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Behavior of a Hypersonic Nozzle Using Finite Rate Chemistry

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BEHAVIOR OF A HYPERSONIC NOZZLE

USING FINITE RATE CHEMISTRY

by

Guillermo Jose Hernandez Paul

A Thesis Submitted to the

School of Graduate Studies and Research

in Partial Fulfillment of the Requirements of the Degree of

Master of Science in Aerospace Engineering

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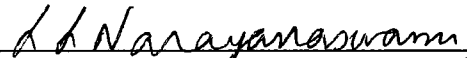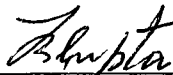
Guillermo Jose Hernandez Paul

This thesis was prepared under the direction of the candidate's thesis committee chairman, Dr. L.L Narayanaswami, Department of Aerospace Engineering, and has been approved by the members of his thesis committee. It was submitted to the School of Graduate Studies and Research and was accepted in partial fulfillment of the requirements for the degree of Master of Science in Aerospace Engineering.

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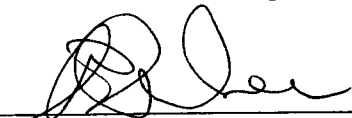
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Above all the author will like to express the most affectionate thanks to his parents and family and dedicate this thesis to them who made it possible to study this lifelong dream (*A mi Madre Thora Paul, a mi Padre Guillermo Hernandez, mi tio Hanim Ali, y a Teresa, por darme esta oportunidad de poder haber estudiado lo que siempre quise desde pequeño, a todos ellos quienes creeron en mi e hicieron posible haber realizado este sueño, les quiero decir grasias y mucho amor. En dedicacion esta Tesis es para ellos*).

ABSTRACT

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Title   :   Behavior of a Hypersonic Nozzle using Finite Rate Chemistry

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This study is concerned with the investigation of the behavior of a hypersonic nozzle with

finite rate chemistry. First, equations describing steady one dimensional flow through a nozzle

are presented. Solution methodologies for frozen, equilibrium and detailed chemistry flow are

then discussed. A hydrogen-air chemical reaction mechanism, which is made up of fourteen

different chemical species, and forty nine chemical reactions is used in this investigation for

obtaining detailed chemistry flow solutions. The investigation also performs a sensitivity

analysis on the reaction mechanism. Results from this may be used to eliminate a particular

reaction from the chemical reaction mechanism that does not significantly affect it. Solutions

for all three flows (frozen, equilibrium, and detailed chemistry) and sensitivity analysis are

obtained from separate computer programs.

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NOMENCLATURE

A	Final area.
A_o	Initial area.
B	Frequency factor equation constant.
C	Frequency factor.
$C_{p,i}$	Specific heat at constant pressure for species i.
$\overline{C_p}$	Mean specific heat at constant pressure of mixture.
$C_{v,i}$	Specific heat at constant volume for species i.
C_v	Mean specific heat of mixture.
e	Internal energy per unit mass.
e_i	Internal energy of species i.
E	Activation energy.
f_i	External body force per unit mass on species i.
F	Jacobian matrix components.
g	Gravitational constant.
g_1, g_2, g_3	Adimensional physical properties.
h	Specific enthalpy of mixture.
h_i	Specific enthalpy of species i.

h_o	Initial specific enthalpy of mixture.
I_{sp}	Specific impulse.
k_f	Forward chemical reaction rate.
k_b	Reverse chemical reaction rate.
k	Net chemical reaction rate.
m	Mass flow rate.
m	Total mass of the mixture.
m_i	Mass of species i.
M_i	Chemical symbol for species i.
n	Frequency factor equation constant.
N	Total number of species in the mixture.
P	Hydrostatic pressure of mixture.
P_{11}, P_{22}, P_{33}	Diagonal components of stress tensor.
Pa	Ambient pressure.
P_e	Exit pressure.
q	Heat flux vector.
R^o	Universal gas constant.
Ro	Initial nozzle radius.
R	Final nozzle radius.

S	Entropy of mixture.
S_o	Initial entropy of mixture.
T	Temperature of mixture.
t	Time.
u	Internal energy per unit mass of mixture.
V	Volume of the mixture.
V_e	Exit velocity.
V_i	Diffusion velocity of species i.
v	Mass average velocity of gas mixture.
$\overline{W}$	Mean molecular weight of mixture.
W_i	Molecular weight of species i.
W	Molecular weight of mixture.
x	Distance along the nozzle.
ω_i	Rate of production of species i by chemical reactions.
Y_i	Mass fraction of species i.
Z	Vector of temperature and mass fractions.
α	Nozzle angle.
κ	Bulk viscosity coefficient.

μ	Coefficient of shear viscosity.
v	Specific volume of the system.
$v`_i$	Stoichiometric coefficients for species i of the reactants.
$v``_i$	Stoichiometric coefficients for species i of the products.
ρ	Density of mixture.
ρ_e	Exit density.

CHAPTER 1

1.0 INTRODUCTION

The design of propulsion systems for hypersonic flight involves consideration of the effects of chemical reactions in all sections of the engine. The analysis of chemically reacting flow is dictated by the relationship between certain characteristic times, called flow and chemical reaction times. The flow time is representative of the time taken for a pocket of gas to pass through the device. The chemical reaction time represents the time required for the chemical reaction to take place. If the chemical reaction time is much smaller than the flow time, the flow may be approximated as one in shifting-equilibrium. If the flow time is much smaller than the chemical reaction time, the flow may be approximated as chemically frozen. In both of these cases, the kinetics of the reactions have no effect on the flow. However, if chemical reaction time and flow time are of the same order of magnitude, chemical kinetics will play a dominant role in determining flow behavior.

The concepts of shifting-equilibrium and frozen flow may be used to investigate flow through rocket nozzles. Since the speeds are relatively low up to the throat, the flow may be

assumed to be in shifting-equilibrium. Downstream of the throat, high velocities prevail, and the flow times will be small. Thus the flow can be approximated to be frozen in this region.

In the case of a hypersonic nozzle, similar assumptions about shifting-equilibrium or frozen flow cannot be made. The high Mach number at the nozzle inlet produces shallow wave angles that require a long nozzle which is integrated with the airframe. Unlike the nozzles for rocket engines and ramjets, this gradual expansion process would result in a significant fraction recovery of the thermal energy from dissociated species present at the combustor exit. Therefore, performance simulations of nozzles for hypersonic propulsion systems should include finite rate chemical kinetics.

Several researchers have considered the behavior of hypersonic nozzle using finite rate chemistry. J.A. Shetz, F.S. Billig, and S. Favin [1] (1985) developed numerical solutions for scramjet nozzle flow. Frozen, equilibrium and flow with chemical kinetics were considered in this study. Their results suggested that frequently chemical reactions could not be neglected during the expansion process. This rapid expansion common in nozzles implied substantial radial pressure gradients. Taken together, these requirements led to the necessity of utilizing the full Navier-Stokes equations for a compressible, multicomponent, turbulent flow with finite rate chemistry.

W.L. Laster and Paul E. Sojka [2] (1987) developed a computer model to predict hydrogen-air ignition delay for various nitrogen concentrations, equivalence ratios, and

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temperatures, factors which may be critical for the study of net thrust in hypersonic nozzles. In this study ignition delay time predictions were presented, along with the contributions from individual elementary reactions to the total production rate of various chemical species. The results of a simple analysis were also presented. Conclusions obtained from this study were that, for low temperatures, nitrogen decreased ignition delay through a chain reaction involving hydrogen and nitrogen. On conducting a sensitivity analysis it was revealed that two chemical reactions containing nitrogen played a predominant role in time delay ignition for nozzle performance (net thrust). This role of nitrogen species may be crucial for designing hypersonic nozzles.

D. R. Reddy and G.J. Harloff [3] (1988) developed a model, using the PARC3D code, to analyze a variety of complex high speed flow configurations for three dimensional viscous flow of high area ratio nozzles for hypersonic propulsion. In this study the shapes considered for code validation were ramps and corners, which are characteristic of inlets and nozzles. Mach numbers of 3 to 14 were considered. This model provided flowfield solutions, which favorably compared with experimental data obtained from an earlier study [4] for hypersonic inlets and nozzles.

Rizkalla, Chinitz and Erdos [5] (1989) developed a method of characteristics computer program for shock free hypersonic nozzles, which included the effects of finite rate chemistry and vibrational relaxation. This model predicted that finite rate chemical recombination is of major consequence in determining nozzle design and performance.

Sangiovanni, Barber and Syed [6] (1991) developed a computer model for describing quasi-one dimensional flow of a gas mixture with area change and finite rate chemical reactions. The model was used to study hydrogen-air chemistry in nozzle performance for a hypersonic nozzle. It predicted that finite rate chemistry should not be neglected in nozzle performance simulations because beneficial chemical processes persisted throughout the entire nozzle length. Also, termolecular recombination reactions represented the principal chemical contribution to nozzle performance.

More recently, Shigeya Watanabe [7] (1992) developed a model to predict both the engine exhaust and the external flowfields of an asymmetric scramjet nozzle. In this study, tests were performed in a hypersonic wind tunnel whose free stream constituted the external flow around an aerospace plane model. Air at room temperature was used to simulate engine exhaust flow. This model established that, in order to predict nozzle performance, a parametric design study, which included interaction effects of external flow, must be made in order to obtain nozzle thrust solutions.

The purpose of this study is to investigate the effect of finite rate chemical reactions on the behavior of a hypersonic nozzle. The attendant release or absorption of energy significantly alters the fluid dynamic behavior of the flow. To properly account for these interactions, it is necessary to supplement the fluid dynamic equations with a detailed description of important chemical reactions. In this study, a set of forty nine chemical reactions is used to model the hydrogen-air chemical reactions in the nozzle. The presence of many chemical reactions makes

the solution of the problem difficult. This is explained in detail in the next chapter. Thus, it is advantageous to minimize the number of reactions describing reaction chemistry without discarding important reaction steps. This may be accomplished by what is known as sensitivity analysis. Sensitivity analysis determines the effect of each chemical reaction step on the outcome of the overall chemical mechanism. Results from this may be used to eliminate from the reaction mechanism a particular chemical reaction that does not significantly affect it.

The material of this investigation is arranged as follows. Chapter 2 describes the development of the model of chemically reacting flow in a hypersonic nozzle. Chapter 3 shows how to perform a sensitivity analysis. Chapter 4 presents a description of the computer codes used for solving the model equations. Chapter 5 discusses the conclusions obtained.

CHAPTER 2

2.0 THEORY AND METHOD OF SOLUTION

This section describes the development of the model of chemically reacting flow. First, the unsteady one dimensional differential equations for mass conservation, momentum, energy, species and state, are presented. These equations are then simplified for the problem being investigated.

