E-10	27	3.00E+13	0.00E+00	0.00E+00
HCN	0.00E+00	0.00E+00	0.00E+00	28	3.00E+13	0.00E+00	0.00E+00
N	0.00E+00	0.00E+00	0.00E+00	29	5.00E+12	0.00E+00	0.00E+00
CN	0.00E+00	0.00E+00	0.00E+00	30	3.00E+13	0.00E+00	0.00E+00
NCO	0.00E+00	0.00E+00	0.00E+00	31	3.00E+13	0.00E+00	0.00E+00
NH	0.00E+00	0.00E+00	0.00E+00	32	1.94E-04	0.00E+00	0.00E+00
HNCO	0.00E+00	0.00E+00	0.00E+00	33	5.87E+12	0.00E+00	0.00E+00
NH2	0.00E+00	0.00E+00	0.00E+00	34	5.87E+12	0.00E+00	0.00E+00
NO	0.00E+00	0.00E+00	0.00E+00	35	7.01E+09	0.00E+00	0.00E+00
HNO	0.00E+00	0.00E+00	0.00E+00	36	9.74E+10	0.00E+00	0.00E+00
NO2	0.00E+00	0.00E+00	0.00E+00	37	1.50E+10	0.00E+00	0.00E+00
N2O	0.00E+00	0.00E+00	1.94E-10	38	2.00E+10	0.00E+00	0.00E+00
HNO2	0.00E+00	0.00E+00	0.00E+00	39	2.03E+09	0.00E+00	0.00E+00
HNO3	0.00E+00	0.00E+00	0.00E+00	40	2.59E+13	0.00E+00	0.00E+00
AR	1.26E-02	9.00E-03	0.00E+00	41	2.59E+13	0.00E+00	0.00E+00
				42	2.00E+13	0.00E+00	0.00E+00
				43	1.10E+12	0.00E+00	0.00E+00
				44	1.00E+14	0.00E+00	0.00E+00
				45	1.00E+13	0.00E+00	0.00E+00
				46	1.00E+14	0.00E+00	0.00E+00
				47	3.00E+13	0.00E+00	0.00E+00
				48	4.17E+12	0.00E+00	0.00E+00
				49	1.00E+13	0.00E+00	0.00E+00
				50	2.80E+13	0.00E+00	0.00E+00
				51	3.13E+12	0.00E+00	0.00E+00
				52	2.52E+12	0.00E+00	0.00E+00
				53	1.51E+12	0.00E+00	0.00E+00

54	3.02E+11	0.00E+00	0.00E+00
55	2.00E+13	0.00E+00	0.00E+00
56	9.69E+11	0.00E+00	0.00E+00
57	7.91E+04	0.00E+00	0.00E+00
58	5.00E+13	0.00E+00	0.00E+00
59	3.66E+11	0.00E+00	0.00E+00
60	2.00E+13	0.00E+00	0.00E+00
61	2.02E+01	0.00E+00	0.00E+00
62	1.71E+13	0.00E+00	0.00E+00
63	8.98E+12	0.00E+00	0.00E+00
64	8.29E+12	0.00E+00	0.00E+00
65	1.02E+11	0.00E+00	0.00E+00
66	2.65E+13	0.00E+00	0.00E+00
67	2.00E+13	0.00E+00	0.00E+00
68	7.62E-02	0.00E+00	0.00E+00
69	3.96E+08	0.00E+00	0.00E+00
70	2.99E+08	0.00E+00	0.00E+00
71	8.43E+13	0.00E+00	0.00E+00
72	4.12E+11	0.00E+00	0.00E+00
73	2.51E+12	0.00E+00	0.00E+00
74	3.30E+13	0.00E+00	0.00E+00
75	8.07E+11	0.00E+00	0.00E+00
76	6.85E+12	0.00E+00	0.00E+00
77	3.47E+08	0.00E+00	0.00E+00
78	4.02E+12	0.00E+00	0.00E+00
79	5.05E+12	0.00E+00	0.00E+00
80	5.00E+12	0.00E+00	0.00E+00
81	3.20E+13	0.00E+00	0.00E+00
82	6.38E+12	0.00E+00	0.00E+00
83	3.00E+13	0.00E+00	0.00E+00
84	3.00E+13	0.00E+00	0.00E+00
85	5.00E+13	0.00E+00	0.00E+00
86	7.34E+13	0.00E+00	0.00E+00
87	9.56E+10	0.00E+00	0.00E+00
88	1.62E+14	3.37E-09	1.00E+00
89	2.06E+03	0.00E+00	0.00E+00
90	2.69E+11	0.00E+00	0.00E+00
91	4.91E+09	0.00E+00	0.00E+00
92	2.20E+10	0.00E+00	0.00E+00
93	1.51E+11	0.00E+00	0.00E+00
94	4.74E+11	0.00E+00	0.00E+00
95	1.75E+13	0.00E+00	0.00E+00
96	2.00E+13	0.00E+00	0.00E+00
97	3.61E+13	1.19E+01	1.00E+00
98	1.01E+14	0.00E+00	0.00E+00
99	1.64E+12	0.00E+00	0.00E+00
100	1.52E+12	0.00E+00	0.00E+00
101	2.65E+11	0.00E+00	0.00E+00
102	2.07E+12	0.00E+00	0.00E+00
103	3.23E+08	0.00E+00	0.00E+00
104	2.01E+12	0.00E+00	0.00E+00
105	6.53E+15	0.00E+00	0.00E+00
106	1.36E-05	4.09E-05	1.00E+00
107	4.35E+14	0.00E+00	0.00E+00
108	1.25E-04	0.00E+00	0.00E+00
109	5.83E-08	1.72E-06	1.00E+00
110	2.45E+07	0.00E+00	0.00E+00
111	2.67E+12	0.00E+00	0.00E+00
112	1.29E+09	0.00E+00	0.00E+00
113	1.51E+11	0.00E+00	0.00E+00
114	3.77E+10	0.00E+00	0.00E+00
115	2.21E+09	0.00E+00	0.00E+00
116	7.70E+13	0.00E+00	0.00E+00
117	4.00E+13	0.00E+00	0.00E+00
118	1.95E+12	0.00E+00	0.00E+00
119	6.81E+11	0.00E+00	0.00E+00
120	7.44E+12	0.00E+00	0.00E+00
121	3.70E+12	0.00E+00	0.00E+00
122	2.35E+13	0.00E+00	0.00E+00

