EVALUATION AND IMPROVEMENT OF LIQUID PROPELLANT
ROCKET CHUGGING ANALYSIS TECHNIQUES: FINAL REPORT PART II

A STUDY OF LOW FREQUENCY COMBUSTION INSTABILITY
IN ROCKET ENGINE PREBURNERS USING A HETEROGENEOUS
STIRRED TANK REACTOR MODEL

PREPARED BY

Timothy A. Bartrand

and presented as a thesis for the Master of Science Degree
The University of Tennessee, Knoxville
August, 1987

Work supported by NASA GRANT NAG8-542
Principal Investigator: Paul E. George, II
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I also thank NASA, Marshall Space Flight Center, Huntsville, AL, for funding this research and Dave Seymour, of Marshal Space Flight Center, for the information he provided me on the space shuttle main engine shutdown.
During the shutdown of the space shuttle main engine, oxygen flow is shut off from the fuel preburner and helium is used to push the residual oxygen (between the oxidizer valve and the preburner combustion chamber) into the combustion chamber. During this process a low frequency combustion instability, or chug, occurs. This chug has resulted in damage to the engine's augmented spark igniter due to backflow of the contents of the preburner combustion chamber into the oxidizer feed system.

To determine possible causes and fixes for the chug, the fuel preburner was modelled as a heterogeneous stirred tank combustion chamber, a variable mass flow rate oxidizer feed system, a constant mass flow rate fuel feed system and an exit turbine. Within the combustion chamber gases were assumed perfectly mixed. To account for liquid in the combustion chamber, a uniform droplet distribution was assumed to exist in the chamber, with the mean droplet diameter determined from an empirical relation. A computer program was written to integrate the resulting differential equations.

Because chamber contents were assumed perfectly mixed, the fuel preburner model erroneously predicted that combustion would not take place during shutdown. The combustion rate model was modified to assume that all liquid oxygen that vaporized instantaneously combusted with fuel. Using this combustion model, the effect of engine parameters on chamber pressure oscillations during the SSME shutdown was calculated. These studies showed that decreasing the
pressure downstream of the preburner's exit turbine, decreasing the fuel temperature, increasing the helium temperature and decreasing the length of the line connecting the helium storage tank to the helium check valve all had adverse effects on engine stability.
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LIST OF ABBREVIATIONS AND SYMBOLS

ABBREVIATIONS

CS : Control Surface
CV : Control Volume
FPOV : Fuel Preburner Oxidizer Valve
LOX : Liquid Oxygen
SSME : Space Shuttle Main Engine
STR : Stirred Tank Reactor
TSTR : Transient Stirred Tank Reactor

VARIABLES

A : Area (m²)

a₁, a₂, a₃ : Constants (dimensionless)
b : Constant (dimensionless)

C : Reaction Rate Coefficient (dimensionless)
c* : Characteristic Propellant Velocity (m/s)
c_{dm} : Constant for finding mean droplet diameter (dimensionless)
c_{ftp} : Constant for finding mass flow rate through the exit turbine (dimensionless)
cₚ : Molar Specific Heat at Constant Pressure (J/kgmole·K)

D : Diameter (m)

E : Total Energy (Joules)
F : Force (N)

F_{f} : The Force on a Pipe due to Friction (N)
f : Constant Used to Find F_{f} (m⁻¹)
\( \Delta H \) : Latent Heat of Vaporization (Joules)

\( h \) : Molar Enthalpy (J/kg·mole)

\( k \) : Thermal Conductivity (W/m·K)

\( L \) : Pipe Length (m)

\( L^* \) : Characteristic Combustion Chamber Length (m)

\( l \) : Length (m)

\( M \) : Molecular Weight (kg/kg·mole)

\( M_g \) : Mass of Product Gases in the Combustion Chamber (kg)

\( m \) : Mass Flow Rate (kg/s)

\( N_j \) : Constant Exponent in a Reaction Rate Expression (dimensionless)

\( N_{NN} \) : Number of Nodes in the Oxidizer Feed System

\( N_{NP} \) : Number of Pipes in the Oxidizer Feed System

\( N_{RXN} \) : Number of Elementary Chemical Reactions

\( N_{S} \) : Number of Species in the Combustion Chamber

\( N_{STRM} \) : Number of Inlet Streams to the Combustion Chamber

\( n \) : Unit Vector

\( O/F \) : Ratio of the Oxidizer and Fuel Mass Flow Rates (dimensionless)

\( P \) : Pressure (Pa)

\( \Delta P \) : Pressure Drop from the Storage Tank to the Combustion Chamber (Pa)

\( P_{HG} \) : Hot Gas Pressure (Downstream of the Preburner Turbine) (Pa)

\( \dot{Q} \) : Heat Transfer Rate out of the Combustion Chamber (J/s)

\( q \) : Volumetric Flow Rate \( (m^3/s) \)

\( R \) : Gas Constant (J/kg·K)
\( R_g \): Universal Gas Constant (J/kgmole·K)

\( \text{Re} \): Reynolds Number (dimensionless)

\( r \): Radius (m)

\( T \): Temperature (K)

\( \Delta T \): Temperature Difference Between a Droplet and the Surrounding Gases (K)

\( t \): Time (sec)

\( u \): Molar Internal Energy (J/kgmole)

\( V \): Volume (m\(^3\))

\( v \): Velocity (m/s)

\( \alpha \): Burning Rate Parameter, \( c \frac{\Delta T}{\Delta \tilde{H}} \) (dimensionless)

\( \beta \): Density of Liquid in the Combustion Chamber (kg/m\(^3\))

\( \varepsilon_{ss} \): Convergence Criterion (kgmoles/kg)

\( \Gamma_i \): Volumetric Rate of Production of Species \( i \) (kgmoles/m\(^3\)·s)

\( \Gamma_j \): Volumetric Rate of Elementary Reaction \( j \) (kgmoles/m\(^3\)·s)

\( \Theta \): Combustion Time Delay (sec)

\( \Theta_g \): In insensitive Combustion Time Delay (sec)

\( \Theta_m \): Mixing Time (sec)

\( \Theta_v \): Vaporization Time (sec)

\( \lambda_n, \omega_n \): Eigenvalues

\( \mu_g \): Viscosity of the Gases In the Combustion Chamber (N·s/m)

\( \phi \): Droplet Age in the Combustion Chamber (sec)

\( \rho \): Density (kg/m\(^3\))

\( \sigma \): Mole Number (kgmoles/kg)

\( \tau \): Sensitive Time Lag (sec)

\( \Omega \): Vaporization Rate (kg/s)
\[ \omega_v \] : Vaporization Rate per Droplet (kg/s/droplet)

**SUBSCRIPTS**

- \( b \) : Burned
- \( c \) : Combustion Chamber
- \( e \) : Exit Flow
- \( f \) : Fuel
- \( i \) : Species \( i \), Inlet Flow
- \( j \) : Reaction \( j \), Stream \( j \)
- \( k \) : Pipe Node \( k \)
- \( m \) : Mixing
- \( o, ox \) : Oxidizer
- \( t \) : Tank
- \( v \) : Volumetric
- \( 1 \) : Upstream
- \( 2 \) : Downstream

**SUPERSCRIPyT**

- \( \cdot \) : Forward Reaction
- \( \cdot \cdot \) : Reverse Reaction
- \( \ast \) : Inlet
CHAPTER I

INTRODUCTION

For start-up and normal operation, the Space Shuttle Main Engine (SSME) fuel preburner maintains stable operation. During shutdown, however, both in ground test firings and actual use, the fuel and oxidizer preburners frequently undergo low frequency combustion instability, or chug. The chug is manifest as pressure oscillations in the preburners and their feed systems. These oscillations have resulted in undesirable turbopump bearing loads and have damaged the augmented spark igniter oxidizer supply piping due to backflow of fuel and oxidizer from the preburner combustion chamber into the feed system. This study is concerned with modelling the SSME fuel preburner and predicting its behavior during chug.

Following is an overview of the SSME and fuel preburner, an account of the engine shutdown process and a description of the model to be used.

1.1 THE SSME AND FUEL PREBURNER

Figure 1.1 shows a schematic of the SSME. Liquid hydrogen, stored at 19 K (34°F) and 0.21 MPa (30 psia), and liquid oxygen, stored at 90 K (164°F) and 0.69 MPa (100 psia), are the engine's propellants. Both the hydrogen and the oxygen enter the engine via low pressure pumps. These raise the pressure of the propellants to prevent cavitation in the subsequent pumps. After leaving the low
Figure 1.1: Space Shuttle Main Engine Propellant Flow Schematic (From Sutton, 1986)
pressure pumps, the hydrogen and oxygen are pumped to high pressures by the turbopumps driven by the exit flow of the fuel and oxidizer preburners. At full power level the hydrogen leaves the fuel turbopump at 48.25 MPa (7000 psia) and the oxidizer leaves the oxidizer turbopump at 30.33 MPa (4400 psia).

Most of the oxygen (86% at full power level) flows directly to the main combustion chamber. The remainder flows to the two preburners. Upon leaving the high pressure pump, 76% (at full power level) of the hydrogen flows directly to the preburners. The remainder flows through the engine, cooling the preburner combustion chambers, the main combustion chamber and the nozzle.

The oxidizer and fuel preburners serve two purposes in the SSME: to drive the turbines which supply power to the high pressure pumps and to preheat the hydrogen for combustion in the main combustion chamber. At full power level, the fuel preburner operates at around 1090 K (1960°R) and 39.01 MPa (5660 psia) and the oxidizer preburner operates at around 830 K (1500°R) and 38.60 MPa (5600 psia). During the fuel preburner chug, the pressure in the fuel preburner varies around 4.48 MPa (650 psia). Actual average chamber temperature data is not available, but the Marshall Space Flight Center SSME transient model predicts mean temperatures between 440 K and 800 K (800°R and 1400°R) during the chug.

Injection of liquid oxygen and supercritical hydrogen into the fuel preburner is accomplished by means of 264 coaxial injectors. To cool the plate, hydrogen also is injected through small orifices
across the face plate. At full power level, just before injection, the hydrogen is at about 160 K (284°F) and 43.08 MPa (6250 psia) and the oxygen is at about 120 K (214°F) and 48.4 MPa (7020 psia).

At full power level, the fuel preburner operates at an equivalence ratio \( \frac{\text{fuel/oxidizer}}{\text{fuel/oxidizer} \text{ stoichiometric}} \) of about 8. Mass flow rates of hydrogen and oxygen into the fuel preburner are 36.4 kg/s (80 lb/s) and 37.7 kg/s (83 lb/s), respectively. Hot gases from the preburners exit the preburner combustion chambers through turbines and enters the main combustion chamber via the hot gas manifold and the main injection plate. In the main combustion chamber the products from the two preburners are burned with oxygen. The equivalence ratio in the main combustion chamber is about 1.33.

1.2 SSME SHUTDOWN AND THE FUEL PREBURNER CHUG

When the SSME shuts down, it is important that combustion ceases in the preburners and that oxidation does not begin in the feed system, so a helium purge is used to push oxygen from the feed system and preburners and assure that the system is above the rich limits of combustion of hydrogen with oxygen. It is during the helium purge that the fuel preburner chug takes place. Figure 1.2 shows the fuel preburner manifold. The helium purge orifice is a small pipe that links the helium supply piping to the pipes that reach the helium check valves. The helium check valves restrain the
Figure 1.2: Fuel Preburner Manifold and Feed System Schematic (From Rockwell International Corp., Rocketdyne Div.)
helium until the pressure downstream of the valves drops below 5.17 MPa (750 psia).

Shutdown is accomplished and controlled by the closing of the oxidizer preburner oxidizer valve, the fuel preburner oxidizer valve, the main oxidizer valve and the main fuel valve and the opening of the helium purge check valves. Table 1.1 (adapted from George, 1984) gives the valve sequence and the resulting events during the SSME shutdown. Two points should be noted from Table 1.1. First, before chugging begins in the fuelside preburner, both the fuelside preburner oxidizer valve and the main oxidizer valve are closed; the fuelside preburner is isolated from the oxidizer feed system. Second, no valve openings or closings coincide with the onset or ending of chug. These points are further discussed in Chapter II.

When the fuelside preburner chug begins is dependent on the power level from which the engine is cut off and the diameter of the helium purge orifice. Pressure traces for typical fuelside preburner chugs for SSME test firings are found in Figure 1.3. These traces are plots of the deviation of the chamber pressure from the mean chamber pressure versus time. The traces were filtered to show only frequencies between 50 and 200 Hz. Figure 1.3 (a) is a pressure trace for a small helium purge orifice diameter (0.17 cm [0.068 inches]) and Figure 1.3 (b) is a trace for a large helium purge orifice diameter (0.74 cm [0.291 inches]). Using the small helium purge orifice resulted in a short chug whose amplitude is about 2.89
Table 1.1: Sequence of Events During the SSME Shutdown

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<th>TIME AFTER CUTOFF (SEC)</th>
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| 1.4                     | OXIDIZER PREBURNER OXIDIZER VALVE SEALS CLOSE  
                           | OXIDIZER PREBURNER PRESSURE DROPS SMOOTHLY FROM  
                           | 800 PSIA TO 500 PSIA  |
| 1.8                     | HELIUM CHECK VALVES OPEN, PUSHING OXIDIZER  
                           | FROM THE OXIDIZER PREBURNER MANIFOLD INTO  
                           | COMBUSTION CHAMBER  
                           | OXIDIZER PREBURNER CHAMBER PRESSURE RISES TO  
                           | 750 PSIA AND STABILIZES.  
                           | HELIUM FLOW SUBSIDES AFTER THE INITIAL SPIKE  |
| 2.2                     | FUEL PREBURNER OXIDIZER VALVE SEALS CLOSE  
                           | HELIUM FLOW RATE IMMEDIATELY RISES  
                           | MAIN OXIDIZER VALVE CLOSES (AFTER THE FUEL  
                           | PREBURNER OXIDIZER VALVE)  |
| 2.3                     | HELIUM FLOW STABILIZES, AS DO THE FUEL PREBUR-  
                           | NER AND OXIDIZER PREBURNER CHAMBER PRESSURES  
                           | FOR THE SMALL ORIFICE TESTS  
                           | HELIUM FLOW RATE CONTINUES TO INCREASE FOR THE  
                           | LARGE ORIFICE TESTS  |
| 2.3 - 2.5               | CHUGGING BEGINS IN THE FUELSIDE PREBURNER;  
                           | LARGE AMPLITUDE FOR THE LARGE ORIFICE  
                           | AND SMALL AMPLITUDE FOR THE SMALL ORIFICE  
                           | LOW LEVEL CHUGGING MAY ALSO BEGIN IN THE OXI-  
                           | DIZER PREBURNER  |
| 2.5                     | LARGE AMPLITUDE CHUG BEGINS FOR THE SMALL  
                           | HELIUM PURGE ORIFICE TESTS  
                           | A TEMPORARY REDUCTION IN THE AMPLITUDE OF THE  
                           | THE FUELSIDE PREBURNER CHUG OCCURS DURING  
                           | THE LARGE ORIFICE TESTS  |
| 3.0                     | CHUGGING ENDS  |
| 3.7                     | THE MAIN FUEL VALVE CLOSES  |
Figure 1.3: Pressure Traces for the SSME Fuel Preburner Chug (From George, 1984)

(Pressure Traces Were Filtered to Show Only Frequencies Between 50 and 200 Hz)
MPa (420 psi). Using the large orifice resulted in a longer but less severe chug. About three seconds after cutoff the chug ends and the chamber pressure and temperature decrease smoothly. The main fuel valve closes after the purge is complete.

Because the chug takes place after the fuel preburner and its piping are isolated from the oxidizer feed system and before the main fuel valve is closed, George (1984) concluded that the chug was not directly related to or triggered by valve openings and closings and that it was associated with the oxidizer purge process. As helium replaces oxygen in the oxidizer feed system, the fluid in the pipes becomes more compressible and propellant feed rates to the preburners become more sensitive to chamber pressure. This effect is described in greater detail in Chapter II.

1.3 MODELLING THE SSME FUEL PREBURNER AND FEED SYSTEM

Because of high mass flow rates, very reactive propellants, high chamber pressure and the fact that combustion takes place on many diffusion flames surrounding droplets throughout the combustion chamber, combustion in a liquid propellant rocket engine can be considered to take place homogeneously through the combustion chamber (Summerfield, 1951). Consequently, the present study modelled the fuelside preburner combustion chamber as a stirred tank reactor; contents are considered well mixed and properties are considered uniform throughout the chamber. Liquid droplets were distributed evenly through the combustion chamber and all had the
same characteristic diameter. The heterogeneous stirred tank reactor is more fully described in Chapter III.

The governing equations for the combustion chamber were derived from the conservation of mass applied to the liquid in the combustion chamber, the conservation of mass applied to the gases in the combustion chamber, the conservation of species, the conservation of energy and the perfect gas law. Auxiliary relations used to obtain terms in the governing equations included empirical expressions for average droplet diameter, droplet evaporation rate, thermodynamic properties for the gases in the combustion chamber and elementary reaction rates. Exhaust mass flow rate from the preburner was given as a function of the ratio of the pressure downstream of the exit turbine to the combustion chamber pressure. At each time, combustion chamber pressure, temperature, density (excluding liquid mass, which is assumed to occupy negligible volume), liquid density (kg of liquid per unit volume of the combustion chamber) and mole number of each species (kgmoles of the species per total mass (kg) in the combustion chamber) were calculated.

In the feed system the effects of the compressibility of helium were important, as was the feed system geometry, so a multiple pipe, multiple node feed system containing distinct liquid and gaseous phases was used to predict the transient feed system behavior. Governing equations for the feed system included the conservation of momentum along each pipe and the conservation of mass at each node. Time dependent variables were the fluid velocity in each pipe, the
liquid/vapor interface position in each pipe and the density at each node.

The combustion chamber and feed system governing equations were solved numerically on a digital computer, integrating over time. Since the equations are stiff (i.e., characterized by widely differing time constants for the dependent variables (Pratt and Radhakrishnan, 1986)) steps were taken to make the equations solvable without using an excess of computer time. In addition to using an integration routine written for solving systems of stiff differential equations, a steady state approximation was made for the concentrations of radicals and atoms in the combustion chamber to facilitate the solution of the governing equations.

Derivation and solution of the governing equations is given in Chapter III.

Success of this model is determined by its ability to predict a chug as encountered in the SSME fuel preburner during shutdown and its ability to vary engine parameters and find a way in which the fuel preburner chug can be lessened in severity or eliminated.
CHAPTER II

LITERATURE SURVEY

2.1 OVERVIEW OF DIFFERENT INSTANCES OF COMBUSTION INSTABILITY, THEIR CAUSES AND EFFECTS.

The phenomenon of combustion instability exists to some degree in all combustion processes. The sputtering of a match, the crackling of a log on a fire and the flickering of a candle are all everyday examples of combustion instability. Such early scientists as Rayleigh and Farraday noted pressure oscillations as sound waves generated during the burning of substances in a tube. Rayleigh (1945) described these oscillations as

... vibrations maintained by heat, the heat being communicated to the mass of air confined in the sounding tube at a place where, in the course of vibration, the pressure varies.

He concluded that "In consequence of the variable pressure within the resonator, the issue of gas, and therefore, the development of heat, varies during vibration." This is an apt description of the processes involved in a periodic combustion instability.

Combustion instability can be classified in a number of different ways. First, it can be either periodic or random. An example of a periodic instability is a pressure wave travelling around a combustion chamber due to varying combustion rates. Spikes or pops (spontaneous explosions) in rocket combustion chambers are examples of random instability. Second, combustion instabilities are
either chamber, system or intrinsic instabilities (Williams, 1985). Chamber instabilities involve only the processes that occur within a combustion chamber, while system instabilities involve interaction between processes occurring in a combustion chamber with processes occurring elsewhere in the system, such as in propellant feed lines or at the combustion chamber exit. An intrinsic instability involves only the combustion process and occurs whether or not there is a combustion chamber. Finally, periodic combustion instability can be classified according to its frequency. In rocket motor combustion instability, there exist three fairly distinct instability frequency ranges. High frequency instabilities (normally greater than 1000 Hz) are chamber instabilities involving longitudinal, transverse or radial waves within the rocket combustion chamber. Low frequency instabilities (normally less than 300 Hz) are system instabilities which couple changes in the propellant feed rate with changes in combustion rate in the combustion chamber. Intermediate frequency instabilities (frequencies between 300 Hz and 1000 Hz) involve aspects of both system and chamber instabilities: waves propagate within the combustion chamber and also within the feed system.

Periodic combustion instability is observed in ramjet engines and solid rocket engines as well as in monopropellant and bipropellant liquid rocket engines. Low frequency combustion instability in ramjet engines is a result of vortices in the combustion chamber and is very dependent upon chamber geometry (Yang and Culick, 1986). There are a number of parallels between liquid
rocket and solid rocket engine low frequency combustion instabilities. Schoyer (1986) describes the physical processes involved in solid rocket chugging as follows:

The basic idea is that due to oscillatory combustion there is a fluctuating heat transfer into the propellant which superimposes an oscillation on the steady state profile in the pyrolyzing propellant. Because the solid propellant depends on the (fluctuating) surface temperature, the pyrolysis rate will also vary, causing a fluctuating mass flow into the combustion chamber. If this fluctuating mass flow is more or less in phase with the pressure fluctuations, the two effects may enhance each other (causing resonance) and lead to oscillatory combustion.

Just as heat transfer and pyrolysis provide gaseous reactants in the burning of solid propellants, heat transfer and vaporization provide the gaseous reactants in the burning of liquid propellants. Combustion in solid and liquid rockets differs in two important ways. First, combustion can be considered to take place on a single planar flame front in a solid rocket combustion chamber, whereas combustion in a liquid propellant combustion chamber involves many diffusion flames that surround droplets. Second, the liquid propellant feed rates must also be considered for a liquid rocket engine.

As mentioned above, liquid rocket engines can undergo low, intermediate and high frequency combustion instability. The physical manifestations of these include noise, pressure and temperature oscillations in the combustion chamber (longitudinal, radial and transverse), changes or even reversals in the mass flow rate of the feed system, increased rates of heat transfer to engine components,
decreased engine performance and possibly severe vibrational loads on engine components.

For a liquid rocket engine, the most destructive type of combustion instability is high frequency instability, sometimes called screech, scream or acoustic instability. Screech can result in vibrational loads on rocket components and, more importantly, increased rates of heat transfer to chamber walls. Lawhead and Combs (1963) observed burnout of the injector face of a liquid rocket combustion chamber between 200 and 300 msec after the beginning of screech. Penner and Datner (1955) stated that performance might be improved by screech, although this would not offset the negative effects of screech.

During screech oscillations of pressure and temperature usually take place only within the combustion chamber of a rocket motor, although oscillations can also occur in the feed system (Coultas, 1972). Upon a perturbation, thermodynamic properties and chemical composition can change in a part of the combustion chamber, leading to a local change in the rate of combustion (Crocco et al., 1960). This change initiates a wave which propagates through the combustion chamber. The wave can be linear (discrete) or nonlinear (coupled with other waves) and radial, longitudinal or circumferential. The propellant feed system is usually not directly involved in the propagation of pressure and temperature waves, but is important in that it determines the amount and distribution of reactants in the combustion chamber. The mass flow rate in the feed...
system does not oscillate during screech because oscillations in the chamber take place at a higher frequency than those to which the feed system can respond.

Among possible sustaining mechanisms for screech are the physical delays associated with the combustion process (atomization, vaporization and reaction rate), the sensitivity of the rate of combustion to pressure and temperature changes and the "explosion" of liquid droplets which are heated to temperatures above their critical temperatures (Coultas, 1972). Reardon, McBride and Smith (1966) showed that spatial nonuniformities in propellant injection rates across the injector were also, at times, responsible for screech. Their work was verified by experiment.

To prevent destructive high frequency combustion instability, liquid propellant rockets may need baffles or liners to cause combustion chamber conditions (pressure, temperature, distribution of propellants) to be more uniform or to change the resonant frequency of the engine (Williams, 1985). A change in the propellant spray field can also prevent destructive scream (Coultas, 1972). Both of these fixes involve local control of combustion rates.

Less common in liquid rocket motors, intermediate frequency instability, or buzz, involves waves in the propellant feed system as well as spatial combustion chamber pressure variations (Coultas, 1972). Buzz differs from screech in that it involves lower frequency disturbances and oscillations in the feed system. It differs from low frequency instability in that spatial variations in pressure,
temperature and chemical composition exist in the combustion chamber. Buzz causes structural loads on engine components and standing waves in the feed system pipes and may initiate high frequency instability.

Scream involves pressure and temperature waves that propagate in the combustion chamber as a result of spatially varying rates of combustion. Buzz is characterized by standing waves in the propellant feed system and spatial variations in combustion rate in the combustion chamber. In contrast to scream and buzz, combustion chamber pressure can be considered uniform during low frequency instability, or chug. In chug, aggregate oscillations in chamber pressure couple with oscillations in propellant feed rate, resulting in loss of performance, structural loads and possible failure of engine parts. The coupling of oscillations in chamber pressure and propellant feed rate is a result of the time delay between the injection of propellants into the combustion chamber and their combustion. Chugging in liquid bipropellant rocket engines is further described in section 2.2.

2.2 LOW FREQUENCY COMBUSTION INSTABILITY IN LIQUID BIPROPELLANT ROCKET ENGINES

Chugging in liquid bipropellant rocket engines is characterized by pulsations in the rate of propellant injection into the combustion chamber and variations in combustion chamber pressure (Penner and Datner, 1955). These pulsations are generally taken to be the result of the time lag that exists between the injection of
liquid propellants into the combustor and their conversion to hot product gases, as proposed by Summerfield (1951). Because of the inertia of the propellant mass in the feed lines, mass flow rates into a combustion chamber are not immediately responsive to changes in chamber pressure. Because of the combustion time lag, combustion chamber temperature, pressure and composition are not immediately responsive to changes in propellant mass flow. When response delays in the feed system and combustion system become coupled, large amplitude chugs can result. Figure 2.1 shows the coupling of the feed system and combustion chamber for a chugging rocket engine.

Because the conversion of low temperature propellants to high temperature products in a liquid bipropellant rocket engine is such a complex process, it would be difficult for a chug model to incorporate all facets of the process. An effort must be made to determine the most important parts of the process. In the SSME fuelside preburner, liquid oxygen and gaseous hydrogen combust. This involves injection of the hydrogen and oxygen, atomization and vaporization of the oxygen, mixing of the gaseous hydrogen and oxygen vapor and chemical reaction of the gaseous species. In his study of screech in liquid bipropellant rockets, Priem (1966) took atomization, vaporization and chemical reaction as the most important processes in combustion instability. In the current study, the author will also take these three processes to be the most important parts of the combustion process and neglect other parts such as gas phase mixing and wall catalyzed reactions. Atomization,
Figure 2.1: Processes Involved in Flow Fluctuation Instabilities
(From Penner and Datner, 1955)
vaporization and chemical reaction and their effect on chugging are briefly described below.

The atomization of a propellant stream is primarily dependent upon the way the stream is injected into the combustion chamber. Propellants can be premixed or distinct upon injection and injection can be accomplished by parallel jets, impinging streams or coaxial streams. After injection, streams may be deflected by a splashplate. The SSME fuelside preburner employs coaxial injectors. Coaxial injectors are primarily used when one of the injected fluids is gaseous and the other is a liquid, since they are well adapted to mixing a gaseous stream with a liquid one (Dykema, 1972).

During atomization, streams break into ligaments which break into droplets. Droplets can either evaporate, shatter or interact with each other. Priem (1966) said that atomization rate is proportional to the mass of unatomized liquid in the combustion chamber and a less strong function of chamber density and axial velocity of the liquid propellant upon injection. The mass of unatomized propellant in the combustion chamber at a given instant is a function of the injection rate previous to that time, so a change in injection rate of propellant will affect the atomization rate only after a time delay.

Spatial injection droplet distribution has been shown to have a great effect on screech (Reardon et al., 1966), but does not greatly affect chugging, since it is aggregate chamber pressure oscillations and not spatial pressure oscillations that are able to couple with
the feed system. Webber (1972) showed that gross changes (for example, not including any small droplets in the droplet distribution in the combustion chamber) in the estimation of droplet sizes in a chug model drastically changed his predicted pressure oscillation amplitudes and frequencies.

The vaporization rate for a liquid propellant in a rocket engine combustion chamber is dependent on the atomization process (droplet size and surface area), the heat transfer rate to the droplet and the rate at which propellant diffuses away from the droplet. To prevent chug, the part of the combustion time delay associated with vaporization should be made as short as possible. In the SSME fuelside preburner, coaxial injectors inject high speed hydrogen around a jet of liquid oxygen. The greater the speed of the hydrogen, the more shear on the liquid oxygen jet, the finer the atomization, the greater the vaporization rate and the shorter the vaporization delay time. Higher chamber temperatures also result in greater rates of vaporization of liquid propellants due to greater rates of heat transfer to droplets. Another way to increase the vaporization rate is to increase the temperature of the liquid propellant. For higher temperature liquid propellants, less energy must be transferred to the droplets to raise their temperature and vaporize them.

Chemical reaction rates, or equivalently, propellant combinations, can greatly influence combustion stability in a rocket engine, though often chemical reaction rate is taken as a less
important factor (Priem, 1966, and Reardon, 1972). Reaction rate can be important if it is sufficiently slow and makes up a significant fraction of the combustion time delay. Summerfield (1951) suggested that chug could be eliminated in some engines through the use of either more reactive propellants or some sort of catalysis.

A number of experimental investigations have been conducted to determine how rocket design parameters such as combustion chamber pressure, propellant combination, injector pressure drop, chamber length, number of injectors, feed system mass flow rates and propellant mixture ratio influence chugging. The results of two papers will be highlighted below.

Both Barrere and Moutet (1956) and Heidmann et al. (1967) noted that higher chamber pressure leads to higher frequency but lower amplitude pressure oscillations (Figures 2.2(a) and 2.2(b)). Temperature and pressure oscillations were roughly in phase during chug (Barrere and Moutet).

As characteristic chamber length (usually defined as the chamber volume divided by the area of the exit nozzle throat) is increased, the range of stable operating conditions is decreased (Heidmann et al.) while the frequency of pressure oscillations decreases (Barrere and Moutet). Chambers of the same characteristic length but different volumes were studied by Barrere and Moutet. Both chambers exhibited roughly the same pressure oscillation frequency, with the smaller chamber undergoing oscillations of slightly higher amplitudes.
Figure 2.2: Effect of Chamber Pressure on Chug Amplitude and Frequency (Barrere and Moutet, 1956)
Increasing the number of jets (injectors) of a combustion chamber decreased the range of stable operating conditions (Heidmann et al.), presumably because of droplet and stream interactions driven by the pressure changes.

Changing the mixture ratio within a moderate range \(0.9 < \frac{m}{m_s} < 1.4\), where \(m\) is the fuel/oxidizer mixture ratio and \(m_s\) is the stoichiometric mixture ratio) had very little effect on chug frequencies for an engine whose propellants were nitric acid and furfurylic alcohol. The lowest amplitude pressure oscillations occurred for a stoichiometric mixture. This is due to a reduced combustion delay time, since collisions between appropriate molecules of reactants are most likely for a stoichiometric mixture.

2.3 CONTROLLING LOW FREQUENCY COMBUSTION INSTABILITY

Having described the processes involved in chugging, a number of methods for controlling chugging will be presented. First, combustion chamber geometry (characteristic length) can be changed. In many cases, as with the SSME, chug is encountered only after the engine has been built, so changing the chamber geometry is not a viable alternative. In addition, since chugging only occurs in the SSME during shutdown, extensive changes in chamber geometry is not merited.

Second, the pressure drop across the injectors can be increased. A larger pressure drop across the injectors means that a change in downstream (chamber) pressure will be a smaller fraction
of the upstream pressure (behind the injector) and will not effect feed system mass flow rates very much. Friction in the feed system and injectors damps oscillations in propellant flow. Any increase in the energy of the propellant stream will be reduced by the feed system and injector friction. Consequently, choosing an injector with much friction could result in a more stable engine. On the other hand, a greater pressure loss for the stream entering the combustion chamber would be the cost.

2.4 THE SSME FUELSIDE PREBURNER CHUG

There are a number of factors peculiar to the SSME fuelside preburner that contribute to the onset of chugging. First, as described in the introduction, the chug occurs during the SSME shut-down while helium progressively replaces liquid oxygen in the oxidizer feed system. The presence of helium in the oxidizer feed system makes the oxidizer mass flow rate more sensitive to changes in the chamber pressure than if there were no helium in the feed system. Gaseous helium is more compressible than liquid oxygen, so an increase in chamber pressure results in compression of the helium and a greater reduction in the oxidizer mass flow rate than if no helium were present. For a temperature and pressure near those at which the chug occurs (5.0 MPa and 100 K), the density and bulk modulus of oxygen are about 1000 kg/m$^3$ (62.4 lbm/ft$^3$) and 221 MPa (32,000 psia), respectively. For helium they are about 17 kg/m$^3$ (1.06 lbm/ft$^3$) and 12.4 MPa (1800 psia), respectively.
In the SSME fuelside preburner, liquid oxygen is burned at a low equivalence ratio (about 8.0 at rated power level) with hydrogen. Hydrogen has a very low critical temperature (33.3 K [60°R]) and pressure (1.29 MPa [188 psia]), so it enters the combustion chamber as a supercritical gas. The critical pressure of oxygen is about 5.09 MPa (738 psia), so during the SSME fuelside preburner chug, which takes place at pressures which vary around 4.83 MPa (700 psia), oxygen is a near critical liquid.

The conversion of gaseous hydrogen and oxygen to water vapor occurs as a chain reaction involving the radicals and atoms OH, O, H, HO₂ and H₂O₂ (Kuo, 1986). At high pressures, the radicals HO₂ and H₂O₂ dissociate and for high temperatures and high mass flow rates, reactions at the wall are not very important. Since the SSME fuelside preburner operates at high pressures, mass flow rates and temperatures, the following reactions can be considered to be the elementary steps in the overall conversion of H₂ and O₂ to water vapor:

\[
\begin{align*}
\text{H}_2 + \text{O}_2 & \rightarrow 2\text{OH} \\
\text{H}_2 + \text{M} & \rightarrow 2\text{H} + \text{M} \\
\text{OH} + \text{H}_2 & \rightarrow \text{H}_2\text{O} + \text{H} \\
\text{H} + \text{O}_2 & \rightarrow \text{OH} + \text{O} \\
\text{O} + \text{H}_2 & \rightarrow \text{OH} + \text{H} \\
\text{H} + \text{H} + \text{M} & \rightarrow \text{H}_2 + \text{M} \\
\text{H} + \text{O} + \text{M} & \rightarrow \text{OH} + \text{M} \\
\text{O} + \text{O} + \text{M} & \rightarrow \text{O}_2 + \text{M}
\end{align*}
\]
\[ \text{H} + \text{OH} + \text{M} \rightarrow \text{H}_2\text{O} + \text{M} \]

where M represents a third body, inert to the reaction. For a rocket engine combustion chamber, which operates at high temperatures and pressures, the atoms and radicals produced in the chain branching reactions will be consumed in the termination reaction nearly as soon as they are produced.