The unsteady one dimensional differential equations for mass conservation, momentum, energy, species and state, can be written as follows [8] :

Mass conservation Equation :

$$\frac{\partial \rho}{\partial t} + \frac{1}{g_2 g_3} \frac{\partial}{\partial x} (\rho \, v \, g_2 g_3) = 0 \qquad (2\text{-}1)$$

Momentum Equation :

$$\frac{\partial v}{\partial t} + v\frac{\partial v}{\partial x} = -\frac{1}{\rho}\frac{\partial P_{11}}{\partial x} + \frac{(P_{22} - P_{11})}{\rho}\frac{1}{g_2}\frac{\partial g_2}{\partial x} + \frac{(P_{33} - P_{11})}{g_3}\frac{1}{g_3}\frac{\partial g_3}{\partial x} + \sum_{i=1}^{N} Y_i f_i \qquad (2-2)$$

Energy Equation :

$$\frac{\partial u}{\partial t} + v\frac{\partial v}{\partial x} = -\frac{1}{\rho g_2 g_3}\frac{\partial}{\partial x}(q\,g_2\,g_3) - \frac{P_{11}}{\rho}\frac{\partial v}{\partial x} - \frac{v}{\rho}\left(\frac{P_{22}}{g_2}\frac{\partial g_2}{\partial x} + \frac{P_{33}}{g_3}\frac{\partial g_3}{\partial x}\right) + \sum_{i=1}^{N} Y_i f_i V_i$$

$$(2-3)$$

Species Equation :

$$\frac{\partial Y_i}{\partial t} + v\frac{\partial Y_i}{\partial x} = \frac{\omega_i}{\rho} - \frac{1}{\rho g_2 g_3}\frac{\partial}{\partial x}(\rho Y_i V_i g_2 g_3) \quad , \qquad (2-4)$$

$$i=1,2,3...,N.$$

State Equation :

$$P = \rho R^0 T \sum_{i=1}^{N} \frac{Y_i}{W_i} \qquad (2-5)$$

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The assumptions introduced for modeling a hypersonic nozzle are as follows

    a) the flow is quasi-one dimensional,

    b) transport by diffusion is negligible,

    c) transport by heat conduction is negligible,

    d) the flow is inviscid, resulting in all diagonal elements of pressure tensor

       reducing to the hydrostatic pressure $P_{11}=P_{22}=P_{33}=P$,

    e) body forces are negligible $f_i = 0$,

    f) effect of radiation is neglected $q_R = 0$,

    g) shock waves are neglected

After assumptions a) through g) are introduced to equations (2-1),(2-2),(2-3),(2-4) and (2-5), the equations for mass conservation, momentum, energy, species and state can be written as follows

Mass conservation Equation

$$\frac{1}{\rho}\frac{d\rho}{dx} + \frac{1}{v}\frac{dv}{dx} + \frac{1}{A}\frac{dA}{dx} = 0 \qquad (2-6)$$

Momentum Equation

$$\rho v \frac{dv}{dx} + \frac{dP}{dx} = 0 \qquad (2-7)$$

Energy Equation :

$$\rho v \overline{C_p} \frac{dT}{dx} + \sum_{i=1}^{N} h_i \omega_i W_i + \rho v^2 \frac{dv}{dx} = 0 \quad . \tag{2-8}$$

Species Equation :

$$\rho v \frac{dY_i}{dx} = \omega_i W_i \quad , \tag{2-9}$$

$$i=1,2,3...,N.$$

State Equation :

$$\frac{1}{P}\frac{dP}{dx} + \frac{1}{W}\frac{dW}{dx} = \frac{1}{\rho}\frac{d\rho}{dx} + \frac{1}{T}\frac{dT}{dx} \tag{2-10}$$

Solutions of equations (2-6),(2-7),(2-8),(2-9) and (2-10) provides the variations of temperature, density, velocity and pressure with respect to distance along a nozzle of specified geometry.

In this investigation a conical nozzle is used. Figure 1.0 schematically illustrates such a nozzle, where A_0 and A are the initial and final areas, and α is the nozzle angle. The variation of
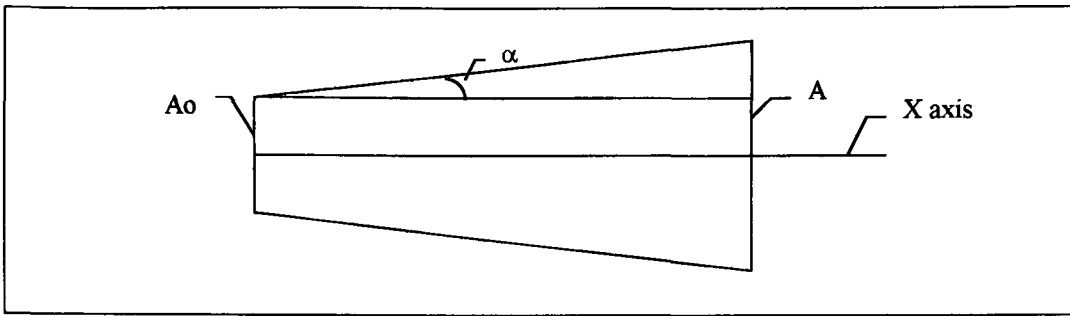
Figure 1.0. Schematic of a Nozzle.

area with distance for this nozzle is given by

$$\frac{dA}{dx} = 2\pi Ro \tan\alpha + 2\pi x \tan^2\alpha \quad , \tag{2-11}$$
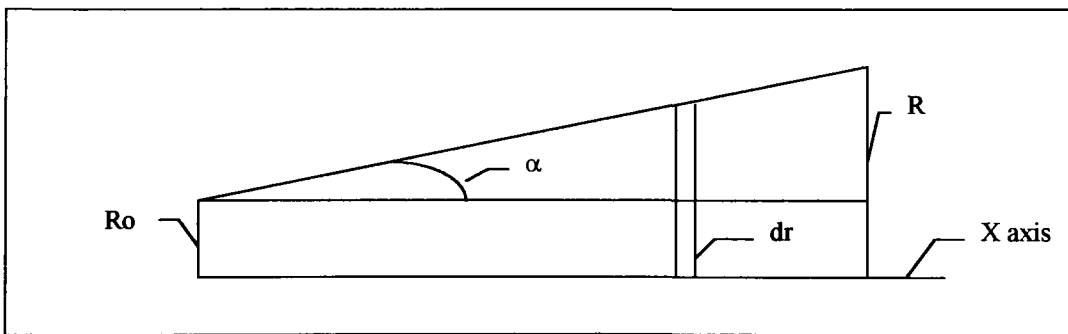
Figure 2.0. Schematic Interior Cut of a Conical Shape Nozzle.

where Ro and R are the initial and final radii, see figure 2.0. Equation (2-11) is used simultaneously with the corresponding equations of flow to solve flow characteristics along the nozzle. The chemical reaction process is represented in this investigation by the Hydrogen-Air chemical reaction. This chemical reaction mechanism involves fourteen different chemical

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species and forty nine chemical reaction steps. While the primary purpose of the investigation was the study of nozzle behavior with finite rate chemistry, the cases of shifting-equilibrium and frozen flows were also investigated as important limiting cases. These cases provide the upper and lower performance bounds of nozzle performance. Accordingly, in what follows, the two limiting cases are first presented. This is followed by a discussion of nozzle flow with finite rate chemistry.

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2.1 FROZEN FLOW

The first case studied is the chemically frozen flow through a hypersonic nozzle. This flow case models flow behavior when the flow time is much smaller than the chemical reaction time.

In obtaining equations for chemically frozen flow, molecular translation of all species and molecular rotation of polyatomic species are taken to be in equilibrium at their fully excited values [9] This assumption has the consequence that the composition is fixed at some arbitrary initial value for a partially dissociated gas. This situation of fixed composition can be explained if in some way chemical reactions could become inhibited so that, molecular collisions still take place, but there is no accompanying change in molecular structure.

With the assumptions mentioned above, the mixture of perfect gases of now fixed composition will be thermally and calorically perfect. Calculations can be carried out on the basis of perfect gas equations, with R, Cv, Cp and γ given constant values appropriate to the assumed situation. As mentioned earlier, chemically frozen flow provides one performance bound of the nozzle.

All chemical rates, ω_i, vanish in this case. The steady one dimensional differential equations (2-6), (2-7), (2-8), (2-9) and (2-10) simplify as follows.

Mass conservation Equation :

$$\frac{1}{\rho}\frac{d\rho}{dx}+\frac{1}{v}\frac{dv}{dx}+\frac{1}{A}\frac{dA}{dx}=0 \qquad (2.1\text{-}1)$$

Momentum Equation :

$$\rho\,v\frac{dv}{dx}+\frac{dP}{dx}=0 \quad . \qquad (2.1\text{-}2)$$

Energy Equation :

$$\rho\,v\overline{Cp}\frac{dT}{dx}+\rho\,v^2\frac{dv}{dx}=0 \quad . \qquad (2.1\text{-}3)$$

Species Equation :

$$\frac{dY_i}{dx}=0 \quad , \qquad (2.1\text{-}4)$$

$$i=1,2,3...,N.$$

State Equation :

$$\frac{1}{P}\frac{dP}{dx}=\frac{1}{\rho}\frac{d\rho}{dx}+\frac{1}{T}\frac{dT}{dx} \quad . \qquad (2.1\text{-}5)$$

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Equations (2.1-1) through (2.1-5), are the basic equations to be solved for chemically frozen flow case. They constitute (N+5) first order, ordinary differential equations, which take into account the number of chemical species that the chemical reaction mechanism is made of. As mentioned before, this investigation makes use of fourteen different chemical species. This will bring the total of nineteen first order differential equations to be solved at each x-distance along the nozzle with area change. Of course, the fourteen species equations (2.1-4) have trivial solutions; $Y_i = Y_{i,initial}$, i=1,2,3...,N.

Although calculations for obtaining flow characteristics of pressure, density, temperature, and velocity can be carried out using perfect gas equations, it was preferred to solve the first order differential equations pertinent for this flow case, equations (2.1-1) through (2.1-5). It was decided to solve the equations in this manner by utilizing the software CHEMKIN II [10] package.

2.2 EQUILIBRIUM FLOW

The second case studied in this investigation deals with shifting-equilibrium flow through a nozzle. This case models the flow in which the chemical reaction time is much smaller than the flow time. The resulting flow, is in complete local thermodynamic equilibrium and is referred to, for brevity, as equilibrium flow. This implies that all molecular processes take place within the gas infinitely rapidly, i.e., that the gas can instantaneously adjust to changes in its environment.