123	2.00E+13	0.00E+00	0.00E+00
124	5.40E+13	0.00E+00	0.00E+00
125	3.00E+13	0.00E+00	0.00E+00
126	5.00E+13	0.00E+00	0.00E+00
127	2.00E+13	0.00E+00	0.00E+00
128	9.42E+12	0.00E+00	0.00E+00
129	2.00E+13	0.00E+00	0.00E+00
130	2.60E+12	0.00E+00	0.00E+00
131	4.33E+12	0.00E+00	0.00E+00
132	5.13E+15	0.00E+00	0.00E+00
133	1.13E+14	0.00E+00	0.00E+00
134	6.92E+04	0.00E+00	0.00E+00
135	6.00E+04	0.00E+00	0.00E+00
136	5.81E-01	0.00E+00	0.00E+00
137	4.00E+12	0.00E+00	0.00E+00
138	6.85E+03	0.00E+00	0.00E+00
139	1.24E+10	3.97E-05	1.00E+00
140	1.16E+09	0.00E+00	0.00E+00
141	1.14E+11	0.00E+00	0.00E+00
142	7.40E+07	0.00E+00	0.00E+00
143	1.58E+16	0.00E+00	0.00E+00
144	1.18E+16	0.00E+00	0.00E+00
145	5.39E+13	0.00E+00	0.00E+00
146	5.90E+15	0.00E+00	0.00E+00
147	1.29E+13	0.00E+00	0.00E+00

Derivs (cgs units): T -1.24E+08 RHO 6.80E+04 V -7.26E+08

Mix Mol Wt. 28.454 Total Energy Exch Rate (cal-cm**3/g**2/s) 3.88E+11 Mass Fr. Sum 1.00000

CPU Time for initialization of LSENS = 0.00 s

Time 3.59E-04 s Axial Position 2.88E+00 cm Area 1.51E+00sq cm

Thermodynamic Properties

Pressure (atm)	2035.639
Velocity (cm/s)	10475.71
Density (g/cm**3)	3.930E-01
Temperature (K)	1796.22
Mass Flow Rate (g/s)	6.204E+03
Entropy (cal/g/K)	1.646E+00
Mach Number	1.275E-01
Gamma (Frozen)	1.286
Enthalpy (cal/g)	1.859E+02
Sp. heat, cp (cal/g/K)	3.144E-01

Integration Indicators

Steps from last print	318
Average step size	1.33E-02
Method Order	1
Incr. CPU Time	0.00 s
Total number of steps	318
Funct evaluations	595
Jacobian evaluations	117
Total CPU Time	0.00 s