George (1984) observed during test firings of the SSME that using a 0.068 inch diameter helium purge orifice for the SSME fuelside preburner as opposed to a 0.291 inch orifice resulted in a 34% increase in maximum peak to peak amplitudes of pressure oscillations (from 335 psia) and a 38% decrease in chug duration (from 0.72 sec). Changing the purge orifice diameter did not substantially change the chug's center counted frequency (the average frequency at the chug's temporal center). The center counted frequency for the small and large orifices were 117 Hz and 117.5 Hz, respectively. Traces of pressure for small and large orifice engine test firings are shown in Figures 1.3(a) and 1.3(b) (page 8). Chug ending time was not affected by the change of the helium purge orifice diameter, but chug starting time was. Because of this, George ruled out oxygen depletion as the chug terminating mechanism. Helium flow rate and compressibility are evidently important in determining the character of the SSME fuelside preburner chug.

The only opening or closing of a valve that occurs near the chug's end is the closing of the main oxidizer valve. As described in Chapter I, during chug the fuelside preburner is isolated from
the oxidizer feed system, so valve openings and closings are probably not a concern in the SSME fuelside preburner chug. The valves that restrain the helium before the purge begins are poppet type valves that remain open even when the pressure drop across the valve is less than the cracking pressure (George, 1985). Therefore, helium purge valve clatter probably does contribute to the chug.

Because of the fuelside preburner turbine blade inertia, the exit mass flow rate does not respond immediately to a change in combustion chamber pressure. A relation for exit mass flow rate as a function of chamber pressure and temperature and pressure downstream of the turbine was given by Nguyen (1981) and is found in Chapter III.

Because of the above considerations, the model of the SSME fuelside preburner allows for the compressibility of helium in the piping system, a combustion time lag due to the atomization and vaporization times for oxygen and turbine blade inertia.

2.5 ROCKET ENGINE STABILITY PREDICTION MODELS

Most chug models have attempted to predict the domain of operating conditions within which a rocket engine can operate without undergoing destructive oscillations in pressure and temperature. By varying inputs such as combustion chamber pressure, injector pressure drop, combustion time delay or instability frequency to these models, stability boundaries for specific engines and general criteria for rocket engine stability can be found.
Figure 2.3 shows the rocket engine model used by Summerfield (1951). He related the rate of change of combustion chamber pressure with respect to time, \( t \), at a given instant, to the propellant injection rate at a time \( t-\theta \), using the equation:

\[
\frac{dP}{dt} = \frac{R}{V} \frac{T_c}{\rho_c} A_2 v_2(t-\theta) - \frac{R}{L^* c^*} \frac{T_c}{P_c}
\]  

[2.2]

where \( T_c \) is the combustion chamber temperature (K), \( \rho_c \) is the combustion chamber density (kg/m\(^3\)), \( V \) is the combustion chamber volume (m\(^3\)), \( L^* \) is the characteristic chamber length (m), \( c^* \) is the characteristic propellant velocity (m/s), \( R \) is the gas constant for the gases in the combustion chamber (J/kg*K), \( A_2 \) is the area (m\(^2\)) at station 2 in Figure 2.3 and \( v_2(t-\theta) \) is the propellant velocity (m/s) at station 2 at time \( t-\theta \). This implies that a mass of propellant injected into the combustion chamber occupies negligible volume and does not react at all until \( \theta \) seconds later when it is converted to products instantaneously. \( \theta \) is the combustion time delay and can be a function of chamber pressure, temperature and composition and of propellant composition and velocity. Characteristic chamber length, \( L^* \), is defined as the volume of the chamber divided by the average cross sectional area. Summerfield defined the characteristic propellant velocity, \( c^* \), as

\[
c^* = f(\gamma) \sqrt{R T_c}
\]

where \( \gamma \) is the ratio of the specific heats in the chamber.
Figure: 2.3 Schematic of Summerfield's Liquid Propellant Rocket System (Summerfield, 1951)
Summerfield used conservation of energy for the control volume bounded by surfaces $A_1$ and $A_2$ along with continuity and equation [2.2]. Differentiating the result with respect to time and linearizing by saying that $v_2(t) - v_2(t-\theta)$ is small, gave an equation of the form

$$u''(t) + A u'(t) + B u(t) + C u(t-\theta) = 0$$  \[2.3\]

where $u = d(v_2)/dt$. Solutions of [2.3] are of the form

$$u = \sum U_n \exp((\lambda_n + \omega_n) t)$$  \[2.4\]

Substituting [2.4] into [2.3], the values of $\lambda_n$ and $\omega_n$ which satisfy [2.3] can be found.

Analyzing the eigenvalues of [2.3], Summerfield determined that the following condition must be met for a liquid rocket engine to be stable (i.e., to not undergo undamped pressure oscillations):

$$\frac{\frac{1}{2} \frac{m}{A_2}}{P_c} + \frac{c_s L^*}{R T_c} \frac{2 \Delta P}{P_c} > \Theta$$  \[2.5\]

where $\Delta P$ is the pressure difference between the propellant storage tank and the combustion chamber (psi) and $l_2$ is the length of the propellant feed line (Figure 2.3).

Inequality [2.5] indicates that an unstable rocket engine can be made stable by

1. increasing the feed system pipes length,

2. increasing the propellant feed mass flow rate,
3. increasing the pressure drop from the storage tank to the combustion chamber,

4. decreasing the combustion chamber pressure or

5. increasing the characteristic chamber length.

Evaluation of \([2.5]\) with the appropriate SSME fuelside preburner shutdown values \((l_2 = 0.5 \text{ m} [1.64 \text{ ft}], m = 33.91 \text{ kg/s})\) \([74.8 \text{ lb/s}]\), \(P_c = 4.825 \text{ MPa} [700 \text{ psia}]\), \(A_2 = 0.0025 \text{ m}^2 [0.027 \text{ ft}^2]\), \(c^* = 60 \text{ m/s} [197 \text{ ft/s}] \) [estimated from calculations by VanOverbeke and Claus, 1986], \(L^* = 0.1 \text{ m} [0.328 \text{ ft}]\), \(R = 2080 \text{ J/kg-K} [0.497 \text{ Btu/lbm-°R}]\), \(\Delta P = 0.345 \text{ MPa} [50 \text{ psia}]\) and \(T_c = 700 \text{ K} [1260°\text{R}]\)) yields the stability criterion

\[
\Theta < 0.0014 \text{ s}
\]

(i.e., the combustion time delay must be less than 440 \(\mu\text{s}\)).

Crocco (1951) began his stability analysis for a monopropellant rocket engine using conservation of mass in the combustion chamber. Assuming, like Summerfield, that propellants have negligible volume until burned and that the mass burned over the time interval \(dt\) is equal to the mass of propellant injected over the time interval \(d(t-\Theta)\), continuity for the combustion chamber can be written

\[
\frac{dM}{dt} + \dot{m}_e(t) = (1 - \frac{d\Theta}{dt}) \dot{m}_i(t-\Theta)
\]

\[2.6\]
where \(m_e\) and \(m_i\) are the mass flow rates out of and into the combustion chamber and \(M\) is the mass of product gases in the combustion chamber.

Crocco divided the combustion delay time, \(\Theta\), into an insensitive part, \(\Theta_g\), which does not vary with small variations in chamber conditions and a sensitive part, \(\tau\).

\[
\Theta = \Theta_g + \tau \quad [2.7]
\]

\(\Theta_g\) can be given, for instance, by \(L^*[c*/R\cdot T_c]\). Crocco assumed that \(\tau\) obeys the relation

\[
\tau \cdot p^n_c = \text{const.} \quad [2.8]
\]

Using [2.8] and [2.7], Crocco nondimensionalized and linearized [2.6].

Applying the conservation of mass and momentum to the feed system, piping system behavior was seen to be dependent on three dimensionless groups: one involving the pressure drop across the injectors, the second involving the inertia of the propellant in the pipes and the third giving the relative elasticity of the pipes and the propellant within.

Using a version of [2.6] and the feed system equations, Crocco formulated a characteristic equation for a monopropellant rocket engine and found the stability boundaries that corresponded to various values of \(n\) in equation [2.8]. He concluded that using a varying time lag changed stability predictions, predicting a greater
range of stable operating conditions, but the changes were not great.

Using an annular section of a liquid bipropellant rocket engine combustion chamber, Priem determined the effect that atomization, vaporization and chemical kinetics had on screech. Though this model was for screech, the way that the combustion rate was modelled can be extended to a chug model.

Priem calculated combustion rate in three different ways. First, he assumed that chemical kinetics was the most important part of the combustion process. Atomization and vaporization times were assumed short enough that the propellants that were injected into the combustion chamber were immediately available for chemical reaction. In the second model vaporization was the controlling process. Atomization was considered very fast, so the liquid injected into the combustion chamber immediately assumed a given, nonvarying droplet distribution profile. Chemical reaction time was also considered negligible. Consequently, the combustion rate was equal to the vaporization rate. Finally, the times required for atomization and chemical reaction were considered very small and the combustion rate was set equal to the atomization rate.

Using conservation of mass, energy and axial momentum, Priem generated stability boundaries. The physical processes of vaporization and atomization were shown to be more important than chemical kinetics for screech. Stability was shown to be very
sensitive to the mass of unburned propellant in the combustion chamber. Priem confirmed his stability boundaries experimentally.

In a companion study to this one, Lim (1986) determined the stability boundaries of the SSME fuel side preburner during shutdown. Lim assumed

1. combustion chamber pressure is uniform and oscillates about a steady state value,
2. combustion chamber temperature is uniform,
3. the combustion delay time is the same for both propellants and
4. reaction rate is infinite and chemical kinetics can be ignored.

Like Summerfield, Lim assumed that the rate that propellants are burned is equal to their rate of injection at a previous time, \( t-\theta \), where

\[
\Theta = \Theta_v + \Theta_m \tag{2.9}
\]

\( \Theta_v \) corresponds to vaporization time and \( \Theta_m \) to mixing time.

Conservation of mass was applied to the combustion chamber, leading to

\[
\frac{d}{dt} (\rho_c V) = \dot{m}_{fb}(t-\theta) + \dot{m}_{ob}(t-\theta) - \dot{m}_e(t) \tag{2.10}
\]

where \( \dot{m}_{fb} \) and \( \dot{m}_{ob} \) are fuel and oxidizer burning rates, respectively (determined by conditions at time, \( t-\theta \)) and \( \dot{m}_e \) is the chamber exit mass flow at time \( t \). The system variables \( \dot{m}_{fb}, \dot{m}_{ob}, \dot{m}_e \) and \( \rho_c \) were
expressed in terms of a steady state value plus a perturbation and substituted into [2.10] which was linearized. The resulting characteristic equation was solved and stability boundaries were generated.

In generating stability boundaries. Lim varied chamber pressure, fuel mass flow rate, oxidizer mass flow rate, fuel injection temperature and oxidizer injection temperature. Lim made the following conclusions from his stability boundaries.

1. The preburner system is generally more stable at lower chamber pressures.
2. For oxidizer and fuel temperatures of 40K, the system is inherently unstable. For oxidizer and fuel temperatures of 120 K, stability can be achieved only for \( P_c < 3.79 \text{ MPa (550 psia)} \). Chugging could not be avoided for low fuel temperatures.
3. Fuel flow rates did not influence stability.
4. High oxidizer flow rates (or high helium purge rates) made the system stable.

2.6 STIRRED TANK REACTOR MODELS

A chemical reactor can be modelled as a batch reactor, a plug flow reactor or a stirred tank reactor (STR). In a batch reactor (Figure 2.4 (a)) reactants are fed into the reactor and left to react. After some time, the reactor is emptied. A plug flow reactor is shown in Figure 2.4 (b). Elements of fluid travel in an orderly
Figure 2.4: Ideal Chemical Reactors
way through the chamber with no element overtaking any other element (i.e., no mixing in the direction of the flow, but infinite radial mixing). A STR is a reactor for which contents are considered well mixed and properties of the contents are uniform throughout the combustion chamber (Figure 2.4 (c)). One ramification of the STR assumption is that some unburned reactants will always be present in the chamber outflow.

Webber (1972) used a heterogeneous STR to determine the transient behavior of a liquid rocket engine undergoing chug. His model included a simple feed system, injectors, a combustion chamber and a nozzle.

A lumped parameter approach was used for the feed system, resulting in the equation

$$\frac{dq}{dt} = \frac{P_t - P_c - (1/2) f \rho_c q |q|}{\rho \sum_{n=1}^{NP} \left( \frac{1}{n} / A_n \right)} \tag{2.11}$$

where \( q \) is the volumetric flow rate (m\(^3\)/s) of the propellant, \( f \) is a coefficient chosen to approximate the sum of the turbulent line losses and the nozzle losses in the feed system (m\(^{-4}\)), \( l_n \) and \( A_n \) are the length (m) and area (m\(^2\)) of pipe \( n \), respectively, \( P_t \) is the pressure in the propellant storage tank, \( P_c \) is the pressure in the combustion chamber and \( NP \) is the total number of pipes in the feed system.

Injector calculations included determination of the droplet size distribution and velocity upon injection. Relying heavily upon
empirical correlations, Webber found the droplet size distribution and velocities associated with a self-impinging doublet injector.

In the combustion chamber, the liquid and gaseous states were treated separately. Liquid propellants were divided into droplet size groups whose diameters and velocities were followed over time. Vaporization rate per droplet, \( \omega_v \) (kg/sec per droplet), was given as

\[
\omega_v = \frac{\pi k}{c_p} D (2 + 0.5 Re^{0.5}) \ln(1 + \alpha) \quad [2.12]
\]

where \( k \) is the droplet thermal conductivity (W/m·K), \( c_p \) is the specific heat of the vapor surrounding the droplet (J/kg·K) and \( D \) is the droplet diameter (m). \( \alpha \) is the burning rate parameter, given as

\[
\alpha = \frac{c_p \Delta T}{\Delta H} \quad [2.13]
\]

where \( c_p \) is the specific heat at constant pressure of the droplet (J/kg·K), \( \Delta T \) is the temperature difference between the droplet and the surrounding gases (K) and \( \Delta H \) is the droplet's latent heat of vaporization (J/kg). \( Re \) is the droplet Reynolds number, given as:

\[
Re = \frac{\rho D |v_g - v_{in}|}{\mu_g} \quad [2.14]
\]

where \( v_g \) is the velocity of the gas in the chamber (m/s), \( v_{in} \) is the injection velocity and \( \mu_g \) is the gas viscosity (N·s/m²).
The gas state in the combustion chamber was considered well mixed and to be a perfect gas. Gas velocity was allowed to vary in the combustion chamber. Gas behavior was determined by conservation of mass in the combustion chamber, the perfect gas law and an expression for the expansion of gas through a choked nozzle.

Webber integrated his equations numerically using a fixed time step integration. The size of the time step was seen to be relatively unimportant. He was able to predict a 66 Hz chug whose maximum amplitude was about 200 psia for an average chamber pressure of 400 psia. From his study, Webber concluded that:

1. chug is sensitive to predicted temperature (he used empirical data to give chamber temperature as a function of stoichiometry) and
2. small variations in the droplet size distribution were not very important, but gross changes drastically changed the model's predictions.

Calculated frequencies were within 7% of experimental values and amplitudes were within 5%.

Courtney (1960) used a much simpler approach to determine combustion intensity (mass of propellant burned per volume per time in a combustion chamber) in a heterogeneous STR. He began with an assumed droplet size distribution and assumed steady state conditions and infinitely fast chemical kinetics. Droplet evaporation rate was given as:
where $k$ was assumed constant (but not explicitly given), $r$ is the droplet radius and $\phi$ is the droplet age in the combustion chamber. Overall evaporation rate was determined by integrating [2.15] for $0 < r < r_{\text{max}}$. For a monodisperse spray, Courtney showed that combustion intensity is a strong function of droplet size; intensity increases rapidly with decreasing droplet size.

2.7 SUMMARY

Low frequency combustion instability in a liquid bipropellant rocket engine involves a coupling of oscillations in chamber pressure with oscillations in propellant flow rate. This coupling is possible because of the combustion time lag in the combustion chamber and the inertia of the propellant in the feed lines.

A number of models have predicted the domain of operating conditions in which a rocket engine will undergo stable operation. (Summerfield, Crocco, Lim and others). These models involve linearized equations from which either stability or instability of an engine can be predicted. In general, it has been shown from these models that higher propellant temperatures, lower chamber pressures and longer propellant feed lines lead to more stable rocket engines.

Other models have predicted either the steady state operation or transient behavior of rocket engines (Webber and Courtney). These
types of models generally involve nonlinear equations which are solved over time numerically for variables such as chamber pressure and temperature, droplet size distribution and combustion rate. The advantage of these models is that amplitudes and frequencies of oscillations in pressure, temperature and oxidizer mass flow rate can be calculated. These models have shown the STR model to be sufficient for modelling rocket engine combustion chambers undergoing chug.

The author has modelled the SSME fuelside preburner as a perfectly mixed reactor and has predicted its behavior during engine shutdown. Derivations of the governing equations for this model are found in Chapter III.
CHAPTER III

MODELLING THE SSME FUEL PREBURNER

The SSME fuel preburner is modelled as a multi-pipe, multi-node oxidizer feed system, a transient stirred tank reactor (TSTR) combustion chamber and an exit turbine, as shown in Figure 3.1. This approach is similar to that used by Webber (1972) and employs most of the same governing equations as those used by Pratt and Radhakrishnan (1986). Using a TSTR model allows the frequency and amplitude of oscillations in chamber pressure and oxidizer mass flow rate to be calculated. Using a multi-pipe, multi-node oxidizer feed system allows the position of a liquid/vapor interface in the feed system to be calculated at each integration time step.

The governing equations for the TSTR and oxidizer feed system are partially derived below and their solution is described. Full derivations are given in Appendix A.

The governing equations were solved on a digital computer. A program flowchart, listing and sample input and output files are found in Appendix B.

3.1 THE COMBUSTION CHAMBER

The TSTR model for the combustion chamber assumes that at any given time the combustion chamber can be considered a stirred tank reactor (properties and composition are uniform throughout the combustion chamber). With time, though, chamber composition and
Figure 3.1: Schematic of the Fuelside Preburner Model
properties are allowed to vary. Using a TSTR to model a chugging rocket combustion chamber is justified, in that oscillations in the combustion chamber have long periods in comparison to the amount of time it takes a disturbance to travel through the combustion chamber. Also, it is aggregate, not local changes in pressure in the chamber that are able to couple with oscillations in the propellant feed rate to produce a low frequency system instability.

The TSTR model was used because it is simple, requiring a minimal number of calculations to determine the conditions at each time, because it can accommodate heterogeneous combustion and because a coupling of oscillations in feed system propellant flow with chamber pressure oscillations is possible.

Heterogeneous combustion of liquid oxygen with gaseous hydrogen occurs within the fuel preburner combustion chamber. This is accommodated by the TSTR model by the imposition of a uniform oxidizer droplet distribution throughout the combustion chamber. Droplets were assumed to all have the same diameter and an equal number of droplets are found in any part of the combustion chamber volume. The instantaneous average droplet diameter \( D_m \) was calculated using a relation given by Hersch and Rice (1967). For a coaxial injector with gaseous hydrogen injected through an annulus around a central stream of liquid oxygen,

\[
D_m = c_{dm} \left( \frac{D}{\overline{D}} \right) \sqrt{\frac{N_i}{R_i \rho_j \rho_i}} \frac{A_{H_2}}{T_{H_2}} \frac{p_c}{p}
\]  

[3.1]
$c_{dm}$ is a dimensionless constant equal to 0.485. $(O/F)$ is the mass ratio of oxidizer flow to fuel flow, $M_{H_2}$ is the molecular weight of hydrogen (kg/kgmole), $A_{H_2}$ is the area of the anulus through which hydrogen is injected ($m^2$), $R_g$ is the universal gas constant $(J/kgmole\cdot K)$, $\rho_j$ is the density of the oxygen jet (kg/m$^3$), $T_{H_2}$ is the temperature of the hydrogen on injection (K) and $P_c$ is the chamber pressure (Pa). Equation [3.1] gives the mean droplet diameter of liquid oxygen droplets immediately after injection. In reality, the mean droplet diameter in the combustion chamber is less than that just after injection, however, equation [3.1] was used to give the mean droplet diameter throughout the chamber since no data were available for determination of the droplet distribution in the chamber. The effect that mean droplet diameter has on preburner operation is shown in Chapter IV.

The evaporation rate of a single droplet, $\omega_v$ (kg/sec/droplet), was given by Webber (1972) in equation [2.12]. For an average liquid density of $\beta$ (mass of liquid per unit volume of the combustion chamber), the total vaporization rate, $\Omega$ (kg/s), including the contributions from all droplets, is

$$\Omega = \frac{6 \beta V}{\rho_1 \pi D_m^3} \omega_v \quad [3.2]$$

$V$ is the combustion chamber volume ($m^3$).

Combustion rate was calculated in two different ways. First, all the oxygen that vaporized was assumed to combust immediately
with hydrogen to form water vapor. This implies that diffusion of oxygen vapor into the chamber contents and chemical reaction both occur instantaneously. Since oxygen is consumed as soon as it vaporizes, its rate of production by combustion $\Gamma_{O_2}$ (kgmoles/s) is equal to negative its rate of production by vaporization:

$$\Gamma_{O_2} = - \frac{\Omega}{M_{O_2}}$$

[3.3]

From conservation of atoms,

$$\Gamma_{H_2} = 2 \Gamma_{O_2}$$
$$\Gamma_{H_2O} = -2 \Gamma_{O_2}$$

For the second combustion model, atomization was assumed infinitely fast. Oxygen vaporized according to [2.12] then instantaneously mixed with the gaseous species in the combustion chamber. The production of water vapor from hydrogen and oxygen occurred via a chain reaction involving nine elementary reactions and the species $H_2$, $O_2$, $H_2O$, $H$, $O$ and $OH$.

To aid in the solution of the governing equations, the very reactive species $H$, $O$ and $OH$ were assumed to be consumed as soon as they were produced. In other words, their mole numbers, $\sigma_i$ (kgmoles of species $i$ per total mass in the combustion chamber) were constant at any time:
\[
\frac{d\sigma_H}{dt} = \frac{d\sigma_O}{dt} = \frac{d\sigma_{OH}}{dt} = 0
\]

This condition fixed the values of the \(\sigma_H\), \(\sigma_O\) and \(\sigma_{OH}\) at each time step. A full derivation of reaction rate involving chemical kinetics is found in Appendix A.

The governing equations for the combustion chamber were derived from the conservation of mass for the gaseous and liquid contents of the combustion chamber, conservation of species, conservation of energy and the ideal gas relation.

Conservation of mass for the gaseous contents of the chamber is shown in Figure 3.2 and described analytically by equation [3.4].

\[
\begin{align*}
\text{inflow} & \quad \text{TSTR} & \quad \text{outflow} \\
\text{NSTRM} \cdot \Sigma m_j & \quad d(\rho C V) / dt, \Omega & \quad \Sigma m_j & \quad m_g \\
j = 1 & \quad & \quad & \quad \end{align*}
\]

Figure 3.2: Conservation of Mass for the Gas Phase

\[
\frac{d(\rho C V)}{dt} = \left( \Sigma m_j \cdot \right) - m + \Omega \quad [3.4]
\]

\(m_g\) is mass flow rate of gases out of the combustion chamber (kg/s),
\( \rho_c \) is combustion chamber density \((\text{kg/m}^3)\), \( t \) is time \((\text{s})\), \( V \) is volume \((\text{m}^3)\), \( \text{NSTRM} \) is the number of inlet streams to the TSTR, the subscript \( g \) denotes the gaseous state and superscript * denotes an inlet quantity.

Conservation of mass for the liquid contents of the chamber is shown in Figure 3.3 and described analytically by equation [3.5].

\[
\frac{\text{d}(\beta V)}{\text{d}t} = \sum_{j=1}^{N\text{STRM}} \frac{\beta}{\rho_c^g} - \Omega
\]

**Figure 3.3: Conservation of Mass for the Liquid Phase**

The subscript \( 1 \) denotes the liquid phase. Since the liquid density is uniform throughout the combustion chamber, the liquid outflow is given by \( \beta m^g / \rho_c \).

Conservation of species is shown in Figure 3.4 and described analytically by equation [3.6].
$\frac{d(\sigma_i \rho c)}{dt} = \sum_{j=1}^{NSTRM} \sum_m m_j \sigma_{ij} - \sum_m m_i \sigma_i + \Gamma_i, \ i=1,2,3,...NS \ [3.6]$
\[
\frac{dE}{dt} = \sum_{i=1}^{NS} \sum_{j=1}^{NSTM} m_{ij} h_{ij} - \sum_{i=1}^{NS} \dot{m}_i \sigma_i h_i - \dot{Q} \quad [3.7]
\]

\[E\] is the total (chemical plus sensible) energy (Joules) in the combustion chamber, \(h_i\) is the molar enthalpy of species \(i\) (J/kgmole) and \(\dot{Q}\) is the heat transfer rate out of the combustion chamber (Joules/s).

Liquids in the chamber were assumed to occupy negligible volume. The volume occupied by liquid in the combustion chamber after a long time at a steady oxidizer mass flow rate of 5 kg/s and a chamber temperature of 1000K was calculated. At these conditions, the ratio of the volume occupied by liquid to the total chamber volume was 1 : 47,000. Gases were assumed to obey the ideal gas relation, which took the form

\[P_c = \rho_c \left( \Sigma \sigma_i \right) R T_c \quad [3.8]\]

\(\Sigma \sigma_i\) gives the average molecular weight of the chamber gases.

Equations [3.6], [3.7] and [3.8] were expressed in terms of the logarithmic variables \(\ln T_c\), \(\ln P_c\) and \(\ln \sigma_i\), \(i=1,2,3,\ldots\NS\). This prohibited negative values and facilitated integration by altering the time constants associated with these variables. In their final form, the conservation of mass for the liquid phase, the conservation of species, the conservation of energy and the ideal gas relation are
\[
\frac{d\beta}{dt} = \frac{\text{NSTRM}_*}{\rho_c} - \beta
\]

\[
\frac{d(ln \sigma_i)}{dt} = \frac{1}{\rho_c \sigma_i} \sum_{j=1}^{\text{NSTRM}_*} (\sigma_{ij}^* - \sigma_i) + \Gamma_{iv} \quad i=1,2,3,...,\text{NS}
\]

\[
\frac{d(ln T_c)}{dt} = \sum_{i=1}^{\text{NS}} \sum_{j=1}^{\text{NSTRM}_*} \frac{m_{ijv} \sigma_{ij}^* h_{ij}}{\rho_c \sigma_i - R_g} - \frac{\rho_c}{\Sigma_i \sigma_i (c_{pi} - R_g)}
\]

\[
\frac{d(ln P_c)}{dt} = \frac{d(ln T_c)}{dt} + \frac{\dot{Q}/V}{\rho_c} + \frac{d \rho_c}{dt} \frac{1}{\rho_c} \sum_{i=1}^{\text{NS}} (\Sigma_i \sigma_i)
\]

The superscript \( v \) denotes a volumetric quantity (1/m³), \( c_{pi} \) is the specific heat at constant pressure for species \( i \) (J/kgmole·K) and \( R_g \) is the universal gas constant (J/kgmole·K). The combustion chamber equations are derived in greater detail in Appendix A.

3.2 THE OXIDIZER FEED SYSTEM

Before shutdown begins, the fuel preburner oxidizer feed system is completely filled with liquid oxygen. During shutdown, gaseous
helium progressively replaces oxygen in the pipes. To create a feed system which was simple, yet responsive to changes in combustion chamber pressure and fluid compressibility in the pipes, the following assumptions were made.

1. Liquid oxygen is incompressible.
2. Helium behaves as a perfect gas.
3. Temperature is constant throughout the feed system.
4. Pipes have a characteristic cross sectional area; area is taken as constant throughout a given pipe.
5. There is no accumulation of mass at pipe nodes; the nodes have negligible volume.
6. If a pipe contains both the liquid and the gas phases, a distinct interface exists between them.
7. Fluid velocity is constant within a given pipe (i.e., if there is an interface in the pipe, the liquid, the vapor and the interface are all assumed to be moving at the same velocity.
8. Flow resistance in a pipe is lumped at the pipe exit, so the flow resistance for a pipe containing a liquid/vapor interface is the same as that for a pipe which contains only liquid, until all of the liquid is expelled.

Time dependent variables in the feed system include the fluid velocity in each pipe, the density at each pipe node and the position of the liquid/vapor interface in each pipe.

Figure 3.6 shows a pipe containing a liquid/vapor interface.
Figure 3.6: Schematic of a Pipe Containing a Liquid/Vapor Interface

\[ V \text{ is volume (m}^3\text{), } L \text{ is pipe length (m), } v_1 \text{ and } v_2 \text{ are upstream and downstream velocities (m/s), respectively, } P_1 \text{ and } P_2 \text{ are upstream and downstream pressures (Pa), respectively, } A \text{ is pipe Area (m}^2\text{) and } F_f \text{ accounts for turbulent and shear head losses in the pipe.} \]

Subscripts 1 and g denote the liquid and gas phases, respectively.

Since pipe length is constant,

\[ \frac{dL_g}{dt} = -\frac{dL_1}{dt} = v \quad [3.13] \]

Conservation of momentum, expressed in integral form, is

(White, 1979)
\[ \Sigma F = \frac{\partial}{\partial t} \left( \iiint_{CV} \rho v dV \right) + \iiint_{CS} \rho v(v \cdot n) \, dA \]  

[3.14]

\[ \Sigma F \] is the sum of the longitudinal forces on the pipe. From Figure 3.6, one can see that

\[ \Sigma F = (P_1 - P_2) A - F_f \]  

[3.15]

\( F_f \) is given as

\[ F_f = f L \rho v^2 A \]  

[3.16]

where \( f \) is a constant (1/m) corresponding to the longitudinal force that either the gas or the liquid within the pipe is exerting on the pipe. Recall that if any liquid is in the pipe, it is as though there is only liquid in the pipe.

Using equations [3.13], [3.15] and [3.16], equation [3.14] can be written

\[ L_g \frac{d \rho_g}{dt} + L_1 \frac{d \rho_1}{dt} + \left( \frac{\rho_g L_g}{v} + \frac{\rho_1 L_1}{v} \right) \frac{dv}{dt} = \frac{P_1 - P_2}{v} - f L \rho v^2 \]  

[3.17]

Equation [3.17] is applied to each pipe, leading to NP equations (NP is the number of pipes in the feed system).

Figure 3.7 shows a pipe node.
Since mass is not allowed to accumulate at the node, for NPN pipes connected at the node, conservation of mass for the node can be written

\[ \sum_{n=1}^{\text{NPN}} (\rho A_n v_n) = 0 \]  \[ [3.18] \]

Equivalently,

\[ \sum_{n=1}^{\text{NPN}} \frac{d}{dt} (\rho A_n v_n) = 0 \]  \[ [3.19] \]

Taking the derivative in [3.19] and assuming that the fluid in each pipe has the same density as the fluid in the others, equal to the density in the node, leads to
\[ \frac{d \rho_n}{dt} + \sum_{n=1}^{NN} A_n v_n + \rho_n \sum_{n=1}^{NP} A_n \left( \frac{dv_n}{dt} \right) = 0 \]  [3.20]

[3.20] is applied to NN nodes, where NN is the number of nodes in the oxidizer feed system. The piping system equations are derived in greater detail in Appendix A.

Equations [3.17] and [3.20] constitute NN+NP equations in the NN unknown nodal densities and the NP unknown pipe velocities. This set of equations is linear and, at each time step, can be solved for \( \frac{dv_n}{dt} \) \( (n=1,2,3,\ldots, NP) \) and \( \frac{d\rho_k}{dt} \) \( (k=1,2,3,\ldots, NN) \).

3.3 THE EXIT TURBINE

Hot product gases pass through a turbine when exiting the fuel preburner. The mass flow rate of the gases through the turbine is a function of the pressure downstream of the turbine (PHG) and the inertia of the turbine blades, as well as the pressure in the combustion chamber. An equation which gives the mass flow rate through the turbine was given in the Dynamic Balance Model for the SSME (Nguyen, 1981) as

\[ m = c_{ftp} \left( \frac{P_c}{T_c} \right)^{0.5} \left[ \left( \frac{PHG}{P_c} \right)^{1.43} - \left( \frac{PHG}{P_c} \right)^{1.71} \right]^{0.5} \]  [3.21]
The parameter \( c_{ftp} \) is an empirical function of turbine geometry and speed. For this model, \( c_{ftp} \) is assumed to be constant during the short time duration of the chug. This implies that turbine speed decreases slowly.

3.4 SOLUTION OF THE GOVERNING EQUATIONS

Equations [3.9], [3.10], [3.11], [3.12], [3.17] and [3.20] were integrated numerically to give the values of \( T_c, P_c, \sigma_i \) (\( i=1,2,3,...NS \)), \( \rho_k \) (\( k=1,2,3,...NN \)), \( v_j \) (\( j=1,2,3,...NP \)) and \( L_g \) (position of the liquid/vapor interface in pipe \( j \)) (\( j=1,2,3,...NP \)) over time. The TSTR equations are nonlinear in the reaction rate expressions and the expression that give thermodynamic properties. Since the set of equations is also stiff (involving widely varying time constants), the IMSL math subroutine DGEAR was used to integrate the equations. DGEAR finds approximations to the solution of ordinary differential equations of the form

\[
\dot{y}' = f(x,\dot{y})
\]

for given initial conditions. The function \( f(x,\dot{y}) \) was calculated in a user supplied subroutine which was declared external in the main program and was accessed by DGEAR for each time step in the integration. A number of different integration methods were available in the DGEAR package. For most executions, the stiffness methods of Gear were used. Where possible, initial conditions were chosen to agree with experimental data. In other cases, when
experimental data were not available, "steady state" conditions were used as initial conditions. The selection of initial conditions is further discussed in Chapter IV.

Flow charts showing the solution process, a listing of program TRNCHG which was developed to solve the governing equations using DGEAR, a sample input file and sample output files are found in Appendix B.
CHAPTER IV

RESULTS

In Chapter III a Transient Stirred Tank Reactor (TSTR) model was proposed for predicting the transient behavior of the SSME fuelside preburner during the helium purge of the engine shutdown. Fuel feed rate is assumed constant, while the oxidizer feed system is modeled as a series of pipes and nodes and an injector resistance. The exiting fluid from the combustion chamber, containing gaseous products, gaseous reactants and liquid droplets, passes through an exit turbine.