The various equations reduce to algebraic form [8] [11] and are as follows:

Entropy Equation :

$$S = S_o = \text{constant} .$$

(2.2-1)

Mass conservation Equation :

$$m = \rho\, v\, A = \text{constant} .$$

(2.2-2)

Energy Equation :

$$h_o = h + \frac{v^2}{2} = \text{constant} .$$

(2.2-3)

The species equations can be replaced by an appropriate set of atom conservation and chemical equilibrium equations. Again, these equations were solved with the aid of the CHEMKIN II software package.

2.3 DETAILED CHEMISTRY FLOW

The primary case studied in this investigation is concerned with detailed chemistry flow. This case represents a flow in which when the chemical reaction time and the flow time are of the same order of magnitude. As mentioned earlier, chemical kinetics will play a dominant role in this situation.

In solving detailed chemistry flow problems there are two difficulties. The first is to determine the chemical reaction mechanism, i.e. to decide what chemical reactions are needed for simulating chemistry. Hydrogen is the fuel of choice in hypersonic propulsion. Accordingly, the mechanism describing H_2-O_2-N_2 chemistry was chosen to represent chemical reactions in this analysis [6] [12] [13]. This chemical mechanism (shown later in this chapter) covers mixture compositions with either fuel or air in excess, as well as stoichiometric mixtures of Hydrogen-air. It is formed by a homogeneous mixture of fourteen chemical species (H, N, O, OH, H_2, O_2, H_2O, HO_2, H_2O_2, NO, N_2, NO_2, N_2O and HNO), and consists of forty nine elementary chemical reaction steps.

The second difficulty in solving this flow is to obtain the values of the specific rate constant k for each elemental chemical reaction that forms the chemical reaction mechanism. In

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this investigation the specific rate constant k must be calculated at each x-distance along the nozzle, for obtaining the solutions of temperature, density, pressure and velocity.

The basic idea behind detailed chemistry flow is, if somehow there is an instantaneous change of temperature from the initial condition, this will have the direct consequence of changing the chemical composition via molecular collisions. This process takes time to be completed. During this adjustment period, chemical reactions are taking place at a definite net rate.

Consider the general case of a reacting mixture of n different species. The general chemical reaction may be written as follows :

$$\sum_{i=1}^{N} \nu'_i M_i \underset{k_b}{\overset{k_f}{\Longleftrightarrow}} \sum_{i=1}^{N} \nu''_i M_i \ . \tag{2.3-1}$$

Where ν'_i and ν''_i represent the stoichiometric coefficients for chemical species i of the reactants and products respectively, and M_i is the chemical symbol for species i.

The forward rate, reverse rate, and net rate of the reaction above, equation (2.3-1), can be written as follows :

Forward rate :

$$\frac{\partial [M_1]}{\partial t} = (v''_1 - v'_1) k_f \prod_1 [M_1]^{v'_1} .$$

(2.3-2)

Reverse rate :

$$\frac{\partial [M_1]}{\partial t} = -(v''_1 - v'_1) k_b \prod_1 [M_1]^{v''_1}$$

(2.3-3)

Net reaction rate

$$\frac{\partial [M_1]}{\partial t} = (v''_1 - v'_1) \{ k_f \prod_1 [M_1]^{v'_1} - k_b \prod_1 [M_1]^{v''_1} \}$$

(2.3-4)

Equation (2.3-4), is a generalized net reaction rate equation, for a particular elementary chemical reaction; it is a general form of the law of mass action. The chemical rate constants are generally measured experimentally. Although methods exist for their theoretical estimation, the resulting values are imprecise. The empirical results for many reactions can be correlated in the form :

$$k = C \exp^{\frac{E}{R^o T}} .$$

(2.3-5)

Here E is the activation energy, R^o is the universal gas constant, T is the temperature and C is the frequency factor. The constant C may depend on the temperature as follows :

$$C = B T^{n} .$$

(2.3-6)

Here B is a constant, n is another constant. Equation (2.3-5), is called the Arrhenius equation. Table 1.0 shows the reaction mechanism used in this analysis. The constant values of B and n for equation (2.3-6) and the activation energy E are also provided for each chemical reaction in the table. The mechanism and the reaction constants were obtained from literature [6].

The equations for mass, momentum, energy, species and state, for detailed chemistry flow, are presented below:

Mass conservation Equation :

$$\frac{1}{\rho} \frac{d\rho}{dx} + \frac{1}{v} \frac{dv}{dx} + \frac{1}{A} \frac{dA}{dx} = 0 .$$

(2.3-7)

Momentum Equation :

$$\rho v \frac{dv}{dx} + \frac{dP}{dx} = 0$$

(2.3-8)

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N	Reaction	B	n	E
1.	H2+O2=OH+OH	5.50E+13	0.0	5.78E+4
2.	H+O2=O+OH	1.20E+17	-0.91	1.65E+4
3.	H2+O=H+OH	1.50E+07	2.0	7.55E+3
4.	OH+OH=O+H2O	3.40E+13	0.0	5.02E+3
5.	OH+H2=H+H2O	1.00E+08	1.6	3.30E+3
6.	H2O2+OH=H2O+HO2	7.00E+12	0.0	1.43E+3
7.	HO2+O=O2+OH	2.00E+13	0.0	0.0
8.	H+HO2=OH+OH	1.50E+14	0.0	1.00E+3
9.	H+HO2=H2O+O	3.00E+13	0.0	0.0
10.	H+HO2=H2+O2	2.50E+13	0.0	6.93E+2
11.	OH+HO2=H2O+O2	2.00E+13	0.0	0.0
12.	HO2+HO2=H2O2+O2	2.00E+12	0.0	0.0
13.	HO2+H2=H2O2+H	7.30E+11	0.0	1.87E+4
14.	O+O+M=O2+M O2/0.0/ N2/0.0/ H2/3.67/ N2O/4.38/	1.00E+17	-1.0	0.0
15.	O+O+O2=O2+O2	7.98E+19	-1.5	0.0
16.	O+O+N2=O2+N2	6.17E+15	-0.5	0.0
17.	H2+M=H+H+M	2.20E+14	0.0	9.60E+4
18.	H+O+M=OH+M	6.00E+16	-0.6	0.0
19.	OH+OH+M=H2O2+M H2O/6.3/ H2O2/6.0/ O2/0.8/	1.30E+22	-2.0	0.0
20.	H+OH+M=H2O+M H2O/6.3 / H/2.0/	2.20E+22	-2.0	0.0
21.	H+O2+M=HO2+M	6.42E+18	-1.0	0.0
22.	H+H2O2=H2O+OH	1.00E+13	0.0	3.59E+3
23.	O+H2O2=OH+HO2	2.80E+13	0.0	6.41E+3
24.	NO+M=N+O+M N/20 /NO/20 / O/20/	4.00E+20	-1.5	1.50E+5
25.	N2O+M=N2+O+M N2/1.22 /O2/1.22 / N2O/5.56/	6.92E+23	-2.5	6.50E+4
26.	NO2+M=NO+O+M H2O/6.1 /NO/2.9 /N2/1.4 /O2/1.0 /N2O/2.1/	1.10E+16	0.0	6.56E+4
27.	N2+M=N+N+M N/6.0 /H2/2.0 /H2O/1.4/	3.72E+21	-1.6	2.25E+5
28.	N2+O=NO+N	1.82E+14	0.0	7.62E+4
29.	NO+O=N+O2	3.80E+09	1.0	4.14E+4

Units are moles, cubic centimeters, seconds, kelvins, and calories/mole.

Table 1.0. Hydrogen-Air chemical reaction mechanism.

N	Reaction	B	n	E
30.	N2O+O=NO+NO	6.92E+13	0.0	2.66E+4
31.	N2O+O=N2+O2	1.00E+14	0.0	2.80E+4
32.	NO2+O=NO+O2	1.00E+13	0.0	6.00E+2
33.	NO2+N=NO+NO	4.00E+12	0.0	0.0
34.	NO2+N=N2O+O	5.00E+12	0.0	0.0
35.	N2O+N=N2+NO	1.00E+13	0.0	1.99E+4
36.	NO+N2O=N2+NO2	1.00E+14	0.0	4.97E+4
37.	NO2+NO2=NO+NO+O2	2.00E+12	0.0	2.68E+4
38.	HNO+O=NO+OH	5.01E+11	0.5	1.99E+3
39.	N2O+OH=N2+HO2	6.31E+11	0.0	9.93E+3
40.	HNO+OH=NO+H2O	1.26E+12	0.5	1.99E+3
41.	N+HO2=NO+OH	1.00E+13	0.0	1.99E+3
42.	NO+HO2=HNO+O2	1.99E+11	0.0	1.99E+3
43.	NO+HO2=NO2+OH	2.09E+12	0.0	-4.77E+2
44.	HNO+HO2=NO+H2O2	3.16E+11	0.5	1.99E+3
45.	NO+H=N+OH	2.63E+14	0.0	5.04E+4
46.	NO2+H=NO+OH	3.47E+14	0.0	1.47E+3
47.	N2O+H=N2+OH	7.59E+13	0.0	1.51E+4
48.	HNO+H=NO+H2	1.26E+13	0.0	3.97E+3
49.	H+NO+M=HNO+M H2/1.86 /N2O/2.21 /H2O/6.15/	2.92E+15	0.0	-5.96E+2

Units are moles, cubic centimeters, seconds, kelvins, and calories/mole.

Table 1.0. Hydrogen-Air chemical reaction mechanism.

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Energy Equation :

$$\rho v \overline{C}_p \frac{dT}{dx} + \sum_{i=1}^{N} h_i \omega_i W_i + \rho v^2 \frac{dv}{dx} = 0 \ . \tag{2.3-9}$$

Species Equation :

$$\rho v \frac{dY_i}{dx} = \omega_i W_i \ , \tag{2.3-10}$$

i=1,2,3...,N.

State Equation :

$$\frac{1}{P}\frac{dP}{dx} + \frac{1}{W}\frac{dW}{dx} = \frac{1}{\rho}\frac{d\rho}{dx} + \frac{1}{T}\frac{dT}{dx} \tag{2.3-11}$$

Equations (2.3-7) through (2.3-11) constitute (N+5) first order differential equations, where N represents the number of chemical species, in this case 14. These equations have to be simultaneously solved at each x-location for determining the flow variables.

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In general, the time scales associated with the various reactions in a mechanism are widely different. For instance, the rate of reaction 6 in table 1.0 may be very high, while for reaction 27 may be very slow. To properly track the effect of these reactions in a numerical scheme, it is necessary to choose a time step that is small enough to follow the faster reaction, yet not too small to make the entire computational process very slow. More importantly, widely varying time scales may also introduce instability in solutions unless proper care is taken. Differential equations that present widely varying time scales are known as stiff-problems, and special methods are needed to solve them.[14] In this investigation the B.D.F (backward differentiation formula) method is used to handle stiffness (explained later in chapter 3).