Chemical Properties

Wi = Net molar production rate per unit volume of species i (mole/cm**3/s)
kj = Forward rate const for reaction j (cgs units)
XH,j = Net energy exch rate for reaction j (cal-cm**3/g**2/s)
Eq,j = Equilibration factor for reaction j (= Net rate/Positive dir rate)

Species i	Mass Fr.	Mole Fr.	Wi	Reac No,j	kj	XH,j	Eq,j
CH4	1.85E-16	3.28E-16	1.84E-11	1	3.93E+06	-3.43E-10	2.06E-03
CH3	6.63E-17	1.26E-16	-1.86E-11	2	5.92E+12	-1.06E-14	2.02E-03
H	1.25E-10	3.54E-09	-4.29E-10	3	1.00E+12	-6.31E-06	2.06E-03
H2	1.52E-08	2.15E-07	-7.52E-10	4	6.98E+12	-1.43E-11	2.09E-03
O2	1.60E-01	1.42E-01	-8.94E-05	5	6.72E+12	6.37E-09	2.08E-03
HO2	1.13E-05	9.76E-06	-1.23E-08	6	8.39E+09	5.29E-06	1.00E+00

O	5.48E-07	9.74E-07	-1.47E-08
OH	4.67E-05	7.82E-05	-1.76E-06
H2O	4.48E-02	7.07E-02	-3.92E-07
CH3O	2.19E-19	2.01E-19	-2.59E-16
CH2O	4.98E-15	4.72E-15	6.52E-14
C2H6	1.23E-23	1.16E-23	-3.74E-18
C2H5	4.27E-24	4.18E-24	4.73E-17
C2H4	1.20E-18	1.22E-18	-7.50E-16
CH2	2.86E-18	5.81E-18	1.15E-14
C2H3	1.05E-18	1.11E-18	-1.95E-15
C2H2	3.29E-13	3.60E-13	1.32E-12
HCO	1.48E-15	1.45E-15	-7.10E-14
C2H2O	4.26E-15	2.88E-15	1.52E-14
C2H	5.47E-18	6.22E-18	8.48E-14
CO	3.36E-07	3.41E-07	-2.08E-08
C2HO	2.92E-16	2.02E-16	2.04E-14
CH2CO	8.02E-06	5.43E-06	-1.57E-08
CO2	4.59E-02	2.97E-02	5.23E-08
CH	7.12E-22	1.56E-21	5.63E-18
H2O2	1.27E-06	1.06E-06	1.51E-08
N2	7.37E-01	7.48E-01	-8.21E-05
HCN	1.15E-14	1.21E-14	-6.38E-12
N	1.08E-13	2.20E-13	1.63E-13
CN	3.56E-21	3.90E-21	3.16E-16
NCO	1.03E-15	6.98E-16	-3.51E-13
NH	4.93E-14	9.35E-14	2.53E-14
HNCO	2.39E-13	1.58E-13	2.77E-12
NH2	7.74E-16	1.38E-15	2.82E-13
NO	9.28E-07	8.80E-07	1.48E-04
HNO	6.61E-12	6.06E-12	1.02E-09
NO2	1.35E-07	8.36E-08	1.40E-05
N2O	1.30E-05	8.38E-06	-1.24E-08
HNO2	9.78E-09	5.92E-09	2.41E-06
HNO3	1.98E-10	8.96E-11	1.46E-07
AR	1.26E-02	9.00E-03	0.00E+00