A computer program, TRNCHG (Appendix B), was written to numerically integrate the resulting differential equations. From the results of TRNCHG it was possible to calculate the amplitude and frequency of oscillations in combustion chamber pressure and oxidizer mass flow rate. A number of engine parameters were varied to determine the role they play in the fuelside preburner chug and to demonstrate the reliability of TRNCHG. The parameters that were varied include the rate of heat transfer from the walls of the combustion chamber to the contents of the chamber, the mean droplet diameter, the fuel mass flow rate, the fuel temperature, the liquid oxygen (LOX) temperature, the temperature of the helium, and the length of the helium purge line (the pipe connecting the helium storage tank to the helium check valve (Figure 3.1, p. 43)) and the diameter of the helium purge line.
This chapter is a summary of the results of TRNCHG. All marked data points in the figures that follow were generated mathematically and were marked either to differentiate between curves on the same graph or to specify calculation points on curves drawn using few data points.

4.1 OPERATION OF THE FUELSIDE PREBURNER DURING THE SSME SHUTDOWN HELIUM PURGE

As described in Chapter I, during the SSME shutdown, gaseous helium pushes liquid oxygen from the oxidizer feed system of the fuelside preburner and into the combustion chamber. As outlined in Table 1.1 (page 7), just before the helium purge of the fuelside preburner begins, the fuelside preburner oxidizer valve (FPOV) is closed, so the velocity of the LOX in the preburner oxidizer feed system was set at 0.001 m/s (it was not set equal to zero because of the numerical difficulties arising from setting the velocity equal to zero). It is possible that a small amount of LOX enters the preburner combustion chamber between the time that the FPOV is closed and the valve that restrains the helium is opened. This is due to the heating and expansion of LOX in the pipe connecting the FPOV to the preburner manifold.

The pressure throughout the combustion chamber, oxidizer feed system and helium supply piping was assumed uniform and equal to the cracking pressure of the helium check valve, 5.17 MPa (750 psia).
The NASA SSME transient model predicts that the temperature in the fuelside preburner decreases at a rate of about 50 K/s (90°R/s) (Seymour, 1986) at the beginning of shutdown. Without any heat transfer from the chamber walls, TRNCHG predicts that the fuelside preburner temperature falls at a rate of 280,000 K/s when the helium check valves first open. Because the rate at which TRNCHG predicts the chamber temperature decays was too high, a rate of heat transfer to the chamber contents of $6.5 \times 10^7$ J/s ($6.2 \times 10^4$ Btu/s) was selected for the TRNCHG helium purge simulation. This value was chosen because it made the initial temperature gradient predicted by TRNCHG closer to that predicted by the SSME transient model yet did not fix the chamber temperature. The selection of heat transfer rate will be further discussed in section 4.2.

At the beginning of the fuelside preburner helium purge, the pressure downstream of the exit turbine (PHG) is 2.41 MPa (350 psia). By the time the helium purge is over, PHG is 1.03 MPa (150 psia). The average value of PHG, 1.72 MPa (250 psia), was used for the helium purge simulation. The exit mass flow rate coefficient, $c_{ftp}$, was calculated using equation [3.21] (page 56). $c_{ftp}$ was algebraically isolated and calculated by setting the initial exit mass flow rate equal to the fuel mass flow rate (which is constant during shutdown) and setting the chamber pressure equal to the initial chamber pressure, 5.17 MPa (750 psia). $c_{ftp}$ was assumed constant during the short time duration of the chug.
No data on helium temperature in the helium line were available, so the temperature of the helium purge was set equal to the oxidizer temperature, 120 K (216°R).

A summary of inputs to TRNCHG for the SSME shutdown is given in Table 4.1.

Figure 4.1 shows TRNCHG's prediction for combustion chamber temperature during the helium purge. Time equal to zero corresponds to the time that the helium check valves are opened for this graph and all graphs generated for the SSME shutdown simulation. Chamber temperature falls until it reaches a fairly constant value, around 400 K (720°R). The steady value that the temperature reached was determined largely by the rate of heat transfer to the chamber contents. With no heat transfer, the steady state temperature is 188 K (338°R). Figure 4.1 includes only the first 25 msec of TRNCHG's predictions although the program was run until the helium/LOX interface in the oxidizer feed system reached the combustion chamber. Figure 4.2 is a plot of the mole number of oxygen vapor (kgmoles of oxygen vapor per mass (kg) in the combustion chamber) in the combustion chamber during shutdown versus time. The amount of oxygen vapor in the chamber rises sharply (from the program's minimum allowable value of 1.0 x 10^{-12} kgmoles/kg) to a steady value around 5 x 10^{-3} kgmoles/kg. The mole number of water vapor did not change significantly from the minimum allowable mole number.
Table 4.1: Inputs to TRNCHG for the SSME Shutdown Simulation

<table>
<thead>
<tr>
<th>PARAMETER</th>
<th>VALUE AT THE BEGINNING OF THE SSME SHUTDOWN SIMULATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chamber Temperature</td>
<td>550 K (990°R)</td>
</tr>
<tr>
<td>Chamber Pressure</td>
<td>5.17 MPa (750 psia)</td>
</tr>
<tr>
<td>PHG</td>
<td>1.72 MPa (250 psia)</td>
</tr>
<tr>
<td>LOX Temperature</td>
<td>120 K (216°R)</td>
</tr>
<tr>
<td>Fuel Temperature</td>
<td>160 K (288°R)</td>
</tr>
<tr>
<td>Helium Temperature</td>
<td>120 K (216°R)</td>
</tr>
<tr>
<td>Fuel Mass Flow Rate</td>
<td>21.0 kg/s (46.3 lbm/s)</td>
</tr>
<tr>
<td>Heat Transfer Rate</td>
<td>6.5 x 10^7 J/s (6.2 x 10^4 Btu/s)</td>
</tr>
<tr>
<td>Pipe Length from the Helium Storage Tank to the Check Valve</td>
<td>1.5 m (4.9 ft)</td>
</tr>
</tbody>
</table>
Figure 4.1: Temperature v. Time for SSME Shutdown
Figure 4.2: Mole Number of Oxygen Vapor in the Combustion Chamber v. Time for SSME Shutdown
As shown by Figures 4.1 and 4.2, TRNCHG predicts that ignition will not take place in the SSME fuelside preburner during the shutdown helium purge, contrary to the findings of test firings. There are two explanations for TRNCHG's incorrect prediction. First, using a TSTR model results in the overprediction of the equivalence ratio at which combustion takes place. In the heterogeneous stirred tank reactor, LOX vaporizes and the oxygen vapor is assumed to instantaneously mix with the gaseous contents of the combustion chamber. In actual droplet combustion, though, oxidizer and fuel burn on a diffusion flame surface around the droplet at a position where oxidizer and fuel meet in stoichiometric proportion. Thus, the TSTR model overpredicts the equivalence ratio at which combustion takes place; the mixture of gases is beyond the rich limits of combustion. Second, the kinetic mechanism and elementary reaction rate data used in TRNCHG may be inaccurate at the temperatures and pressures that are found in the preburner during the helium purge.

Since use of chemical kinetics in the calculation of combustion rate resulted in erroneous predictions, a second combustion model was used to predict preburner behavior during shutdown. All the LOX that was vaporized was assumed to immediately combust with hydrogen to form water vapor (i.e., chemical kinetics were assumed to be infinitely fast). Figure 4.3 shows TRNCHG's prediction of chamber pressure using this second combustion model and Figure 4.4 shows the predicted oxidizer mass flow rate. The symbols mark each third analytically generated data point. TRNCHG was allowed to run until
Figure 4.3: Chamber Pressure v. Time for the SSME Shutdown (Infinitely Fast Chemical Kinetics)
Figure 4.4: Oxidizer Mass Flow Rate v. Time for the SSME Shutdown (Infinitely Fast Chemical Kinetics)
the helium/LOX interface entered the combustion chamber, but only the first 25 msec of the run is shown in Figures 4.3 and 4.4, since no oscillations took place after that time. The initial peak to peak amplitude of the pressure oscillation is 1.4 MPa (200 psia) and the frequency of the oscillation is 111 Hz. The amplitude and frequency of pressure oscillations during an actual typical preburner chug are 2.41 MPa (350 psia) and 117 Hz, respectively. Oscillations in the chamber pressure and oxidizer mass flow rate are about 1/5 cycle more than 180° out of phase, due to the vaporization time delay.

To investigate the possibility that a disturbance in chamber pressure (for example, due to a change in the oxidizer preburner combustion chamber pressure) incites the fuel side preburner chug when the helium/LOX interface has progressed nearly to the combustion chamber, a perturbation was applied in TRNCHG at 50 msec. The system was perturbed by changing the constant, $c_{dm}$, in the expression for mean droplet diameter (equation [3.1], page 44). $c_{dm}$ was changed from 0.485 to 20.0 at time equal to 50 msec. After 2.5 msec the value of $c_{dm}$ was returned to 0.485. While $c_{dm}$ was equal to 20.0, the vaporization rate decreased since the droplets were larger and the ratio of the surface area of liquid to the mass of liquid in the combustion chamber decreased. Because of the subsequent decrease in the evaporation rate of the LOX, liquid accumulated in the combustion chamber. When the value of $c_{dm}$ was returned to 0.485, the accumulated liquid burned quickly and the chamber pressure rose sharply. The resulting chamber pressure
oscillations are shown in Figure 4.5. Once again, chamber pressure oscillations damped quickly.

Assuming infinitely fast chemical kinetics, TRNCHG did not predict sustained oscillations in chamber pressure. As described earlier, a number of the engine parameters used in this base case simulation of the SSME shutdown were selected as best guesses of the actual conditions that exist in the fuelside preburner during shutdown. To determine whether or not a change in engine parameters could incite a chug, engine parameters were varied, one at a time. In many cases a small change in an engine parameter had a large influence on preburner stability. Following is a summary of the predictions of TRNCHG when engine parameters were varied.

4.2 THE EFFECT OF HEAT TRANSFER RATE ON PREBURNER OPERATION

As discussed in section 4.1, in order for TRNCHG's prediction of initial temperature gradient to be equal to that predicted by the NASA SSME transient model, there must be heat transfer to the combustion chamber contents. Care had to be taken in choosing this rate of heat transfer, since data from which heat transfer rate could be calculated was not available and since heat transfer rate has such a large effect on the chamber temperature.

TRNCHG was executed using different rates of heat transfer and no oxidizer mass flow to find the temperature that the chamber contents would eventually reach. These steady state temperatures are
Figure 4.5: Preburner Response to a Perturbation During Shutdown (Infinitely Fast Chemical Kinetics)
plotted against heat transfer rate in Figure 4.6. High heat transfer rates have the effect of fixing chamber temperatures; even in the absence of combustion, the chamber temperature will never fall below the steady state temperature for a given heat transfer rate.

Figure 4.7 is a plot of chamber pressure versus time for heat transfer rates of 0 J/s, $7.5 \times 10^7$ J/s and $1.0 \times 10^8$ J/s. For higher heat transfer rates there is less oscillation in the chamber pressure than for the lower rates. Frequency of the oscillations remains the same for all the rates of heat transfer.

4.3 THE EFFECT OF DROPLET SIZE ON PREBURNER OPERATION

Mean droplet diameter proved very important in determining the operation of the fuelside preburner. To vary the mean droplet diameter, the constant, $c_{dm}$, in equation [4.1], was given the values 0.0485, 0.97, 1.94 and 3.88. These droplet coefficient values resulted in mean droplet diameters (averaged over the 25 msec shown in Figure 4.8) of 1.2 μm, 24.4 μm, 63 μm and 440 μm, respectively. Note that changing $c_{dm}$ changed the droplet diameter both directly and indirectly, since different values of $c_{dm}$ lead to different values of average chamber pressure and oxidizer mass flow rate. Figure 4.8 shows predicted chamber pressure for the four values of the droplet coefficient and Figure 4.9 shows oxidizer mass flow rate. For $c_{dm}$ below 1.0, pressure oscillations damp quickly. For $c_{dm}$ greater than 1.0, oscillations become more sustained, until droplet size becomes
Figure 4.6: Steady State Temperature v. Heat Transfer Rate
Figure 4.7: The Effect of Heat Transfer Rate on Chamber Pressure Oscillations
Figure 4.8: The Effect of Mean Droplet Diameter on Chamber Pressure Oscillations
Figure 4.9: The Effect of Mean Droplet Diameter on Oxidizer Mass Flow Rate
so large that vaporization rate becomes very small (due to limited
droplet surface area) and reaction blows off, as shown by the curve
for \( c_{dm} = 3.88 \). For \( c_{dm} = 0.0485 \) the frequency of the pressure
oscillation is 116 Hz. For \( c_{dm} = 1.97 \) the frequency is 83 Hz. For
\( c_{dm} = 1.97 \) backflow of combustion chamber contents into the oxidizer
feed system is predicted, as shown in Figure 4.9.

As seen in Figure 4.8, there is probably some critical mean
droplet diameter (or equivalently, some critical combustion delay
time) at which the fuelside preburner begins to undergo unstable
operation. The critical diameter could be reached by changing the
injector geometry or the fuel mass flow rate. The effect of fuel
mass flow rate on the fuelside preburner is described in section
4.5. Since, in the absence of chemical kinetics, the value of \( c_{dm} \)
determines the combustion time delay, \( c_{dm} \) could be raised to
increase the combustion time delay and account for chemical
kinetics. The exact amount that \( c_{dm} \) would have to be raised was not
calculated by the author.

4.4 THE EFFECT OF THE OXIDIZER FEED SYSTEM ON PREBURNER OPERATION

TRNCHG was executed for LOX temperature equal to 90 K, 100 K,
120 K and 150 K (162°R, 180°R, 216°R and 270°R). All the other
engine parameters were the same as those given in Table 4.1 (page
64). Decreasing the LOX temperature increases the LOX density and
decreases the LOX vaporization rate in the combustion chamber.
Predicted chamber pressure is plotted against time in Figure 4.10. As predicted by Lim (1986), lower oxidizer temperatures resulted in less stable preburner operation (i.e., larger amplitude pressure oscillations that damped more slowly).

The frequency of chamber pressure oscillations is plotted against LOX temperature in Figure 4.11. As LOX temperature is decreased, oscillation frequency decreases slightly.

In this study, the term amplitude ratio refers to the ratio of the peak to peak amplitude of the second chamber pressure oscillation to the peak to peak amplitude of the first oscillation. It is used as a measure of the rate at which pressure oscillations damp out. Amplitude ratio is plotted against LOX temperature in Figure 4.12. The amplitude ratio rises linearly as LOX temperature is decreased from 150 K to 100 K. As LOX temperature is decreased below 100 K, the amplitude ratio increases more slowly.

4.5 THE EFFECT OF THE FUEL FEED SYSTEM ON PREBURNER OPERATION

Two fuel feed system parameters, the fuel temperature and the fuel mass flow rate, were varied in TRNCHG. As predicted by Lim (1986), lower fuel temperature led to sustained pressure oscillations. Contrary to Lim's predictions, fuel mass flow rate also influenced the preburner's stability.

TRNCHG was executed for fuel temperatures of 50 K, 100 K and 200 K (90°R, 180°R and 360°R). The resulting chamber pressure was
Figure 4.10: The Effect of Oxidizer Temperature on Chamber Pressure Oscillations
Figure 4.11: Pressure Oscillation Frequency v. LOX Temperature

Figure 4.12: Amplitude Ratio v. LOX Temperature
plotted against time in Figure 4.13. Lower fuel temperatures resulted in more slowly damped pressure oscillations of greater amplitude and lower frequency. Oscillation frequency is plotted against fuel temperature in Figure 4.14. Frequency does not change much with temperature until the temperature becomes less than about 120 K, where frequency decreases rapidly as fuel temperature is decreased.

In Figure 4.15, chamber pressure was plotted against time for executions of TRNCHG using fuel mass flow rates of 12 kg/s, 18 kg/s and 25 kg/s. So that the results of these executions were not obscured by heat transfer rate to the chamber contents, the heat transfer rate was assumed to be 0.0 J/s for these runs. The fuel mass flow rate did not effect the pressure oscillation frequency, but did influence the rate at which the oscillations damped. The average oxidizer mass flow rate is plotted against the fuel mass flow rate in Figure 4.16.

The average oxidizer mass flow rate rises almost linearly with fuel mass flow rate. For high mass flow rates (greater combustion chamber throughput), more energy is needed to heat the fuel that does not participate in combustion and hot product gases are quickly swept from the combustion chamber. This leads to lower chamber pressures which lead to higher oxidizer mass flow rates.

As mentioned above, Lim (1986) predicted that fuel mass flow rate is not important in the fuelside preburner chug. The unexpected behavior of chamber pressure oscillations as mass flow rate is
Figure 4.13: The Effect of Fuel Temperature on Chamber Pressure Oscillations
Figure 4.14: Pressure Oscillation Frequency v. Fuel Temperature
Figure 4.15: The Effect of Fuel Mass Flow Rate on Chamber Pressure Oscillations

- △ Fuel Mass Flow Rate = 12 kg/s
- ○ Fuel Mass Flow Rate = 18 kg/s
- □ Fuel Mass Flow Rate = 25 kg/s
Figure 4.16: Oxidizer Mass Flow Rate v. Fuel Mass Flow Rate
changed is attributed to oscillations in chamber temperature. Recall that the fuelside preburner operates very fuel rich and that the incoming fuel is quite cold (160 K [288°R]). For a high fuel mass flow rates, much of the energy liberated by combustion raises the temperature of the hydrogen (most of which does not participate in chemical reactions) to the chamber temperature; there is not enough energy to raise the temperature much above the chamber temperature and sustain oscillations. For a lower mass flow rate, less energy is needed to heat the incoming hydrogen to the chamber temperature, so an oscillation in chamber temperature and an oscillation in chamber pressure can be sustained.

4.6 THE EFFECT OF THE EXIT TURBINE ON PREBURNER OPERATION

During shutdown, the pressure downstream of the exit turbine, PHG, falls from 2.41 MPa (350 psia) to 1.03 MPa (150 psia). It is possible that this change plays a part in inciting the fuel preburner chug. Figure 4.17 contains plots of chamber pressure versus time for PHG equal to 1.03 MPa, 1.72 MPa and 2.41 MPa. Frequency of the pressure oscillations is the same for all three values of PHG. The rate at which the oscillations are damped is smaller for lower values of PHG, as shown in Figure 4.18. Although changing the pressure downstream of the exit turbine did not produce chugging by itself, this change probably plays a part in the onset of chug.
Figure 4.17: The Effect of the Pressure Downstream of the Exit Turbine on Chamber Pressure Oscillations

- PHG = 1.03 MPa
- PHG = 1.72 MPa
- PHG = 2.41 MPa
Figure 4.18: Amplitude Ratio v. Pressure Downstream of the Exit Turbine
4.7 THE EFFECT OF THE HELIUM PURGE ON PREBURNER OPERATION

At the onset of this research, it was thought that oscillations in helium density in the oxidizer feed system were at least partly responsible for the occurrence of the fuelside preburner chug. In section 4.1 it was shown that, even when the oxidizer feed system was almost completely filled with helium, a perturbation did not result in chug, so the presence of helium does not single-handedly bring about chug. To see what effect the presence of helium does have on fuel preburner operation, the temperature of the helium (assumed to be uniform and constant) and the helium purge line diameter and length were varied.

No data were available for the temperature of the helium at the helium check valve, so the temperature was initially assumed to be equal to the LOX temperature, 120 K (216°R). In Figure 4.19, chamber pressure is plotted against time for helium temperatures of 50 K, 150 K, 200 K and 300 K. Figure 4.20 shows the variation of the frequency of chamber pressure oscillations with helium temperature and Figure 4.21 shows the variation with helium temperature of the ratio of the peak to peak amplitudes of the second and first pressure oscillations. Higher helium temperatures lead to higher frequency pressure oscillations that damp more slowly. In the absence of helium, higher temperatures in the oxidizer feed system lead to more stable operation. Helium temperature reverses this
Figure 4.19: The Effect of Helium Temperature on Chamber Pressure Oscillations
Figure 4.20: Pressure Oscillation Frequency v. Helium Temperature

Figure 4.21: Amplitude Ratio v. Helium Temperature
trend. The presence of helium in the oxidizer feed system results in less stability for higher temperatures in the oxidizer feed system. The initial amplitude of pressure oscillations differed only slightly for the different helium temperatures.

As predicted by Summerfield (1951), shorter pipe lengths lead to chug. Figure 4.22 is a plot of chamber pressure versus time for the fuelside preburner for no helium purge line (i.e., for the helium tank mounted directly on the helium check valve). Execution of TRNCHG was halted after 8.3 msec because execution became very slow. For no helium line, the preburner undergoes undamped oscillations in chamber pressure and backflow of chamber contents into the oxidizer feed system.

Figure 4.23 is a plot of chamber pressure versus time for helium purge line lengths of 0.5 m and 2.0 m. Oscillation frequency and the ratio of the peak to peak amplitude of the second oscillation to that of the first are plotted against helium line length in Figures 4.24 and 4.25, respectively. Both the frequency and amplitude ratio rise sharply for helium line lengths below 0.5 m.

TRNCHG was executed using helium purge line diameters of 1.029 cm, 0.739 cm, 0.381 cm and 0.178 cm (0.4", 0.291", 0.381" and 0.15"). The resulting plots of chamber pressure versus time are found in Figure 4.26. For a helium purge line diameter of 0.178 cm, TRNCHG was unable to dependably calculate chamber pressure after about 5 msec because of numerical instability. The velocity of the
Figure A.22: Chamber Pressure v. Time, No Helium Purge Line

Figure 4.22: Chamber Pressure v. Time, No Helium Purge Line
Figure 4.23: The Effect of Helium Line Length on Chamber Pressure Oscillations
Figure 4.24: Pressure Oscillation Frequency v. Helium Line Length

Figure 4.25: Amplitude Ratio v. Helium Line Length
Figure 4.26: The Effect of Helium Line Diameter on Chamber Pressure Oscillations

- HELIUM LINE DIAM = 1.029 cm
- HELIUM LINE DIAM = 0.739 cm
- HELIUM LINE DIAM = 0.381 cm
- HELIUM LINE DIAM = 0.178 cm
fluid in the purge line began to undergo undamped high frequency numerical oscillations. To try to prevent numerical instability, the maximum error allowable in the IMSL integration routine, DGEAR, was reduced and the number of pipes in TRNCHG that represented the purge line was increased. Both of these changes resulted in slightly longer periods of numerical stability accompanied by considerably longer CPU times. The CPU time necessary for TRNCHG to give an accurate solution for a small diameter helium purge line was deemed too high and only the limited solution shown in Figure 4.26 was generated for a helium purge line diameter equal to 0.178 cm.

From Figure 4.26, one can see that a larger diameter helium purge line results in higher frequency chamber pressure oscillations of greater amplitude and which damp more slowly. The average chamber pressure decreases with decreases helium purge line diameter. For a given helium line length, the greater the volume of helium in the line, the less stable the preburner.

4.8 PREBURNER OPERATION AT FULL POWER LEVEL

TRNCHG was used to simulate fuelside preburner operation at full power level (with no helium purge) both to validate the program and to determine the part that chemical kinetics play in the preburner chug. Care had to be taken in choosing TRNCHG's initial conditions, since poor choices resulted in large derivatives and numeric overflows. Species mole numbers and the initial mass of
liquid in the combustion chamber were set equal to the values they 
would reach in a transient stirred tank reactor, after a long period 
of time, at constant chamber pressure, chamber temperature and 
oxidizer and fuel mass flow rates. The oxidizer mass flow rate was 
set equal to the oxidizer mass flow rate that would be reached in 
the pipes after a long period of time at constant upstream and 
chamber pressures. A summary of inputs to TRNCHG for the full power 
level simulation is given in Table 4.2

TRNCHG was first run assuming infinitely fast chemical kinetics 
and was then run taking chemical kinetics into account (as described 
in Chapter III and Appendix A). Chamber pressure for these runs is 
plotted against time in Figure 4.27. Just as in actual operation, 
the preburner does not undergo sustained chug at full power level. 
The initial pressure oscillations are due to the choice of the 
initial values of chamber pressure and chamber temperature. The 
presence of chemical kinetics has a pronounced effect on chamber 
pressure and temperature: pressure oscillations damp more slowly and 
the temperature and pressure that the combustion chamber reaches 
after a long time are lower when chemical kinetics are considered. 
The frequency of the pressure oscillations for the run involving 
kinetics is 164 Hz.

A perturbation was applied to the preburner, at full power 
level, with chemical kinetics included, to see if chug could be 
incited by a large disturbance. At 30 msec, the mean droplet 
diameter coefficient, $c_{\text{dm}}$, of equation [4.1], was reduced from 0.485
Table 4.2: Inputs to TRNCHG for Full Power Level

<table>
<thead>
<tr>
<th>PARAMETER</th>
<th>VALUE AT THE BEGINNING OF THE FULL POWER LEVEL SIMULATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chamber Temperature</td>
<td>1106 K (1991°R)</td>
</tr>
<tr>
<td>Chamber Pressure</td>
<td>38.0 MPa (5500 psia)</td>
</tr>
<tr>
<td>Mass of Liquid in the Chamber</td>
<td>2.71x10^{-2} kg (5.01x10^{-2} lbm)</td>
</tr>
<tr>
<td>Oxidizer Mass Flow Rate</td>
<td>32.08 kg/s (70.72 lbm/s)</td>
</tr>
<tr>
<td>Fuel Mass Flow Rate</td>
<td>34.40 kg/s (75.84 lbm/s)</td>
</tr>
<tr>
<td>Pipe Length</td>
<td>0.12 m (0.39 ft)</td>
</tr>
<tr>
<td>Mass Fractions:</td>
<td></td>
</tr>
<tr>
<td>He</td>
<td>0.0</td>
</tr>
<tr>
<td>H\textsubscript{2}</td>
<td>5.40x10^{-1}</td>
</tr>
<tr>
<td>O\textsubscript{2}</td>
<td>6.59x10^{-3}</td>
</tr>
<tr>
<td>H\textsubscript{2}O</td>
<td>4.54x10^{-1}</td>
</tr>
<tr>
<td>H</td>
<td>5.76x10^{-6}</td>
</tr>
<tr>
<td>O</td>
<td>1.53x10^{-7}</td>
</tr>
<tr>
<td>OH</td>
<td>1.15x10^{-7}</td>
</tr>
</tbody>
</table>
Figure 4.27: Chamber Pressure v. Time at Full Power Level
to 0.364 for 0.5 msec, and then returned to 0.485. The resulting chamber pressure oscillation is shown in Figure 4.28. Initially, when $c_{\text{dm}}$ is reduced, the mean droplet size becomes smaller and more oxygen vaporizes and is available for combustion. During this time the pressure rises. Next, when the amount of liquid in the chamber and the injection rate of LOX into the chamber become small, the combustion rate and pressure fall. The oxidizer mass flow rate then increases and the oscillation in chamber pressure continues. Within seven cycles, the peak to peak amplitude of the pressure oscillations is damped to 16% of its original value.

4.9 CONDITIONS THAT RESULT IN INSTABILITY

Aside from reducing the helium line length to zero, it was not possible to incite chug by varying just one engine parameter, so it is a combination of engine parameters that cause the fuelside preburner chug. TRNCHG was run with various combinations of engine parameters. The purpose of these runs was not to determine the domain of engine parameters that give rise to chugging, but to demonstrate that TRNCHG can predict chug and to show that only small deviations from the engine parameters used for the SSME shutdown simulation can result in chug. Two runs that resulted in instability are described below.

Figure 4.29 is a plot of chamber pressure v. time for hydrogen temperature equal to 120K, helium temperature equal to 200 K, PHG equal to 1.03 MPa, fuel mass flow rate equal to 18 kg/s and mean
Figure 4.28: Preburner Response to a Perturbation at Full Power Level
droplet diameter coefficient equal to 0.585. All other engine parameters were the same as those listed in Table 4.1. Execution was halted after 49 msec because time for each integration step became too long. Using a mean droplet diameter of 0.485 and all other engine parameters the same as those described for Figure 4.29, TRNCHG predicted stable operation.

Figure 4.30 is a plot of chamber pressure versus time for hydrogen temperature equal to 70 K, fuel mass flow rate equal to 15 kg/s, heat transfer rate to the chamber contents equal to $8.5 \times 10^7$ J/s, PHG equal to 1.03 MPa and helium temperature equal to 200 K. All other engine parameters were the same as those listed in Table 4.1. This run was made stable by lowering the helium temperature to 150 K.

4.10 SUMMARY OF RESULTS

The program TRNCHG, which was written to solve the governing equations derived in Chapter III for heterogeneous preburner operation, was supplied with the approximate conditions at the opening of the helium check valves and was executed. When chemical kinetics were allowed to proceed according to a chemical kinetic mechanism, the model erroneously predicted that ignition would not take place in the preburner. When chemical kinetics were assumed infinitely fast, the model predicted that a quickly damped pressure oscillation with a frequency of 111 Hz would take place immediately after the helium check valves were opened. An oscillation in
Figure 4.30: Unstable Preburner Operation (b)
oxidizer mass flow rate into the preburner combustion chamber was also predicted and it was about 1/5 cycle more than 180° out of phase with the pressure oscillation.

To determine their effect on engine stability, the following engine parameters were varied: heat transfer rate from the chamber walls, mean droplet diameter, oxidizer temperature, fuel temperature, fuel mass flow rate, pressure downstream of the fuel preburner exit turbine (fuel turbo-pump), helium temperature, helium line length and helium line diameter. It was found that small variations in a number of these parameters had a large effect on preburner operation. A summary of the effect that each of these parameters has on preburner operation is given in Table 4.3.

TRNCHG was also used to predict conditions in the fuel preburner at full power level. This was both to validate the model and to allow comparison of different reaction rate models. As expected, TRNCHG predicted stable operation at full power level. Assuming that rates of production of the species in the combustion chamber could be calculated using elementary reaction rates resulted in much more slowly damped oscillations in chamber pressure than assuming chemical kinetics were infinitely fast.

Finally, it was demonstrated that, after changing a small number of engine parameters by only a small amount, TRNCHG was able to predict unstable preburner operation.
Table 4.3: Summary of the Effects of Engine Parameters on Fuelside Preburner Operation

<table>
<thead>
<tr>
<th>ENGINE PARAMETER</th>
<th>EFFECT ON PREBURNER OPERATION</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Heat Transfer Rate</strong></td>
<td>Heat transfer rate had a large effect on average chamber pressure and temperature, but very little effect on the rate at which pressure oscillations damped.</td>
</tr>
<tr>
<td><strong>Q</strong> = 6.5x10^7 J/s</td>
<td></td>
</tr>
<tr>
<td>0.0 J/s &lt; Q &lt; 1.0x10^8 J/s</td>
<td></td>
</tr>
<tr>
<td><strong>Mean Droplet Diameter Coefficient</strong></td>
<td>Higher values of c_{dm} lead to large amplitude pressure oscillations which damp more slowly and have lower frequencies. For some value of c_{dm} between 1.94 and 3.88, there is a critical value of c_{dm} for which the preburner is unstable. Above that value liquid droplets become too large and ignition does not occur.</td>
</tr>
<tr>
<td>c_{dm} = 0.485</td>
<td></td>
</tr>
<tr>
<td>0.0485 &lt; c_{dm} &lt; 3.88</td>
<td></td>
</tr>
<tr>
<td><strong>LOX Temperature</strong></td>
<td>Lower oxidizer temperatures lead to higher frequency chamber pressure oscillations which damp relatively quickly. The amplitude ratio for T_{ox} = 150 K is 54.4% of that for T_{ox} = 90 K.</td>
</tr>
<tr>
<td>T_{ox} = 120 K</td>
<td></td>
</tr>
<tr>
<td>90 K &lt; T_{ox} &lt; 150 K</td>
<td></td>
</tr>
<tr>
<td><strong>Fuel Temperature</strong></td>
<td>Below 120 K fuel temperature has a large effect on preburner stability. The frequency of chamber pressure oscillations for T_{fuel} = 50 K is 68% of that for T_{fuel} = 150 K. Oscillations damp more slowly and have greater amplitudes for lower fuel temperatures</td>
</tr>
<tr>
<td>T_{fuel} = 160 K</td>
<td></td>
</tr>
<tr>
<td>50 K &lt; T_{fuel} &lt; 200 K</td>
<td></td>
</tr>
</tbody>
</table>
Table 4.3: (continued)

<table>
<thead>
<tr>
<th>ENGINE PARAMETER</th>
<th>EFFECT ON PREBURNER OPERATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel Mass Flow Rate</td>
<td>Decreasing the fuel mass flow rate caused chamber pressure oscillations to damp more slowly, but did not change the oscillation frequency. Higher fuel mass flow rates resulted in higher oxidizer mass flow rates.</td>
</tr>
<tr>
<td>( m_f = 21.0 \text{ kg/s} )</td>
<td></td>
</tr>
<tr>
<td>( 12.0 &lt; m_f &lt; 25.0 )</td>
<td></td>
</tr>
<tr>
<td>Pressure Downstream of the Exit Turbine</td>
<td>Decreasing the pressure downstream of the exit turbine resulted in more slowly damped chamber pressure oscillations, but did not change the frequency. The amplitude ratio for ( \text{PHG} = 1.03 \text{ MPa} ) is 4.9 times that for ( \text{PHG} = 2.41 \text{ MPa} ).</td>
</tr>
<tr>
<td>( \text{PHG} = 1.72 \text{ MPa} )</td>
<td></td>
</tr>
<tr>
<td>( 1.03 \text{ MPa} &lt; \text{PHG} &lt; 2.41 \text{ MPa} )</td>
<td></td>
</tr>
<tr>
<td>Helium Temperature</td>
<td>Changing the helium temperature changed both the amplitude ratio and the oscillation frequency; Higher helium temperatures lead to higher frequency pressure oscillations that damped more slowly. The frequency at 200 K is 1.3 times that at 120 K. The amplitude ratio at 200 K is 1.5 times that at 120 K.</td>
</tr>
<tr>
<td>( T_{\text{He}} = 120 \text{ K} )</td>
<td></td>
</tr>
<tr>
<td>( 50 \text{ K} &lt; T_{\text{He}} &lt; 300 \text{ K} )</td>
<td></td>
</tr>
<tr>
<td>Helium Line Length</td>
<td>If the helium storage tank were mounted directly on the helium check valves, the fuelside preburner would be unstable. Longer helium line lengths lead to more stable operation. Above 1.5 m, increasing the helium line length had only a small effect on oscillation frequency or amplitude ratio.</td>
</tr>
<tr>
<td>( L_{\text{He}} = 1.5 \text{ m} )</td>
<td></td>
</tr>
<tr>
<td>( 0.01 \text{ m} &lt; L_{\text{He}} &lt; 2.0 \text{ m} )</td>
<td></td>
</tr>
<tr>
<td>ENGINE PARAMETER</td>
<td>EFFECT ON PREBURNER OPERATION</td>
</tr>
<tr>
<td>------------------</td>
<td>-------------------------------</td>
</tr>
<tr>
<td><strong>BASE VALUE</strong></td>
<td></td>
</tr>
<tr>
<td><strong>RANGE OF VALUES USED IN TRNCHG</strong></td>
<td></td>
</tr>
<tr>
<td>Helium Line Diameter</td>
<td>Large helium line diameters volumes of helium in the line) lead to higher chamber pressures and oscillations which have higher frequencies and damp more slowly. For the smallest helium line diameter, a full solution could not be generated because numerical instability was encountered.</td>
</tr>
<tr>
<td>$D_{He} = 0.739$ cm</td>
<td></td>
</tr>
<tr>
<td>$0.173 \text{ cm} &lt; D_{He} &lt; 1.029$ cm</td>
<td></td>
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CHAPTER V

CONCLUSIONS

The objectives of this study were to evaluate the validity of the TSTR model for modelling a rocket engine combustion chamber, to predict the amplitude and frequency of the SSME fuelside preburner shutdown chug and to determine the processes and engine parameters that give rise to the chug.