It follows from the above discussion that it is advantageous to have only a minimum number of reactions in a mechanism. Reactions in a mechanism may not, however, be arbitrarily eliminated. Sensitivity analysis provides a logical means for reducing the number of steps in a reaction mechanism without compromising accuracy, and is described in the next chapter.

CHAPTER 3

3.0 SENSITIVITY ANALYSIS

This Chapter describes the sensitivity analysis performed in this investigation. Sensitivity analysis is a collection of methods used for evaluating how sensitive the model output is to changes in parameter or input values. The major purposes of sensitivity analysis are :

i) guiding future research by highlighting the most important processes,

ii) parameter estimation by showing which combination of parameters leads to realistic model behavior, and

iii) evaluating the magnitude of the effects of input data error on model performance.

In this investigation results from sensitivity may be used to eliminate particular chemical reactions that do not significantly affect the chemical reaction mechanism. Results may also be used to observe the effects of chemical reactions on nozzle inlet or outlet conditions.

To obtain a sensitivity analysis of the model being used, first order sensitivity coefficients must be obtained for building the sensitivity matrix $\omega_{j,i}$. This matrix, formed by solutions of the studied problem shows which parameters have to change simultaneously for a maximum change of the concentration of one or several chemical species (this is explained in more detail later in this chapter). The information contained in this matrix is useful for uncertainty analysis, parameter estimation, experimental design, and chemical reaction mechanism reduction.

In nearly all models, the solutions depend both on initial and boundary conditions, and on certain parameters that go into defining the model itself. Often the modeler is uncertain of the values of some of the parameters and would like to know how sensitive the results of the model are to these parameters. This is why sensitivity analysis is needed for those particular parameters in the model formulation. Considered here as parameters are the elementary reaction rate constants. Thus, without solving the problem respectively with different values for the rate constants, the sensitivity analysis allows one to understand how the model will respond to changes in the rate parameters. It also provides insight about how important certain reaction pathways are to the model's predictions. The computer program used for obtaining the results of sensitivity analysis is called Senkin [14]. The program determines first-order sensitivity coefficients with respect to elementary reaction rate parameters.

In this investigation, sensitivity analysis solutions are obtained for an adiabatic system with the volume being a specified function of time. To obtain the governing equations for the system, the equations for mass and energy conservation have to be described. The reacting

mixture is treated as a closed system with no mass crossing the boundary, so the total mass of the mixture $m = \Sigma\ m_i$, where i=1,2,3...,N, m is constant, and dm/dt = 0. Here m_i is the mass of the ith species and N is the total number of species in the mixture. The individual species are produced or consumed according to :

$$\frac{dm_i}{dt} = V\omega_i W_i \ ,$$

(3-1)

i=1,2,3...,N,

where t is time, ω_i is the molar production rate of the ith species by elementary reaction, W_i is the molecular weight of the ith species, and V is the volume of the system, which may vary in time. Since the total mass is constant, this equation can be written in terms of the mass fraction as :

$$\frac{dY_i}{dt} = v\omega_i W_i \ ,$$

(3-2)

i=1,2,3...,N,

where $Y_i = mi\ /\ m$, is the mass fraction of the ith species and v = V / m, is the specific volume.

The first law of thermodynamics for a pure substance in a adiabatic, closed system states that :

$$de + Pdv = 0 \ ,$$

(3-3)

where e is the internal energy per unit mass, and P is the pressure. This general relation holds for an ideal mixture of gases, with the internal energy of the mixture given by :

$$e = \sum_{i=1}^{N} e_i Y_i \quad , \tag{3-4}$$

$$i=1,2,3...,N,$$

where e_i is the internal energy of the ith species. Differentiating the internal energy of the mixture leads to the expression :

$$de = \sum_{i=1}^{N} Y_i de_i + \sum_{i=1}^{N} e_i dY_i \quad , \tag{3-4}$$

$$i=1,2,3...,N.$$

Assuming calorically perfect gases, $de_i = C_{v,i} dT$, where T is the temperature of the mixture, and $C_{v,i}$ is the specific heat of the ith species evaluated at constant volume.

Defining the mean specific heat of the mixture, $C_v = \Sigma\, C_{v,i}\, Y_i$, and differentiating with respect to time, the energy equation becomes :

$$C_v \frac{dT}{dt} + \sum_{i=1}^{N} e_i \frac{dY_i}{dt} + \frac{p\,dv}{dt} = 0 \quad , \tag{3-6}$$

$$i=1,2,3...,N.$$

Substitution of equation (3-1), for the species production rate gives :

$$C_v \frac{dT}{dt} + P \frac{d\upsilon}{dt} + \upsilon \sum_{i=1}^{N} e_i \, \omega_i \, W_i = 0 \quad , \tag{3-7}$$

where $C_v = \Sigma \, Y_i \, C_{v,i}$, for i=1,2,3...,N . The ideal gas equation of state is used to compute the pressure:

$$P = \frac{\rho R T}{W} \quad , \tag{3-8}$$

where R is the universal gas constant, W is the mean molecular weight of the mixture, and ρ is the mass density of the mixture

In this investigation, equations (3-7), and (3-2) for the species mass fractions are to be used simultaneously. The net chemical production rate ω_i of each species results from a competition among all chemical reactions involving that species. Each reaction proceeds according to the law of mass action, and rate coefficients are given in the Arrhenius form (2.3-5).

To obtain the first order sensitivity coefficients, the system of ordinary differential equations that describes the physical problem are cast in the following form

$$\frac{dZ}{dt} = f(Z, t, B) \quad , \tag{3-9}$$

where, in this case, $Z = (T, Y_1, Y_2, \ldots, Y_k)^t$ is the vector of temperature and mass fractions. The parameter B represents the pre-exponential constants for each of the elementary reactions.

The first order sensitivity coefficient matrix is defined as .

$$\omega_{j,i} = \frac{\partial Z_j}{\partial B_i} \quad , \tag{3-10}$$

where the indices j and i refer to the dependent variables and reactions respectively. Differentiating equation (3-9) with respect to the parameters B_i yields :

$$\frac{d\omega_{j,i}}{dt} = \frac{\partial F}{\partial Z} \omega_{j,i} + \frac{\partial F_j}{\partial B_i} \quad , \tag{3-11}$$

$$i=1,2,3\ldots,N \; ; j=1,2,3\ldots,N.$$

When equation (3-11) is solved using the B.D.F (backward differentiation formula) method, the solution is efficient due to the existence of linearity between the sensitivity coefficients.

The Jacobian matrix $\partial F / \partial Z$ that appears in equation (3-11), is exactly the one that is required by the B.D.F method in solving the original problem. Each column corresponds to the sensitivities with respect to one of the reaction pre-exponential constants. The solution will

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proceed column by column. The Jacobian matrix is the same for each column of $\omega_{j,i}$. However, since the $\partial F_j / \partial B_i$ matrix describes the explicit dependence of F on each of its columns, this $\partial F_j / \partial B_i$ matrix must be formed prior to solving a column of $\omega_{j,i}$

To normalize the sensitivity coefficients used in this study, the following equation is implemented:

$$\omega_{j,i} = \frac{B_i}{Z_j} \frac{\partial Z_j}{\partial B_i}$$

(3-12)

Equation (3-12) is used to determine the normalized sensitivity coefficients for the production of water with respect to the rate constants for the chemical reactions. In this investigation water which is the primary product of reaction is used as the dependent variable or jth species. The normalized sensitivity coefficients for all forty nine chemical reactions comprising forms the chemical reaction mechanism are computed with respect to time. However, only those chemical reactions that show the most sensitivity are plotted in the production of water are plotted.

Three cases using sensitivity analysis have been considered. The first case is obtained by using sensitivity analysis throughout the nozzle length, temperature and pressure changing at each x-distance along the nozzle. The second case is obtained by keeping the initial nozzle inlet conditions of pressure and temperature constant. Finally the third case is obtained by keeping

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nozzle outlet conditions of pressure and temperature constant. It must be mentioned that the chemical reactions and time interval obtained in the first case are also used for the second and third cases. This is done with the purpose of observing what behavior will be exhibited by the same chemical reactions at different nozzle conditions of pressure and temperature.

CHAPTER 4

4.0 DESCRIPTION OF THE COMPUTER PROGRAM

In this investigation, various driver programs were used for obtaining the different exit

nozzle parameters, and also for performing sensitivity analysis. The main driver program used is

called Chemkin II [10] which is a chemical kinetics package for the analysis of gas phase

chemical kinetics.

This chemical kinetics package should not be considered as a program in the ordinary

sense, i.e., it is not designed to accept input, or to solve a particular problem and report the

answer. Instead, it is a tool intended to help a user work efficiently with large systems of

chemical reactions.

The general structure of the Chemkin II package is composed of two blocks of Fortran

code and two files:

- The Interpreter (Fortran code).

- The Gas-Phase Subroutine Library (Fortran code).

- The Thermodynamic Database (file).

- The Linking File (file).

The Interpreter is a program which reads a symbolic description of a chemical reaction mechanism and then extracts the needed thermodynamic data for each species involved from a Thermodynamic Database (LTHRM). The file LTHRM contains information on many species most of which are not needed for any given problem.

The primary output from the Interpreter is a binary file called the Linking File. This file contains all required information regarding the elements, species, and reactions in the chemical reaction mechanism. The Linking File is named LINKCK. The logical file number for LINKCK must be declared both in the interpreter (so it can be written) and in user's code (so that it can be read by the initialization subroutine).

In addition to the Linking File, three other files are needed by the Interpreter: an input file, an output file, and the thermodynamic database file. The input to the Interpreter is read from file LIN, and printed output is directed to the file LOUT. The printed output contains a listing of the elements, species, and the chemical reaction mechanism. It also provides diagnostic error messages should they be needed.

Once the Interpreter has been executed and the Linking File created, the user is ready to use the Gas-Phase Subroutine Library. Subroutines from this library are called from the user's Fortran code. The user's first step must be to dimension three work arrays (one integer, one floating point, and one character data type) and then call the initialization subroutine CKINIT to create the work arrays from the Linking File. One or more of these arrays is required input to every subroutine in the Chemkin II package.

Selection of Chemkin II subroutines for any given problem begins by finding the appropriate set of governing equations. In this investigation, it constitutes finding the governing equations for frozen, equilibrium, and detailed chemistry flows. Depending on the type of flow problem to be solved, only a few of the subroutines in the package would be called.