7	2.94E+09	-3.45E-06	1.00E+00
8	3.20E+12	4.60E-07	1.00E+00
9	1.39E+11	7.09E-07	1.00E+00
10	1.20E+13	5.25E-14	1.00E+00
11	5.42E+11	-1.35E-17	9.93E-01
12	2.13E+13	-6.25E-18	9.39E-01
13	3.23E+13	-1.82E-15	9.39E-01
14	2.20E+13	-4.91E-13	9.39E-01
15	1.69E+13	-1.09E-11	3.22E-03
16	2.84E+11	8.68E-15	3.22E-03
17	2.00E+12	7.65E-21	3.18E-03
18	2.00E+13	8.62E-17	9.87E-01
19	7.35E+12	7.43E-15	7.16E-02
20	5.84E+07	-6.49E-09	6.39E-01
21	5.77E+12	9.13E-10	7.16E-02
22	1.53E+12	-2.64E-09	1.00E+00
23	1.63E+13	-6.40E-10	1.00E+00
24	6.16E+12	-6.67E-11	1.00E+00
25	3.83E+11	-3.64E-05	6.12E-01
26	4.26E+12	-6.56E-05	1.00E+00
27	3.00E+13	1.37E-11	6.12E-01
28	3.00E+13	-3.23E-09	1.00E+00
29	5.00E+12	6.31E-08	6.12E-01
30	3.00E+13	4.58E-21	2.27E-01
31	3.00E+13	1.23E-18	9.83E-01
32	4.02E+03	2.17E-07	9.56E-01
33	1.93E+13	-4.00E-04	1.00E+00
34	1.93E+13	-1.94E-04	1.00E+00
35	3.56E+11	3.66E-06	9.56E-01
36	2.15E+12	5.70E-04	9.56E-01
37	3.51E+11	-2.78E-04	1.00E+00
38	1.27E+11	2.32E-03	9.58E-01
39	8.81E+09	-1.69E-05	1.00E+00
40	3.28E+13	-1.12E-03	1.00E+00
41	3.28E+13	-5.21E-03	1.00E+00
42	2.00E+13	-5.77E-07	1.00E+00
43	1.26E+12	-3.67E-03	1.00E+00
44	1.00E+14	-2.41E-06	1.00E+00
45	1.00E+13	-5.28E-06	1.00E+00
46	1.00E+14	-2.19E-09	1.00E+00
47	3.00E+13	-4.12E-18	9.94E-01
48	5.71E+12	-2.36E-19	9.72E-01
49	1.00E+13	-3.83E-17	1.00E+00
50	2.80E+13	-1.19E-04	1.00E+00
51	4.28E+12	-1.27E-05	6.17E-01
52	4.33E+12	-1.76E-09	1.00E+00
53	5.32E+12	-9.12E-11	6.17E-01
54	1.06E+12	-7.66E-10	6.17E-01
55	2.00E+13	-7.10E-06	1.00E+00
56	1.20E+12	-2.07E-07	1.00E+00
57	1.00E+09	2.76E-04	1.00E+00
58	5.00E+13	-2.74E-08	1.00E+00
59	6.22E+12	-6.82E-06	1.00E+00
60	2.00E+13	-1.47E-12	1.00E+00
61	6.98E+06	3.58E-06	9.77E-01
62	2.69E+13	-3.48E-04	9.77E-01
63	2.40E+13	-6.78E-09	9.77E-01
64	1.45E+13	-9.74E-07	9.77E-01
65	8.97E+11	-9.38E-18	9.77E-01
66	2.65E+13	-1.16E-17	2.18E-02
67	2.00E+13	-6.69E-07	1.00E+00
68	1.40E+05	-2.35E-09	4.97E-01
69	3.05E+10	-9.01E-14	4.97E-01
70	2.32E+10	-2.53E-11	4.97E-01
71	8.43E+13	-8.91E-07	1.00E+00
72	1.98E+12	2.27E-07	4.97E-01
73	2.80E+12	-1.02E-08	1.00E+00
74	3.30E+13	-6.48E-07	1.00E+00
75	3.02E+12	-1.86E-04	1.00E+00