To meet the first two objectives the fuelside preburner was modelled as a heterogeneous TSTR combustion chamber, a variable mass flow rate oxidizer feed system, a constant mass flow rate fuel feed system and an exit turbine. A computer program, TRNCHG, was written to integrate the resulting differential equations numerically. For full power level simulations TRNCHG predicted stability and executed without difficulty. For SSME engine shutdown conditions, chemical kinetics were assumed infinitely fast and TRNCHG predicted quickly damped chamber pressure and oxidizer mass flow rate oscillations.

To meet the third objective, engine parameters which had been shown in literature to influence the stability of liquid rocket engine combustion were varied. This procedure was quite successful, showing that small changes in some engine parameters resulted in large changes in preburner operation and pointing out two engine parameters that have a larger role in the SSME fuelside preburner chug than predicted by Lim's (1986) linearized model.
Three questions are answered in this chapter: which engine parameters are the key parameters in the SSME fuelside preburner chug? how could the preburner model be extended or modified? and how well does the fuelside preburner model work?

5.1 KEY ENGINE PARAMETERS AND THEIR EFFECT ON PREBURNER STABILITY

As stated in Chapter IV, it is probably a combination of factors that result in the fuelside preburner chug. The most important factors and their influence on the preburner chug, as predicted by the program TRNCHG, are given below.

1. Mean droplet diameter. Mean droplet diameter is a function of injector geometry, chamber pressure and the ratio of the oxidizer and fuel mass flow rates. As mean droplet diameter is increased, pressure oscillations in the combustion chamber damp more slowly. This is due to an increase in the combustion delay time (or decrease in the vaporization rate) associated with large droplets. For a sufficiently large droplet diameter, reaction blows off.

2. Pressure downstream of the exit turbine (PHG). During engine shutdown, PHG falls from 2.41 MPa to 1.03 MPa (350 psia to 150 psia). Pressure oscillations were shown to damp more slowly for lower values of PHG.

3. Fuel temperature. As described in Chapter I, fuel cools the
main combustion chamber and nozzle before being injected into the fuelside preburner combustion chamber. During shutdown, the fuel mass flow rate to the combustion chamber is less than at full power level, but the main combustion chamber and nozzle are also cooler, so the temperature of the fuel injected into the fuelside preburner may be lower during shutdown. Lower fuel temperatures result in a less stable fuelside preburner. When the fuel temperature is reduced below 120 K, pressure oscillation frequency decreases rapidly and the oscillations become less damped.

4. Fuel mass flow rate. Contrary to the predictions of Lim (1986), lower fuel mass flow rates were predicted to cause oscillations in chamber pressure to damp out more slowly. There are two reasons for this. First, for lower fuel mass flow rates there is less cold fuel to heat to the chamber temperature and more energy is available (from combustion) to sustain pressure oscillations. Second, the mean droplet diameter is a function of the fuel mass flow rate: as fuel mass flow rate decreases, the mean droplet diameter increases. As shown in figure 4.10 (page 75), as mean droplet diameter is increased, preburner operation becomes less stable.

5. Helium temperature. Changing the Helium temperature did not substantially change the amplitude of pressure oscillations, but did influence their frequency. Frequencies of pressure
oscillations for helium temperatures of 120 K and 300 K were 111 Hz and 175 Hz, respectively.

6. Helium purge line geometry. The length and diameter of the pipe connecting the helium storage tank to the helium check valve both have a strong influence on the preburner's operation during shutdown. As predicted by Summerfield (1951), as the length of the helium line was increased, the preburner became more stable. Above a helium purge line length of about 1.0m, a large change in pipe length is necessary to accomplish a small change in frequency or the rate at which oscillations damp out.

It was not possible to obtain solutions from TRNCHG for small helium purge line diameters. In general, small helium purge line diameters lead to reduced chamber pressures and greater stability. For a given helium line length, the volume of helium between the helium storage tank and the combustion chamber is important in determining whether fuelside preburner will be stable.

Comparing the results generated by the non-linear model used in this study to the results generated by the linear model used by Lim (1986) to model the SSME fuelside preburner, the non-linear model showed the preburner's stability to be sensitive to engine parameters to which the linearized model predicted the preburner would be insensitive. One instance of the greater sensitivity of the non-linear model is that the inclusion of chemical kinetics in the calculation of reaction rates at full power level resulted in more
slowly damped pressure oscillations than for chemical kinetics being considered infinitely fast (figure 4.28, page 100). Lim assumed that chemical kinetics were infinitely fast. Reaction rate is a non-linear function of chamber temperature and the mole number of the species in the combustion chamber. A second instance in which the predictions of the non-linear and linearized models differ is in the effect that fuel mass flow rate has on chamber pressure oscillations. Lim stated that chug could not be eliminated by changing the mass flow rate. As shown in figure 4.18 (page 86), the non-linear model predicts a pronounced effect of fuel mass flow rate on the rate at which oscillations are damped. Chamber temperature, droplet vaporization rate and mean droplet diameter are all functions of the fuel mass flow rate.

Using a linearized model, Lim was able to predict the effect that a number of engine parameters had on the stability of the SSME fuelside preburner. The results of the linearized model were concise, required a relatively small amount of computer time and in most cases proved accurate. The non-linear model used in the current study was able to show that chemical kinetics and fuel mass flow rate play a greater role in determining whether or not the preburner undergoes stable operation than predicted by the linearized model. These predictions show that a non-linear model is necessary in a detailed study of chug and offset the greater computer time necessary to predict how the preburner operates.
5.2 POSSIBLE EXTENSIONS OF THIS RESEARCH

There are number of ways the fuelside preburner model could be changed to increase its accuracy and to enable it to be used to model different rocket engine phenomena.

To improve the accuracy of the fuelside preburner model, the oxidizer feed system could be more faithfully represented, adding pipes and an oxidizer manifold. A finer grid of pipes would also increase accuracy, although for most cases this is not necessary. Within the oxidizer feed system the compressibility of LOX could be taken into account.

In the combustion chamber, a droplet distribution, which, like Webber's (1972) could contain different sized droplets whose size is followed over time, could be added. Given temperature data for the combustion chamber walls, the rate of heat transfer from the combustion chamber walls to the chamber contents could be more accurately calculated.

Finally, if it were desired to study spatial variations in chamber pressure, temperature and composition, it would be possible to use multiple TSTR's to model the combustion chamber. TSTR's could be distributed longitudinally and radially throughout the combustion chamber. The exit mass flow rate from the face of one TSTR would be an inlet mass flow rate through the face of an adjacent TSTR. Such a scheme could prevent the mixture ratio from being overestimated.
severely in sections of the combustion chamber that contain many liquid droplets.

It is reiterated here that the above alterations of the TSTR model were not necessary in the study of the SSME fuelside preburner chug and are presented as ways in which the fuelside preburner model can be extended to be used in different applications.

5.3 EVALUATION OF THE FUELSIDE PREBURNER MODEL

The TSTR model of the fuelside preburner combustion chamber is simple, yet has been shown capable of predicting low frequency combustion instability. With the proper assumptions, the model can be used over a wide domain of operating conditions and engine parameters.

Among the strengths of the fuelside preburner model are,
1. the frequency of pressure oscillations in the preburner is predicted to within 6% of typical measured frequencies,
2. the effect that various engine parameters and combinations of these parameters has on preburner operation was shown,
3. the presence of liquid in the combustion chamber is included,
4. chemical kinetics may be included for high temperatures and pressures and
5. the fuel preburner is predicted to maintain stable operation at full power level.
The preburner model's weaknesses are

1. chemical kinetics are not modelled during the SSME shutdown,
2. solutions cannot be generated when the diameter of the pipe connecting the helium storage tank to the helium check valve is too small,
3. accurate initial conditions are required and
4. long CPU times are required to generate solutions when large derivatives are encountered (e.g., when backflow of combustion chamber contents into the oxidizer feed system occurs).

Despite the model's limitations, the objectives of this research were basically met. The TSTR model was able to predict transient conditions in a rocket engine preburner. The model predicted that, during the SSME shutdown the fuelside preburner would not undergo unstable operation, yet when key engine parameters were changed by a small amount instability resulted. It is also possible, as a worst case, that the inclusion of chemical kinetics in the model for shutdown would result in unstable preburner operation. The frequency of the SSME preburner chug was accurately predicted, but the amplitude was not, since sustained oscillations were not predicted by TRNCHG. Finally, the model not only showed the influence that engine parameters and processes have on chug, but also pointed out, contrary to the predictions of a linearized model, that fuel mass flow rate and chemical kinetics are important.

The program, TRNCHG, was written for the SSME fuelside preburner. However, by altering the oxidizer feed system
calculations and changing the way that exit mass flow rate is calculated, TRNCHG could be applied to many other rocket engine combustion chambers to study low frequency combustion instability. Using such a program has been shown valuable in an in-depth study of chug.
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APPENDIX A

COMBUSTION CHAMBER AND OXIDIZER FEED

SYSTEM DERIVATIVES
A.1 DERIVATION OF THE TSTR GOVERNING EQUATIONS

The conservation of mass for the gas and the liquid phases is fully derived in Chapter III. The conservation of species and energy for a TSTR and the ideal gas law as used in the present study are derived below.

The Conservation of Species

Equation \[3.6\] can be written

\[
\frac{d(\sigma_i \rho_c)}{dt} = \frac{\text{NSTRM}}{i} \sum_{j=1}^{\text{NSTRM}} \left( \dot{m}_{ij}^* \sigma_{ij}^* - \dot{m}_{giv} \sigma_i + \Gamma_{iv} \right) \tag{[A.1]}
\]

for \(i=1,2,3\ldots\text{NS}\.\) The subscript \(v\) denotes a volumetric quantity.

The derivative in \([A.1]\) is expanded, giving

\[
\rho_c \frac{d\sigma_i}{dt} + \sigma_i \frac{d\rho_c}{dt} = \frac{\text{NSTRM}}{i} \sum_{j=1}^{\text{NSTRM}} \left( \dot{m}_{ij}^* \sigma_{ij}^* - \dot{m}_{giv} \sigma_i + \Gamma_{iv} \right) \tag{[A.2]}
\]

From equation \([3.4]\),

\[
\frac{d\rho_c}{dt} = \frac{\text{NSTRM}}{i} \sum_{j=1}^{\text{NSTRM}} \left( \dot{m}_{ij}^* - \dot{m}_{giv} \right) \tag{[A.3]}
\]

\([A.3]\) is substituted into \([A.2]\) and the result is simplified, yielding

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For any variable, $x$, 

$$\frac{d(ln x)}{dt} = \frac{1}{x} \frac{dx}{dt} \tag{A.5}$$

\[A.5\] is applied to \[A.4\], giving the conservation of species for the TSTR in its final form:

$$\frac{d(ln \sigma_i)}{dt} = \frac{1}{\sigma_i \rho_c} \sum_{j=1}^{NSTRM} \left[ m_{ij}^*(\sigma_{ij}^* - \sigma_i) \right] + \Gamma_{iv} \tag{A.6}$$

\[i=1,2,3 \ldots NS\]

**Conservation of Energy**

Conservation of energy is given by equation \[3.7\] as 

$$\frac{dE}{dt} = \sum_{i=1}^{NS} \sum_{j=1}^{NSTRM} \left( m_{ij}^* \sigma_{ij}^* h_{ij}^* \right) - \sum_{i=1}^{NS} \left( m_i \sigma_i h_i \right) - \dot{Q} \tag{A.7}$$

assuming that changes in the kinetic and potential energies of the chamber contents are negligible,

$$\frac{dE}{dt} = \frac{dU}{dt} = \frac{d}{dt} \left( \sum_{i=1}^{NS} \rho_c \sigma_i u_i \right) \tag{A.8}$$

where $E$ is the total energy (Joules) of the chamber contents, $U$ is the internal energy (Joules) of the chamber contents and $u_i$ is the
specific molar internal energy \((J/\text{kgmole})\) of species \(i\). Expanding the derivative,

\[
\frac{dE}{dt} = \frac{d\rho_c}{dt} \sum_{i=1}^{NS} \rho V_i \sigma_i \frac{d\sigma_i}{dt} + \frac{d\rho_c}{dt} \sum_{i=1}^{NS} \rho V_i \sigma_i \frac{du_i}{dt} \tag{A.9}
\]

Assuming that the contents of the chamber behave as a mixture of perfect gases and that their specific heats at constant pressure, \(c_{pi} \,(J/\text{kgmole}\cdot\text{K})\) do not vary,

\[
\frac{du_i}{dt} = \frac{d}{dt} \left( h_i - R T_c \right) = \frac{dT_c}{dt} \left( c_{pi} - R_g \right) \tag{A.10}
\]

Using \([A.10]\), \([A.9]\) becomes

\[
\frac{dE}{dt} = \frac{d\rho_c}{dt} \sum_{i=1}^{NS} \rho V_i \sigma_i \frac{d\sigma_i}{dt} + \frac{d\rho_c}{dt} \sum_{i=1}^{NS} \rho V_i \sigma_i \frac{du_i}{dt} + \rho_c \frac{dT_c}{dt} \sum_{i=1}^{NS} \sigma_i (c_{pi} - R_g) \tag{A.11}
\]

\([A.11]\) is substituted into \([A.7]\) and \([A.5]\) is applied, giving

\[
\frac{d(ln T_c)}{dt} = \left[ \sum_{i=1}^{NS} \sum_{j=1}^{NSTRM} m_{ji}^* \sigma_i^* \sigma_j^* h_{ij} - \sum_{i=1}^{NS} \sum_{j=1}^{NSTRM} m_{ij}^* \sigma_i^* \sigma_j^* h_{ij} \right] \rho_c \frac{d\rho_c}{dt} \sum_{i=1}^{NS} \sigma_i u_i
\]

\[
\rho_c \frac{d\sigma_i}{dt} \sum_{i=1}^{NS} \sigma_i u_i + \frac{d}{dt} \left( h_i - R T_c \right) / T_c \rho_c \sum_{i=1}^{NS} \sigma_i (c_{pi} - R_g) \right] \tag{A.12}
\]

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The Ideal Gas Law

For the combustion chamber, the ideal gas law can be written

\[ P_c = \rho_c \sigma_m R T_c \]

where \( \sigma_m = \sum_{i=1}^{NS} \sigma_i \). Alternatively,

\[ \frac{dP}{dt} = \rho_c \sigma_m R \frac{dT}{dt} + \rho_c R T_c \frac{d\sigma_m}{dt} \tag{A.13} \]

Equation [A.5] is applied to [A.13], giving

\[ \frac{d(\ln P_c)}{dt} = \frac{\sigma_m R T_c}{P_c} \frac{d\rho_c}{dt} + \frac{\rho_c \sigma_m R}{P_c} \frac{dT}{dt} + \frac{\rho_c R T_c}{P_c} \frac{d\sigma_m}{dt} \tag{A.14} \]

or,

\[ \frac{d(\ln P_c)}{dt} = \frac{1}{\rho_c} \frac{d\rho_c}{dt} + \frac{1}{T_c} \frac{dT}{dt} + \frac{1}{\sigma_m} \frac{d\sigma_m}{dt} \tag{A.15} \]

A.2 DERIVATION OF THE REACTION RATE FROM ELEMENTARY KINETICS

The volumetric forward and reverse reaction rates for an elementary reaction, \( j \), can be written (Pratt and Woomack, 1976)

\[ R'_{jv} = A' \frac{T'_{ij}}{c} \exp\{ -T'_{ij}/T_c \} (\rho_c \sigma_m)^{\nu'_i}{\sum_{i=1}^{NS}}(\rho_c \sigma_i)^{\nu'_i} \tag{A.16} \]

\[ R''_{jv} = A'' \frac{T''_{ij}}{c} \exp\{ -T''_{ij}/T_c \} (\rho_c \sigma_m)^{\nu''_i}{\sum_{i=1}^{NS}}(\rho_c \sigma_i)^{\nu''_i} \tag{A.17} \]
where $A_j$, $N_j$ and $T_{aj}$ are empirically determined coefficients, $T_c$ is the combustion chamber temperature, $\nu_{ij}$ is the stoichiometric coefficient of species $i$ in reaction $j$, $\nu_m$ is the stoichiometric coefficient for a third body, and the superscripts $'$ and $''$ denote forward and reverse reaction, respectively. The overall rate of production of species $i$ by a chain of NRXN elementary reactions is

$$R_{iv} = \sum_{j=1}^{NRXN} (\nu''_{ij} R''_{jv} - \nu'_{ij} R'_{jv})$$

The following elementary reactions made up the overall conversion of $H_2$ and $O_2$ to water vapor in the TSTR model of the SSME fuelside preburner:

$$O_2 + H_2 \rightleftharpoons OH + OH$$
$$OH + H_2 \rightleftharpoons H_2O + H$$
$$O_2 + H \rightleftharpoons OH + O$$
$$O + H_2 \rightleftharpoons OH + H$$
$$O + H_2O \rightleftharpoons OH + OH$$
$$H + H + M \rightleftharpoons H_2 + M$$
$$O + O + M \rightleftharpoons O_2 + M$$
$$O + H + M \rightleftharpoons OH + M$$
$$H + OH + M \rightleftharpoons H_2O + M$$

Because the atoms $O$ and $H$ and the radical $OH$ are so reactive, they are consumed nearly as soon as they are produced, so their mole
numbers were assumed to be constant at any given time, or

\[ \frac{d\sigma_O}{dt} = \frac{d\sigma_H}{dt} = \frac{d\sigma_{OH}}{dt} = 0 \quad \text{[A.19]} \]

Using equation [A.19], equation [A.4] can be written for \( O \), \( H \) and \( OH \), giving

\[ f_H = \sum_{j=1}^{m_N} \sigma_{Hj} \left( \sigma_{Hj} - \sigma_H \right) + R_{Hv} = 0 \quad \text{NSTRM} \]

\[ f_O = \sum_{j=1}^{m_N} \sigma_{Oj} \left( \sigma_{Oj} - \sigma_O \right) + R_{Ov} = 0 \quad \text{[A.20]} \]

\[ f_{OH} = \sum_{j=1}^{m_N} \sigma_{OHj} \left( \sigma_{OHj} - \sigma_{OH} \right) + R_{OHv} = 0 \quad \text{NSTRM} \]

Since there are no radicals present in the inlet streams,

\[ f_H = -\sigma_H \left( \sum_j \sigma_{Hj} \right) + R_{Hv} = 0 \]

\[ f_O = -\sigma_O \left( \sum_j \sigma_{Oj} \right) + R_{Ov} = 0 \quad \text{[A.21]} \]

\[ f_{OH} = -\sigma_{OH} \left( \sum_j \sigma_{OHj} \right) + R_{OHv} = 0 \]

At each time, values for \( \sigma_H \), \( \sigma_O \), \( \sigma_{H0} \), \( T_c \), \( P_c \) and \( \sigma_{OH} \) are known (these are the combustion chamber variables which are being integrated), so equations [A.21] constitute three equations in the three unknown mole numbers \( \sigma_H \), \( \sigma_O \) and \( \sigma_{OH} \).
The roots of equations [A.21] were found using a Newton iteration. The functions, \( f_i \), were expanded in a Taylor series about the assumed solution and second order and higher terms were truncated (George, 1982), giving

\[
f_i = f_{i,old} + \sum_{k=1}^{\text{NRAD}} \frac{\partial f_{i,old}}{\partial \sigma_k} \sigma_k \quad i=1,\text{NRAD} \quad [A.22]
\]

where NRAD is the number of species whose mole number is assumed constant at each time step (Nrad=3 for the SSME TSTR model). If the correct values of the radical mole numbers are chosen, \( f_i = 0 \) for \( i=1,\text{NRAD} \). [A.22] can then be written

\[
\sum_{k=1}^{\text{NRAD}} \frac{\partial f_i}{\partial \sigma_k} \Delta \sigma_k = -f_{i,old} \quad i=1,\text{NRAD}
\]

or,

\[
\begin{bmatrix}
\frac{\partial f_H}{\partial \sigma_H} & \frac{\partial f_H}{\partial \sigma_0} & \frac{\partial f_H}{\partial \sigma_{\text{OH}}} \\
\frac{\partial f_O}{\partial \sigma_H} & \frac{\partial f_O}{\partial \sigma_0} & \frac{\partial f_O}{\partial \sigma_{\text{OH}}} \\
\frac{\partial f_{\text{OH}}}{\partial \sigma_H} & \frac{\partial f_{\text{OH}}}{\partial \sigma_0} & \frac{\partial f_{\text{OH}}}{\partial \sigma_{\text{OH}}}
\end{bmatrix}
\begin{bmatrix}
\Delta \sigma_H \\
\Delta \sigma_0 \\
\Delta \sigma_{\text{OH}}
\end{bmatrix}
= \begin{bmatrix}
-f_{H,old} \\
-f_{O,old} \\
-f_{\text{OH},old}
\end{bmatrix} \quad [A.23]
\]

Equation [A.23] is solved for the correction variables \( \Delta \sigma_i \), \( i=1,\text{NRAD} \). New estimates for \( \sigma_i, i=1,\text{NRAD} \), are

\[
\sigma_{\text{new}} = \sigma_{\text{old}} + \Delta \sigma_i \quad [A.24]
\]

The results of [A.24] are successively substituted into [A.23] until
the condition

\[ \sigma_i < \varepsilon_{ss} \quad i=1, \text{NRAD} \]  

is met. \( \varepsilon_{ss} \) was set at 1.0 \( \times \) 10\(^{-5} \) in the program TRNCHG.

When condition [A.25] was met, reaction rate for \( \text{H}_2\text{O} \) was calculated using the known values for mole numbers, temperature, pressure and density, the steady state values for the radical mole numbers and equations [A.16], [A.17] and [A.18]. By conservation of atoms,

\[ R_{\text{H}_2\text{v}} = -R_{\text{H}_2\text{Ov}} \]
\[ R_{\text{O}_2\text{v}} = 0.5 \ R_{\text{H}_2\text{Ov}} \]  

[A.26]

In all observed cases, the approximate values for \( R_{\text{H}_2\text{v}} \) and \( R_{\text{O}_2\text{v}} \) were close (within an estimated 5%) of the values calculated directly using [A.16], [A.17] and [A.18].

A.3 DERIVATION OF THE OXIDIZER FEED SYSTEM EQUATIONS

In integral form, the conservation of linear momentum for a control volume is (White, 1979)

\[ \Sigma F = \frac{\partial}{\partial t} \left( \iiint \rho \mathbf{v} \, d\mathbf{V} \right) + \iint \rho \mathbf{v} (\mathbf{v} \cdot \mathbf{n}) \, d\mathbf{A} \]  

[A.27]

As shown in figure 3.6, using equations [3.15] and [3.16],

\[ \Sigma F = (P_1 - P_2) A - fL \rho \mathbf{v}^2 A \]  

[A.28]

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For a pipe containing a liquid/vapor interface, [A.27] can be written
\[ (P_1 - P_2)A - fL\rho v^2A = \frac{d}{dt} (\rho_l v\dot{v} + \rho_g v\ddot{v}) + \rho_l v^2A - \rho_g v^2A \] [A.29]

Note that
\[ \frac{dl}{dt} = \frac{dl}{dt} = v \] [A.30]

Divide by A and group terms for
\[ P_1 - P_2 - fL\rho v^2 = (\rho_l \dot{v} + \rho_g \ddot{v}) \frac{dv}{dt} + (\frac{d\rho_l}{dt} + \frac{d\rho_g}{dt}) + \frac{l}{g} \frac{dv}{dt} \] [A.31]

For each pipe node, k, equation [3.20] is written
\[ \rho_k \sum_{n=1}^{NPN} A_n (\frac{dv}{dt})_n + (\frac{d\rho_k}{dt}) \sum_{n=1}^{NPN} A_n v_n = 0 \] [A.32]

Equations [A.31] and [A.32] constitute \( NN+NP \) linear equations in the \( NN+NP \) unknowns: \( \frac{dv}{dt}_n, n=1,2,3 \ldots NP, \) and \( \frac{d\rho_k}{dt}, k=1,2,3, \ldots NN. \) [A.31] and [A.32] can be expressed as the matrix equation \([A] \{X\} = \{B\}\) where matrix \([A]\) contains the coefficients of the unknowns, \(\{X\}\) contains the values of the unknowns and \(\{B\}\) contains \( P_1 - P_2 - fL\rho v^2 \) for rows 1,2,3 ...NP and zero for rows NP+1, NP+2, ... NP+NN. In the program written for this study, \(\{X\}\) was found via a call to IMSL subroutine LEQT1F.
APPENDIX B

FLOWCHARTS, PROGRAM LISTING AND SAMPLE INPUT

AND OUTPUT FILES FOR PROGRAM TRNCHG
Initialize variables and arrays
Read thermodynamic property and reaction rate data
[TSTR (main), subroutines BLKDATA and NPT]

Define the integration step
TM = Present time  TMNX = time following integration
TMEND = time at the termination of the run
STEP = integration step size (can be fixed or variable)
[subroutines TSTR2 and DTSTR or DGEAR]

Calculate the derivatives of the system variables
(see figure A. 2 for a flow chart of these calculations)
[subroutines CSLOPE, COMBRT, THERPS, RADS and RATES]

Calculate and update the values of the system variables
for TM = TM + STEP
[subroutine DTSTR or DGEAR]

Is TM = TMNX ?

yes
Output the values of the system variables to a plot file
and a text file
[files TSTR.PLT and TSTR.OUT]

no

Is TM = TMEND ?

yes
STOP

Figure B.1: Flowchart for Program TRNCHG
CALL FROM INTEGRATION SUBROUTINE

Reset derivative array to zero
Calculate useful variables
[subroutine CSLOPE]

Calculate the evaporation rate of liquid oxygen
[subroutines COMBRT and THERPS]

Calculate the rate of production of each species according to a kinetic mechanism
[subroutines RADSS, RATES, COMBRT AND THERPS]

Are chemical kinetics considered?
yes
no

Assume all vaporized oxygen immediately reacts
Calculate the rate of production of each species
[subroutine COMBRT]

Calculate YPRIME for the species mole numbers, and combustion chamber temperature and pressure
[subroutine CSLOPE]

Calculate piping system variable derivatives
[subroutine PIPES]

Is oxidizer mass flow rate constant?
no
yes

Set all piping system derivatives equal to zero
[subroutine CSLOPE]

RETURN TO THE INTEGRATION SUBROUTINE

Figure B.2: Flowchart for the Calculation of Derivatives
TRNCHG:MAIN (AUGUST, 1987)

TRNCHG was written to predict the transient behavior of the space shuttle main engine fuelside preburner during the shutdown helium purge. It is also capable of predicting engine behavior during operation at full power level.

Initial programming for TRNCHG was by Dr. P. George II, currently at Battelle Lab, Columbus, OH. Subsequent programming was by T. Bartramd, Master's candidate, U. of Tennessee, Knoxville.

The preburner combustion chamber was modelled as a stirred tank reactor. Fuel mass flow rate was taken as constant. Oxidizer enters the combustion chamber via a multi-pipe multi-node feed system with a constant pressure at the furthest upstream node.

The TRNCHG system variables, which are integrated over time, fall into two categories: the chamber variables and the oxidizer feed system variables.

Chamber variables include:
- \( S_2(I) \): Mole number of species I (kg moles of I/kg)
- \( T_K \): Temperature (K)
- \( P_A \): Pressure (Pa)
- \( D_{LIQ} \): Liquid density in the combustion chamber (kg/m**3)

Feed system variables include:
- \( V(J) \): Velocity in pipes j (m/s)
- \( FVI(J) \): Position of the liquid/vapor interface in pipe j (% of the pipe length)
- \( RHO(K) \): Density at node K (kg/m**3)
- \( FVI2 \): Position of the backflow interface in the last pipe (% of the pipe length)

Execution of TRNCHG involves 11 subroutines (written for the program) and the use of two IMSL subroutines: DGEAR, for numerical integration of differential equations and LEQTIF, for solution of matrix equation \( A \times X = B \) for the vector \( X \). A listing of the subroutines used in the execution of TRNCHG and a brief explanation of the function that each performs follows.

COMMONSS: Common block included in most of the subroutines called in the execution of TRNCHG.

YCAL: Used to call the integration routine and call subroutine OUTPT.

NPT: Reads most of the necessary data for execution. Initializes variables, calculates thermodynamic properties and forms reaction rate expressions.

DTSTR: Runge-Kutta integration subroutine to be used in the absence of IMSL subroutine DGEAR. To select DTSTR the vari-
ABLE NDGEAR (NAMELIST ICONS) IS SET EQUAL TO 1. TO USE DGEAR
LET NDGEAR = 0.

CSLOPE: CALCULATES THE DERIVATIVES WITH RESPECT TO TIME FOR
THE SYSTEM VARIABLES ON A CALL FROM THE INTEGRATING ROUTINE.
CALLS SUBROUTINES COMBRT, PIPES AND THERPS.
THERPS: CALCULATES ENTHALPY, INTERNAL ENERGY AND SPECIFIC HEAT
AT CONSTANT PRESSURE FOR GASEOUS CONSTITUENTS WITHIN THE
COMBUSTION CHAMBER.
COMBRT: CALCULATES THE RATE OF PRODUCTION OF THE MAJOR SPECIES
IN THE COMBUSTION CHAMBER DUE TO VAPORIZATION AND COMBUSTION.
COMBRT CALLS BOTH RADSS AND THERPS.
PIPES: CALCULATES THE DERIVATIVES OF THE PIPING SYSTEM VARI-
ABLES ON A CALL FROM CSLOPE. ACCESSES IMSL SUBROUTINE LEQT1F.
INPUTS TO PIPES ARE FOUND IN NAMELIST INPIP AND COMMON BLOCK
CPIPE.
RADSS: CALCULATES THE RATE OF PRODUCTION OF THE MAJOR SPECIES IN
THE COMBUSTION CHAMBER DUE TO COMBUSTION. ASSUMES THE MOLE
NUMBERS OF THE VERY REACTIVE SPECIES (ATOMS AND RADICALS) ARE
CONSTANT AT ANY TIME. RADSS ACCESSES IMSL SUBROUTINE LEQT1F
AND SUBROUTINE RATES.
RATES: CALCULATES THE RATE OF PRODUCTION OF RADICALS AND ATOMS
AND THE DERIVATIVE OF THESE RATES. RATE FOR A GIVEN SPECIES
IS FOUND BY SUMMING THE CONTRIBUTIONS TO RATE BY EACH ELEMENTARY REACTION.
OUTPT: OUTPUTS VALUES TO THE TEXT FILE TSTR.OUT AND THE PLOT
FILES TSTR.PLT1 AND TSTR.PLT2 ON RETURN FROM THE INTEGRATION
SUBROUTINE OR IF THE EXECUTION MUST BE STOPPED.
OUTPUT IS CONTROLLED BY THE PARAMETER NDEBUG. FOR NDEBUG(I) EQUAL
TO 1 THE OUTPUT OF OUTPUT GROUP I IS PRINTED IN THE APPROPRIATE
FILE. OTHERWISE NDEBUG(I) SHOULD EQUAL 0.
OUTPUT GROUPS ARE:

NDEBUG(1) ---» PROBLEM PARAMETERS FROM NAMELISTS PARAM, ICONS,
SSRXN AND PIPES.
NDEBUG(2) ---» THERMODYNAMIC PROPERTY DATA.
NDEBUG(3) ---» REACTION RATE DATA.
NDEBUG(4) ---» INITIAL CONDITIONS OF THE INLET STREAMS
AND IN THE COMBUSTION CHAMBER.
NDEBUG(5) ---» INPUTS TO THE INTEGRATING ROUTINE.
NDEBUG(6) ---» OUTPUTS FROM THE INTEGRATING ROUTINE TO
THE OUTPUT TEXT FILE (TSTR.OUT)
NDEBUG(7) ---» OUTPUTS FROM THE INTEGRATING ROUTINE TO
THE OUTPUT PLOT FILE (TSTR.PLT)
NDEBUG(8) ---» TERMS USED IN THE CALCULATION OF DERIVATIVES
TIVES IN SUBROUTINE CSLOPE.
NDEBUG(9) ---» DERIVATIVE ESTIMATES AT THE END OF
SUBROUTINE CSLOPE.
NDEBUG(10) ---» OUTPUTS VALUES OF TEMP, PRESS, AND MOLE NO. TO
THE SCREEN IN CSLOPE (FOR INTERACTIVE USE)

NDEBUG(11) --> CONVERGENCE SUMMARY FOR SUBROUTINE RADSS
NDEBUG(12) --> SUMMARY OF THE DERIVATIVES CALCULATED IN
    SUBROUTINE PIPES.
NDEBUG(13) --> OUTPUTS FROM SUBROUTINE RATES, INCLUDING
    A LISTING OF THE RXNS WHOSE REACTION RATES
    ARE SMALL AND SET EQUAL TO ZERO.
NDEBUG(14) --> OUTPUTS VALUES OF TIME, STEP, TEMPERATURE
    AND MOLE NUMBERS OF THE MAJOR SPECIES TO
    THE SCREEN ON RETURN TO YCAL FROM THE INTEG-
    RATION SUBROUTINE.
NDEBUG(15) --> SUMMARY OF DERIVATIVE ESTIMATES, OLD AND
    NEW SYSTEM VARIABLE VALUES FROM THE RUNGE-
    KUTTA INTEGRATION SUBROUTINE DTSTR.

THREE SETS OF COMBUSTION CHAMBER CONSTITUENTS ARE
    CONSIDERED IN TRNCHG:

    (1) INLET STREAM CONSTITUENTS (REACTANTS) WHICH ARE
        PRESENT IN SIGNIFICANT AMOUNTS IN THE COMBUSTION
        CHAMBER,
    (2) REACTION PRODUCTS WHICH ARE PRESENT IN SIGNIFICANT
        AMOUNTS IN THE COMBUSTION CHAMBER AND
    (3) RADICALS AND ATOMS, WHICH ARE CONSIDERED TO HAVE
        SMALL CONCENTRATIONS RELATIVE TO REACTANTS AND
        PRODUCTS AND WHOSE MOLE NUMBER IS TAKEN CONSTANT
        AT ANY INSTANT OF TIME.

TRNCHG IS DOUBLE PRECISION FOR ALL REAL VARIABLES. THE MAXI-
MUM NUMBER OF SYSTEM VARIABLES IS 50, BUT CAN BE EASILY
INCREASED BY INCREASING THE DIMENSIONS OF ARRAYS Y, YPRIME,
WK AND IWK.