Another important subroutine used in this investigation simultaneously with Chemkin II package is called LSODE [15]. This subroutine solves initial value problems for stiff or nonstiff systems of first order ordinary differential equations. This subroutine, used for the frozen and detailed chemistry flow cases, is based on the Gear method. In this investigation a main program is written which calls the subroutine lsode at each point where answers such as density, temperature, velocity, and pressure are desired. Each point will be the x-distance along the hypersonic nozzle. For equilibrium flow, a separate software package is used for obtaining the desired nozzle characteristics. This software package is called STANJAN and was developed by Stanford University.

For the sensitivity analysis, the driver program used is called SENKIN [14] as described in

the last chapter. This program is to be used in conjunction with Chemkin II for performing the

sensitivity analysis. As mentioned before, this involves computations of the first order

sensitivity coefficients with respect to the elementary reaction rate parameters.

CHAPTER 5

5.0 DISCUSSION OF RESULTS

This chapter presents the results obtained in this investigation. Profiles of various flow properties such as specific impulse, temperature, density, velocity and pressure along the x-distance of the hypersonic nozzle are presented. Also, sensitivity analysis results are presented.

In order to obtain the various flow properties at each x-distance along the hypersonic nozzle, the three programs developed were executed with various initial conditions. A conical nozzle with an area ratio of 50 was chosen for this study. The half angle of the nozzle was 12.431° and its length was 8.50 meters. The initial conditions imposed on the model under investigation, which were taken from literature for a hypersonic nozzle [16] [17] are as follows .

Nozzle Inlet Flow Conditions

- Velocity 5634 m/s

- Pressure 1 atm

- Temperature 3072 ^{0}K

Other separate input parameters will be the initial x-distance, which will serve as an initial point for incrementing the length of the hypersonic nozzle, and the initial concentrations in mole fraction for the fourteen chemical species involved in this study. These initial concentrations are shown in table 2.0.

[H]= 0.87059E-01	[HO2]= 0.44573E-05
[N]= 0.14647E-04	[H2O2]= 0.23341E-06
[O]= 0.80033E-02	[NO]= 0.50908E-02
[OH]= 0.30143E-01	[N2]= 0.46517E+00
[H2]= 0.20225E+00	[NO2]= 0.30478E-06
[O2]= 0.31803E-02	[N2O]= 0.19957E-06
[H2O]= 0.19909E+00	[HNO]= 0.10668E-05

Table 2.0. Concentrations in mole fraction at nozzle inlet.

Input parameters for sensitivity analysis are the initial concentrations in mole fraction for the fourteen chemical species, and a time interval which ranges from 0 milliseconds to 1.5 milliseconds. It must be mentioned that this time interval has been obtained from literature [16] and has the purpose of obtaining profiles of chemical reactions which show the most sensitivity.

Figure 3.0 depicts the variation of specific impulse (I_{sp}) of the three flows considered in this study along the hypersonic nozzle. Specific impulse can be defined as the impulse delivered to the rocket or aircraft per unit weight of propellant ejected. Propellants with large values of specific impulse are desirable, hence the exit value of velocity is relevant for practical cases. The higher the exit velocity, the higher the specific impulse value of the rocket.

The specific impulse is obtained by employing the usual static pressure balance [16] across the nozzle. The resulting equation for the specific impulse is (see also figure 1.0):

$$I_{sp} = \frac{V_e}{g} + \frac{P_e}{\rho_e V_e g} \quad .$$
(5-1)

Observe that in equation (5-1) the ambient pressure Pa is eliminated and has no effect for obtaining specific impulse. This is due to the fact that the hypersonic nozzle expands into vacuum, Pa=0. Figure 3.0 shows that the contribution of chemical reaction to the increase in impulse persists throughout the entire nozzle length, and nozzle performance depends on the extent of chemical reaction, as well as on the fluid dynamic expansion process.
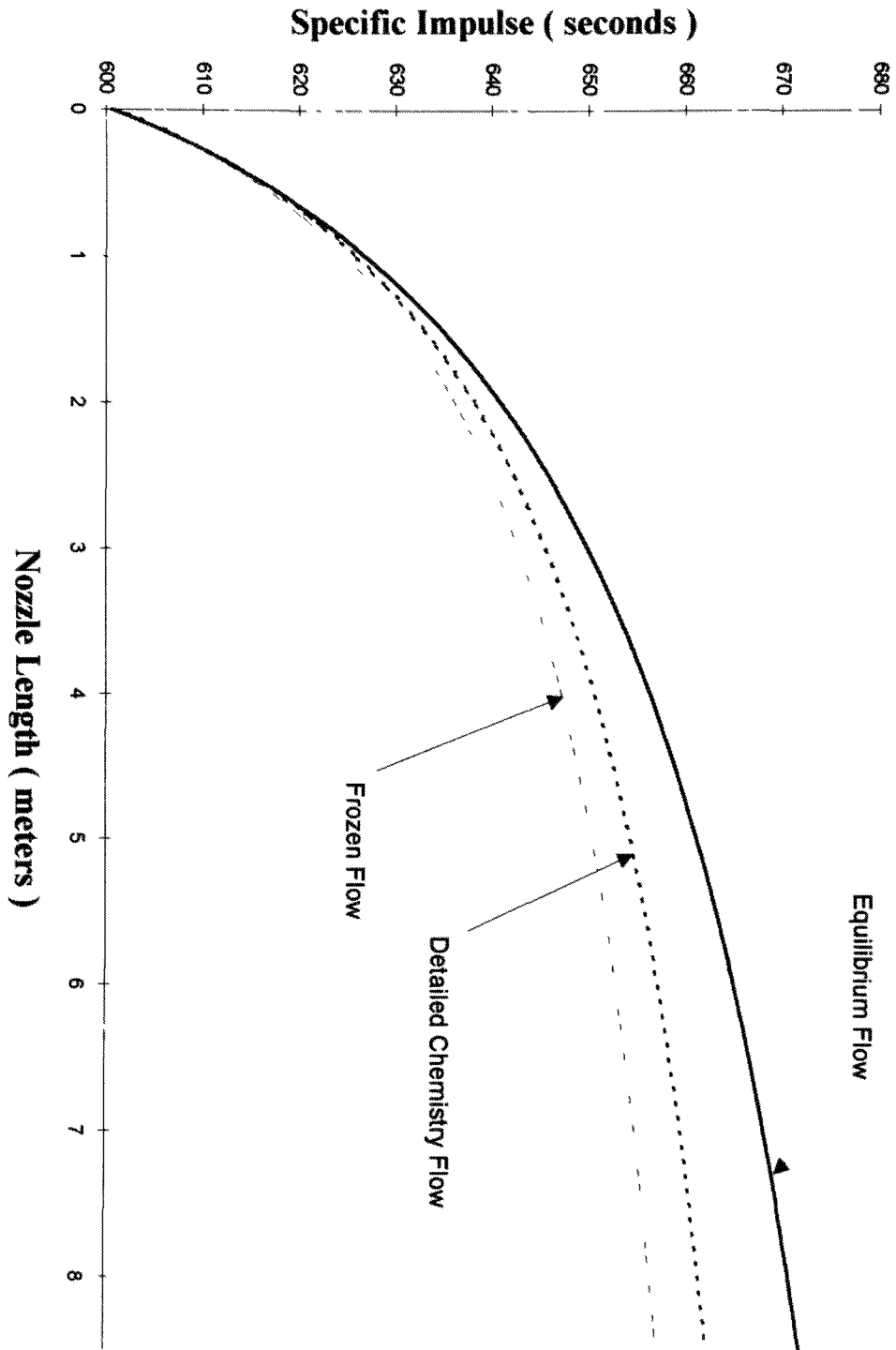
Figure 3.0. Specific Impulse against nozzle length.

Figure 3.0 which is of great importance clearly shows which flows constitute the two limiting bounds. Equilibrium flow is the higher limiting bound, and frozen flow is the lower limiting bound. The detailed chemistry flow solution lies between these two limiting bounds.

Although figure 3.0 shows that up to a nozzle length of approximately 0.5 meters all three flow cases seem to produce the same results, this is not entirely correct. The chemical processes do not reach a frozen state at any point along the nozzle expansion. Similarly, the chemical processes do not attain a chemical equilibrium state anywhere in the nozzle expansion. It must also be mentioned that at this nozzle length of 0.5 meters, for simplification one may use any of the three flows at inlet conditions, for obtaining nozzle performance simulations. The chemistry effects at a nozzle location beyond 0.5 meters will be very significant, therefore, for any of the three flow conditions, parameter results must be obtained. Beyond a nozzle location of 0.5 meters, a singular flow solution cannot be presumed since this may lead to significant errors in nozzle performance simulations.

The results obtained in this figure may vary for each nozzle, depending on the inlet initial conditions, chemical reaction mechanism, and nozzle geometry. Figure 3.0 clearly shows that finite rate chemistry cannot be neglected in nozzle performance simulations.

Figure 4.0 depicts the variation of specific impulse with respect to nozzle length. For different chemical reaction mechanisms, this figure clearly shows that one must be careful to avoid simplifications which neglect important chemical reaction paths. By making simplifications, certain species may be prevented from participating in the chemical reaction mechanism. Also, important reaction pathways contributing to nozzle performance may be eliminated by the simplifications.

In figure 4.0, four cases of species simplification are presented. First, eliminating nitrogen from the chemical reaction mechanism, will result in a lowered specific impulse from the hypersonic nozzle. The second case shows that, on eliminating HO2, H2O2, HNO, N2O species from the chemical reaction mechanism, the specific impulse is somewhat lower than using detailed chemistry flow. Nonetheless, it still decreases the hypersonic nozzle performance. The third case, eliminating HNO species from the chemical reaction mechanism does not produce significant difference to nozzle performance. Hence, nozzle performance does not depend heavily on HNO species. In the fourth and last case, by eliminating all nitrogen species NO_x from the chemical reaction mechanism, only an oxygen and hydrogen environment will exist. Nozzle performance dramatically increases in this case.