76	8.67E+12	-6.42E-04	1.00E+00
77	2.75E+10	-1.12E-13	9.95E-01
78	1.57E+13	-1.53E-07	9.95E-01
79	1.51E+13	-9.36E-13	9.95E-01
80	5.00E+12	6.01E-19	9.76E-01
81	3.20E+13	1.86E-17	9.91E-01
82	6.79E+12	-1.24E-03	1.98E-02
83	3.00E+13	-8.99E-08	1.97E-02
84	3.00E+13	-1.16E-07	1.97E-02
85	5.00E+13	-1.44E-05	1.97E-02
86	7.34E+13	-8.20E-10	1.98E-02
87	8.89E+11	4.82E-04	1.98E-02
88	2.60E+14	6.79E-03	3.63E-05
89	3.82E+06	-7.45E-04	4.04E-04
90	4.70E+11	2.07E-04	5.38E-07
91	2.02E+11	-1.81E-02	3.71E-04
92	3.96E+11	-9.51E+00	1.67E-05
93	1.46E+12	6.16E+00	4.04E-04
94	4.20E+12	-1.46E-04	7.20E-05
95	2.08E+13	-1.85E-03	3.96E-05
96	2.00E+13	3.86E-01	3.24E-05
97	3.34E+13	3.33E+01	1.57E-05
98	1.12E+14	-6.05E-02	3.72E-04
99	9.10E+12	1.50E-01	3.35E-04
100	1.60E+12	2.18E+00	3.91E-04
101	2.05E+11	-3.04E-01	3.75E-04
102	3.65E+12	2.18E-05	1.89E-05
103	4.18E+11	4.15E+00	1.12E-07
104	6.78E+12	1.17E-01	5.53E-05
105	4.45E+15	1.89E+01	3.33E-06
106	2.10E+02	1.20E-01	1.90E-05
107	2.78E+14	5.99E-05	3.57E-05
108	4.59E+02	-1.33E-06	3.63E-05
109	4.38E+00	4.02E-02	4.40E-04
110	4.88E+08	2.30E-12	1.00E+00
111	5.61E+12	1.15E-10	9.99E-01
112	1.71E+11	5.33E-08	9.99E-01
113	1.07E+12	-2.57E-08	9.99E-01
114	2.68E+11	-1.45E-07	1.00E+00
115	1.66E+10	-2.67E-07	1.00E+00
116	7.70E+13	-2.66E-11	9.58E-01
117	4.00E+13	-1.64E-10	4.71E-01
118	8.03E+12	-4.77E-09	3.11E-01
119	2.64E+12	-1.61E-08	9.98E-01
120	6.95E+12	-1.42E-08	4.71E-01
121	3.70E+12	4.31E-10	4.71E-01
122	2.35E+13	-2.02E-06	1.00E+00
123	2.00E+13	-2.03E-13	3.02E-01
124	5.40E+13	-5.66E-09	9.64E-01
125	3.00E+13	-2.05E-12	1.00E+00
126	5.00E+13	-3.36E-12	5.52E-01
127	2.00E+13	-2.49E-12	1.00E+00
128	1.61E+13	6.33E-03	5.54E-01
129	2.00E+13	-2.49E-03	9.98E-01
130	2.41E+12	-2.02E-01	1.64E-03
131	4.17E+12	3.22E-02	1.67E-03
132	2.73E+15	-3.60E+00	1.23E-03
133	1.19E+14	1.61E-03	1.27E-03
134	1.93E+08	-4.55E-02	9.99E-01
135	6.32E+07	-2.67E+00	9.99E-01
136	9.50E+04	6.44E+00	1.00E+00
137	4.00E+12	-7.03E-06	9.99E-01
138	6.25E+07	-1.78E+01	6.88E-04
139	6.77E+10	6.09E-02	1.13E-03
140	4.42E+10	-1.58E+01	1.00E+00
141	2.22E+12	3.67E-03	7.24E-04
142	7.11E+09	-5.17E-06	1.30E-03
143	8.70E+15	-4.69E-02	1.02E-06
144	9.02E+15	-7.80E-01	1.48E-06

145	8.24E+13	-1.03E-07	8.60E-04
146	3.68E+15	8.00E-03	8.24E-04
147	2.59E+13	-8.50E-04	8.05E-04

Derivs (cgs units): T -2.54E-03 RHO 5.93E-07 V -1.58E-02

Mix Mol Wt. 28.454 Total Energy Exch Rate 2.13E+01 Mass Fr. Sum 1.00000
(cal-cm**3/g**2/s)

Time 6.34E-04 s Axial Position 5.75E+00 cm Area 1.51E+00sq cm

Thermodynamic Properties

Pressure (atm)	2035.640
Velocity (cm/s)	10475.66
Density (g/cm**3)	3.930E-01
Temperature (K)	1796.22
Mass Flow Rate (g/s)	6.204E+03
Entropy (cal/g/K)	1.646E+00
Mach Number	1.275E-01
Gamma (Frozen)	1.286
Enthalpy (cal/g)	1.859E+02
Sp. heat, cp (cal/g/K)	3.144E-01

Integration Indicators

Steps from last print	2
Average step size	7.69E+00
Method Order	1
Incr. CPU Time	0.00 s
Total number of steps	320
Funct evaluations	598
Jacobian evaluations	118
Total CPU Time	0.00 s

Chemical Properties

Wi = Net molar production rate per unit volume of species i (mole/cm**3/s)
kj = Forward rate const for reaction j (cgs units)
XH,j = Net energy exch rate for reaction j (cal-cm**3/g**2/s)
Eq,j = Equilibration factor for reaction j (= Net rate/Positive dir rate)