***** TRNCHG USES SI FOR ALL CALCULATIONS *****

INCLUDE 'INIT.FOR/LIST'
DIMENSION S2P(10),Y(50),IWK(50),WK(9000)
INCLUDE 'COMMONSS.FOR/LIST'

NAMELIST
* /RUNNO/ NMON,NDAY,NYR,NRUN,
* /PARAM/ VOL,Q,S2MIN,EMS,TKS,TMSD,RGMX,RHOGAS,RHOLIQ,
*        RHOH2,AH2IN,A02IN,FVI2MN,DLIQMN,DMIN,DMC,
*        CFTP,PHG,XPER,TEMPR,CVR,
* /INIC/ XMASS,TK,PA,DM,
* /INDX1/ NDEBUG,MCON,KINET,
* /ICONS/ METH,MITER,NDGEAR,IER,STEP,TMI,TPRNT,TMEND,
* INDEX, EPSI,
* /SSRRT/ EPSISS, RLX, RLX2, ITMAXS, IDGT, JER
* /INPIP/ V, FVI, RHO, FVI2, PL, AREA, RFLIQ, RFGAS, RFLHO,
* RFGHO, RFLV, RFGV, PS, CDIN, SM1MIN,
* /INDX2/ N1, N2, NP, NN, NHHEO, NFVI

DATA RGAS/ 8314.4 /, JJ/ 9 /, TENLN/ 2.302585093 /

OPEN (UNIT=20, FILE='[BART.TSTR.WORK]TSTR.IN', READ ONLY,
* STATUS='OLD')
OPEN (UNIT=30, FILE='[BART.TSTR.WORK]TSTR.OUT', STATUS='OLD')
OPEN (UNIT=31, FILE='[BART.TSTR.WORK]TSTR.PLT1', STATUS='NEW')
OPEN (UNIT=32, FILE='[BART.TSTR.WORK]TSTR.PLT2', STATUS='NEW')

C --- READ AND WRITE PROBLEM PARAMETERS FROM NAMELISTS.

READ (20, RUNNO)
READ (20, PARAM)
READ (20, INITC)
READ (20, INDX1)
READ (20, ICONS)
READ (20, SSRRT)
READ (20, INPIP)
READ (20, INDX2)

WRITE (30, 1000) NMON, NDAY, NYR, NRUN

IF (NDEBUG(1)) THEN
  WRITE (30, 1100) VOL, Q, S2MIN, XMASS, DM, DMMIN, CFTP, PHG,
* NDEBUG
  WRITE (30, 1150) DMC, AH2IN, AO2IN, MCON, KINET
  WRITE (30, 1200) METH, MITER, NDGEAR, IER, EPSI, STEP, TMI,
* TMPRTN, TMEND, TMSD
  WRITE (30, 1300) EPSISS, RLX, ITMAXS, IDGT, JER
  WRITE (30, 1400) NP, NN, NHHEO, NFVI, RF LIQ, RFGAS, RFLHO,
* RFGHO, RFLV, RFGV, CDIN, PS, FVI2
  WRITE (30, 1500) (I, N1(I), N2(I), AREA(I), PL(I), PL(I), I=1, NP)
  WRITE (30, 1600) (I, V(I), FVI(I), I=1, NP)
  WRITE (30, 1700) (I, RHO(I), I=1, NN)
END IF

S2MLG = DLOG(S2MIN)
PAMAX = 1.0D+03 * PA

C --- ARATIO IS THE RATIO OF THE TOTAL AREA OF THE OXYGEN
C INJECTORS TO THE AREA OF THE LAST PIPE IN THE OXIDIZER
C FEED SYSTEM.

ARATIO = 264.0 * AO2IN/AREA(NP)
ARATSQ = ARATIO*ARATIO
CALL NPT

--- DEFINE THE ISIDE ARRAY. ISIDE(KK,LL) TELLS THE SIDE OF RXN LL ON WHICH SPECIE KK IS FOUND. IF KK ON THE LHS, ISIDE IS NEGATIVE. IF KK IS ON THE RHS, KK IS POSITIVE.

IF KK APPEARS TWICE, ISIDE=2. IF KK APPEARS ONCE, ISIDE=1. FOR KK NOT PRESENT, ISIDE=0.

DO 120 LL=1,JJ
  DO 110 KK=1,NSRATE
    DO 100 MM=1,4
      IF (KK.EQ.ID(MM,LL)) THEN
        IF (MM.LE.2.AND.ID(1,LL).EQ.ID(2,LL)) THEN
          ISIDE(KK,LL) = -2
        ELSE IF (MM.LE.2) THEN
          ISIDE(KK,LL) = -1
        ELSE IF (ID(3,LL).EQ.ID(4,LL)) THEN
          ISIDE(KK,LL) = 2
        ELSE
          ISIDE(KK,LL) = 1
        END IF
      END IF
      GO TO 110
    ENDDO
  ENDDO
  ISIDE(KK,LL) = 0
  110 CONTINUE
  120 CONTINUE

--- WRITE THERMODYNAMIC AND REACTION RATE DATA TO THE OUTPUT TEXT FILE.

IF (NDEBUG(2)) THEN
  WRITE (30,1900) (I,ANAM(I),SMW(I),I=1,NS)
  WRITE (30,2000) (I,ANAM(I),SMW(I),I=NS+1,NSRATE)
  WRITE (30,2100) (ANAM(I),(Z(J),J=(I-1)*14+1,I*14),I=1,NSRATE)
END IF

IF (NDEBUG(3)) THEN
  WRITE (30,2200) (J,(ID(K,J),K=1,4),J=1,JJ)
  WRITE (30,2300) (J,(ISIDE(K,J),K=1,NSRATE),J=1,JJ)
  WRITE (30,2400)
  DO 125 J=1,JJ
    TM1 = BX(J)/TENLN
    TM2 = BX2(J)/TENLN
    WRITE (30,2450) J,MODR(J),TM1,TEN(J),TACT(J),TM2,
* TEN2(J),TACT2(J)

125 CONTINUE
END IF

C --- PUT MOLE NUMBER WITHIN THE PROBLEM DOMAIN
C (S2MIN < S2 < 1/SMW), SUMMARIZE INPUTS AND WRITE INITIAL
C CONDITIONS TO THE PLOT AND TEXT OUTPUT FILES.
C
SM = 0.0
DO 130 I=1,NS
   IF(S2(I).LT.S2MIN) S2(I) = S2MIN
   SM = SM + S2(I)
130 CONTINUE

C --- DEFINE USEFUL CONSTANTS
C
TKINV = 1.0/TK
SMINV = 1.0/SM
RGASIN = 1.0/RGAS
OMV = EMS(1)/VOL
FMV = EMS(2)/VOL
PMV = EMS(3)/VOL
EMV = OMV + FMV + PMV
RHOCC = PA*SMINV*RGASIN*TKINV

C --- WRITE INITIAL PIPE AND COMBUSTION CHAMBER CONDITIONS TO
C THE TEXT FILE AND THE PLOT FILE.
C
IF(NDEBUGU)) THEN
   WRITE (30,2500) (I,ANAM(I),S2(I),ISTRM(I),S1(ISTRM(I),
               I),AST(I),I=1,NSRATE)
   WRITE (30,2600) TK,PA,RHOCC,SM,VOL,(I,ANST(I),TKS(I),
               EMS(I),SF(I),HS(I),SH(I),I=1,3)
END IF

C
C --- SET PIPES INITIAL CONDITIONS AND INDICIES. NOTE THAT
C
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THE LOG VARIABLE FORM IS NOT USED IN THE FORMULATION
OF THE PIPING SYSTEM OF EQUATIONS.

NN    NO. OF NODES
NP    NO. OF PIPES
NHEO  NO. OF PIPES THAT MAKE UP THE HELIUM PURGE ORIFICE
NPV   INDEX FOR THE PIPE THAT ACTS AS THE HELIUM CHECK VALVE
NFVI  INDEX FOR THE PIPE IN WHICH THE LIQUID/VAPOUR INTERFACE IS LOCATED
NS4   --> NS5 INDICES FOR PIPE FLUID VELOCITIES.
NS6   --> NS7 INDICES FOR PIPE FLUID/VAPOUR INTERFACES.
NS8   --> NS9 INDICES FOR NODAL DENSITIES
NS10  INDEX OF THE SYSTEM VARIABLE THAT FOLLOWS THE PROGRESS OF A LIQUID/VAPOUR INTERFACE THAT RESULTS FROM BACKFLOW FROM THE COMBUSTION CHAMBER INTO THE OXIDIZER FEED SYSTEM.
NV    TOTAL NUMBER OF DEPENDENT (SYSTEM) VARIABLES WHICH MUST BE INTEGRATED.

NODE 1 IS THE FURTHEST UPSTREAM NODE. PRESSURE FOR NODE 1 IS TAKEN AS CONSTANT. NODE NN IS THE FURTHEST DOWNSTREAM NODE. IT IS THE JUNCTION OF THE PIPING SYSTEM WITH THE COMBUSTION CHAMBER. ONLY ONE UPSTREAM AND ONE DOWNSTREAM BOUNDARY ARE PROGRAMMED.

PIPE 1 IS TAKEN AS THE FURTHEST UPSTREAM PIPE. PIPE NP IS THE FURTHEST DOWNSTREAM PIPE, CONNECTED TO THE COMBUSTION CHAMBER VIA NODE NN.

NS4 = NS3 + 1
NS5 = NS3 + NP
NS6 = NS5 + 1
NS7 = NS5 + NP
NS8 = NS7 + 1
NS9 = NS7 + NN
NS10 = NS9 + 1
NV = NS10
NPV = NHEO + 1

--- N AND NWK ARE THE DIMENSIONS OF THE SYSTEM VARIABLES USED IN THE INTEGRATION.

N = NV
IF(METH.EQ.1) NMETH = NV*13
IF(METH.EQ.2) NMETH = NV*6
IF(MITER.EQ.1.OR.MITER.EQ.2) NMITER = NV*(NV+1)
IF(MITER.EQ.3) NMITER = NV
IF(MITER.EQ.-1.OR.MITER.EQ.-2) MITER=NV*(2*NLC+NUC+3)
IF(MITER.EQ.0) NMITER = 1
NWK = 4*NV + NMETH + NMITER

--- YCAL CARRIES OUT THE INTEGRATION AND OUTPUTS RESULTS TO A
--- PLOT FILE AND TEXT FILE ON RETURNS FROM THE INTEGRATION
--- ROUTINE.

CALL YCAL(Y,WK,IWK,N,NWK)

STOP

1000 FORMAT(//2X,'***** TSTR OUTPUT TEXT FILE *****'/,
             * 12X,12,2X,I2,2X,I2,2X,I4,12X,'RUN NUMBER',2X,I3,11)
1100 FORMAT(2X,'***** SOLUTION PARAMETERS *****'/,
             * 4X,'CC VOLUME = ',1PD9.2,' M**3'/,
             * 4X,'CC HEAT TRANS. RATE = ',1PD12.5,' J/S'/,
             * 4X,'MIN ALLOWABLE MOLE NO. = ',1PD12.5,' KMOL/KG'/,
             * 4X,'INITIAL MASS OF LIQ IN THE COMB CHAMBER = ',1PD12.5,
             * ' KG'/,4X,'INITIAL DROPLET DIAMETER = ',1PD12.5,' M'/,
             * 4X,'MIN ALLOWABLE DROPLET DIAMETER = ',1PD10.3,' M'/,
             * 4X,'EXIT TURBINE FLOW RATE CONSTANT = ',1PD10.3,/,
             * 4X,'HOT GAS MANIFOLD PRESSURE = ',1PD10.3,' PA'/,
             * /4X,'NDEBUG (1 FOR PRINITING, 0 FOR SUPRESSING OUTPUT)'*
             * /,(8X,10(I1,2X))
1150 FORMAT(/4X,'DROPLET DIAMETER COEFFICIENT = ',1PD11.4/, *
             * 4X,'AREA OF HYDROGEN INJECTOR ANULUS = ',D11.4/, *
             * 4X,'AREA OF THE OXIDIZER INJECTOR = ',1PD11.4,' 4X', *
             * 'MCON (=0 FOR CONSTANT MASS FLOW; =1 FOR PIPING SYSTEM)'*,
             * I1,4X,'KINET (=0 FOR NO KINETICS; =1 FOR CALL TO RADSS)'*,
             * I1)
1200 FORMAT(4X,'INTEGRATION PARAMETERS:/', *
             * 6X,'MITER, METH, NDGEAR',2X,3(I1,3X)/,6X,'IER, EPSI', *
             * 2X,I3,2X,1PD9.2/6X,'INPUT STEP SIZE = ',1PD9.2,' SEC/', *
             * 6X,'INITIAL TIME = ',D9.2,' SEC',/6X,'OUTPUT INTERVAL', *
             * '=' ',D9.2,' SEC'/6X,'FINAL TIME = ',D9.2,' SEC'/, *
             * 6X,'TIME SHUTDOWN BEGINS = ',D9.2)
1300 FORMAT(4X,'FOR SS RATE APPROXIMATION:/',6X, *
             * 'CONVERGENCE CRITERION (MAX % CHANGE) = ',1PD9.2,'/6X, *
             * 'RELAXATION PARAMETER = ',OPF10.5,6X,'MAX NO ITERATIONS', *
             * '=' ',17,6X,'ERROR CHECK IDGT = ',I2/, *
             * 6X,'IMSL ERROR FLAG JER = ',I3)
1400 FORMAT(4X,'OXIDIZER FEED SYSTEM INPUTS:/', *
             * 6X,'NO. OF PIPES',2X,I2,2X,'NO. OF NODES',2X,I2/, *
             * 6X,'NO. OF HELIUM ORIFICE PIPES',2X,I2/, *
             * 6X,'PIPE IN WHICH THE INTERFACE IS INITIALLY LOCATED', *
             * 2X,I2,6X,'RFLIQ FOR THE OX PIPES = ',1PD10.3/, *
             * 6X,'RFGAS FOR THE OX PIPES = ',D10.3/, *
             * 6X,'RFLIQ FOR THE HE ORIFICE = ',D10.3/, *
             * 6X,'RFGAS FOR THE HE ORIFICE = ',D10.3/, *
             * 6X,'RFLIQ FOR THE HE VALVE = ',D10.3/)
* 6X,'RFGAS FOR THE HE VALVE   = ',D10.3/,
* 6X,'INJECTOR AND MANIFOLD CD = ',D10.3/,
* 6X,'UPSTREAM SOURCE PRESSURE = ',D12.5,' PA'/,
* 6X,'INITIAL BACKFLOW INTERFACE POSITION = ',1PD10.3)
1500 FORMAT(4X,'PIPE GEOMETRY:/',
* 6X,'PIPE',2X,'NODE 1',2X,'NODE 2',2X,'AREA (M**2)',
* 2X,'LENGTH (M)'/,(7X,I2,5X,I2,6X,I2,5X,1PD10.4,
* 3X,0PF10.5))
1600 FORMAT(4X,'PIPE INITIAL CONDITIONS:/',6X,'PIPE',2X,
* 'VELOCITY (M/SEC)'/,2X,'LIQUID/VAP INT. POSITION'
* '(' LENGTH)'/,(7X,I2,5X,1PD11.4,4X,1PD11.4))
1700 FORMAT(4X,'INITIAL NODAL DENSITIES:/',6X,'NODE',2X,
* 'DENSITY (KG/M**3)'/,(7X,I2,6X,1PD11.4))
1800 FORMAT(12(A4,2X))
1900 FORMAT(2X,'***** SPECIES PROPERTIES *****',/
* 4X,'MAJOR CONSTITUENTS:/',6X,'INDEX',2X,'NAME',
* 4X,'MOLEC. WT.'/,(8X,I2,3X,A4,4X,1PD11.4))
2000 FORMAT(4X,'RATE DETERMINING RADICALS',/,
* 6X,'INDEX',2X,'NAME',4X,'MOLEC. WT.'/,
* (8X,I2,3X,A4,4X,1PD11.4))
2100 FORMAT(2X,'***** "Z" ARRAY OF THERMO PROPERTY POLYNOMIAL',
* 'COEFFICIENTS *****',/
* (6X,A4,5(2X,1PD12.5),10X,5(2X,1PD12.5))/,10X,
* 4(2X,1PD12.5))/)
2200 FORMAT(2X,'***** REACTION RATE INDICES AND DATA *****',/
* 4X,'REACTION INDICES',/
* (9X,I2,8X,4(I2,7X)))
2300 FORMAT(2X,'***** CC AND INLET INITIAL CONDITIONS *****',/
* 'SPECIE',2X,'NAME',2X,'S2 (KGMOLE/KG)',2X,'ISTRM',2X,
* 'SI (KGMOLE/KG)',2X,'STATE',/
* (6X,I2,4X,A4,3X,1PD12.5,5X,I1,5X,1PD12.5,4X,A4))
2400 FORMAT(2X,'CC TEMPERATURE = ',OPF12.4,' K'/,
* 'CC PRESSURE   = ',1PD12.4,' PA'/,
* 'CC DENSITY    = ',1PD12.5,' KG/M**3'/,
* 'AVG. MOL. WT. = ',1PD12.5,' KG/KGMOLE'/,
* 'CC VOLUME     = ',1PD12.5,' M**3'/,
* '6HSTREAM',X,4HNAME,2X,4HTEMP,8X,4HMDOT,9X,2HSF,12X,2HHS,
* 12X,2HSH,18X,3H(K),6X,8H(KG/SEC),3X,12H(KGMOLE/SEC),3X,
* 10H(J/KGMOLE),3X,7H(J/SEC)/,(6X,I1,4X,A4,2X,0PF6.2,2X,
* 'SI (KGMOLE/KG)',2X,'STATE',/
* (6X,I2,4X,A4,3X,1PD12.5,5X,I1,5X,1PD12.5,4X,A4))
2500 FORMAT(2X,'CC TEMPERATURE = ',0PF12.4,' K'/,
* 'CC PRESSURE   = ',1PD12.4,' PA'/,
* 'CC DENSITY    = ',1PD12.5,' KG/M**3'/,
* 'AVG. MOL. WT. = ',1PD12.5,' KG/KGMOLE'/,
* 'CC VOLUME     = ',1PD12.5,' M**3'/,
* '6HSTREAM',X,4HNAME,2X,4HTEMP,8X,4HMDOT,9X,2HSF,12X,2HHS,
* 12X,2HSH,18X,3H(K),6X,8H(KG/SEC),3X,12H(KGMOLE/SEC),3X,
* 10H(J/KGMOLE),3X,7H(J/SEC)/,(6X,I1,4X,A4,2X,0PF6.2,2X,
* 'SI (KGMOLE/KG)',2X,'STATE',/
* (6X,I2,4X,A4,3X,1PD12.5,5X,I1,5X,1PD12.5,4X,A4))
2750 FORMAT(4X,'TIME',3X,'TEMPERATURE',X,'PRESSURE',X,'OX MDOT',
* 2X,'LIQ DEN',4X,'DROP DIAM ',2X,'VAP RATE',/3X,'(MSEC)',6X,
* '(K)',6X,'(MPA)',4X,'(KG/S)',4X,'(KG/M3)',4X,'(MICRONS)',2X,
* '(KG/M3 S)')
* OPF8.3,3X,F8.2)
END
FILE INIT: INITIALIZATIONS OF VARIABLES

IMPLICIT REAL*8 (A-H,P-Z)
IMPLICIT INTEGER*4 (I-O)
REAL*8 OMV
CHARACTER*4 ANAM(20),AST(20),ASTNST(10),ANST(10),ALIQ,AGAS
COMMONS.FRC

COMMON

* /CPARA/ SMW(10), AST, ANAM, RATE(10), YPP(10), OMV, FMV, PMV,
   EMV, SMEMV, RGAS, RGASIN, VOL, Q, S2MIN, S2MLG, SM, SMINV,
   TMSD, RGMX, ALIQ, AGAS, VR, RHOGAS, RHOLIQ, RHOH2, CPSUM,
   AH2IN, AO2IN, VH2, DM, DMIN, DMC, CFTP, PHG, DFIN, RPX,
   DLIQMN, FVI2MN, XPER, TMRER, PAMAX, CVR,
   /CSVAR/ S2(10), TK, TKINV, PA, RHOCC, RHINV, DLIQ, XMASS,
   /CSTRM/ S1(3,30), ISTRM(10), TKS(3), ENS(3), DHF(10),
   INST(10), HS(3), ASTNST, ANST, SH(3), SF(3),
   /CINTE/ TMEND, TMI, TMRNRT, STEP, EPSI, METH, MITER, INDEX,
   IER, NDGEAR,
   /CIDX1/ NDEBUG(20), NREA, NPROD, NRAD, NSRATE, JJ, NSTRM,
   NV, NS, NS1, NS2, NS3, NS4, NS5, NS6, NS7, NS8, NS9, NS10, MCON,
   KINET,
   /CRATE/ ID(4,20), ISIDE(10,20), MODR(20), BX(20), BX2(20),
   TEN(20), TEN2(20), TACT(20), TACT2(20), ARR(10), RIP(10,10),
   X1(20), X2(20),
   /CPROP/ Z(200), H(10), CP(10), U(10), S(10), DCP(10), HO(10),
   CPO(10), SO(10),
   /CSSR/ EPSISS, RLX, ITMAXS, IDGT, JER,
   /CFIPE/ V(15), FVI(15), RHO(15), P(15), AREA(15), PL(15),
   PS, FVI2, CDIN, S1MIN, RFLIQ, RGAS, RFLV, RFGV, RFGHO, RFLHO,
   /CIDX2/ N1(15), N2(15), NN, NP, NHEO, NFVI, NFV
SUBROUTINE CSLOPE(N,T,Y,YPRIME)

CSLOPE CALCULATES THE DERIVATIVES WITH RESPECT TO TIME OF
THE SYSTEM VARIABLES.

N IS THE TOTAL NUMBER OF DEPENDENT VARIABLES.

YPRIME(1:NS) --> D(LOG(S2(I)))/DT
YPRIME(NS1) --> D(DLIQ)/DT
YPRIME(NS2) --> D(LOG(TK))/DT
YPRIME(NS3) --> D(LOG(PA))/DT
YPRIME(NS4:NS5) --> D(V(J))/DT
YPRIME(NS6:NS7) --> D(FVI(J))/DT
YPRIME(NS8:NS9) --> D(RHO(K))/DT
YPRIME(NS10) --> D(FVI2)/DT

SYSTEM VARIABLES INCLUDE COMBUSTION CHAMBER VARIABLES AND
FEED SYSTEM VARIABLES:

S2(I) IS MOLE NUMBER OF SPECIES I (KGMOLES I/KG TOTAL)
DLIQ IS THE COMBUSTION CHAMBER LIQUID DENSITY (KG/M**3)
TK IS COMBUSTION CHAMBER TEMPERATURE (K)
PA IS COMBUSTION CHAMBER PRESSURE (PA)
V(J) IS FLUID VELOCITY IN PIPE J.
FVI(J) IS POSITION OF THE LIQUID/VAPOR INTERFACE IN PIPE J.
RHO(K) IS DENSITY OF NODE K.
FVI2 IS THE POSITION OF THE BACKFLOW INTERFACE (FROM THE
COMBUSTION CHAMBER INTO THE OXIDIZER FEED SYSTEM.

OTHER VARIABLES:

OMV = VOLUMETRIC MASS FLOW RATE THROUGH THE OXIDIZER
      FEED SYSTEM
FMV = VOLUMETRIC MASS FLOW RATE THROUGH THE FUEL FEED
      SYSTEM (CONSTANT)
PMV = VOLUMETRIC MASS FLOW RATE OF HELIUM INTO THE
      COMBUSTION CHAMBER.
EMV = EXIT VOLUMETRIC MASS FLOW RATE (THE THE EXIT
      TURBINE
SM = AVERAGE MOLECULAR WEIGHT IN THE COMBUSTION CHAMBER
     (DOES NO TAKE LIQUID SPECIES INTO ACCOUNT)

INCLUDE 'INIT.FOR/LIST'

DIMENSION Y(N),YPRIME(N),ALG(20)

INCLUDE 'COMMONS.FOR/LIST'

---_RESET YPRIME ARRAY

150
DO 100 I=1,N
100 YPRIME(I) = 0.0
C --- IF THE HELIUM/OXYGEN INTERFACE IS AT THE LAST NODE STOP
C EXECUTION
C IF(FVI(NP).GE.1.0) THEN
   WRITE (30,1000)
   CALL OUTPT(Y,TM,N,NSTEPS)
   STOP
ENDIF
C --- COUNT ITERATIONS AT EACH TIME STEP
C IF(T.EQ.TMOLD) THEN
   ITER = ITER + 1
ELSE
   ITER = 1
   TMOLD = T
ENDIF
C --- COMPUTE MOLE NUMBERS. NO SPECIES MOLE NUMBER MAY EXCEED
C 1.0/SMW(I) (SMW(I) IS THE MOLECULAR WEIGHT OF SPECIES I)
C TMRAT = 0.0
SM = 0.0
DO 110 I=1,NS
   ALG(I) = DLOG(1.0/SMW(I))
   IF(Y(I).LT.ALG(I).AND.Y(I).GT.S2MLG) THEN
      S2(I) = DEXP(Y(I))
   ELSE IF(Y(I).GE.ALG(I)) THEN
      S2(I) = DEXP(ALG(I))
      Y(I) = ALG(I)
   ELSE
      S2(I) = S2MIN
      Y(I) = S2MLG
   ENDIF
   TMRAT = TMRAT + S2(I)*SMW(I)
110 CONTINUE
C --- NORMALIZE MOLE NUMBERS
C DO 120 I=1,NS
   SM = SM + S2(I)
   S2(I) = S2(I)/TMRAT
120 CONTINUE
SMINV = 1./SM
C --- FIND TEMPERATURE, PRESSURE, DENSITY AND THE LIQUID DENSITY
C FOR THE COMBUSTION CHAMBER AND BACKFLOW INTERFACE POSITION.

151
DLIQ = Y(NS1)
IF(DLIQ.LT.DLIQMN) THEN
  DLIQ = DLIQMN
ENDIF
TK = DEXP(Y(NS2))
IF(TK.GT.1.0D+04) THEN
  TK = 1.0D+04
ELSE IF(TK.LT.100.0) THEN
  TK = 90.0
ENDIF
PA = DEXP(Y(NS3))
IF(PA.GT.PAMAX) THEN
  PA = PAMAX
ELSE IF(PA.LT.1.0D+03) THEN
  PA = 1.0D+03
ENDIF
TKINV = 1.0 / TK
FVI2 = Y(NS10)
RHOCC = PA*R GASIN*SMINV*TKINV
IF(RHOCC.LT.0.01) RHOCC = 0.01
RHINV = 1.0/RHOCC

--- FILL ARRAYS FOR V, RHO AND FVI
DO 130 I=1,NP
  V(I) = Y(NS3+I)
  FVI(I) = Y(NS5+I)
130 CONTINUE
DO 140 I=1,NN
  RHO(I) = Y(NS7+I)
140 CONTINUE

--- DETERMINE MASS FLOW RATE IN THE OXIDIZER FEED SYSTEM AND
RATE OF ENERGY INFLUX TO THE CHAMBER FROM THE OXIDIZER
FEED SYSTEM.

IF(FVI(NP).LT.1.0) THEN
  PMV = 0.0
  SF(3) = 0.0
  SH(3) = 0.0
ELSE
  OMV = RHOLIQ * AREA(NP) * V(NP) / VOL
  SH(1) = OMV * HS(1) / SMW(3)
  SF(1) = 0.0
END IF
DO 150 I=1,NS
    SH(1) = SH(1) + OMV*S2(I)*H(I)
150 CONTINUE
ENDIF
ELSE
    OMV = 0.0
    PMV = RHO(NN)*AREA(NP)*V(NP)/VOL
    SF(3) = PMV/SMW(1)
    SH(3) = SF(3)*HS(1)
ENDIF

C --- DETERMINE THE VOLUMETRIC EXIT MASS FLOW RATE (EMV)
C
    PR = PHG/PA
    PB = PR**1.4286 - PR**1.7143
    IF(PB.LE.0.0) THEN
        EMV = 0.0
    ELSE
        EMV = CFTP*DSQRT(PA*PB/TK)
    ENDIF
    EMV = EMV/VOL
    IF (EMV.LT.0.0) EMV = 0.0

C --- COMBRT CALCULATES THE RATE OF PRODUCTION OF EACH SPECIES IN
C THE CHAMBER DUE TO COMBUSTION AND VAPORIZATION.
C
    CALL COMBRT(T,Y,YPRIME)
C
C --- LOOPS TO CALCULATE YPRIMES C C --- YPP(I) ARE THE TERMS USED
C TO FIND D(TEMP)/D(TIME)
C
    DO 160 IB = 1,10
160     YPP(IB) = 0.0
C
C --- CALL THERPS FOR THE SPECIFIC MOLAR INTERNAL ENERGY AND
C ENTHALPY FOR EACH SPECIES C
C CALL THERPS(NS,TK)
C
C --- CONSERVATION OF MASS FOR THE GAS PHASE
C
    IF(V(NP).GE.0.0.AND.RHO(NN).GE.RGMX) THEN
        SUMM = VR + FMV + PMV
    ELSE
        SUMM = VR + OMV + FMV + PMV
    ENDIF
    RPX = SUMM - EMV

C --- OUTPUT VALUES TO THE SCREEN IF NDEBUG(10) = 1
C
    IF(NDEBUG(10)) THEN
WRITE (6,1100) T,V(NP),TK,VR,DM,DLIQ
ENDIF
C
C --- CONSERVATION OF SPECIES
C
NOTE: IF THERE IS BACKFLOW INTO THE PIPES OR THERE IS
AN INTERFACE IN THE PIPES DUE TO BACKFLOW (FVI2>0.0),
OMV ACCOUNTS FOR THE INFLOW OR OUTFLOW OF CHAMBER CONTENTS.
CHAMBER GAS IN THE PIPES IS ASSUMED TO HAVE THE SAME
DENSITY AND TEMPERATURE AS THE CHAMBER CONTENTS.
C
DO 170 I=1,NS
  IF(OMV.LT.O.O.AND.RHO(NN).LT.RGMX) THEN
    IF(ISTRM(I).GT.O) THEN
      YP = (SF(ISTRM(I))-(SUMM-OMV)*S2(I)+RATE(I))*RHINV
    ELSE
      YP = (-SUMM-OMV)*S2(I)+RATE(I))*RHINV
    ENDIF
  ELSE
    IF(ISTRM(I),GT.O) THEN
      YP = (SF(ISTRM(I))-SUMM*S2(I)+RATE(I))*RHINV
    ELSE
      YP = (-SUMM*S2(I)+RATE(I))*RHINV
    ENDIF
  ENDIF
  YPRIME(I) = YP/S2(I)
  IF(Y(I).GE.ALG(I).AND.YP.GT.O.O) THEN
    YPRIME(I) =0.0
    YP = 0.0
  ENDIF
170 CONTINUE
YPP(1) = SH(1)
YPP(2) = SH(2)
YPP(3) = SH(3)
YPP(5) = YPP(5)*RPX
YPP(6) = YPP(6)*RHOCC
YPP(7) = Q/VOL
YPP(8) = YPP(8)*RHOCC
C
C --- CONSERVATION OF ENERGY
C
TP = (YPP(1)+YPP(2)+YPP(3)-YPP(4)-YPP(5)-YPP(6)-YPP(7))/YPP(8)
YPP(8) = YPP(8) * TK
YPRIME(NS2) = TP/TK
C
154
C --- CONSERVATION OF MASS FOR THE LIQUID PHASE
C
IF (ASTNST(1).EQ.AGAS) THEN
  YPRIME(NS1) = 0.0
ELSE
  IF (V(NP).GE.0.0.AND.RHO(NN).GE.RGMX) THEN
    YPRIME(NS1) = OMV-VR-EMV*DLIQ/RHOCC
  ELSE
    YPRIME(NS1) = -VR-(EMV-OMV)*DLIQ/RHOCC
  ENDIF
ENDIF

C --- THE IDEAL GAS LAW
C
YPRIME(NS3) = YPRIME(NS2) + RPX * RHINV + YPP(9) * SMINV

C --- SUBROUTINE PIPES DETERMINES YPRIME FOR THE PIPING SYSTEM
C DEPENDENT VARIABLES. PIPES IS CALLED IF MCON = 1. OTHERWISE
C OXIDIZER FEED RATE REMAINS CONSTANT
C
IF (MCON) CALL PIPES(Y, YPRIME, T)
C
C --- WRITE A SUMMARY OF THE TERMS USED TO CALCULATE DERIVATIVES
C
IF (NDEBUG(8).EQ.1) THEN
  WRITE(30,1200) T, ITER, TK, PA, RHOCC, EMV, DLIQ, VR,
  *(I, EMS(I), SF(I), SH(I), I=1, 3)
  WRITE(30,1300) (IS, H(IS), U(IS), CP(IS), RATE(IS), IS=1, NS)
  WRITE(30,1400) ((IB, YPP(IB)), IB=1, 9)
ENDIF
C
C --- WRITE A SUMMARY OF YPRIME VALUES CALCULATED IN CSLOPE
C
IF (NDEBUG(9).EQ.1) THEN
  WRITE(30,1500) T, ITER
  WRITE(30,1600)
  WRITE(30,1700) ((I, S2(I), Y(I), YPRIME(I)), I=1, NS),
  * NS1, DLIQ, Y(NS1), YPRIME(NS1), NS2, Y(NS2),
  * YPRIME(NS2), NS3, PA, Y(NS3), YPRIME(NS3), NS10,
  * FV12, YPRIME(NS10)
  WRITE(30,1800) (J, V(J), YPRIME(NS3+J), FVI(J),
  * YPRIME(NS5+J), J=1, NP)
  WRITE(30,1900) (K, RHO(K), YPRIME(K+NS7), K=1, NN)
ENDIF
C
RETURN
C
1000 FORMAT(2X,'***** INTERFACE HAS REACHED THE LAST NODE *****'/,,
  * 2X,'***** EXECUTION HALTED *****'//)
1100 FORMAT(X,'T ',1PD8.2,X,'V, TK, VR, DM, DLIQ ',D8.1,X,
* OPF6.1,3(X,1PD8.1))

1200 FORMAT(/2X, '***** DEPENDENT VARIABLE DERIV. PARAMS *****' //,
* 4X, 'TIME = ',1PD12.5,2X,'ITERATION = ',I5/,4X,
* 'TEMPERATURE = ',OPF15.4,2X,'PRESSURE = ',1PD12.5/,4X,
* 'DENSITY = ',1PD12.5,2X,'EXIT VOLUMETRIC MASS FLOW = '
* 1PD12.5/,4X,'LIQ DENSITY = ',1PD12.5,' (KG/M**3)'//,4X,
* 'VAPORIZATION RATE = ',1PD11.4,' KG/S M**3'//,4X,'STREAM',2X,
* ' MASS FLOW ',2X,' MOLE FLOW ',2X,'ENTHALPY FLOW'/,14X,
* '(KG/SEC)',2X,'(KGMOLE/SEC)',3X,'(JOULES/SEC)'//,
* 3(7X,11,4X,1PD11.4,2X,1PD11.4,2X,1PD11.4))

1300 FORMAT(/4X, 'IN CSLOPE THERMO PROPS AND RXN RATES ARE: '/,
* 4X, ' I',2X,' H ',2X,' U ',2X,' __ CP ',
* 4X, ' A ',//,(4X,I2,4(2X,1PD12.5)))

1400 FORMAT(/4X, 'TEMPERATURE DERIVATIVE TERMS ARE: '/,
* (4X, 'YPP('I',') = MPD12.5,2X,'YPP('I',') = ',1PD12.5))

1500 FORMAT(//2X, '***** CLSOPE YPRIME ESTIMATES *****'//,
* 4X,'TIME = ',1PD12.5,2X,'ITERATION = ',I5,//)

1600 FORMAT(4X,3H I ,2X,12H S2(I) ,2X,12H Y(l) ,2X,
* 13H YPRIME(I) ,//)

1700 FORMAT(4X,I3,2X,1PD12.5,2X,1PD12.5,2X,1PD12.5)

1800 FORMAT(/4X, 'PIPE',2X,' VELOC. (M/S) ',2X,'D(VELOC.)/D(T)',
* 2X,'FL/V INTERFACE',2X,'D(FVI)/D(TIME)'/,
* (5X,I2,X,4(5X,1PD11.4)))

1900 FORMAT(/4X, 'NODE',2X,'DENSITY (M**3)',2X,'D(RHO)/D(TIME)'//,
* (5X,I2,X,2(5X,1PD11.4)))

END
SUBROUTINE COMBRT(TM,Y,YPRIME)

COMBRT FINDS THE RATE OF PRODUCTION OF EACH OF THE SPECIES IN
THE COMBUSTION CHAMBER DUE TO REACTION RATE AND VAPORIZATION.