Figures 3.0 and 4.0 conclusively shows that specific impulse will depend on the species considered in the chemical reaction mechanism. This is observed when taking into consideration
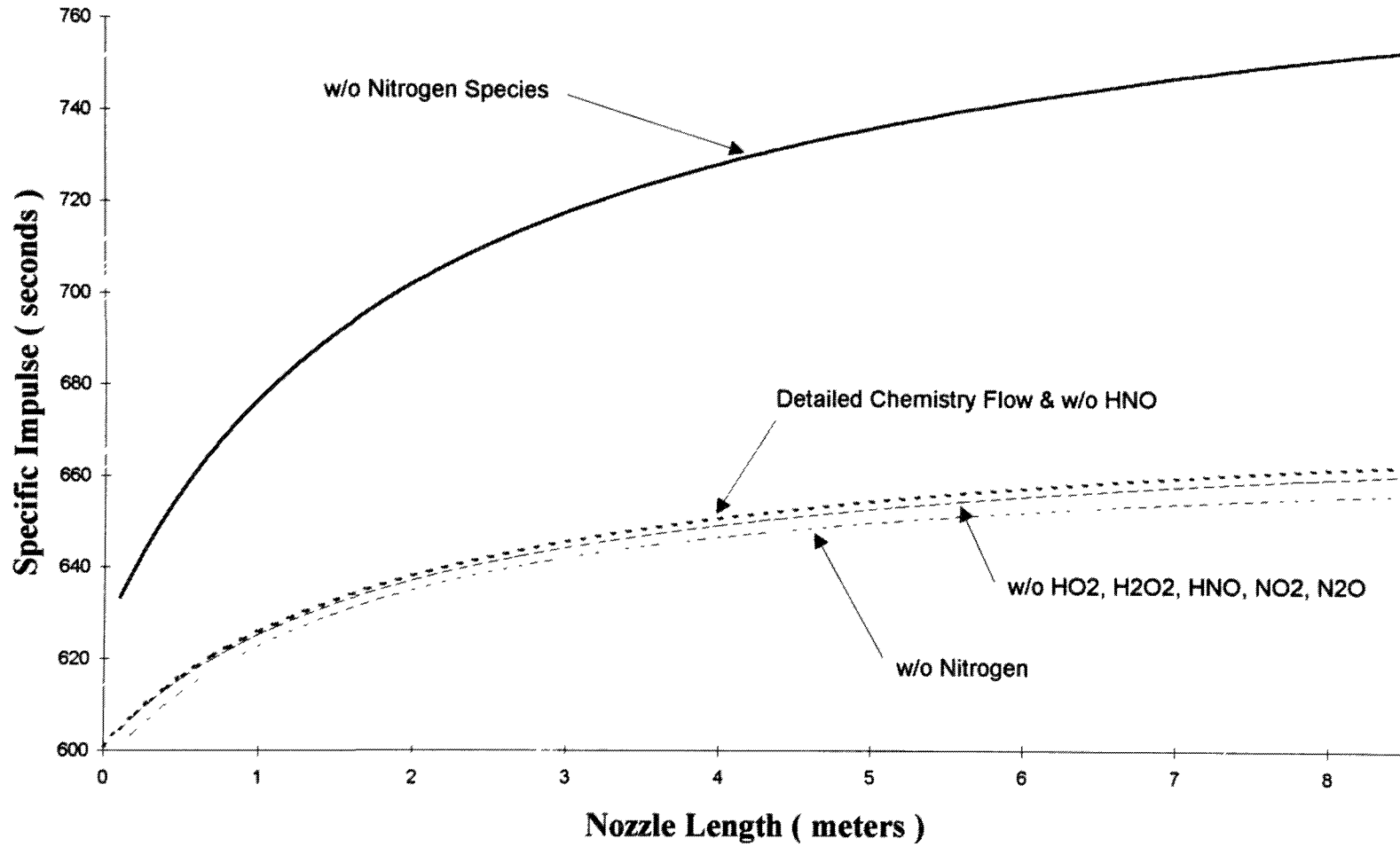
Figure 4.0. Variation of nozzle performance against nozzle length for different chemical reaction mechanisms.

the nitrogen species in the chemical reaction mechanism. Depending on whether some or all of nitrogen species is eliminated, nozzle performance varies by increasing or decreasing specific impulse. As mentioned before, one must take into account the contributions of all chemical species that form the chemical reaction mechanism. This contribution of chemical species can be observed in Table 3.0, which shows a summary of the different cases presented for obtaining specific impulse for the hypersonic nozzle.

One way of solving the simplification problem of important chemical pathways is to tune the reduced chemical reaction mechanism, that is, by properly compensating or adjusting the chemical reactions in the reduced chemical reaction mechanism, which will produce the same results as the original chemical reaction mechanism. Although this approach can be used to solve the reduction problem, it is advisable not to depend on it very much due to the complexities in employing the method and obtaining the proper adjustments for the reactions.

CASE	Specific Impulse (seconds)
Frozen	657.35
Equilibrium	672.19
Detailed Chemistry	662.50
w/o HNO	662.50
w/o HO2,H2O2,HNO,NO2,N2O	656.20
w/o Any Nitrogen Species	753.50
w/o N	660.50

Table 3.0. Summary table for different chemical reaction mechanism
for a hypersonic nozzle of 8.5 meters length.

Figure 5.0 depicts the variation of temperature along the nozzle. As expected, in a nozzle expansion the temperature decreases along the nozzle length for all three flows. Where equilibrium flow is the lower bound, frozen flow is the higher bound and detailed chemistry flow lies between the two.

Figure 6.0 depicts the variation of density along the nozzle. This particular graph shows a very interesting case. As expected, density decreases along the nozzle length, but the variation is independent of the chemical reaction. All the three flows show the same density variation.

Figure 7.0 depicts the variation of velocity along the nozzle. This graph shows that velocity increases along nozzle length. Again, equilibrium flow provides the upper bound, frozen flow provides the lower bound, and detailed chemistry flow velocity falls between the two.