Species i	Mass Fr.	Mole Fr.	Wi	Reac No,j	kj	XH,j	Eq,j
CH4	1.84E-16	3.27E-16	4.69E-15	1	3.93E+06	4.51E-13	2.72E-06
CH3	6.61E-17	1.25E-16	-4.86E-15	2	5.92E+12	1.91E-16	3.66E-05
H	1.25E-10	3.54E-09	-1.51E-08	3	1.00E+12	-1.43E-09	4.68E-07
H2	1.52E-08	2.15E-07	-7.48E-10	4	6.98E+12	-2.23E-13	3.27E-05
O2	1.60E-01	1.42E-01	-8.94E-05	5	6.72E+12	4.92E-11	1.61E-05
HO2	1.13E-05	9.76E-06	-5.42E-09	6	8.39E+09	5.27E-06	1.00E+00
O	5.48E-07	9.74E-07	7.82E-08	7	2.94E+09	-3.43E-06	1.00E+00
OH	4.67E-05	7.82E-05	1.69E-05	8	3.20E+12	4.58E-07	1.00E+00
H2O	4.48E-02	7.07E-02	-3.91E-07	9	1.39E+11	7.06E-07	1.00E+00
CH3O	2.18E-19	2.00E-19	2.52E-16	10	1.20E+13	3.13E-15	9.93E-01
CH2O	4.98E-15	4.72E-15	8.21E-18	11	5.42E+11	-1.34E-17	9.94E-01
C2H6	7.36E-25	6.96E-25	-9.55E-22	12	2.13E+13	7.57E-21	1.86E-02
C2H5	4.27E-24	4.18E-24	1.03E-20	13	3.23E+13	2.21E-18	1.87E-02
C2H4	1.19E-18	1.21E-18	1.10E-19	14	2.20E+13	5.96E-16	1.87E-02
CH2	2.86E-18	5.81E-18	-1.09E-17	15	1.69E+13	-3.72E-15	1.10E-06
C2H3	1.05E-18	1.11E-18	-6.04E-19	16	2.84E+11	1.15E-17	4.29E-06
C2H2	3.29E-13	3.60E-13	-2.45E-15	17	2.00E+12	-7.86E-23	3.28E-05
HCO	1.48E-15	1.45E-15	-8.61E-16	18	2.00E+13	8.57E-17	9.87E-01
C2H2O	4.26E-15	2.88E-15	-1.99E-17	19	7.35E+12	7.88E-15	7.59E-02
C2H	5.47E-18	6.22E-18	4.65E-17	20	5.84E+07	-6.50E-09	6.41E-01
CO	3.36E-07	3.41E-07	-1.36E-09	21	5.77E+12	9.68E-10	7.60E-02
C2HO	2.92E-16	2.02E-16	9.02E-18	22	1.53E+12	-2.63E-09	1.00E+00
CH2CO	8.01E-06	5.42E-06	-1.57E-08	23	1.63E+13	-6.36E-10	1.00E+00
CO2	4.59E-02	2.97E-02	3.28E-08	24	6.16E+12	-6.64E-11	1.00E+00
CH	7.11E-22	1.55E-21	-1.29E-20	25	3.83E+11	-3.64E-05	6.12E-01
H2O2	1.27E-06	1.06E-06	3.34E-08	26	4.26E+12	-6.56E-05	1.00E+00
N2	7.37E-01	7.48E-01	-8.20E-05	27	3.00E+13	1.37E-11	6.12E-01
HCN	3.18E-16	3.35E-16	-1.76E-13	28	3.00E+13	-3.23E-09	1.00E+00
N	1.08E-13	2.20E-13	2.85E-12	29	5.00E+12	6.31E-08	6.12E-01
CN	1.86E-22	2.04E-22	-3.98E-18	30	3.00E+13	4.50E-21	2.24E-01
NCO	7.63E-17	5.17E-17	-9.73E-15	31	3.00E+13	1.23E-18	9.83E-01
NH	4.96E-14	9.40E-14	2.85E-14	32	4.02E+03	2.17E-07	9.56E-01
HNCO	2.35E-13	1.56E-13	-3.32E-13	33	1.93E+13	-4.00E-04	1.00E+00