INCLUDE 'INIT.FOR/LIST'

DIMENSION Y(NV),YPRIME(NV)

INCLUDE 'COMMONSS.FOR/LIST'

--- FIND THE VAPORIZATION RATE, VR (KG/M**3 S) AND YPRIME(NS1)

CPSUM = THE AVERAGE SPECIFIC HEAT AT CONSTANT PRESSURE FOR
THE COMBUSTION CHAMBER GASES.

XK = THERMAL CONDUCTIVITY OF HYDROGEN (LEAST SQUARES LINEAR
FIT FOR XK AS A FUNCTION ONLY OF TEMPERATURE)

XMU = VISCOSITY OF HYDROGEN (LEAST SQUARES LINEAR FIT FOR
XMU AS A FUNCTION ONLY OF TEMPERATURE)

DATA PI/3.141592654/

TAV = (TKS(1) + TK)/2.0
CALL THERPS(NS,TAV)
CPSUM = 0.0
DO 100 I=1,NS
   CPSUM = CPSUM + CP(I)*S2(I)
100 CONTINUE
CALL THERPS(NS,TKS(1))
XK = 5.282D-02 + 4.117D-04*TAV
XMU = 5.0767D-06 + 1.4884D-08*TAV

(B) FIND THE AVERAGE DROPLET DIAMETER, DM (M), THE RATE OF
VAPORIZATION, VR (KG/M3 S), AND THE TOTAL NUMBER OF
DROPLETS IN THE COMBUSTION CHAMBER, XNDR.

THE EXPRESSION USED TO CALCULATE EVAPORATION RATE WAS
ADAPTED FROM WEBBER (1972) (J. OF THE ARS)

IF(ASTNST(1).EQ.AGAS) THEN
   VR = OMV
   GO TO 110
ENDIF

DM = DMC*OMV/FMV*DSQRT(SMW(2)*AH2IN*PA/RGAS/RHOLIQ/TKS(2))
IF(DM.LT.DMIN) DM = DMIN
DM3 = DM**3
REN = RHOC*VH2*DM/XMU
ALPH = 1.0 + CVR * (TK-TKS(1))
IF(ALPH.GT.1.0) THEN
   VRD = PI*XK*DM*(2.0+0.5*REN**0.5)*DLOG(ALPH)/CPSUM
   GO TO 117
ENDIF
VRD = VRD/1000
RETURN
END

110 VR = 0.000
GO TO 200
117 VR = VRD/1000
GO TO 200
ELSE
VRD = 0.0
ENDIF
XNDR = 6.0*DLIQ*VOL/RHOLIQ/DM**3/PI
VR = 6.0*VRD*DLIQ/PI/RHOLIQ/DM3
IF(VR.LE.0.0) THEN
VR = 0.0
ENDIF
110 CONTINUE
C
C — DETERMINE THE RATES OF PRODUCTION DUE TO COMBUSTION AND
C VAPORIZATION
C (A) IF KINET = 1, CHEMICAL KINETICS ARE CONSIDERED. REACTION
C RATE IS CALCULATED IN RADSS ASSUMING THAT ATOM AND RADI-
C CAL CONCENTRATIONS ARE STEADY STATE.
C (B) IF KINET = 0, ALL OXYGEN WHICH VAPORIZES IS ASSUMED TO
C IMMEDIATELY COMBUST.
C
IF(KINET.EQ.1) THEN
CALL RADSS
RATE(3) = RATE(3) + VR/SMW(3)
ELSE IF(KINET.EQ.0) THEN
RATE(3) = 0.0
RATE(4) = 2.0*VR/SMW(3)
RATE(2) = -2.0*VR/SMW(3)
ELSE IF(KINET.EQ.2) THEN
CALL RATES
DO 200 I=1,NS
RATE(I) = ARR(I)
200 CONTINUE
RATE(3) = RATE(3) + VR/SMW(3)
ENDIF
C
IF(NDEBUG(15)) WRITE(30,1000) TM,TK,PA,DM,VRD,XNDR,REN,VR,
* (ANAM(I),RATE(I),I=1,NS)
C
RETURN
C
1000 FORMAT(/,2X,'***** OUTPUT FROM COMBRT *****',/,'4X,'AT TIME ',
* 1PD11.5/,
* 4X,'TEMPERATURE' = ',0PF10.3,' K '/,
* 4X,'PRESSURE' = ',1PD12.5,' PA'/,
* 4X,'DROPLET DIAMETER' = ',D12.5,' M '/,
* 4X,'DROPLET EVAPORATION RATE' = ',D12.5,' KG/S/DROPLET'/,
* 4X,'NO. OF DROPLETS' = ',D12.5,' DROPLETS'/
* 4X,'REYNOLDS NO. OF DROPS' = ',D12.5/',
* 4X,'TOTAL EVAPORATION RATE' = ',D12.5,' KG/M**3 S'/,
* 4X,'HSPECIES,2X,'RATE OF PRODUCTION (KMOLES/M**3 S)'//,
* (5X,A4,5X,1PD12.5))
C
158
SUBROUTINE DTSTR(NV, CSLOPE, TM, STEP, Y, TMNXT, WK, NDEBUG)

C
C THIS IS A RUNGE-KUTTA FOURTH ORDER INTEGRATING SUBROUTINE
C WHICH ANSWERS A CALL MIMICKING A CALL TO IMSL SUBROUTINE
C DGEAR. THE PURPOSE OF DGEAERX IS TO ALLOW DEBUGGING OF
C THE TRANSIENT CHUGGING CODE AT MSFC, WHERE DGEAR IS NOT
C AVAILABLE.
C
C THE SIGNIFICANT VARIABLES ARE
C NV=NUMBER OF VARIABLES
C CSLOPE=NAME OF ROUTINE TO EVALUATE 1ST DERIVATIVE
C TM=INDEPENDENT VARIABLE
C STEP=DELTA TM
C Y=ARRAY OF INDEPENDENT VARIABLES
C SHOULD BE AN INTEGER
C TMNXT=ENDING TM -(TMNXT-TM)/STEP
C WK=WORK VECTOR OF 4*NV SIZE
C OTHERS ARE UNUSED DUMMY PARAMETERS
C
C IMPLICIT REAL*8 (A-H,P-Z)
DIMENSION Y(NV),WK(4,NV),YEND(100),F(100),NDEBUG(20)
C
C NSTEPS=(TMNXT-TM)/STEP
IF(NSTEPS.LE.0) NSTEPS=1
C
C DO 100 J=1,NSTEPS
C
C GET FIRST ESTIMATE OF THE DELTA X'S
C
C CALL CSLOPE (NV,TM,Y,F)
DO 10 I=1,NV
   WK(1,I)=STEP*F(I)
   YEND(I)=Y(I)+WK(1,I)*0.5
10 CONTINUE
C
C GET SECOND ESTIMATE (USING YEND)
C
NE=2
TM2E=TM+STEP*0.5
CALL CSLOPE (NV, TM2E, YEND, F)
DO 20 I=1,NV
   WK(2,I)=STEP*F(I)
   YEND(I)=Y(I)+WK(2,I)*0.5
20 CONTINUE
C
C THIRD ESTIMATE
C
C
160
NE=3
CALL CSLOPE(NV,TM2E,YEND,F)
DO 30 I=1,NV
   WK(3,I)=STEP*F(I)
   YEND(I)=Y(I)+WK(3,I)
30 CONTINUE
C
C LAST ESTIMATE
C
NE=4
TM2E=TM+STEP
CALL CSLOPE(NV,TM2E,YEND,F)
DO 40 I=1,NV
   WK(4,I)=STEP*F(I)
40 CONTINUE
C
C COMPUTE Y'S AT TM + STEP BY WEIGHTED AVERAGE
C
DO 50 I=1,NV
   YEND(I)=Y(I)+(WK(1,I)+2*WK(2,I)+2*WK(3,I)+WK(4,I))/6.0
50 CONTINUE
C
C WRITE VALUES OF THE DERIVATIVE ESTIMATES AND "OLD" AND "NEW" VALUE OF Y IF NDEBUG(15) = 1
C
IF(NDEBUG(15)) THEN
   WRITE(30,1000) TM,STEP
   WRITE(30,1100) (K,(WK(I,K),I=1,4),Y(K),YEND(K),K=1,NV)
ENDIF
C
C ADVANCE Y & TM FOR NEXT STEP
C
DO 60 I=1,NV
   Y(I)=YEND(I)
60 CONTINUE
TM=TM+STEP
C
100 CONTINUE
C
RETURN
C
C FORMATS
C
1000 FORMAT(//,2X,'***** DTSTR OUTPUT *****'//,
   * 6X,'TIME = ',1PD12.5,' SEC',2X,'STEP = ',D12.5,' SEC',//,
   * 4X,'INDEX',X,'ESTIMATE 1',X,'ESTIMATE 2',X,'ESTIMATE 3',
   * X,'ESTIMATE 4',X,' Y OLD ',X,' Y NEW ')//)
   * X,D10.3)
SUBROUTINE NPT

C --- DEFINITION OF INPUT VARIABLES.
C
C ANAM(I) = HOLERITH NAME OF SPECIES I
C S2(I) = MOLE NUMBER OF SPECIES I (KGMOLES OF I/KG (TOTAL))
C XIN(I) = INLET MOLE FRACTION OF SPECIES I
C XCC(I) = INITIAL MOLE FRACTION OF SPECIES I.
C AST(I) = PHASE OF SPECIES I
C ISTRM(I) = NUMBER OF THE INLET STREAM CONTAINING SPECIES I
C INST(J) = NUMBER OF THE SPECIES CONTAINED IN REACTANT STREAM J
C ANST(J) = HOLERITH NAME OF THE SPECIES IN STREAM J
C ASTNST(J) = PHASE OF REACTANT STREAM J
C DHF(J) = LATENT HEAT OF VAP. OF LIQUID IN STREAM J
C HS(J) = ENTHALPY OF THE INCOMING FLUID IN STREAM J
C TKS(J) = TEMPERATURE OF STREAM J (ASSUMED CONSTANT)
C SF(J) = MOLE FLOW (KGMOLE/M^3 SEC) INTO THE CC
C SH(J) = ENTHALPY FLOW (J/M^3 SEC) INTO THE CC

C INCLUDE 'INIT.FOR/LIST'
C
C CHARACTER*4 AXP(10),AXR(10),ASTP(10),DATA(12),ASTR(10),
C AT(7),CMNT,PHAZ,DT1,DT2,ATYP,AX,ASTX,BLANK,
C AREAC,APROD,ARADI,ACOMM,AREVE,AGLOB,AHETE,
C APYRO,ACGS,THIRD
C
C DIMENSION SMWR(10),XIN(20),XCC(20),SMWP(10),XCCP(10),
C TX(50),TY(50)

C INCLUDE 'COMMONSS.FOR/LIST'
C
C DATA BLANK/ ' /,AREAC/'REAC'/,APROD/'PROD'/,ARADI/'RADI'/,
C S2/ 10*0.0/,S1/90*0.0/,XIN/20*0.0/,XCC/20*0.0/,,
C ISTRM/10*0/,NREAC0/,NPROM0/,NRADI0/,NS0/,NSRATE0/,,
C ALIQ/'L '/,AGAS/'G '/,LSI/ 1 /,ACOMM/'COMM'/,
C AREVE/'REVE'/,AGLOB/'GLOB'/,AHETE/'HETE'/,APYRO/'PYRO'/,
C AGCS/'CGS '/,THIRD/'M '/,XMAX/0.00125/,XMIN/0.0005/,
C TENLN/2.302585093/
C
C --- READ RELEVANT SPECIES AND ASSIGN THEM AS REACTANT, PRODUCT OR RATE DETERMINING RADICAL.

C 100 READ(20,1000) ATYP,AX,SMWX,ISTRMX,XINX,XCCX,ASTX,DHFX,HNSTRM
C IF(ATYP.EQ.BLANK) GO TO 110
C IF(ATYP.EQ.AREAC) THEN
C NREAC = NREAC + 1
C ANAM(NREAC) = AX
C ANST(ISTRMX) = AX
C
SMW(NREAC) = SMWX
ISTRM(NREAC) = ISTRMX
XIN(NREAC) = XINX
XCC(NREAC) = XCCX
AST(NREAC) = ASTX
ASTNST(ISTRMX) = ASTX
DHF(ISTRMX) = DHFX
HS(ISTRMX) = HNSTRM
INST(ISTRMX) = NREAC
ELSE IF(ATYP.EQ.APROD) THEN
NPROD = NPROD + 1
AXP(NPROD) = AX
SMWP(NPROD) = SMWX
XCCP(NPROD) = XCCX
ASTP(NPROD) = ASTX
ELSE
NRAD = NRAD + 1
AXR(NRAD) = AX
SMWR(NRAD) = SMWX
ASTR(NRAD) = ASTX
END IF
GO TO 100
110 CONTINUE
C
C --- PUT ALL SPECIES INTO THE S2 AND OTHER ASSOCIATED ARRAYS.
C ORDER IS: FIRST REACTANTS, SECOND PRODUCTS AND THIRD
C RADICALS.
C
NS = NREAC + NPROD
NSRATE = NS + NRAD
NS1 = NS + 1
NS2 = NS1 + 1
NS3 = NS1 + 2
DO 120 I=1,NPROD
II = NREAC + I
ANAM(II) = AXP(I)
SMW(II) = SMWP(I)
XCC(II) = XCCP(I)
AST(II) = ASTP(I)
120 CONTINUE
DO 130 I=1,NRAD
II = NS + I
ANAM(II) = AXR(I)
SMW(II) = SMWR(I)
AST(II) = ASTR(I)
130 CONTINUE
DO 140 I=1,NSRATE
S2(I) = XCC(I)/SMW(I)
IF(S2(I).LT.S2MIN) S2(I) = S2MIN
140 CONTINUE
DO 150 I=1,NREAC
150 S1(ISTRM(I),I) = XIN(I)/SMW(I)
C
C --- DEFINE THE ONE DIMENSIONAL Z ARRAY WHICH HOLDS THE COEFFI-
C CIENTS OF THE POLYNOMIALS THAT GIVE THERMODYNAMIC PROPERTIES.
C
160 READ (20,1100) (DATA(I),I=1,3)
   DO 170 I=1,NSRATE
      IF(DATA(1).EQ.ANAM(I)) THEN
         READ (20,1200) (Z(J),J=(I-1)*14+1,I*14)
         GO TO 160
      ENDIF
   CONTINUE
   IF(DATA(I).EQ.BLANK) THEN
      READ (20,1350)
      GO TO 180
   ENDIF
   READ (20,1300)
   GO TO 160
180 CONTINUE
C
C --- SET INITIAL MOLE AND ENERGY FLOWS (SF AND SH)
C
   DO 190 J=1,3
      SF(J) = EMS(J)/VOL/SMW(INST(J))
      SH(J) = SF(J) * HS(J)
   190 CONTINUE
C
C --- READ AND DETERMINE CONSTANTS USED IN DETERMINING
C CHEMICAL REACTION RATES.
C
C --- READ MECHANISM/RATE DATA CARDS
C COLUMNS 13 THROUGH 48 OF THE MECHANISM CARD ARE USED
C AS A LABEL TO IDENTIFY THE KINETIC MECHANISM USED ON
C THE SOLUTION OUTPUT.
C
THE VARIABLE DT1 (COLUMNS 73/76) IS USED AS A FLAG:
C
CGS ---> CGS UNITS, RATE CONSTANTS IN GM-MOLES, CM,
      SEC AND EACT IN (KCAL/GM-MOLE) OTHERWISE
C THE SI UNITS (KG-MOLES, M,SEC) ARE ASSUMED.
COMM ---> COMMENT CARD, FIRST 48 CHARACTERS PRINTED
REV1 --> REVERSE RATE DATA, IN SAME UNITS AS FORWARD
      DATA
GLOB ---> GLOBAL RATE EXPRESSION DATA IN SI UNITS
PYRO ---> HETEROGENEOUS PYROLYSIS REACTIONS
HETE ---> HETEROGENEOUS CHAR REACTIONS
C
THE HETEROGENEOUS REACTIONS ARE PROGRAMED IN CHAPTERS
C 1 & 2 OF SUBROUTINE CORRECT. BX(J), TEN(J), AND TACT(J)
C ARE READ AS BX(J), ALPHA(1 OR 2), AND TACT(J) FOR PYROLY-
C SIS AND BX(J), TEN(J) AND TACT(J) FOR THE CHAR REACTIONS.
C
C DT1 AMD DT2 (COL 73/80) CANHAVE ANYTHING (COMMENTS) IF
C ABOVE SIX WORDS ARE NOT REQUIRED.
C TACT IS ACTIVATION TEMPERATURE, = EACT/GASCON, DEG K
C
IF(NDEBUG(3)) WRITE (30,1500)
DO 200 I=1,20
    TEN2(I)=0.
    BX2(I)=0.
200 CONTINUE
C
JJ=1
NPYROL=0
NGLOB=0
NHETER=0
C
210 READ (20,1600) (DATA(I),I=1,12),BX(JJ),TEN(JJ),
     TACT(JJ),DT1,DT2
     IF (DATA(I).EQ.BLANK.AND.DTI.NE.ACOMM) GO TO 400
     C
     c... CHECK
     FOR COMMENT CARD
     C
     IF (DTI.NE.ACOMM) GO TO 220
     IF (NDEBUG(3)) WRITE (30,1700) (DATA(I),I=1,12)
     GO TO 210
C
C --- SCAN TO INSURE ALL REACTANTS IN SPECIES LIST
C
220 DO 240 IR=1,6
    I=2*IR-1
    IF (DATA(I).EQ.BLANK.OR.DATA(D.EQ.THIRD) GO TO 240
    DO 230 IS=1,NSRATE
        IF (DATA(I).EQ.ANAM(IS)) GO TO 240
    230 CONTINUE
    IF (NDEBUG(3).NE.l) GO TO 210
        WRITE (30,1800)
        WRITE (30,1900) (DATA(IDD),IDD=1,12)
        WRITE (30,2000) DATA(I)
    GO TO 210
    240 CONTINUE
C
C --- CHECK FOR REVERSE RATE DATA. NOTE:
C (1) ORDER OF CARDS MUST BE CORRECT
C (2) UNITS OF REVERSE DATA ASSUMED SAME AS FORWARD DATA
C
IF (DT1.NE.AREVE) GO TO 250
J = JJ-1
BX2(J) = BX(JJ)
TEN2(J) = TEN(JJ)
TACT2(J) = TACT(JJ)
IF (NDEBUG(3)) WRITE (30,2100) BX2(J),TEN2(J),
* TACT2(J),DT1,DT2
C
C --- CONVERT BX2 FOR INTERNAL CALCULATIONS
C
BX2(J) = BX2(J)*TENLN
IF (LSI) GO TO 210
BX2(J) = BX2(J)-TENLN*3.0
TACT2(J) = TACT2(J)*1000.0/1.987
IF (MODR(J).EQ.2) BX2(J) = BX2(J)-TENLN*3.0
GO TO 210
C
C --- CHECK FOR UNITS
C
250 LSI = 1
IF (DT1.EQ.ACGS) LSI = 0
IF (LSI.EQ.0) TACT(JJ)=TACT(JJ)*1000.0/1.987
IF (NDEBUG(3)) WRITE (30,2200) JJ,(DATA(I),I=1,12),
* DT1,DT2,BX(JJ),TEN(JJ),TACT(JJ)
IF (DT1.NE.APYRO) GO TO 260
NPYROL = NPYROL+1
IF (NPYROL.GT.2) WRITE (30,2300)
NHETER = NHETER+1
NGLOB = NGLOB+1
260 CONTINUE
IF (DT1.NE.AHETE) GO TO 270
NGLOB = NGLOB+1
NHETER = NHETER+1
270 CONTINUE
IF (DT1.EQ.AGLOB) NGLOB=NGLOB+1
C
C --- CONVERT BX FOR INTERNAL CALCULATIONS
C
BX(JJ) = BX(JJ)*TENLN
C
C --- ID(I,J) IS THE INDEX NUMBER OF THE I-TH DISTINCT SPECIES
C IN REACTION J ... I=1,4 AS NO DISTINCT THIRD BODIES ARE
C CONSIDERED
C
DO 280 I=1,4
280 ID(I,JJ) = 0
C
ND = 1
DO 330 N=1,6
K = N**2 - 1
IF (DATA(K).EQ.BLANK) GO TO 330
IF (DATA(K).NE.THIRD) GO TO 290
C
167
DATA(K) = BLANK
GO TO 330

290 CONTINUE
DO 300 I=1,NSRATE
   IF (DATA(K).NE.ANAM(I)) GO TO 300
   II = I
   GO TO 310
300 CONTINUE
IF (K.GT.3) GO TO 320
ID(ND,JJ) = II
ND = ND+1
GO TO 330
320 IF (ND.EQ.2) ND = 3
ID(ND,JJ) = II
ND = ND+1
330 CONTINUE

C
C --- STORE THE TYPE OF REACTION...THREE TYPES
C MODR 1 ... A + B --> C + D
C MODR 2 ... AB + M --> A + B + M
C MODR 3 ... A + B + M --> AB + M
C
MODR(JJ)=1
IF (ID(2,JJ).EQ.0) MODR(JJ)=2
IF (ID(4,JJ).EQ.0) MODR(JJ)=3

C --- THE FOLLOWING SECTION, UP TO STATEMENT 355 INCLUSIVE,
C MAY BE ELIMINATED IF REVERSE (AS WELL AS FORWARD) RATE
C DATA IS SUPPLIED FOR ** ALL ** REACTIONS.
C
C THIS SECTION CALCULATES REVERSE RATE CONSTANTS FROM
C EQUILIBRIUM CONSTANTS AND FORWARD RATE CONSTANTS FOR
C TWENTY POINTS OVER THE TEMPERATURE RANGE 1000K TO 4000K
C
IF (DT1.EQ.AGLOB) GO TO 390
IF (DT1.EQ.AHETE) GO TO 390
IF (DT1.EQ.APYRO) GO TO 390
DX=(XMAX-XMIN)/19.0
SUMX=0.0
SUMY=0.0
IHCPS=2
DO 360 N=1,20
   TX(N)=XMIN + DX*DFLOAT(N-1)
   SUMX=SUMX+TX(N)
   XTKINV=TX(N)
   XTK=1.0/XTKINV
   TLN=DLOG(XTK)
   CALL THERPS(NSRATE,XTK)
   RTKINV = 1./(XTK * RGAS)
360 CONTINUE

168
SUM1 = 0.0
DO 350 ND = 1, 4
  K = ID(ND, JJ)
  IF (K .EQ. 0) GO TO 350
  GF = HO(K) - SO(K)
  IF (ND .LT. 3) SUM1 = SUM1 + GF
  IF (ND .GE. 3) SUM1 = SUM1 - GF
350 CONTINUE
TM1 = 0.0
IF (ID(2, JJ) .EQ. 0) TM1 = TLN - 2.50034
IF (ID(4, JJ) .EQ. 0) TM1 = 2.50034 - TLN

C --- -2.50034 = LN(RGAS) RGAS IN UNITS ATM M**3/KGMOLE K HERE ONLY

TY(N) = TM1 - SUM1 + TEN(JJ) * TLN - TACT(JJ) * TKNINV + BX(JJ)
SUMY = SUMY + TY(N)
360 CONTINUE
XBAR = SUMX / 20.0
YBAR = SUMY / 20.0
SUMX = 0.0
SUM1 = 0.0
SUMY = 0.0
DO 370 N = 1, 20
  SUMX = SUMX + TY(N) * (TX(N) - XBAR)
  SUM1 = SUM1 + (TX(N) - XBAR)**2
  SUMY = SUMY + (TY(N) - YBAR)**2
370 CONTINUE
TEN2(JJ) = 0.0
TACT2(JJ) = -SUMX / SUM1
BX2(JJ) = (YBAR + TACT2(JJ) * XBAR) / TENLN
SUMX = 0.0
DO 380 N = 1, 20
  SUMX = SUMX + (TY(N) + TACT2(JJ) * TX(N) - TENLN * BX2(JJ))**2
380 CONTINUE
SUMY = DSQRT(1.0 - SUMX / SUMY)
SUMX = DSQRT(SUMX / 19.0)
DATAT = TACT2(JJ)
IF (LSI .NE. 1) DATAT = TACT2(JJ) * 1.987 * 0.001
IF (NDEBUG(3)) WRITE (30, 2400) SUMX, SUMY, BX2(JJ),
                      TEN2(JJ), TACT2(JJ)

C --- CONVERT BX2 FOR INTERNAL CALCULATIONS

BX2(JJ) = BX2(JJ) * TENLN

C 390 JJ = JJ + 1

C --- CONVERT ALL RATE DATA TO SI UNITS

C IF (LSI) GO TO 210
J = JJ-1  
BX(J) =BX(J)-TENLN*3.0  
BX2(J) =BX2(J)-TENLN*3.0  
IF (MODR(J).EQ.2) BX2(J) =BX2(J)-TENLN*3.0  
IF (MODR(J).EQ.3) BX(J) =BX(J)-TENLN*3.0  
GO TO 210  

C  
400  JJ=JJ-1  
NPYROP=NPYROL+1  
NGLOB=NGLOB+1  
NHETRP=NHETER+1  

C --- SET CONTACT INDEXES TO UNITY  
C  
DO 410 J=1,JJ  
   X1(J)=1.0  
   X2(J)=1.0  
410 CONTINUE  

C --- RETURN TO TSTR  
C  
RETURN

1000 FORMAT(A4,X,A4,X,F7.4,X,I1,X,1PD11.5,X,D11.5,X,A4,X,  
   * D11.4,X,D11.4)  
1100 FORMAT(3A4)  
1200 FORMAT(5D15.8/,5D15.8/,4D15.8/)  
1300 FORMAT(/)  
1350 FORMAT(/)  
1400 FORMAT((A4,5(X,1PD11.4)))'  
1500 FORMAT(/2X,'****** REACTION RATE DATA FROM NPT *****'//)  
1600 FORMAT(12A4,3F8.3,2A4)  
1700 FORMAT(6X,3H**,12A4,3H**)  
1800 FORMAT(/4X,26HFOLLOWING REACTION IGNORED)  
1900 FORMAT(8X,6A4,5H---->,6X,6A4)  
2000 FORMAT(4X,9REACTANT ,A4,26H NOT FOUND IN SPECIES LIST)  
2100 FORMAT(/14X,17HREVERSE RATE DATA,28X,3F15.3,2A4)  
2200 FORMAT(/4X,9REACTION ,I2,3X,6A4,5H---->,3X,6A4/,  
   * 6X,14HDATA COMMENT: ,2A4/,6X,21HFD DATA RATE DATA: BX = ,  
   * F10.3,X,7HTEN = ,F10.3,X,8HTACT = ,F10.3)  
2300 FORMAT(2X,'****** TOO MANY PYROLYSIS REACTIONS *****')  
2400 FORMAT(6X,3HCALCULATED REVERSE RATE CONSTANTS/,  
   * 6X,16HSTD DEVIATION = ,1PD11.3,X,13HCORR COEFF = ,D11.3/,  
   * 6X,21HREV RATE DATA : BX2 = ,0FF10.3,X,7HTEN2 = ,F10.3,X,  
   * 8HTACT2 = ,F10.3)  
2500 FORMAT(2X,'****** KINETIC REACTION RATE DATA IN SI UNITS '  
   * '*****'//,  
   * 7X,1HJ,6X,4HMODR,12X,2HID,19X,2HBX,10X,3HTEN,9X,4HTACT,13X,  
   * 3HBX2,9X,4HTEN2,9X,5HTACT2/)  
2600 FORMAT((5X,I2,1H.,I8,3X,4I5,2(3X,3F13.3)))

END
SUBROUTINE PIPES(Y,YPRIME,TM)
C
C
C INCLUDE 'INIT.FOR/LIST'
C
C DIMENSION Y(NV),YPRIME(NV),DV(15),DRH(15),FVIC(15),
* SUM1(15),SUM2(15),RF(15),ALEQ(50,50),BLEQ(50),
* WKAREA(IOO)
C
C INCLUDE 'COMMONSS.FOR/LIST'
C
C --- SHUTDOWN IS BEGUN BY SETTING THE DENSITY OF THE FURTHEST
C UPSTREAM NODE IN THE PIPING SYSTEM EQUAL TO THE DENSITY
C OF THE HELIUM AT THE HELIUM SOURCE PRESSURE AND TEMPERATURE. THIS IS DONE AT TIME = TMSD (TIME OF SHUTDOWN).
C
IF(TM.GT.TMSD) THEN
   RHO(1) = RHOGAS
   Y(NS8) = RHOGAS
ENDIF
IF(NDEBUG(12)) THEN
   WRITE(30,1000)
ENDIF
C
C --- FIND THE LIQUID/VAPOR INTERFACE POSITION AND VELOCITY IN
C EACH PIPE. NOTE:
C
C (1) POSITION IS FIXED USING POSITION AND NODAL DENSITIES
C (0.0 < FVI < 1.0).
C (2) IF A NODE HAS JUST BECOME GASEOUS (THE INTERFACE HAS
C JUST PASSED THROUGH) ITS DENSITY IS RECALCULATED USING
C THE PREVIOUS NODAL PRESSURE AND THE IDEAL GAS RELATION.
C (3) D(FVI(J))/DT IS EITHER ZERO (IF THERE IS NO INTERFACE
C IN THE PIPE) OF EQUAL TO THE FLUID VELOCITY IN THE PIPE.
C (4) AN INTERFACE CAN ENTER THE PIPE VIA BACKFLOW FROM THE
C COMBUSTION CHAMBER. THIS OCCURS WHEN THE VELOCITY IN THE
C LAST PIPE IS NEGATIVE. THE INTERFACE THAT RESULTS FROM
C BACKFLOW IS NEVER ALLOWED TO PROCEED PAST THE UPSTREAM
C NODE OF THE LAST PIPE.
C
DO 100 J=1,NP
   ND1 = N1(J)
   ND2 = N2(J)
   IF(J.LE.NHEO) THEN
      RFLX = RFLHO
      RFGX = RFHO
   ELSE IF(J.EQ.NPV) THEN
      RFLX = RFLV
      RFGX = RFGV
   ELSE
C
100 CONTINUE

171
RFLX = RFLIQ
RFGX = RFGAS
ENDIF
C
C --- BOTH PIPE NODES ARE GASEOUS
C
IF(RHO(ND1).LT.RGMX.AND.RHO(ND2).LT.RGMX) THEN
  YPRIME(NS5+J) = 0.0
  FVI(J) = 1.0
  FVIC(J) = 0.0
  RFJ = RFGX*PL(J)*V(J)*V(J)*RHO(ND2)
  RF(J) = DSIGN(RFJ,V(J))
  Y(NS5+J) = 1.0
C
C --- ONLY THE UPSTREAM NODE IS GASEOUS. THREE CASES:
C
1) 0 < FVI < 1.0: THERE IS AN INTERFACE IN THE PIPE
2) FVI > 1.0: THE INTERFACE HAS JUST LEFT THE PIPE.
   THE DOWNSTREAM NODE IS MADE GASEOUS AND FVI IS SET
   AT 1.0.
3) FVI < 1.0: THE INTERFACE HAS RETURNED TO THE UP-
   STREAM PIPE. DENSITY OF NODE ND1 RETURNS TO THE
   CONSTANT LIQUID DENSITY (RHOLIQ). FVI IS RESET TO
   0.0 AND FVI AND ITS VELOCITY ARE RECALCULATED FOR
   THE UPSTREAM PIPE.
ELSE IF(RHO(ND1).LT.RGMX) THEN
C
C THE INTERFACE HAS JUST LEFT THE PIPE
C
IF(FVI(J).GE.1.0) THEN
  YPRIME(NS5+J) = 0.0
  FVI(J) = 1.0
  FVIC(J) = 0.0
  RFJ = RFGX*PL(J)*V(J)*V(J)*RHO(ND2)
  RF(J) = DSIGN(RFJ,V(J))
  Y(NS5+J) = 1.0
  RHO(ND2) = P(ND2)*SMW(1)/RGAS/TKS(3)
  Y(NS7+ND2) = RHO(ND2)
C
C THE INTERFACE IS MOVING WITHIN THE PIPE
C
ELSE IF(FVI(J).GE.0.0) THEN
  NFVI = J
  YPRIME(NS5+J) = V(J)/PL(J)
  FVIC(J) = 1.0 - FVI(J)
  RFJ = PL(J)*V(J)*V(J)*(FVI(J)*RFGX*RHO(ND1) +
    * FVIC(J)*RFLX*RHO(ND2))
  RF(J) = DSIGN(RFJ,V(J))
C
C THE INTERFACE IS RETURNING UPSTREAM
ELSE IF (FVI(J).LT.0.0) THEN
IF (J.EQ.1) THEN
   FVI(J) = 0.0
   YPRIME(NS5+J) = 0.0
   FVIC(J) = 1.0
   RFJ = PL(J)*V(J)*V(J)*RHOLIQ*RFLX
   RF(J) = DSIGN(RFJ,V(J))
ELSE
   FVI(J-1) = 1.0 + FVI(J)
   FVIC(J-1) = 1.0 - FVI(J-1)
   RFJ = PL(J-1)*V(J-1)*V(J-1)*(FVI(-J-1)*RFGX* RHO(ND1-1)+FVIC(J-1)*RFLX*RHO(ND1))
   RF(J-1) = DSIGN(RFJ,V(J-1))
   Y(NS5+J-1) = FVI(J-1)
   YPRIME(NS5+J-1) = V(J-1)/PL(J-1)
   RHO(ND1) = RHOLIQ
   Y(NS7+ND1) = RHOLIQ
   FVI(J) = 0.0
   FVIC(J) = 1.0
   RFJ = PL(J)*V(J)*V(J)*RFLX*RHOLIQ
   RF(J) = DSIGN(RFJ,V(J))
   Y(NS5+J) = 0.0
   YPRIME(NS5+J) = 0.0
ENDIF
ENDIF
C --- BOTH NODES ARE LIQUID
C
ELSE
   YPRIME(NS5+J) = 0.0
   FVI(J) = 0.0
   FVIC(J) = 1.0
   RFJ = PL(J)*V(J)*V(J)*RFLX*RHOLIQ
   RF(J) = DSIGN(RFJ,V(J))
ENDIF
100 CONTINUE
C --- IF THE VELOCITY OF THE FURTHEST DOWNSTREAM PIPE (NP) IS
C NEGATIVE, AN INTERFACE PASSES INTO THE PIPE. THE SYSTEM
C VARIABLE Y(NS10)=FVI2 follows the progress of the inter-
C face upstream in the same way FVI(J) follows the oxygen/
C helium interface. Note:
C
(1) THE INTERFACE THAT ENTERS THE PIPES FROM THE COMBUS-
C TION CHAMBER CAN ONLY GO AS FAR AS THE UPSTREAM NODE
C OF THE FURTHEST DOWNSTREAM PIPE.
C
(2) FVI2 IS VIEWED BACKWORD: AS THE INTERFACE GOES UP THE
C PIPE, FVI2 RANGES FROM 0 TO 0.9999.
IF((V(NP).LE.0.0).OR.(RHO(NN).LE.RGMX).OR.
   *(FVI2.GT.FVI2MN)) THEN
   IF(FVI2.GT.1.0) THEN
     FVI2 = 0.99999
     YPRIME(NS10) = 0.0
     RHO(NN) = RHOCC
     Y(NS7+NN) = RHOCC
   ELSE IF(FVI2.GT.FVI2MN.OR.V(NP).LT.0.0) THEN
     YPRIME(NS10) = -V(NP)/PL(NP)
     RHO(NN) = RHOCC
     Y(NS7+NN) = RHOCC
   ELSE IF(FVI(NP).GE.1.0) THEN
     FVI2 = 0.0
     Y(NS10) = 0.0
     YPRIME(NS10) = 0.0
     RHO(NN) = PA*RGASIN/TKS(3)/SMW(1)
     Y(NS7+NN) = RHO(NN)
   ELSE
     FVI2 = 0.0
     YPRIME(NS10) = 0.0
     RHO(NN) = RHOLIQ
     Y(NS7+NN) = RHOLIQ
   ENDIF
   ELSE
     YPRIME(NS10) = 0.0
   ENDIF
C
C --- FIND PRESSURE AT EACH NODE.
C
(1) IF A NODE IS GASEOUS, PRESSURE IS FOUND USING THE
PERFECT GAS RELATION.
(2) IF A NODE IS LIQUID, PRESSURE IS FOUND BY CALCULATING
THE PRESSURE LOSSES FROM UPSTREAM PIPES AND
SUBTRACTING FROM FURTHEST UPSTREAM PRESSURE.
(3) SOURCE NODE PRESSURES ARE FIXED. PRESSURE AT NODE
NN (WHICH CONNECTS THE PIPING SYSTEM TO THE COMBUSTION
CHAMBER) IS ALSO FIXED.