Figure 8.0 depicts the variation of pressure along the nozzle length. As expected, in a nozzle expansion the pressure decreases along the nozzle length for all three flows. Where equilibrium flow is the lower bound, frozen flow is the higher bound and detailed chemistry flow lies between the limiting cases.
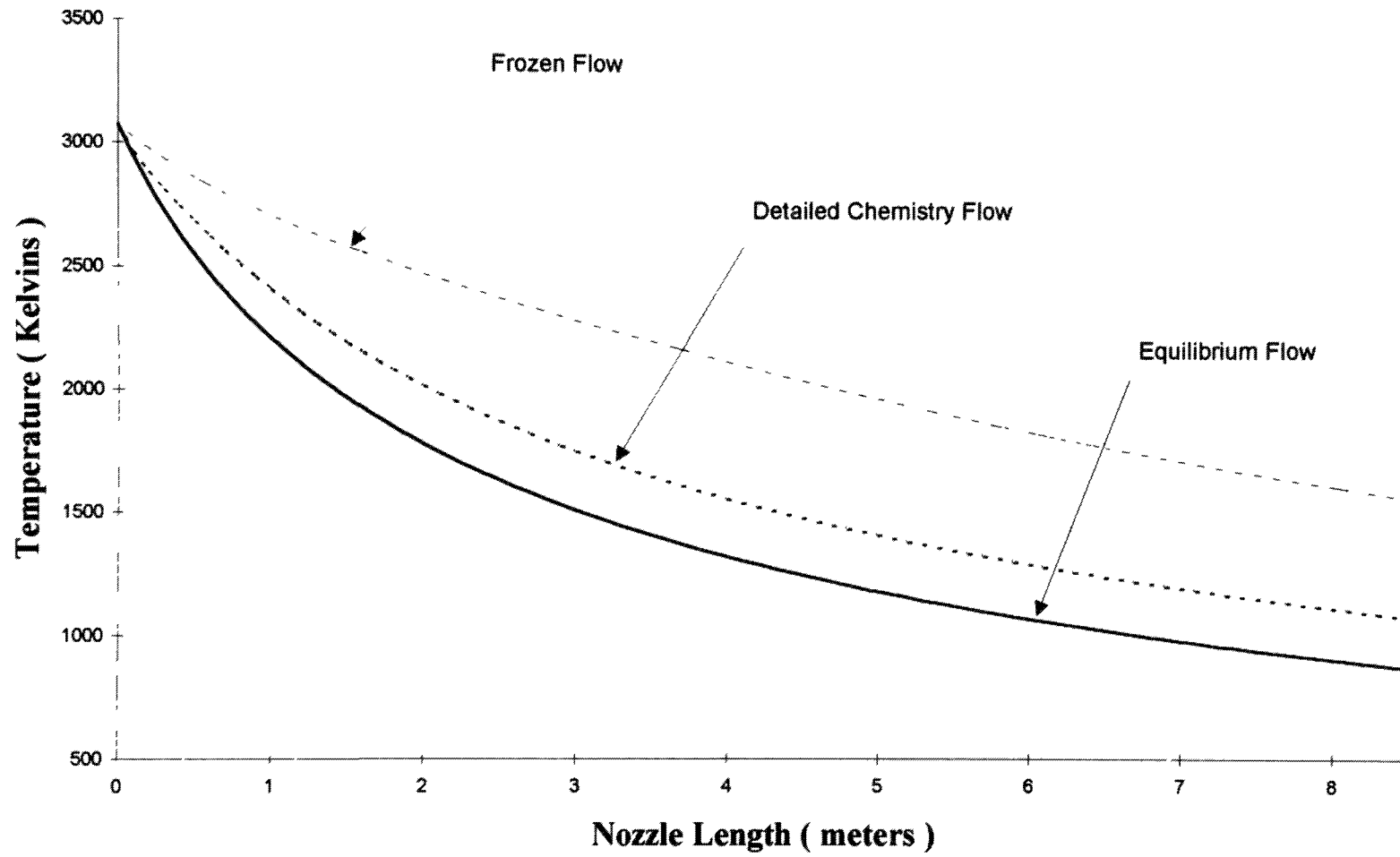
Figure 5.0. Variation of temperature against nozzle length.
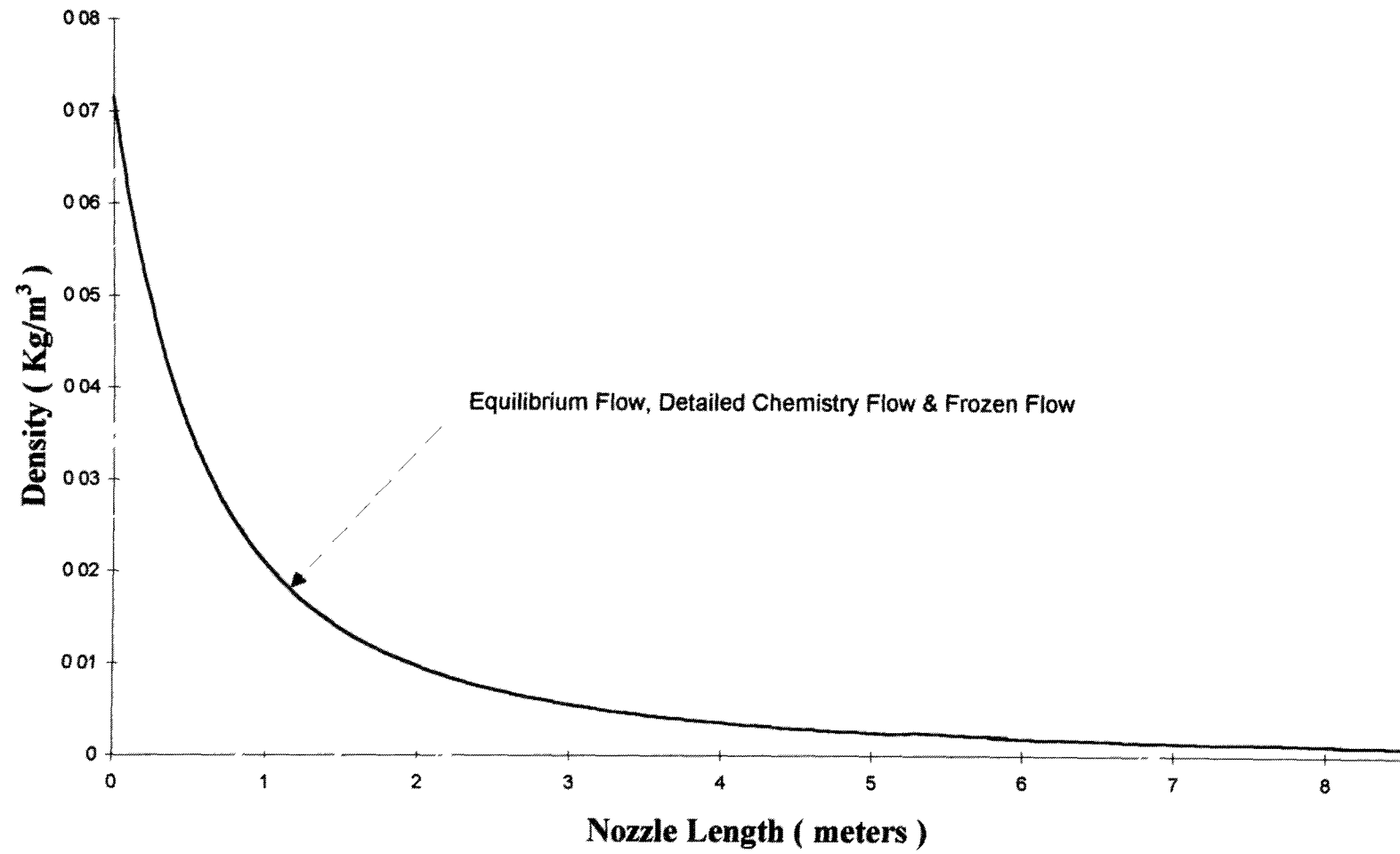
Figure 6.0. Variation of density against nozzle length.
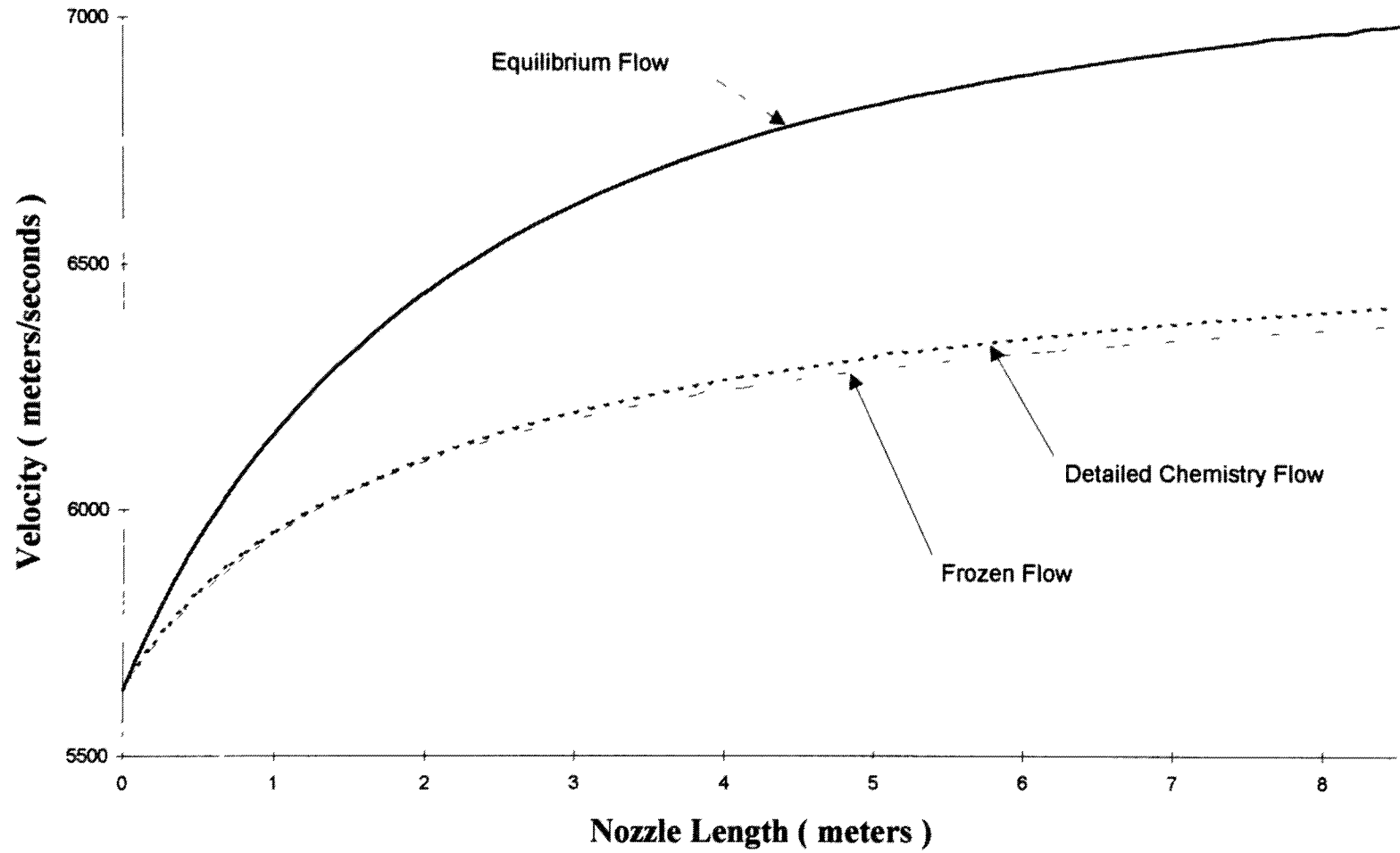
Figure 7.0. Variation of velocity against nozzle length.
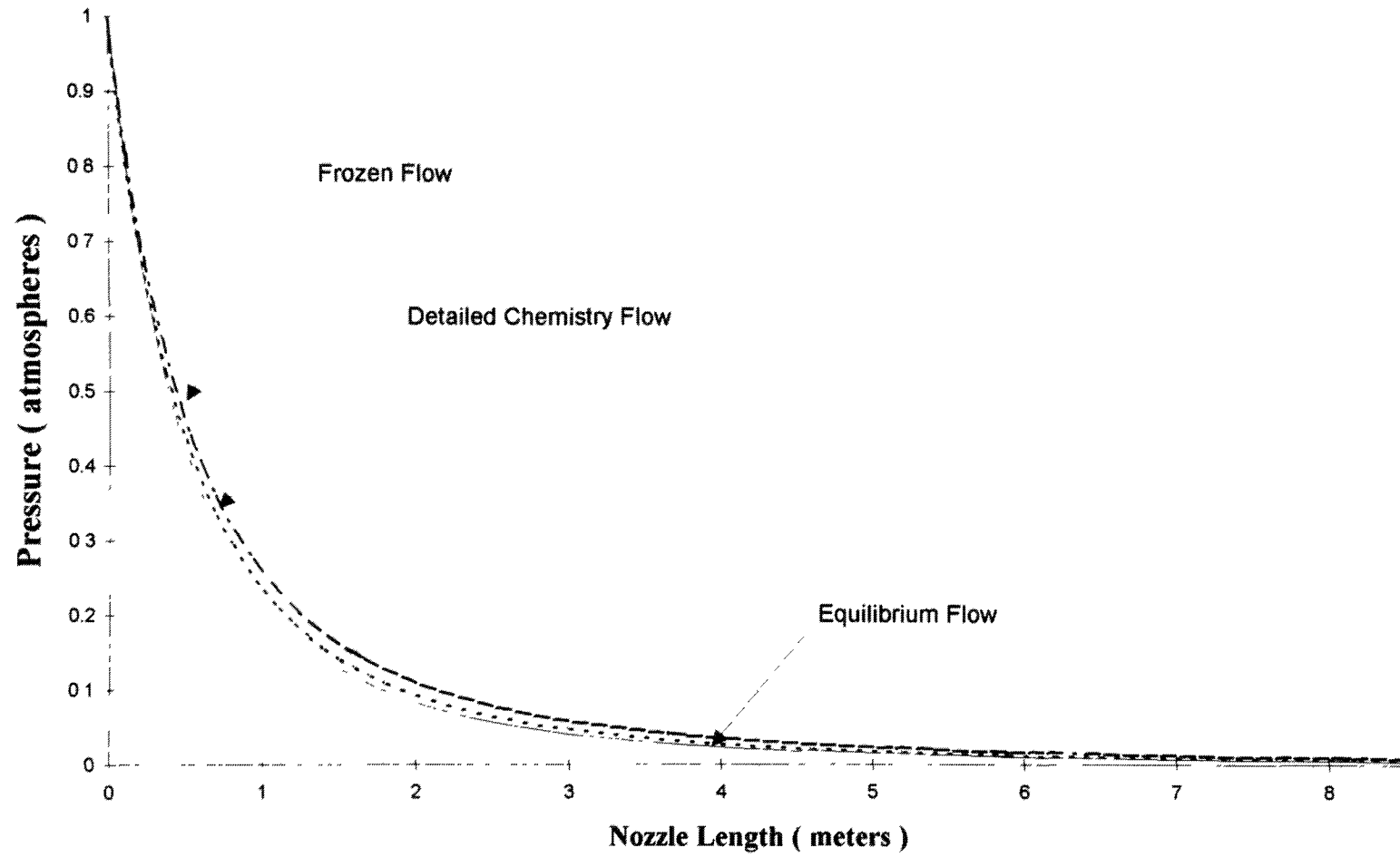
Figure 8.0. Variation of pressure against nozzle length.

Figure 9.0 depicts the variation of normalized sensitivity coefficients for the production

of water, with respect to the rate constants for those chemical reactions which are dominant.

This figure was obtained by using the Senkin[12] subroutine for all forty nine chemical reactions

comprising the chemical reaction mechanism of this investigation. Reactions 20, 17, 21, 2, 3, 5

and 28 exert the most influence and the sensitivity coefficients are shown for these reactions in

figure 9.0.