NH2	3.86E-15	6.86E-15	2.75E-13	34	1.93E+13	-1.94E-04	1.00E+00
NO	4.05E-06	3.84E-06	1.65E-04	35	3.56E+11	3.66E-06	9.56E-01
HNO	2.88E-11	2.64E-11	1.98E-09	36	2.15E+12	5.69E-04	9.56E-01
NO2	5.90E-07	3.65E-07	1.53E-05	37	3.51E+11	-2.78E-04	1.00E+00
N2O	1.30E-05	8.38E-06	-9.95E-09	38	1.27E+11	2.32E-03	9.58E-01
HNO2	4.27E-08	2.58E-08	-1.49E-05	39	8.80E+09	-1.69E-05	1.00E+00
HNO3	8.66E-10	3.91E-10	-1.21E-06	40	3.28E+13	-1.12E-03	1.00E+00
AR	1.26E-02	9.00E-03	0.00E+00	41	3.28E+13	-5.21E-03	1.00E+00
				42	2.00E+13	-5.77E-07	1.00E+00
				43	1.26E+12	-3.67E-03	1.00E+00
				44	1.00E+14	-2.41E-06	1.00E+00
				45	1.00E+13	-5.28E-06	1.00E+00
				46	1.00E+14	-2.18E-09	1.00E+00
				47	3.00E+13	-4.12E-18	9.94E-01
				48	5.71E+12	-2.36E-19	9.72E-01
				49	1.00E+13	-3.83E-17	1.00E+00
				50	2.80E+13	-1.19E-04	1.00E+00
				51	4.28E+12	-1.27E-05	6.17E-01
				52	4.32E+12	-1.76E-09	1.00E+00
				53	5.32E+12	-9.12E-11	6.17E-01
				54	1.06E+12	-7.66E-10	6.17E-01
				55	2.00E+13	-7.10E-06	1.00E+00
				56	1.20E+12	-2.07E-07	1.00E+00
				57	1.00E+09	2.76E-04	1.00E+00
				58	5.00E+13	-2.74E-08	1.00E+00
				59	6.22E+12	-6.79E-06	1.00E+00
				60	2.00E+13	-1.47E-12	1.00E+00
				61	6.97E+06	3.58E-06	9.77E-01
				62	2.69E+13	-3.47E-04	9.77E-01
				63	2.40E+13	-6.78E-09	9.77E-01
				64	1.45E+13	-9.73E-07	9.77E-01
				65	8.97E+11	-9.34E-18	9.77E-01
				66	2.65E+13	-1.05E-17	1.98E-02
				67	2.00E+13	-6.66E-07	1.00E+00
				68	1.40E+05	-2.36E-09	4.99E-01
				69	3.05E+10	-9.04E-14	4.99E-01
				70	2.32E+10	-2.54E-11	4.99E-01
				71	8.43E+13	-8.87E-07	1.00E+00
				72	1.98E+12	2.28E-07	4.99E-01
				73	2.80E+12	-1.02E-08	1.00E+00
				74	3.30E+13	-6.48E-07	1.00E+00
				75	3.02E+12	-1.86E-04	1.00E+00
				76	8.67E+12	-6.41E-04	1.00E+00
				77	2.75E+10	-1.12E-13	9.95E-01
				78	1.57E+13	-1.53E-07	9.95E-01
				79	1.51E+13	-9.35E-13	9.95E-01
				80	5.00E+12	6.01E-19	9.76E-01
				81	3.20E+13	1.86E-17	9.91E-01
				82	6.79E+12	-1.24E-03	1.98E-02
				83	3.00E+13	-8.99E-08	1.97E-02
				84	3.00E+13	-1.16E-07	1.97E-02
				85	5.00E+13	-1.44E-05	1.97E-02
				86	7.34E+13	-8.20E-10	1.98E-02
				87	8.89E+11	4.81E-04	1.98E-02
				88	2.60E+14	7.86E-03	4.19E-05
				89	3.82E+06	-7.01E-04	3.80E-04
				90	4.70E+11	2.51E-03	6.51E-06
				91	2.02E+11	-1.69E-02	3.47E-04
				92	3.96E+11	-9.44E+00	1.66E-05
				93	1.46E+12	5.89E+00	3.86E-04
				94	4.20E+12	-1.40E-04	6.93E-05
				95	2.08E+13	-1.73E-03	3.71E-05
				96	2.00E+13	3.84E-01	3.22E-05
				97	3.34E+13	3.33E+01	1.57E-05
				98	1.12E+14	-5.76E-02	3.54E-04
				99	9.10E+12	1.43E-01	3.20E-04
				100	1.60E+12	2.08E+00	3.73E-04
				101	2.05E+11	-2.89E-01	3.57E-04
				102	3.65E+12	2.16E-05	1.87E-05