P(1) = PS
XDPIN = 0.5*QMV*QM*VOL*VOL/(AO2IN*AO2IN*264.0*264.0*CDIN*CDIN)
IF(FVI(NP).LT.1.0) THEN
   IF(FVI2.GT.FVI2MN.OR.V(NP).LT.0.0) THEN
     DPIN = XDPIN / RHOCC
   ELSE
     DPIN = XDPIN / RHOLIQ
   ENDIF
ELSE
   DPIN = XDPIN / RHOGAS
ENDIF
DPIN = DSIGN(DPIN, V(NP))
P(NN) = PA + DPIN
DO 110 J=2,NP
   ND1 = N1(J)
   IF(RHO(ND1).LT.RGMX) THEN
      P(ND1) = RHO(ND1) * RGAS * TKS(3) / SMW(1)
   ELSE
      SRF = 0.0
      RHLSM = 0.0
      DO 120 JX=J-1,NP
         SRF = SRF + RF(JX)*AREA(JX)
         RHLSM = RHLSM + RHOLIQ * FVIC(JX) * PL(JX)
      CONTINUE
      RHLSM = RHLSM + FVI2*PL(NP)*(RHOCC-RHOLIQ)+
               FVI(J)*PL(J)*RHO(ND1)
      DELP1 = P(ND1-1) - P(NN)
      IF(DABS(SRF).LT.1.0D-04) THEN
         P(ND1) = P(ND1-1)
      ELSE
         P(ND1) = P(ND1-1) - RF(J-1)*AREA(J-1)*DELP1/SRF
      ENDIF
      DELP2 = P(ND1) - P(NN)
      DELPP = DELP2/DFLOAT(NN-ND1)
      DO 130 KX = ND1+1,NN-1
         P(KX) = P(KX-1) - DELPP
      CONTINUE
      GO TO 140
   ENDIF
110 CONTINUE
140 CONTINUE

C --- THE EQUATIONS FOR DRH(K) AND DV(J) ARE LINEAR FOR THE
C DERIVATIVES. A MATRIX EQUATION IS SET UP WITH THE COEF-
C FICIENTS OF DRH AND DV IN MATRIX ALEQ AND THE RHS IN
C VECTOR BLEQ. IMSL SUBROUTINE LEQTIF IS CALLED TO SOLVE
C THE MATRIX EQUATION [ALEQ]*{D> = {BLEQ}. VALUES FOR DV
C AND DRH ARE RETURNED IN BLEQ.
C
C --- CALCULATE THE COEFFICIENTS ALEQ(NP+K,NP+K) = SUM1(K)
C --- RESET SUM1
C
DO 150 K=1,NN
   SUM1(K) = 0.0
150 CONTINUE

C --- CALCULATE SUM1
C
DO 160 J=1,NP
   SUM1(N1(J)) = SUM1(N1(J)) - AREA(J)*V(J)
   SUM1(N2(J)) = SUM1(N2(J)) + AREA(J)*V(J)
160 CONTINUE
160 CONTINUE
    DO 161 K=1,NN
      IF(DABS(SUM1(K)).LT.SM1MIN) SUM1(K)=DSIGN(SM1MIN,
          * SUM1(K))
161 CONTINUE
C
C --- RESET ALEQ AND BLEQ
C
NVP = NN + NP
DO 170 I=1,NVP
   BLEQ(I) = 0.0
DO 180 J=1,NVP
   ALEQ(I,J) = 0.0
180 CONTINUE
170 CONTINUE
C
C --- FILL ALEQ AND BLEQ
C
MLIQ = 0
DO 190 J=1,NP-1
   ND1 = N1(J)
   ND2 = N2(J)
C
C --- BOTH NODES ARE GASEOUS
C
   IF(RHO(ND2).LT.RGMX) THEN
      ALEQ(J,J) = 0.5*PL(J)*(RHO(ND1) + RHO(ND2))
      ALEQ(J,NP+ND1) = 0.5 * PL(J) * V(J)
      ALEQ(J,NP+NN) = PL(NP) * FVI2 * V(NP)
      BLEQ(J) = P(ND1) - AREA(NP)*P(NN)/AREA(J) - SRF/AREA(J) -
          * RHOLIQ*V(J)*V(J) - RHO(NN)*V(NP)*V(NP)*AREA(NP)/
          * AREA(J)
      ALEQ(NP+ND1,NP+ND1) = SUM1(ND1)
      ALEQ(NP+ND1,J) = - RHO(ND1) * AREA(J)
      ALEQ(NP+ND2,J) = RHO(ND2) * AREA(J)
   C
C --- ONLY THE UPSTREAM NODE IS GASEOUS
C
ELSE IF(MLIQ.LT.1) THEN
   MLIQ = 1
   JHE = J
   ALEQ(J,J) = RHLSM
   ALEQ(J,NP+ND1) = PL(J) * FVI(J) * V(J)
   ALEQ(J,NP+NN) = PL(NP) * FVI2 * V(NP)
   BLEQ(J) = P(ND1) - AREA(NP)*P(NN)/AREA(J) - SRF/AREA(J) -
          * RHOLIQ*V(J)*V(J) - RHO(NN)*V(NP)*V(NP)*AREA(NP)/
          * AREA(J)
   ALEQ(NP+ND1,NP+ND1) = SUM1(ND1)
   ALEQ(NP+ND1,J) = - RHO(ND1) * AREA(J)
C
C --- BOTH NODES ARE LIQUID
C
ELSE
    ALEQ(J,J) = 1.0
    ALEQ(J,J-1) = -AREA(J-1)/AREA(J)
    ALEQ(NP+ND1,NP+ND1) = 1.0
ENDIF
190 CONTINUE
C
C --- THE FURTHEST DOWNSTREAM PIPE IS HANDLED SEPARATELY BECAUSE
C OF THE POSSIBILITY OF A BACKFLOW INTERFACE.
C
C --- THE UPSTREAM NODE IS LIQUID
C
IF(RHO(NN-1).GT.RGMX) THEN
    ALEQ(NP,NP) = 1.0
    ALEQ(NP,NP-1) = -AREA(NP-1)/AREA(NP)
    ALEQ(NP+NN-1,NP+NN-1) = 1.0
    ALEQ(NP+NN,NP+NN) = 1.0
ENDIF
C
C --- THE FURTHEST DOWNSTREAM NODE IS LIQUID
C
IF(FVI2.LE.0.0) THEN
    BLEQ(NP+NN) = 0.0
ELSE
    BLEQ(NP+NN) = RPX
ENDIF
C
C --- A BACKFLOW INTERFACE EXISTS
C
ELSE IF(FVI(NP).GE.1.0) THEN
    ALEQ(NP,NP) = 0.5*PL(NP)*(RHO(NN-1) + RHO(NN))
    ALEQ(NP,NP+NN-1) = 0.5 * PL(NP) * V(NP)
    ALEQ(NP,NP+NN) = 0.5 * PL(NP) * V(NP)
    BLEQ(NP) = P(NN-1) - P(NN) - RF(NP)
    ALEQ(NP+NN-1,NP+NN-1) = SUM1(NN-1)
    ALEQ(NP+NN-1,NP) = -RHO(NN-1) * AREA(NP)
    ALEQ(NP+NN,NP+NN) = 1.0
    BLEQ(NP+NN) = YPRIME(NS3) * RHO(NN)
C
C --- AN HELIUM/OXYGEN INTERFACE EXISTS IN THE PIPE
C
ELSE IF(FVI2.LE.0.0) THEN
    ALEQ(NP,NP) = PL(NP)*(RHO(NN-1)*FVI(NP) + RHOLIQ*FVIC(NP))
    ALEQ(NP,NP+NN-1) = PL(NP) * V(NP) * FVI(NP)
    BLEQ(NP) = P(NN-1) - P(NN) - RF(NP)
    ALEQ(NP+NN-1,NP+NN-1) = SUM1(NN-1)
    ALEQ(NP+NN-1,NP) = -RHO(NN-1) * AREA(NP)
    ALEQ(NP+NN,NP+NN) = 1.0
C --- TWO INTERFACES EXIST IN THE LAST PIPE (BACKFLOW AND HE/OX)
C
ELSE

ALEQ(NP,NP) = PL(NP)*(RHO(NN-1)*FVI(NP)+(FVIC(NP)-FVI2)*RHOLIQ + RHOCC * FVI2)

ALEQ(NP,NP+NN-1) = PL(NP)*FVI(NP)*V(NP)

ALEQ(NP,NP+NN) = PL(NP)*FVI2*V(NP)

BLEQ(NP) = P(NN-1) - P(NN) - RF(NP)

ALEQ(NP+NN-1,NP+NN-1) = SUM1(NN-1)

ALEQ(NP+NN-1,NP) = -RHO(NN-1)*AREATNP)

ALEQ(NP+NN,NP+NN) = 1.0

BLEQ(NP+NN) = YPRIME(NS3) * RHOCC

ENDIF

ALEQ(NP+1,NP+1) = 1.0

ALEQ(NP+1,N1) = 0.0

IERP = 10

CALL LEQT1F(ALEQ,1,NVP,50,BLEQ,0,WKAREA,IERP)

IF(IER.GT.IOO) THEN

WRITE (30,1300) IERP,TM,TK,PA,RHOCC,FVI2,YPRIME(NS10)

WRITE (30,1310) (J,FVI(J),YPRIME(NS5-J),V(J),DV(J),J-1,NP)

WRITE (30,1320) (K,RHO(K),P(K),DRH(K),K=1,NN)

STOP

ENDIF

DO 800 J=1,NP

DV(J) = BLEQ(J)

YPRIME(NS3+J) = DV(J)

800 CONTINUE

DO 900 K=1,NN

DRH(K) = BLEQ(NP+K)

YPRIME(NS7+K) = DRH(K)

900 CONTINUE

IF(NDEBUG(12)) THEN

WRITE (30,1400) FVI2,YPRIME(NS10),SRF

WRITE (30,1500) (J,V(J),DV(J),RF(J),J=1,NP)

WRITE (30,1600) (K,RHO(K),DRH(K),P(K),K=1,NN)

ENDIF

RETURN

1000 FORMAT(//'2X,'***** OUTPUT FROM SUBROUTINE PIPES *****'//)

1300 FORMAT(//'2X,'***** CONVERGENCE OF PIPING SYSTEM FAILED',
" ' *****'//,4X,'LEQT1F RETURNED WITH IER = ',I4,
" ', EXECUTION HALTED',4X,'TIME = ',1PD11.4,
" , CHAMBER TEMPERATURE = ',0PF10.2,' K',/
" , CHAMBER PRESSURE = ',1PD11.4,' PA',/
" , CHAMBER DENSITY = ',D11.4,' KG/M**3',/
" , FVI2 = ',D11.4',/
" , YPRIME(FVI2) = ',D11.4')
* 1PD10.3))
1320 FORMAT(/4X,4HNODE,3X,7HDENSITY,3X,8HPRESSURE,4X,
* 9HD(RHO)/DT//,(6X,I1,2X,1PD10.3,X,1PD10.3,X,1PD10.3))
1400 FORMAT(/4X'PIPES DERIVATIVE ESTIMATE SUMMARY'/,
* 4X,'POSITION OF THE BACKFLOW INTERFACE (FVI2) = ',
* 1PD11.4,'D(FVI2)/DT = ',D11.4,4X,'SRF = ',
* D11.4)
1500 FORMAT(/4X,'PIPE',2X,' V ',2X,' D(V)/DT ',2X,
* 'RF '/,(5X,I2,3X,1PD11.4,2X,D11.4,2X,D11.4))
1600 FORMAT(/4X,'NODE',2X,' RHO ',2X,' D(RHO)/DT ',2X,
* 'P '/,(5X,I2,3X,1PD11.4,2X,D11.4,2X,D11.4))
END
SUBROUTINE RADSS

C INCLUDE 'INIT.FOR/LIST'
DIMENSION G1(20),BLEQ(10),WKAREA(10),ALEQ(10,10),S2I(10)

C INCLUDE 'COMMONSS.FOR/LIST'

C ITER = 0

C SMNS = 0.0
DO 100 I=1,NS
   SMNS = SMNS + S2(I)
100 CONTINUE

DO 110 I=NS1,NSRATE
   S2I(I) = S2(I)
110 CONTINUE

C --- DEFINE THE G1 ARRAY: G1(I) = MASS INFLOW OF SPECIES I FROM
C THE PIPES.

G1(2) = FMV / SMW(2)
G1(3) = OMV / SMW(3)

C --- ITERATION BEGINS

120 CALL RATES

ICHK = 0
ITER = ITER + 1
DO 140 I=NS1,NSRATE
   BLEQ(I-NS) = - G1(I) - ARR(I) + EMV * S2(I)
   DO 130 K=NS1,NSRATE
      ALEQ(I-NS,K-NS) = RIP(I,K)
   130 CONTINUE
   ALEQ(I-NS,I-NS) = ALEQ(I-NS,I-NS) - EMV
140 CONTINUE

C --- LEQT1F SOLVES THE MATRIX EQUATION: [ALEQ]DS2=[BLEQ] AND
C RETURNS THE ANSWER IN THE VECTOR (BLEQ).

CALL LEQT1F(ALEQ,1, NRAD, 10, BLEQ, IDGT, WKAREA, JER)

C --- INCREMENT ALL S2 BY DS2 AND KEEP THE RESULT WITHIN THE BOUNDS
C ( S2MIN < S2(I) < 1.0/SMW(I) )

SM = SMNS
DO 150 I=NS1,NSRATE
   ALG = 1.0/SMW(I)
   SCHK = DABS(BLEQ(I-NS)/S2(I))
   IF(SCHK.GT.EPSISS) ICHK = 1
   S2(I) = S2(I) + RLX*BLEQ(I-NS)
150 CONTINUE

C - 3
IF(S2(I).LT.S2MIN) S2(I) = S2MIN
IF(S2(I).GT.ALG) S2(I) = ALG
SM = SM + S2(I)
150 CONTINUE
SMINV = 1.0/SM
C
C --- STOP THE ITERATION IF ITERATION COUNTER ITER IS GREATER
C THAN ITMAXS. IF THE SPECIES MOLE NUMBERS FALL BELOW THE
C MINIMUM ALLOWABLE MOLE NUMBER THE ITERATION CANNOT CON-
C VERGE. IF THIS TAKES PLACE THE MOLE NUMBERS ARE SET TO
C MINIMUM ALLOWABLE MOLE NUMBER AND EXECUTION IS ALLOWED
C TO CONTINUE.
C
IF(ITER.GT.ITMAXS) THEN
  ISTOP = 0
  S2CHK = S2MIN*100.0
  DO 160 I = NS1, NSRATE
    IF(S2(I).LE.S2CHK) THEN
      ISTOP = 1
      S2(I) = S2MIN
    ENDIF
  160 CONTINUE
  IF (ISTOP.EQ.1) GO TO 170
  WRITE (30,1000) ITMAXS, TM, TK, PA, RHOCC, DLIQ, VR
  WRITE (30,1100) (ANAM(I), S2(I), I=1, NS)
  WRITE (30,1200) (ANAM(I), S2(I), BLEQ(I-NS), I=NS1, NSRATE)
  WRITE (30,1300)
  STOP
ENDIF
C
C --- IF ICHK = 1 THE CONVERGENCE CRITERION WAS NOT MET
C
IF(ICHK) GO TO 120
C
C --- CALCULATE THE RATE OF PRODUCTION OF THE PRODUCTS AND INFERENCE
C THE RATE OF CONSUMPTION OF THE REACTANTS FROM THE CONSERVATION
C OF ATOMS
C
170 RATE(4) = ARR(4)
RATE(2) = -RATE(4)
RATE(3) = -RATE(4)*0.5
RATE(1) = 0.0
C
C --- OUTPUT FOR NDEBUG(11) = 1
C
IF(NDEBUG(11)) THEN
  WRITE (30,1400) ITER, RLX, EPSISS
  WRITE (30,1500) TK, PA, RHOCC, OMV, PMV, PMV
WRITE (30,1600)
WRITE (30,1700) (ANAM(I),S2I(I),I=NS1,NSRATE)
WRITE (30,1800)
WRITE (30,1900) (ANAM(I),S2(I),ARR(I),RATE(I),I=1,NSRATE)
ENDIF
C
RETURN
C
1000 FORMAT(/2X,'***** IN RADSS, ITMAX = ',17,' EXCEEDED *****'//,
* 4X,'RADICAL MOLE NUMBER IterATION DID NOT CONVERGE FOR:'//,
* 4X,'TIME = ',1PD11.4,' SEC'//,
* 4X,'CC TEMPERATURE = ',OPF10.3,' K'//,
* 4X,'CC PRESSURE = ',1PD11.4,' PA'//,
* 4X,'CC DENSITY = ',D11.4,' KG/M**3'//,
* 4X,'CC LIQUID DENSITY = ',D11.4,' KG/M**3'//,
* 4X,'CC VAPOR. RATE = ',D11.4,' KG/M**3 SEC'//)
1100 FORMAT(4X,'MAJOR SPECIES MOLE NUMBER (KGMOLES/KG)'//,
* (8X,A4,13X,D11.4))
1200 FORMAT(/4X,'SPECIES MOLE NUMBER (KGMOLES/KG) INCREMENT'//,
* (5X,A4,7X,D11.4,13X,D11.4))
1300 FORMAT(/2X,'***** EXECUTION HALTED *****')
1400 FORMAT(/2X,'***** OUTPUT FROM SSRATE *****'//,
* 4X,'SSRATE SUCCEEDED AFTER ',1PD4,' ITERATIONS.'//,
* 4X,'RELAXATION FACTOR = ',1PD8.2/, 
* 4X,'PERCENT TOLERANCE = ',D8.2)
1500 FORMAT(4X,'TEMPERATURE = ',F8.2/, 
* 4X,'PRESSURE = ',1PD12.4/, 
* 4X,'DENSITY = ',D12.4/, 
* 4X,'OMV, FMV, PMV = ',3(D12.4,2X))
1600 FORMAT(/4X,'SPECIES',2X,'INITIAL MOLE NO.'//)
1700 FORMAT(5X,A4,3X,Q12.5)
1800 FORMAT(/4X,'CONVERGED SOLUTION:'//,
* 4X,'SPECIES',2X,'EFFECTIVE S2',2X,'SS RXN RATE ',2X,
* 'EFFECTIVE RXN RATE',12X,'KGMOLE(I)/KG',X,'KGMOLE/M~3*SEC',X,
* 'KGMOLE/M~3*SEC'//)
1900 FORMAT(5X,A4,3X,1PD12.5,2X,Q12.5,2X,Q12.5,2X,Q12.5)
END
SUBROUTINE RATES
C
C --- CALCULATES RATE OF PRODUCTION OF EACH SPECIES, ARR(I),
C AND THE DERIVATIVE OF THE RATE OF PRODUCTION OF EACH
C SPECIES, I, WITH RESPECT TO THE MOLE NUMBER OF EACH
C SPECIES, K, RIP(I,K).
C
INCLUDE 'INIT.FOR/LIST'
C
DIMENSION RFP(20,20),RRP(20,20),RF2(20),RR(20)
C
INCLUDE 'COMMONSS.FOR/LIST'
C
DATA BIG/46.051/
C
C --- DETERMINE DENSITY AND OFTEN USED CONSTANTS
C
TLN = DLOG(TK)
TKSQ = TK * TK
TKSQIN = 1.0/TKSQ
RHS = PA * RGASIN * TKINV
RHOP = RHS * SMINV
RHSQ = RHOP * RHOP
RHINV = 1.0 / RHOP
C
C --- FIND THE FORWARD AND REVERSE RATES OF EACH OF THE ELEMENTARY
C REACTIONS, J, FOR J=1,JJ (JJ = NO. OF ELEM RXNS)
C
DO 10 J=1,JJ
RF2(J) = 0.0
RR(J) = 0.0
I = ID(1,J)
K = ID(2,J)
M = ID(3,J)
N = ID(4,J)
MODE = MODR(J)
R1 = 0.0
R2 = 0.0
TX1 = TACT(J)*TKINV - BX(J) - TEN(J)*TLN
TX2 = TACT2(J)*TKINV - BX2(J) - TEN2(J)*TLN
R1 = DEXP(-TX1)
R2 = DEXP(-TX2)
C
C --- SECTION FOR FORWARD REACTION RATES
C
IF(DABS(TX1).GT.BIG) THEN
   IF(NDEBUG(13))WRITE(30,1000) ITER,J
   GO TO 50
ENDIF

183
R1 = R1 * X1(J)
IF(MODE-2) 20,30,40
20 RF2(J) = R1 * S2(I) * RHSQ * S2(K)
   GO TO 60
30 RF2(J) = R1 * RHSM * S2(I) * RHOP
   GO TO 60
40 RF2(J) = R1 * RHSM * S2(I) * RHOP
   IF(K.NE.0) RF2(J) = RF2(J) * S2(K) * RHOP
   GO TO 60
50 RF2(J) = 0.0
60 CONTINUE
C
C --- SECTION FOR REVERSE RATES
C
IF(DABS(TX2).GT.BIG) THEN
   IF(NDEBUG(13)) WRITE(30,1100) ITER, J
   GO TO 100
ENDIF
R2 = X2(J) * R2
IF(MODE-2) 70,80,90
70 RR(J) = R2 * S2(M) * RHSQ * S2(N)
   GO TO 10
80 RR(J) = R2 * RHSM * S2(M) * RHSQ * S2(N)
   GO TO 10
90 RR(J) = R2 * RHSM * RHOP * S2(M)
   GO TO 10
100 RR(J) = 0.0
10 CONTINUE
C
C --- FIND THE RATE OF PRODUCTION OF EACH SPECIES I, ARR(I).
C
   DO 110 I=1,NSRATE
      ARR(I) = 0.0
   DO 120 J=1,JJ
      ARR(I) = ARR(I)+DFLOAT(ISIDE(I,J))*(RF2(J)-RR(J))
   120 CONTINUE
110 CONTINUE
C
C --- FIND THE DERIVATIVES OF THE FWD AND REV RXN RATES OF EACH
C ELEMENTARY RXN WITH RESPECT TO EACH MOLE NO. (I.E.
C RFP(J,K)=D(RF2(J))/D(S2(K)) AND RRP(J,K)=D(RR(J))/D(S2(K))
C
   DO 130 J=1,JJ
      DO 140 K=1,NSRATE
         RFP(J,K) = 0.0
         RRP(J,K) = 0.0
         IF(ISIDE(K,J).LT.0)
            RFP(J,K)=-DFLOAT(ISIDE(K,J))*RF2(J)/S2(K)
            RRP(J,K)=DFLOAT(ISIDE(K,J))*RR(J)/S2(K)
      140 CONTINUE
130 CONTINUE
CONTINUE
CONTINUE

C --- FIND THE DERIVATIVE OF THE RATE OF PRODUCTION OF EACH SPECIES
WITH
RESPECT TO THE MOLE NO. OF EACH SPECIES
(RIP(I,K)=D(ARR(I))/D(S2(K)))

DO 150 I=1,NSRATE
   DO 160 K=1,NSRATE
      RIP(I,K) = 0.0
      DO 170 J=1,JJ
         RIP(I,K) = RIP(I,K)+DFLOAT(ISIDE(I,J))*(RFP(J,K)-RRP(J,K))
      170 CONTINUE
   160 CONTINUE
150 CONTINUE
RETURN

1000 FORMAT(4X,'IN RATES, FOR ITERATION ',I4,' FWD RATE = 0 FOR J = ',* I2)
1100 FORMAT(4X,'IN RATES, FOR ITERATION ',I4,' REV RATE = 0 FOR J = ',* I2)
END
SUBROUTINE YCAL(Y,WK,IWK,N,NWK)
C
C TSTR2 RUNS THE CALLING OF THE INTEGRATION ROUTINE AND
C THE OUTPUTTING OF DATA TO THE OUTPUT AND PLOT FILES
C
INCLUDE 'INIT.FOR/LIST'
C
REAL*4 SDUMMY(4)
C
EXTERNAL CSLOPE
C
DIMENSION Y(N),IWK(N),WK(NWK),WK2U(4,100),S2P(10),CHG(50)
C
INCLUDE 'COMMONSS.FOR/LIST'
COMMON / GEAR / DUMMY(48),SDUMMY,IDUMMY(38)
C
C --- PUT MOLE NUMBERS, TEMPERATURE AND DENSITY INTO LOG VARIABLE
C FORM AND INSERT THEM INTO THE VECTOR Y. DENSITY OF LIQUID IN
C THE COMBUSTION CHAMBER IS LEFT IN NON-LOG FORM.
C
DO 100 1=1,NS
100 Y(I) = DLOG(S2(I))
Y(NS1) = XMASS/VOL
Y(NS2) = DLOG(TK)
Y(NS3) = DLOG(PA)
VH2 = EMS(2)/AH2IN/RHOH2/264.0
C
C --- PLACE THE PIPING SYSTEM VARIABLES INTO THE VECTOR Y.
C
DO 110 1=1,NP
   Y(NS3+I) = V(I)
   Y(NS5+I) = 0.0
   IF(N2(I).EQ.NN) OMV = OMV + RHO(NN)*AREA(I)*V(I)
110 CONTINUE
DO 120 1=1,NN
   Y(NS7+I) = RHO(I)
120 CONTINUE
C
C --- GET GOOD INTITIAL ESTIMATES FOR ATOM AND RADICAL MOLE
C NUMBERS VIA A CALL TO RADSS
C
IF(KINET.EQ.1) THEN
   CALL RADSS
ENDIF
C
C --- BEGIN THE INTEGRATION LOOP
C
NSTEPS = JIDINT((TMEND-TMI)/TMPRNT)
DO 150 NX = 1,NSTEPS
   TMNXT = TMNXT + TMRNT
150 CONTINUE

186
IF(TMNX.TGT.TMEND) TMNX = TMEND
IF(NDEBUG(5)) WRITE (30,1000) NX,NSTEPS,TM,TMNX
IF(NDGEAR) THEN
  CALL DTSTR(N,CSLOPE,TM,STEP,Y,TMNX,WK2,NDEBUG)
ELSE
  CALL DGEAR (N,CSLOPE,CHGJ,TM,STEP,Y,TMNX,EPSI,METH,
  MITER,INDEX,IWK,WK,IER)
  IF(IER.GE.128) THEN
    WRITE (30,1100) IER,TM
    DO 140 I=1,NV
    140 — CHG(I) = WK(IDUMMY(11)+I)/WK(I)
    WRITE (30,1200) (I,Y(I),CHG(I),I=1,NV)
    CALL OUTPT(Y,TM,N,NSTEPS)
    STOP
  END IF
END IF
IF (NDEBUG(14))
*  WRITE (6,1300) TM,STEP,TK,PA,RHOCC,(V(J),J=1,3),
*       (RHO(K),K=1,3),(FVI(J),J=NP-2,NP),V(NP),FVI2,
*       (S2(I),I=1,4)
C
C   ON RETURN FROM THE INTEGRATION ROUTINE OUTPUT DEPENDENT
C   VARIABLES AND SIGNIFICANT PROBLEM PARAMETERS TO THE TEXT
C   AND PLOT OUTPUT FILES.
C
CALL OUTPT(Y,TM,N,NSTEPS)
IF(TM.GT.TMPER.AND.IPER.LT.1) THEN
  IPER = 1
  DMCX = DMC
  DMC = XPER * DMC
ELSE IF(TM.GT.TMPER.AND.IPER.LE.5) THEN
  IPER = IPER + 1
ELSE IF(IIPER.GT.5) THEN
  DMC = DMCX
ENDIF
150 CONTINUE
C
RETURN
1000 FORMAT(/2X,'***** INTEGRATING ROUTINE CALLED *****'/,
  * 4X,'CALL FOR STEP ',I7,' OUT OF ',I12,' STEPS'/,
  * 4X,'STEP BEGINS AT TIME = ',1PD12.5,
  * ' AND ENDS AT TIME = ',1PD12.5)
1100 FORMAT(2X,'***** ERROR CONDITION ON RETURN FROM DGEAR
  *****/,
  * 4X,'EXECUTION STOPPED. IER = ',I4,X,'TIME = ',1PD12.5//,
  * 2X,'VARIABLE',2X,'VALUE AT HALT',2X,'RELATIVE CHANGE'/)
1200 FORMAT(5X,12,5X,1PD12.5,4X,1PD12.5)
1300 FORMAT(/2X,'ON RETURN TO YCAL: TIME = ',1PD8.2,' STEP = ',
  * D8.2/,
  * 2X,'TEMP = ',0PF10.2,X,'PRESS = ',1PD8.2,X,'DENS = ',D8.2/,
* 2X,'V(1:3)  = '3D9.2/,
* 2X,'RHO(1:3)  = '3D9.2/,
* 2X,'FVI(NP-2:NP) = '3D9.2/,
* 2X,'V(NP) = 'D9.2,2X,'FVI2 = 'D9.2/,
* 2X,'S2(1:4) = '4D9.2)
END
SUBROUTINE THERPS(NS,XTK)

C
C THERPS CALCULATES THE SPECIFIC MOLAR INTERNAL ENERGY,
C ENTHALPY AND SPECIFIC HEAT AT CONSTANT PRESSURE FOR EACH
C SPECIES, I=1,NS.
C
C H(I) = ENTHALPY (J/KGMOLE)
C U(I) = INTERNAL ENERGY (J/KGMOLE)
C CP(I) = SPECIFIC HEAT AT CONSTANT PRESSURE (J/KGMOLE K)
C
C THERPS IS MODELLED AFTER SUBROUTINE HCPS USED BY DR. PAUL
C GEORGE II (PHD DISSERTATION, PURDUE UNIVERSITY, 1982).
C
IMPLICIT REAL*8 (A-H,P-Z)
IMPLICIT INTEGER*4 (I-O)

DIMENSION H1(20),H2(20),H01(20),H02(20),CP1(20),CP2(20),
* CP01(20),CP02(20),S1(20),S2(20),SO1(20),S02(20),U1(20),
* U2(20)

COMMON
* / CPROP / Z(200),H(10),CP(10),U(10),S(10),DCP(10),HO(10),
* CP0(10),SO(10)

DATA ICIT/14/,RGAS/8314.4/
IT=0
IF (XTK.LT.950.0) THEN
   IT=7
ELSE IF(XTK.GT.1050.0) THEN
   IT = 0
ELSE
   GO TO 70
ENDIF

XTKSQ=XTK**2
XTKCU=XTKSQ*XTK
XTK4=XTKCU*XTK
XTKINV=1./XTK
XTLN=DLOG(XTK)
RTK=RGAS*XTK

C --- H(I), U(I), CP(I), DCP(I) REQUIRED

DO 60 I=1,NS
   K=IT+ICIT*(I-1)
   CP1X=Z(K+1)
   CP2X=XTK*Z(K+2)
   CP3X=XTKSQ*Z(K+3)
   CP4X=XTKCU*Z(K+4)

60 CONTINUE
CP5X = XTK4 * Z(K+5)

H0(I) = 0.2 * CP5X + 0.25 * CP4X + 0.33333333 * CP3X + 0.5 * CP2X + CP1X

* + XTKINV * Z(K+6)

SO(I) = 0.25 * CP5X + 0.33333333 * CP4X + 0.5 * CP3X + CP2X + CP1X * XTLN

CP0(I) = CP1X + CP2X + CP3X + CP4X + CP5X

H(I) = H0(I) * RTK

U(I) = H(I) - RTK

S(I) = SO(I) * RGAS

CP(I) = CP0(I) * RGAS

60 CONTINUE

C

RETURN

C

70 XTKSQ = XTK ** 2

XTKCU = XTKSQ * XTK

XTK4 = XTKCU * XTK

XTKINV = 1 / XTK

XTLN = DLOG(XTK)