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                                        103  4.18E+11  3.95E+00  1.06E-07
                                        104  6.78E+12  1.11E-01  5.28E-05
                                        105  4.45E+15  1.81E+01  3.19E-06
                                        106  2.10E+02  1.18E-01  1.88E-05
                                        107  2.78E+14  5.94E-05  3.54E-05
                                        108  4.59E+02 -1.24E-06  3.39E-05
                                        109  4.38E+00  3.85E-02  4.22E-04
                                        110  4.88E+08  2.30E-12  1.00E+00
                                        111  5.61E+12  3.19E-12  9.98E-01
                                        112  1.71E+11  1.48E-09  9.98E-01
                                        113  1.07E+12 -7.13E-10  9.99E-01
                                        114  2.68E+11 -4.02E-09  9.99E-01
                                        115  1.66E+10 -7.31E-09  9.87E-01
                                        116  7.70E+13 -2.77E-13  1.91E-01
                                        117  4.00E+13 -4.54E-12  2.49E-01
                                        118  8.03E+12  9.25E-09  8.91E-01
                                        119  2.64E+12 -1.57E-08  9.91E-01
                                        120  6.95E+12 -3.93E-10  2.50E-01
                                        121  3.70E+12  1.19E-11  2.49E-01
                                        122  2.35E+13 -1.49E-07  9.96E-01
                                        123  2.00E+13  4.19E-13  8.94E-01
                                        124  5.40E+13 -2.25E-10  5.18E-01
                                        125  3.00E+13 -8.95E-12  1.00E+00
                                        126  5.00E+13 -2.65E-11  9.97E-01
                                        127  2.00E+13 -1.09E-11  1.00E+00
                                        128  1.61E+13  6.33E-03  5.52E-01
                                        129  2.00E+13 -2.49E-03  9.92E-01
                                        130  2.41E+12 -2.98E-01  5.52E-04
                                        131  4.17E+12  4.92E-02  5.85E-04
                                        132  2.73E+15 -2.08E+00  1.63E-04
                                        133  1.19E+14  1.10E-03  1.99E-04
                                        134  1.93E+08 -4.54E-02  9.97E-01
                                        135  6.32E+07 -2.67E+00  9.97E-01
                                        136  9.50E+04  6.43E+00  1.00E+00
                                        137  4.00E+12 -3.07E-05  9.97E-01
                                        138  6.24E+07 -1.78E+01  6.88E-04
                                        139  6.77E+10  5.99E-02  1.11E-03
                                        140  4.42E+10 -1.58E+01  1.00E+00
                                        141  2.22E+12  3.67E-03  7.23E-04
                                        142  7.11E+09 -4.07E-06  2.35E-04
                                        143  8.70E+15  3.88E-01  1.93E-06
                                        144  9.02E+15  4.82E+00  2.09E-06
                                        145  8.24E+13 -1.13E-07  2.17E-04
                                        146  3.68E+15  7.75E-03  1.83E-04
                                        147  2.59E+13 -7.56E-04  1.64E-04

Derivs (cgs units):  T        -3.24E-03  RHO       6.99E-07  V        -1.86E-02

Mix Mol Wt.   28.454  Total Energy Exch Rate  2.73E+01  Mass Fr. Sum   1.00000
                        (cal-cm**3/g**2/s)


(LSENS)  End of this case


            Summary of computational work required for problem:
              Total no. of steps -                      320
              Total no. of derivative evaluations -     598
              Total no. of Jacobian evaluations -       118
              Total CPU Time -                        0.00 s

              Total CPU time (including I/O) =        0.00 s

(LSENS)     Read data for next case
```

```
                          ** Problem Data **

        1         2         3         4         5         6         7         8
2345678901234567890123456789012345678901234567890123456789012345678901234567890

                                Blank Line
                                Blank Line
                                Blank Line
                                Blank Line
                                Blank Line
                                Blank Line
 (CIMAGE) ** Warning: End of problem data, but no
    end of file indicator or incomplete data




(KINP)  ** Error: The ACTION switch (= "    " is illegal **
  Legal values are ADD, NEW, CHANGE, and REPEAT


(LSENS)     A fatal error has occurred - Case terminated
```

VITA

Ashley Owens was born Jackson, Tennessee, to Phillip and Dawn Owens in 1982. She lived in Caruthersville, Missouri for a short time. Her family then moved to Union City, Tennessee, in 1985. Finally , her family moved to Martin, Tennessee in 1986 and remained there. Growing up, Ashley played basketball and softball up until the time she graduated high school. She also played soccer for 5 years. Ashley also enjoyed riding horses. Ashley attended the University of Tennessee at Martin where she earned a bachelor's degree in Engineering. In 2005, she received the degree and decided to take one more step to receive her master's degree.

Friends and family helped to persuade her to try the University of Tennessee Space Institute in Tullahoma, Tennessee. While at UTSI, Ashley had the opportunity to make some great friends. Along with Dr. Schulz, Ashley had the opportunity to be present at J85 testing. Ashley has recently taken a job in Dresden, Tennessee, at Greenfield Products, Inc.