RTK = RGAS * XTK

C

C --- H(I), U(I), CP(I), DCP(I) REQUIRED

C

DO 80 ITK = 1, 2

IT = 0

IF (ITK.EQ.2) IT = 7

DO 90 I = 1, NS

K = IT + ICIT * (I - 1)

CP1X = Z(K+1)

CP2X = XTK * Z(K+2)

CP3X = XTKSQ * Z(K+3)

CP4X = XTKCU * Z(K+4)

CP5X = XTK4 * Z(K+5)

H0(I) = 0.2 * CP5X + 0.25 * CP4X + 0.33333333 * CP3X + 0.5 * CP2X + CP1X

* + XTKINV * Z(K+6)

SO(I) = 0.25 * CP5X + 0.33333333 * CP4X + 0.5 * CP3X + CP2X + CP1X * XTLN

CP0(I) = CP1X + CP2X + CP3X + CP4X + CP5X

H(I) = H0(I) * RTK

U(I) = H(I) - RTK

S(I) = SO(I) * RGAS

CP(I) = CP0(I) * RGAS

IF (ITK.EQ.1) THEN

HO1(I) = H0(I)

SO1(I) = SO(I)

CP01(I) = CP0(I)

HI(I) = H(I)

CP1(I) = CP(I)

U1(I) = U(I)

S1(I) = S(I)

ELSE

HO2(I) = H0(I)

190
\textbf{ENDIF}

90 \textbf{CONTINUE}

80 \textbf{CONTINUE}

FR1 = (XTK - 950.0)/100.0
FR2 = (1050.0 - XTK)/100.0
DO 100 I=1,NS
    HO(I) = FR1*HO1(I) + FR2*HO2(I)
    SO(I) = FR1*SO1(I) + FR2*SO2(I)
    CPO(I) = FR1*CPO1(I) + FR2*CPO2(I)
    H(I) = FR1*H1(I) + FR2*H2(I)
    U(I) = FR1*U1(I) + FR2*U2(I)
    CP(I) = FR1*CP1(I) + FR2*CP2(I)
100 \textbf{CONTINUE}

C \textbf{RETURN}

C \textbf{END}
INPUT FILE TSTR.IN
&RUNNO NMON=06,NDAY=11,NYR=1987,NRUN=1 &END
&PARAM VOL=0.013,Q=-5.5D+07,S2MIN=1.0D-18,EMS=0.0,
18.00,0.0,TKS=120.0,120.0,200.0,TMSD=0.00E+03,
RGNX=65.5,RHOGAS=12.4435,RHOLIQ=990.70,RHOH2=9.86784,
AH2IN=1.329D-05,A02IN=1.09682D-05,FVI2MN=1.0D-08,
DLIQMN=1.0D-07,DLMIN=1.5D-06,DMC=0.585,CFTP=0.96738,
PHO=1.03393D+06,TEMPH=5.0D+02,XPER=20.0,CVR=1.23045D-02
&END
&INITC XMASS=1.00D-15,TK=550.00,PA=5.16964D+06,
DM=1.0D-07 &END
&INDX1 NDEBEG=0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,
MCON=1,KINET=0 &END
&ICONS METH=2,MITER=2,NDGEAR=0,IER=10,STEP=1.0D-12,
TM0=0.0,IMPRNT=5.0D-04,IMEND=1.0D-01,INDEX=1,
EPSI=1.0D-05 &END
&SSRKT EPSISS=1.0D-06,ITMAXS=25,IDGT=0,IER=10 &END
&INPFL V=90.001,FVI=5A1.0,6A0.0,RHO=6A12.4435,
&990.70,FVI2=0.0,PL=5A0.30,0.005,3A0.060,
AREA=5A2.9085D-05,4A2.02683D-03,RFLLQ=0.130294,
RFCAS=0.182725,RFLO=0.836663,RFGO=1.14483,
RFLV=1.72000D+04,RFVG=1.82725D+04,PS=5.16964D+06,
CDIN=0.5O,SM1MIN=0.0D-08 &END
&INDX2 N1=1,2,3,4,5,6,7,8,9,N2=2,3,4,5,6,7,8,9,10,
NP=9,NN=10,NHE0=5,NFVI=6 &END
REAC HE 4.0026 3 1.00000D+00 0.00000D+00 G 0.00000D+00 -3.5416D+06
REAC H2 2.0160 2 1.00000D+00 9.99999D-01 G 0.00000D+00 -3.1432D+06
REAC O2 32.0000 1 1.00000D+00 1.00000D-09 L 2.00000D+05 -2.73000D+05
PROD H2O 18.0160 0 0.00000D+00 1.00000D-09 G 0.00000D+00 0.00000D+00
RADI H 1.0080 0 0.00000D+00 0.00000D-00 G 0.00000D+00 0.00000D+00
RADI O 16.0000 0 0.00000D+00 0.00000D-08 G 0.00000D+00 0.00000D+00
RADI OH 17.0080 0 0.00000D+00 0.00000D-08 G 0.00000D+00 0.00000D+00

HE L 5/66HE 1.00 0.00 0.00 0.0 G 300.000 5000.000 1
0.25000000D+01 0.00000000D+00 0.00000000D+00 0.00000000D+00 0.00000000D+00 0.00000000D+00 2
-0.7453749B+03 0.91534888D+00 0.25000000D+01 0.00000000D+01 0.00000000D+00 3
0.00000000D+00 0.00000000D+00 0.00000000D+00 0.00000000D+00 0.00000000D+00 0.00000000D+00 4
0 2.7080 37.0000 298.0 1200.0 6000.0 HE 5

AR L 5/66AR 1 G 300.000 5000.000
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-0.74537502E+03 0.43660006E+01 0.25000000E+01 0.0 0.0
0.0 0.0 -0.74537498E+03 0.43660006E+01
0 3.4180 124.000 300.0 1200.0 5000.0

CH4 J 3/61C 1H 400 000 0G 300.000 5000.000 1
0.15027072E 01 0.1046798E-01-0.39181522E-05 0.67777899E-09-0.44283706E-13 2
-0.9978708E-04 0.10707143E 02 0.38261932E 01-0.39794821E-02 0.24558340E-04 3
-0.22732925E-07 0.69626957E-11-0.10144950E 05 0.86690073E 00
0. 3.8220 137.0000

CH3 J 6/69C 1H 3 0 OG 300.000 5000.000 1

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<td>H2O(L)</td>
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**C2H6**  0.2  **C2H4**  0.2  **H2**  14.41  0.0  25000.GLOBAL
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</table>
6 11 1987

RUN NUMBER 1

***** SOLUTION PARAMETERS *****

CC VOLUME = 1.30D-02 M^3
CC HEAT TRANS. RATE = -6.50000D+07 J/S
MIN ALLOWABLE MOLE NO. = 1.00000D-18 KGMOLE/KG
INITIAL MASS OF LIQ IN THE COMB CHAMBER = 1.00000D-15 KG
INITIAL DROPLET DIAMETER = 1.00000D-07 M
MIN ALLOWABLE DROPLET DIAMETER = 5.000D-07 M
EXIT TURBINE FLOW RATE CONSTANT = 9.233D-01
HOT GAS MANIFOLD PRESSURE = 1.723D+06 PA

NDEBUG (1 FOR PRINTING, 0 FOR SUPRESSING OUTPUT)

1 1 1 1 1 1 1 0 0 0
0 0 0 1 0 0 0 0 0 0

DROPLET DIAMETER COEFFICIENT = 4.8500D-01
AREA OF HYDROGEN INJECTOR ANULUS = 1.3290D-05
AREA OF THE OXIDIZER INJECTOR = 1.0968D-05
MCON (=0 FOR CONSTANT MASS FLOW; =1 FOR PIPING SYSTEM) 1
KINET (=0 FOR NO KINETICS; =1 FOR CALL TO RADSS) 0

INTEGRATION PARAMETERS:
MIKR, METH, NDGEAR 2 2 0
IER, EPSI 10 5.00D-07
INPUT STEP SIZE = 1.00D-12 SEC
INITIAL TIME = 0.00D+00 SEC
OUTPUT INTERVAL = 5.00D-04 SEC
FINAL TIME = 1.00D-01 SEC
TIME SHUTDOWN BEGINS = 0.00D+00

FOR SS RATE APPROXIMATION:
CONVERGENCE CRITERION (MAX % CHANGE) = 1.00D-06
MAX NO ITERATIONS = 25
ERROR CHECK IDGT = 0
IMSL ERROR FLAG JER = 10

OXIDIZER FEED SYSTEM INPUTS:
NO. OF PIPES 11 NO. OF NODES 12
NO. OF HELIUM ORIFICE PIPES 7
PIPE IN WHICH THE INTERFACE IS INITIALLY LOCATED 8
RFLIQ FOR THE OX PIPES = 1.303D-01
RFGAS FOR THE OX PIPES = 1.827D-01
RFLIQ FOR THE HE ORIFICE = 1.367D-01
RFGAS FOR THE HE ORIFICE = 5.283D-01
RFLIQ FOR THE HE VALVE = 1.720D+04
RFGAS FOR THE HE VALVE = 1.827D+03
INJECTOR AND MANIFOLD CD = 5.000D-01
UPSTREAM SOURCE PRESSURE = 5.1664D+06 PA
INITIAL BACKFLOW INTERFACE POSITION = 0.000D+00

PIPE GEOMETRY:

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PIPE INITIAL CONDITIONS:

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INITIAL NODAL DENSITIES:

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REACTION RATE DATA FROM NPT

FOLLOWING REACTION IGNORED

C3H8 + O2 ----> C2H4 + H2
REACTANT C3H8 NOT FOUND IN SPECIES LIST

FOLLOWING REACTION IGNORED

C8H18 + O2 ----> C2H4 + H2
REACTANT C8H18 NOT FOUND IN SPECIES LIST

FOLLOWING REACTION IGNORED

C2H4 + O2 ----> CO + H2
REACTANT C2H4 NOT FOUND IN SPECIES LIST

FOLLOWING REACTION IGNORED

C6H6 + O2 ----> CO + H2
REACTANT C6H6 NOT FOUND IN SPECIES LIST

FOLLOWING REACTION IGNORED

FUEL + O2 ----> CO + H2
REACTANT FUEL NOT FOUND IN SPECIES LIST

FOLLOWING REACTION IGNORED

H2O(L) ----> H2O
REACTANT H2O(L) NOT FOUND IN SPECIES LIST

REACTION 1

O2 + H2 ----> OH + OH
DATA COMMENT: PRATT
FWD RATE DATA: BX = 11.907 TEN = 0.000 TACT = 22661.000
CALCULATED REVERSE RATE CONSTANTS
STD DEVIATION = 2.428D+00 CORR COEFF = 9.475D-01
REV RATE DATA: BX2 = 19.489 TEN2 = 0.000 TACT2 = 30793.276

REACTION 2

OH + H2 ----> H2O + H
DATA COMMENT: PRATT
FWD RATE DATA: BX = 11.439 TEN = 0.000 TACT = 5187.000
CALCULATED REVERSE RATE CONSTANTS
STD DEVIATION = 4.078D-01 CORR COEFF = 9.939D-01
REV RATE DATA: BX2 = 14.133 TEN2 = 0.000 TACT2 = 15784.008

REACTION 3

O2 + H ----> OH + O
DATA COMMENT: PRATT
FWD RATE DATA: BX = 11.677 TEN = 0.000 TACT = 8712.000
CALCULATED REVERSE RATE CONSTANTS
STD DEVIATION = 1.892D+00 CORR COEFF = 8.664D-01
REACTION 4 O2 + H2 ----> OH + H
DATA COMMENT: PRATT
FWD RATE DATA: BX = 9.352 TEN = 0.000 TACT = 3903.000
CALCULATED REVERSE RATE CONSTANTS
STD DEVIATION = 5.361D-01 CORR COEFF = 9.459D-01
REV RATE DATA : BX2 = 10.976 TEN2 = 0.000 TACT2 = 6690.385

REACTION 5 O2 + H2O ----> OH + OH
DATA COMMENT: PRATT
FWD RATE DATA: BX = 11.095 TEN = 0.000 TACT = 9115.000
CALCULATED REVERSE RATE CONSTANTS
STD DEVIATION = 1.283D-01 CORR COEFF = 9.217D-01
REV RATE DATA : BX2 = 10.025 TEN2 = 0.000 TACT2 = 1305.377

REACTION 6 H + H + M ----> H2 + M
DATA COMMENT: PRATT
FWD RATE DATA: BX = 12.699 TEN = -1.150 TACT = 0.000
CALCULATED REVERSE RATE CONSTANTS
STD DEVIATION = 1.051D+00 CORR COEFF = 1.000D+00
REV RATE DATA : BX2 = 11.955 TEN2 = 0.000 TACT2 = 51707.198

REACTION 7 O + O + M ----> O2 + M
DATA COMMENT: PRATT
FWD RATE DATA: BX = 9.672 TEN = -0.278 TACT = 0.000
CALCULATED REVERSE RATE CONSTANTS
STD DEVIATION = 1.274D+00 CORR COEFF = 9.941D-01
REV RATE DATA : BX2 = 7.667 TEN2 = 0.000 TACT2 = 50190.523

REACTION 8 O + H + M ----> OH + M
DATA COMMENT: PRATT
FWD RATE DATA: BX = 10.627 TEN = 0.000 TACT = -1400.000
CALCULATED REVERSE RATE CONSTANTS
STD DEVIATION = 6.110D-01 CORR COEFF = 9.988D-01
REV RATE DATA : BX2 = 15.564 TEN2 = 0.000 TACT2 = 54467.238

REACTION 9 H + OH + M ----> H2O + M
DATA COMMENT: PRATT
FWD RATE DATA: BX = 10.778 TEN = 0.000 TACT = -252.000
CALCULATED REVERSE RATE CONSTANTS
REV RATE DATA : BX2 = 16.785 TEN2 = 0.000 TACT2 = 63424.861

FOLLOWING REACTION IGNORED
H + O2 + M ----> H02 + M
REACTANT HO2 NOT FOUND IN SPECIES LIST
NODAL DENSITIES AND Pressures:

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NODAL DENSITIES (KG/M$^3$) and PRESSURE (PA):

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<td>4.2119D+06</td>
</tr>
<tr>
<td>12</td>
<td>9.9070D+02</td>
<td>4.2119D+06</td>
</tr>
</tbody>
</table>
***** INTEGRATING ROUTINE CALLED *****

CALL FOR STEP 3 OUT OF 200 STEPS
STEP BEGINS AT TIME = 1.00000D-03 AND ENDS AT TIME = 1.50000D-03

***** CC AND INLET CONDTS ON RETURN *****
FROM THE INTEGRATING SUBROUTINE *****

TIME FOLLOWING INTEGRATION = 1.50000D-03 SEC
FINAL STEP SIZE = 1.75435D-05 SEC
ERROR FLAG, IER = 0

<table>
<thead>
<tr>
<th>SPECIES NAME</th>
<th>S2 (KGMOLE/KG) ISTRM</th>
<th>S1 (KGMOLE/KG) STATE</th>
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<tbody>
<tr>
<td>HE</td>
<td>1.00944D-18</td>
<td>2.49838D-01 G</td>
</tr>
<tr>
<td>H2</td>
<td>4.82805D-01</td>
<td>4.96032D-01 G</td>
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<tr>
<td>O2</td>
<td>1.03397D-11</td>
<td>3.12500D-02 L</td>
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<tr>
<td>H2O</td>
<td>1.48005D-03</td>
<td>0.00000D+00 G</td>
</tr>
<tr>
<td>H</td>
<td>1.00000D-18</td>
<td>0.00000D+00 G</td>
</tr>
<tr>
<td>O</td>
<td>1.00000D-18</td>
<td>0.00000D+00 G</td>
</tr>
<tr>
<td>OH</td>
<td>1.00000D-18</td>
<td>0.00000D+00 G</td>
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DENSITY OF LIQUID IN THE CC = 5.07032D-03 KG
BACKFLOW INTERFACE POSITION = 0.00000D+00
CC TEMPERATURE = 465.0223 K
CC PRESSURE = 4.21058D+06 PA
CC DENSITY = 2.24873D+00 KG/M**3
AVG. MOL. WT. = 4.84285D-01 KG/KGMOLE
CC VOLUME = 1.30000D-02 M**3
OMV, FMV, PMV, EMV = 1.350D+02 1.615D+03 0.000D+00 1.694D+03 KG/M3/S
UPSTREAM PRESSURE = 5.1696D+06 PA
INJECTOR PRESSURE DROP = 7.4206D+02 PA

<table>
<thead>
<tr>
<th>STREAM</th>
<th>TEMP (K)</th>
<th>MDOT (KG/SEC)</th>
<th>SF (KGMOLE/SEC)</th>
<th>SH (JOULES/SEC)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>120.000</td>
<td>1.75556D+00</td>
<td>0.000000D+00</td>
<td>-1.152083D+06</td>
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<tr>
<td>2</td>
<td>160.000</td>
<td>2.10000D+01</td>
<td>8.012821D+02</td>
<td>-2.518590D+09</td>
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<tr>
<td>3</td>
<td>120.000</td>
<td>0.000000D+00</td>
<td>0.000000D+00</td>
<td>0.000000D+00</td>
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PIPE CONDITIONS:

PIPE VELOCITY (M/SEC) LIQUID/VAP INT. POSITION (% LENGTH)
<table>
<thead>
<tr>
<th>SPECIES NAME</th>
<th>S2 (KG MOLE/KG)</th>
<th>S1 (KG MOLE/KG)</th>
<th>STATE</th>
</tr>
</thead>
<tbody>
<tr>
<td>H2</td>
<td>4.90960D-01</td>
<td>2</td>
<td>G</td>
</tr>
<tr>
<td>O2</td>
<td>1.51292D-11</td>
<td>1</td>
<td>L</td>
</tr>
<tr>
<td>H2O</td>
<td>5.67428D-04</td>
<td>0</td>
<td>G</td>
</tr>
<tr>
<td>H</td>
<td>1.00000D-18</td>
<td>0</td>
<td>G</td>
</tr>
<tr>
<td>O</td>
<td>1.00000D-18</td>
<td>0</td>
<td>G</td>
</tr>
</tbody>
</table>

**Density of Liquid in the CC** = 1.11943D-03 KG

**Backflow Interface Position** = 0.00000D+00

**CC Temperature** = 467.4076 K

**CC Pressure** = 4.28538D+06 PA

**CC Density** = 2.24344D+00 KG/M**3**

**Avg. Mol. Wt.** = 4.91528D-01 KG/KG MOLE

**CC Volume** = 1.30000D-02 M**3**

**OMV, PMV, EMV, ENV** = 7.201D+01 1.615D+03 0.00000D+00 1.698D+03 KG/M3/S

**Upstream Pressure** = 5.1696D+06 PA

**Injector Pressure Drop** = 2.1102D+02 PA

**Pipe Conditions:**

**Pipe Velocity (M/SEC)**

<table>
<thead>
<tr>
<th>NODE</th>
<th>VELOCITY (M/SEC)</th>
<th>LIQUID/VAP Int. Position (% Length)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.1627D+01</td>
<td>1.0000D+00</td>
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<td>2</td>
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<td>1.0000D+00</td>
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<tr>
<td>3</td>
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<td>1.0000D+00</td>
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<td>4</td>
<td>1.1627D+01</td>
<td>1.0000D+00</td>
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<td>5</td>
<td>1.1627D+01</td>
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<tr>
<td>6</td>
<td>1.1627D+01</td>
<td>1.0000D+00</td>
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<td>7</td>
<td>1.1627D+01</td>
<td>1.0000D+00</td>
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<td>8</td>
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<td>3.3539D-02</td>
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<td>0.0000D+00</td>
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<tr>
<td>10</td>
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<td>0.0000D+00</td>
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<tr>
<td>11</td>
<td>4.6623D-01</td>
<td>0.0000D+00</td>
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**Nodal Densities and Pressures:**

<table>
<thead>
<tr>
<th>NODE</th>
<th>DENSITY (KG/M<strong>3</strong>)</th>
<th>PRESSURE (PA)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.0739D+01</td>
<td>5.1696D+06</td>
</tr>
<tr>
<td>2</td>
<td>2.0260D+01</td>
<td>5.0501D+06</td>
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<tr>
<td>3</td>
<td>1.9793D+01</td>
<td>4.9339D+06</td>
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<tr>
<td>4</td>
<td>1.9340D+01</td>
<td>4.8210D+06</td>
</tr>
</tbody>
</table>
STREAM   TEMP (K)   MDOT (KG/SEC)   SF (KGMOLE/SEC)   SH (JOULES/SEC)
1   120.000   2.71235D-01   0.000000D+00   -1.779982D+05
2   160.000   2.10000D+01   8.012821D+02   -2.518590D+09
3   120.000   0.000000D+00   0.000000D+00   0.000000D+00

PIPE CONDITIONS:

PIPE VELOCITY (M/SEC) LIQUID/VAP INT. POSITION (% LENGTH)

1   3.3503D+00   1.0000D+00
2   3.3503D+00   1.0000D+00
3   3.3503D+00   1.0000D+00
4   3.3503D+00   1.0000D+00
5   3.3503D+00   1.0000D+00
6   3.3503D+00   1.0000D+00
7   3.3503D+00   1.0000D+00
8   1.3508D-01   4.6974D-03
9   1.3508D-01   0.0000D+00
10  1.3508D-01   0.0000D+00
11  1.3508D-01   0.0000D+00

NODAL DENSITIES AND Pressures:

NODE DENSITY (KG/M**3) PRESSURE (PA)

1   2.0739D+01   5.1696D+06
2   2.0427D+01   5.0918D+06
3   2.0121D+01   5.0156D+06
4   1.9822D+01   4.9410D+06
5   1.9529D+01   4.8681D+06
6   1.9243D+01   4.7967D+06
7   1.8962D+01   4.7268D+06
8   1.8688D+01   4.6583D+06
9   9.9070D+02   4.5941D+06
10  9.9070D+02   4.5941D+06
11  9.9070D+02   4.5941D+06
12  9.9070D+02   4.5941D+06

***** INTEGRATING ROUTINE CALLED *****

CALL FOR STEP 2 OUT OF 200 STEPS
STEP BEGINS AT TIME = 5.000000D-04 AND ENDS AT TIME = 1.000000D-03

***** CC AND INLET CONDTNS ON RETURN *****
****** FROM THE INTEGRATING SUBROUTINE ******

TIME FOLLOWING INTEGRATION = 1.000000D-03 SEC
FINAL STEP SIZE = 1.02457D-05 SEC
ERROR FLAG, IER = 0
<table>
<thead>
<tr>
<th>CC TEMPERATURE</th>
<th>550.000 K</th>
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<tbody>
<tr>
<td>CC PRESSURE</td>
<td>5.1696D+06 PA</td>
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<tr>
<td>CC DENSITY</td>
<td>2.27907D+00 KG/M^3</td>
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<tr>
<td>AVG. MOL. WT.</td>
<td>4.96031D-01 KG/KGMOLE</td>
</tr>
<tr>
<td>CC VOLUME</td>
<td>1.30000D-02 M^3</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>STREAM NAME</th>
<th>TEMP (K)</th>
<th>MDOT (KG/SEC)</th>
<th>SF (KGMOLE/SEC)</th>
<th>HS (J/KGMOLE)</th>
<th>SH (J/SEC)</th>
</tr>
</thead>
<tbody>
<tr>
<td>O2</td>
<td>120.00</td>
<td>0.00000D+00</td>
<td>0.00000D+00</td>
<td>-2.73000D+05</td>
<td>0.00000D+00</td>
</tr>
<tr>
<td>H2</td>
<td>160.00</td>
<td>2.10000D+01</td>
<td>8.01282D+02</td>
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<td>-2.51859D+09</td>
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<tr>
<td>HE</td>
<td>120.00</td>
<td>0.00000D+00</td>
<td>0.00000D+00</td>
<td>-3.54160D+06</td>
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</table>

**** INTEGRATING ROUTINE CALLED ****

CALL FOR STEP 1 OUT OF 200 STEPS
STEP BEGINS AT TIME = 0.00000D+00 AND ENDS AT TIME = 5.00000D-04

**** CC AND INLET CONDINS ON RETURN ****
FROM THE INTEGRATING SUBROUTINE ****

TIME FOLLOWING INTEGRATION = 5.00000D-04 SEC
FINAL STEP SIZE = 3.17799D-06 SEC
ERROR FLAG, IER = 0

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<tr>
<th>SPECIES NAME</th>
<th>S2 (KGMOLE/KG)</th>
<th>ISTRM</th>
<th>S1 (KGMOLE/KG)</th>
<th>STATE</th>
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</thead>
<tbody>
<tr>
<td>HE</td>
<td>1.00146D-18</td>
<td>3</td>
<td>2.49838D-01</td>
<td>G</td>
</tr>
<tr>
<td>H2</td>
<td>4.95236D-01</td>
<td>2</td>
<td>4.96032D-01</td>
<td>G</td>
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<tr>
<td>O2</td>
<td>2.18638D-11</td>
<td>1</td>
<td>3.12500D-02</td>
<td>L</td>
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<td>H2O</td>
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<td>0</td>
<td>0.00000D+00</td>
<td>G</td>
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<tr>
<td>H</td>
<td>1.00000D-18</td>
<td>0</td>
<td>0.00000D+00</td>
<td>G</td>
</tr>
<tr>
<td>O</td>
<td>1.00000D-18</td>
<td>0</td>
<td>0.00000D+00</td>
<td>G</td>
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</table>

DENSITY OF LIQUID IN THE CC = 4.84393D-05 KG
BACKFLOW INTERFACE POSITION = 0.00000D+00
CC TEMPERATURE = 493.6106 K
CC PRESSURE = 4.59581D+06 PA
CC DENSITY = 2.26077D+00 KG/M^3
AVG. MOL. WT. = 4.95325D-01 KG/KGMOLE
CC VOLUME = 1.30000D-02 M^3
OMV, FMV, PMV, EMV = 2.086D+01 1.615D+03 0.000D+00 1.681D+03 KG/M^3/S
UPSTREAM PRESSURE = 5.1696D+06 PA
INJECTOR PRESSURE DROP = 1.7713D+01 PA
ISIDE ARRAY

RXN  ISIDE(K,RXN)
1  0  -1  -1  0  0  0  2
2  0  -1  0  1  1  0  -1
3  0  0  -1  0  -1  1  1
4  0  -1  0  0  1  -1  1
5  0  0  0  -1  0  -1  2
6  0  1  0  0  -2  0  0
7  0  0  1  0  0  -2  0
8  0  0  0  0  -1  -1  1
9  0  0  0  1  -1  0  -1

REACTION RATE DATA IN SI UNITS

RXN  MODE  BX  TEN  TACT
1  1  FWD  11.903  0.000  22661.000
   REV  19.489  0.000  30793.276
2  1  FWD  11.439  0.000  5187.000
   REV  14.133  0.000  15784.008
3  1  FWD  11.677  0.000  8712.000
   REV  17.639  0.000  14056.891
4  1  FWD  9.352  0.000  3903.000
   REV  10.976  0.000  6690.385
5  1  FWD  11.095  0.000  9115.000
   REV  10.025  0.000  1305.377
6  3  FWD  12.699  -1.150  0.000
   REV  11.955  0.000  51707.198
7  3  FWD  9.672  -0.278  0.000
   REV  7.667  0.000  50190.523
8  3  FWD  10.627  0.000  -1400.000
   REV  15.564  0.000  54467.238
9  3  FWD  10.778  0.000  -252.000
   REV  16.785  0.000  63424.861

CC AND INLET INITIAL CONDITIONS

SPECIE  NAME  S2 (KGMOLE/KG)  ISTRM  S1 (KGMOLE/KG)  STATE
1  HE  1.00000D-18  3  2.69838D-01  G
2  H2  4.96031D-01  2  4.96032D-01  G
3  O2  3.12500D-11  1  3.12500D-02  L
4  H2O  5.55062D-11  0  0.00000D+00  G

206
### "Z" Array of Thermo Property Polynomial Coefficients

<table>
<thead>
<tr>
<th>NAME</th>
<th>COEFFICIENTS</th>
</tr>
</thead>
<tbody>
<tr>
<td>HE</td>
<td>2.500000D+00 0.000000D+00 0.000000D+00 0.000000D+00 0.000000D+00</td>
</tr>
<tr>
<td></td>
<td>-7.45375D+02 9.15349D+01 2.500000D+00 0.000000D+00 0.000000D+00</td>
</tr>
<tr>
<td></td>
<td>0.000000D+00 0.000000D+00 -7.45375D+02 9.15349D+01 0.000000D+00</td>
</tr>
<tr>
<td>H2</td>
<td>3.10019D+00 5.11195D+01 5.26442D-01 -3.49100D-11 5.69453D-15</td>
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<td>-8.77380D+02 -1.96294D+00 3.05744D+00 2.67652D-03 -5.80991D-06</td>
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<td>5.52103D-09 -1.81277D-12 -9.88560D+02 3.60582D+00</td>
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<tr>
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<td>3.62195D+00 7.36183D-04 -1.96522D-07 3.62016D-11 -2.89456D-15</td>
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</tr>
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<td>H2O</td>
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<td></td>
<td>-2.99058D+04 6.63057D+00 4.07013D+00 -1.10845D-03 4.15212D-06</td>
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<tr>
<td>H</td>
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<tr>
<td></td>
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<tr>
<td>O</td>
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### Reaction Rate Indices and Data

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<tr>
<th>REACTION INDICES</th>
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<tbody>
<tr>
<td>RXN (J)</td>
</tr>
<tr>
<td>---------</td>
</tr>
<tr>
<td>1</td>
</tr>
<tr>
<td>2</td>
</tr>
<tr>
<td>3</td>
</tr>
<tr>
<td>4</td>
</tr>
</tbody>
</table>

207
CH30 M ---+ CH20 H M
REACTANT CH30 NOT FOUND IN SPECIES LIST

FOLLOWING REACTION IGNORED
CH20 M ---+ CHO H M
REACTANT CH20 NOT FOUND IN SPECIES LIST

FOLLOWING REACTION IGNORED
CH20 O ---+ CHO OH
REACTANT CH20 NOT FOUND IN SPECIES LIST

FOLLOWING REACTION IGNORED
CH20 H ---+ CHO H2
REACTANT CH20 NOT FOUND IN SPECIES LIST

FOLLOWING REACTION IGNORED
CH20 OH ---+ CHO H20
REACTANT CH20 NOT FOUND IN SPECIES LIST

FOLLOWING REACTION IGNORED
CHO M ---+ CO H M
REACTANT CHO NOT FOUND IN SPECIES LIST

FOLLOWING REACTION IGNORED
CHO H ---+ CO H2
REACTANT CHO NOT FOUND IN SPECIES LIST

FOLLOWING REACTION IGNORED
CHO OH ---+ CO H20
REACTANT CHO NOT FOUND IN SPECIES LIST

FOLLOWING REACTION IGNORED
CHO O ---+ CO OH
REACTANT CHO NOT FOUND IN SPECIES LIST

***** SPECIES PROPERTIES *****

MAJOR CONSTITUENTS:
INDEX NAME MOLEC. WT.
1 H2 4.0026D+00
2 H2 2.0160D+00
3 O2 3.2000D+01
4 H20 1.8016D+01

RATE DETERMINING RADICALS
INDEX NAME MOLEC. WT.
5 H 1.0080D+00
6 O 1.6000D+01
7 OH 1.7008D+01

208
FOLLOWING REACTION IGNORED
\[
\text{CO} + \text{OH} \rightarrow \text{H} + \text{CO}_2
\]
REACTANT CO NOT FOUND IN SPECIES LIST

FOLLOWING REACTION IGNORED
\[
\text{CO} + \text{O}_2 \rightarrow \text{CO}_2 + \text{M}
\]
REACTANT CO NOT FOUND IN SPECIES LIST

FOLLOWING REACTION IGNORED
\[
\text{CO}_2 + \text{O}_2 \rightarrow \text{CO}_2 + \text{M}
\]
REACTANT CO NOT FOUND IN SPECIES LIST

FOLLOWING REACTION IGNORED
\[
\text{CH}_4 + \text{H} \rightarrow \text{CH}_3 + \text{H}_2
\]
REACTANT CH NOT FOUND IN SPECIES LIST

FOLLOWING REACTION IGNORED
\[
\text{CH}_4 + \text{OH} \rightarrow \text{CH}_3 + \text{H}_2\text{O}
\]
REACTANT CH NOT FOUND IN SPECIES LIST

FOLLOWING REACTION IGNORED
\[
\text{CH}_3 + \text{CHO} \rightarrow \text{CH}_4 + \text{CO}
\]
REACTANT CH NOT FOUND IN SPECIES LIST

FOLLOWING REACTION IGNORED
\[
\text{CH}_3 + \text{CH}_2\text{O} \rightarrow \text{CHO} + \text{CH}_4
\]
REACTANT CH NOT FOUND IN SPECIES LIST

FOLLOWING REACTION IGNORED
\[
\text{CH}_3 + \text{O}_2 \rightarrow \text{CHO} + \text{H}
\]
REACTANT CH NOT FOUND IN SPECIES LIST

FOLLOWING REACTION IGNORED
\[
\text{CH}_3 + \text{OH} \rightarrow \text{CHO} + \text{H}_2
\]
REACTANT CH NOT FOUND IN SPECIES LIST

FOLLOWING REACTION IGNORED
\[
\text{CH}_3 + \text{H}_2\text{O} \rightarrow \text{CHO} + \text{CH}_4
\]
REACTANT CH NOT FOUND IN SPECIES LIST

FOLLOWING REACTION IGNORED
\[
\text{CH}_3 + \text{M} \rightarrow \text{CHO} + \text{M}
\]
REACTANT CH NOT FOUND IN SPECIES LIST

FOLLOWING REACTION IGNORED
\[
\text{CH}_3 + \text{O} \rightarrow \text{CHO} + \text{H}_2\text{O}
\]
REACTANT CH NOT FOUND IN SPECIES LIST

FOLLOWING REACTION IGNORED
\[
\text{CH}_3 + \text{O}_2 \rightarrow \text{CH}_3\text{O} + \text{H}_2\text{O}
\]
REACTANT CH NOT FOUND IN SPECIES LIST

FOLLOWING REACTION IGNORED

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VITA

Timothy A. Bartrand was born in [redacted] on [redacted]. In June, 1979, he received a diploma from Rogers High School, Wyoming, Michigan and in August, 1979, began studies at the University of Notre Dame, Notre Dame, Indiana. He received a Bachelor of Science degree in Aerospace Engineering from Notre Dame in May, 1983.

In June, 1983, Mr. Bartrand joined the United States Peace Corps and, after an intensive language, technical and cross cultural training, taught secondary school Mathematics and Physics in Bachuo Akagbe, a rural village in the Southwest Province of Cameroon.

After completing his Peace Corps service, Mr. Bartrand began study toward a Master of Science degree in Mechanical Engineering at the University of Tennessee, Knoxville. This degree will be awarded in December, 1987.

The author will work toward a Ph.D. in Mechanical Engineering at Purdue University, beginning in August, 1987.