This figure shows that chemical reaction 20 is by far the most important chemical

reaction for nozzle performance contribution. It can be observed that this reaction has the

highest sensitivity coefficient 4.4E-03 at 1.04E-04 milliseconds. After this maximum the

reaction sensitivity coefficient value decreases with time. Also, chemical reaction 17 which has

a maximum sensitivity value of 1.0E-03 at 1.04E-04 milliseconds, and chemical reaction 21

which has a maximum sensitivity value of 0.26E-03 at 1.04E-04 milliseconds, are of importance

to nozzle performance contribution. It must be mentioned also that the last two chemical

reactions 17 and 21 behave in the same way as chemical reaction 20, i.e., attaining a maximum

sensitivity value in a short time period, and decreasing after this point as time increases.

Reactions 2,3,5, and 28 also become important pathways for nozzle performance. It can

be observed that, for these chemical reactions, the sensitivity coefficient values increase in a

steady manner as time increases.
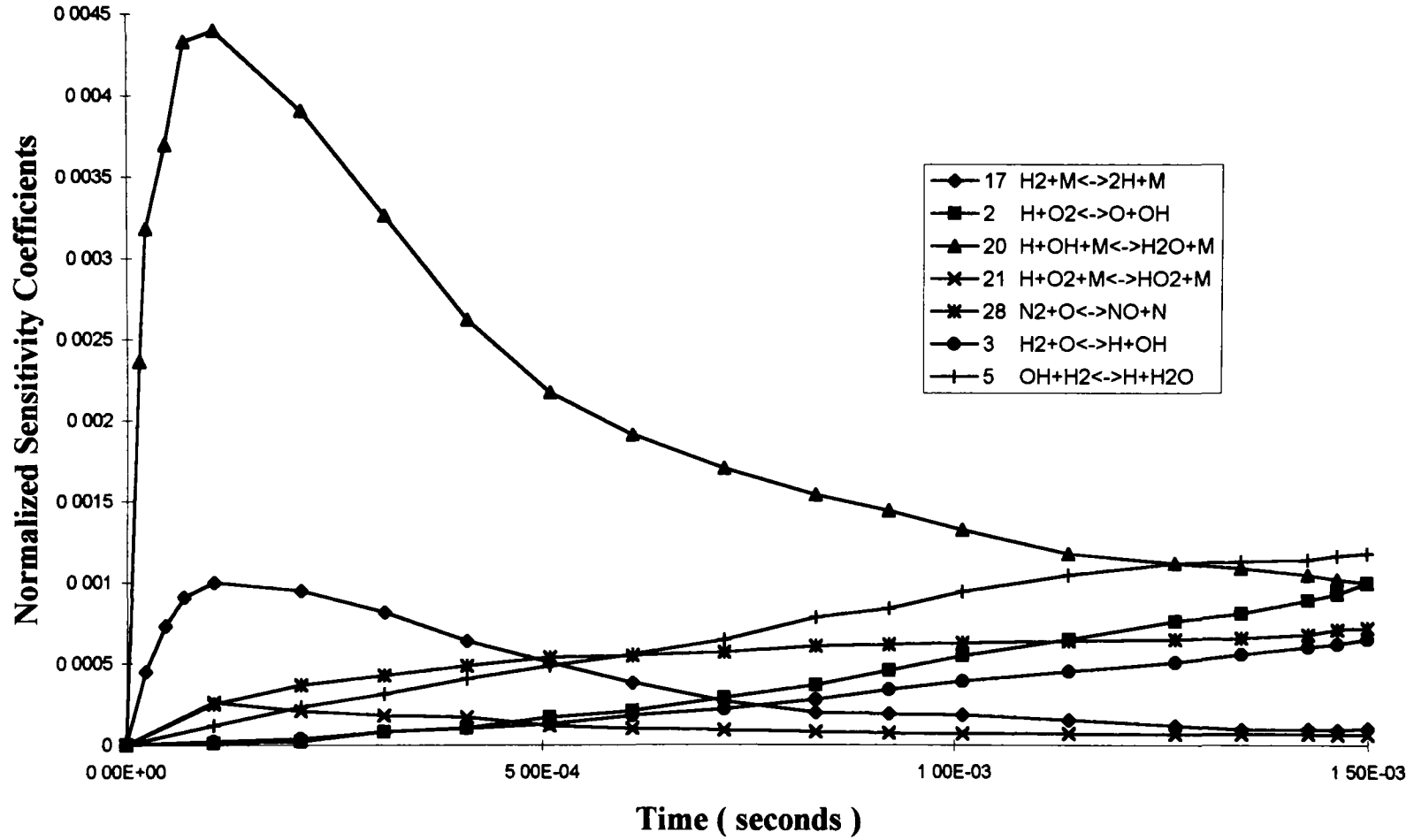
Figure 9.0. Normalized sensitivity coefficients against time through nozzle length.

Figure 10.0 depicts the variation of normalized sensitivity coefficients for the production of water with respect to the rate constants at nozzle entrance. This plot was obtained by maintaining a constant temperature of 3072 K, and a constant pressure of 1 atmosphere at the nozzle entrance. Again, as in figure 9.0 chemical reactions 20, 17, 21, 2, 3, 5 and 28 are the most influential and thus shown in this plot. Results are presented for time ranging from 0 milliseconds to 1.5 milliseconds.

Figure 10.0 shows that chemical reactions 21 and 17 are the most important chemical pathways because their sensitivity coefficient values increases in time. Also chemical reactions 2 and 28 are of importance because their sensitivity coefficient values also increases with time, but at a lower rate than chemical reactions 21 and 17. Chemical reactions 20,3 and 5 do not contribute to the formation of water. For these three chemical reactions, the sensitivity coefficient values decrease with time.

Figure 11.0 depicts the variation of normalized sensitivity coefficients for the production of water with respect to the rate constants for nozzle outlet conditions. Again, as in figure 9.0 and figure 10.0 chemical reactions 20, 17, 21, 2, 3, 5 and 28 are used for this plot. Results are presented for time ranging from 0 milliseconds to 1.5 milliseconds.

Results for this plot were obtained by keeping temperature constant at 1073.63 K, and pressure constant at 0.00532 atmospheres, which constitute nozzle outlet conditions at 8.5
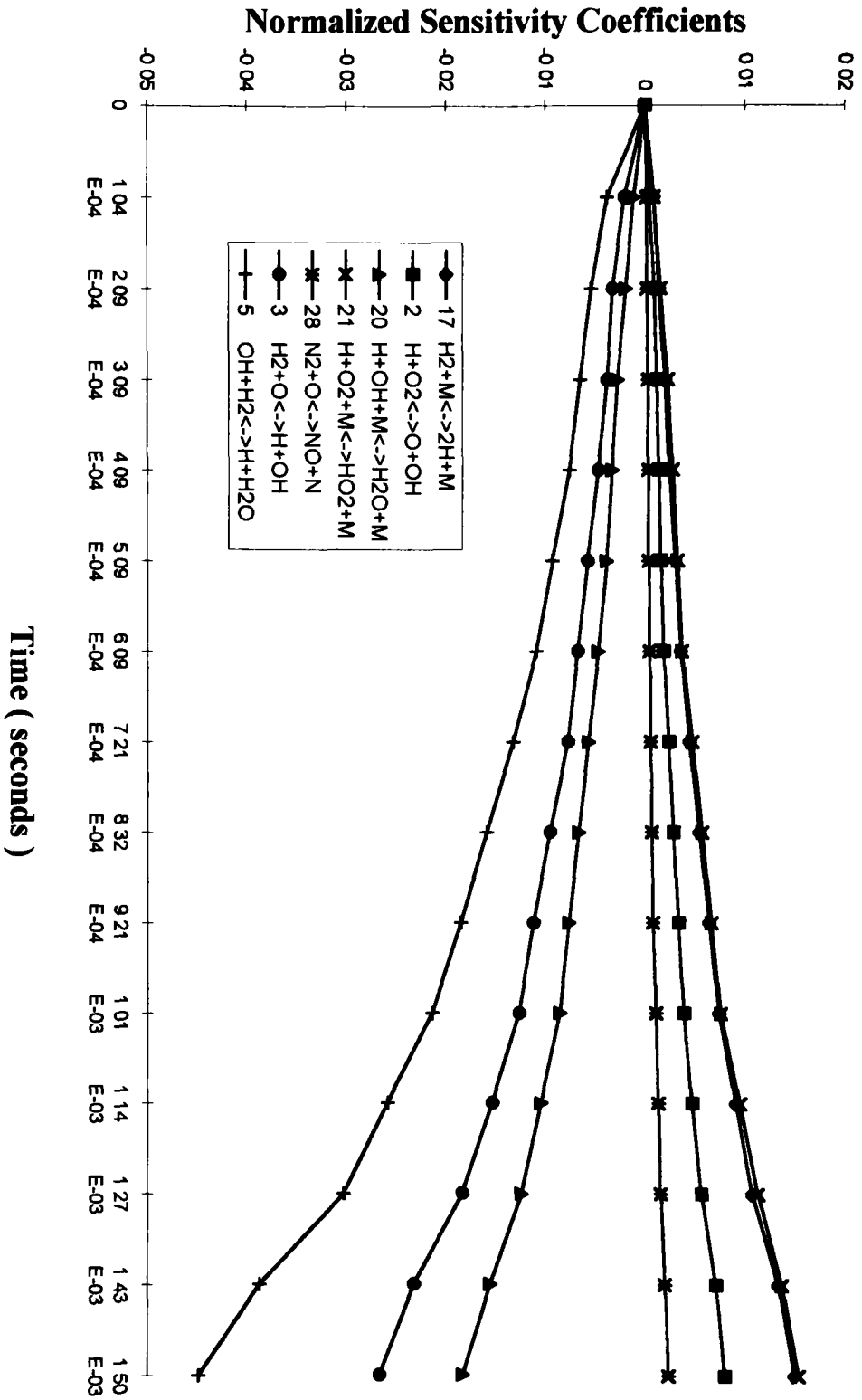
Figure 10.0. Normalized sensitivity coefficients against time for constant nozzle inlet conditions.

Normalized Sensitivity Coefficients

0 035

0 03

0 025

0 02

0 015

0 01

0 005

0

-0 005

Legend:
- 17 H2+M<->2H+M
- 2 H+O2<->O+OH
- 20 H+OH+M<->H2O+M
- 21 H+O2+M<->HO2+M
- 28 N2+O<->NO+N
- 3 H2+O<->H+OH
- 5 OH+H2<->H+H2O

| 0 | 1 04 E-04 | 2 09 E-04 | 3 09 E-04 | 4 09 E-04 | 5 09 E-04 | 6 09 E-04 | 7 21 E-04 | 8 32 E-04 | 9 21 E-04 | 1 01 E-03 | 1 14 E-03 | 1 27 E-03 | 1 43 E-03 | 1 50 E-03 |

Time (seconds)
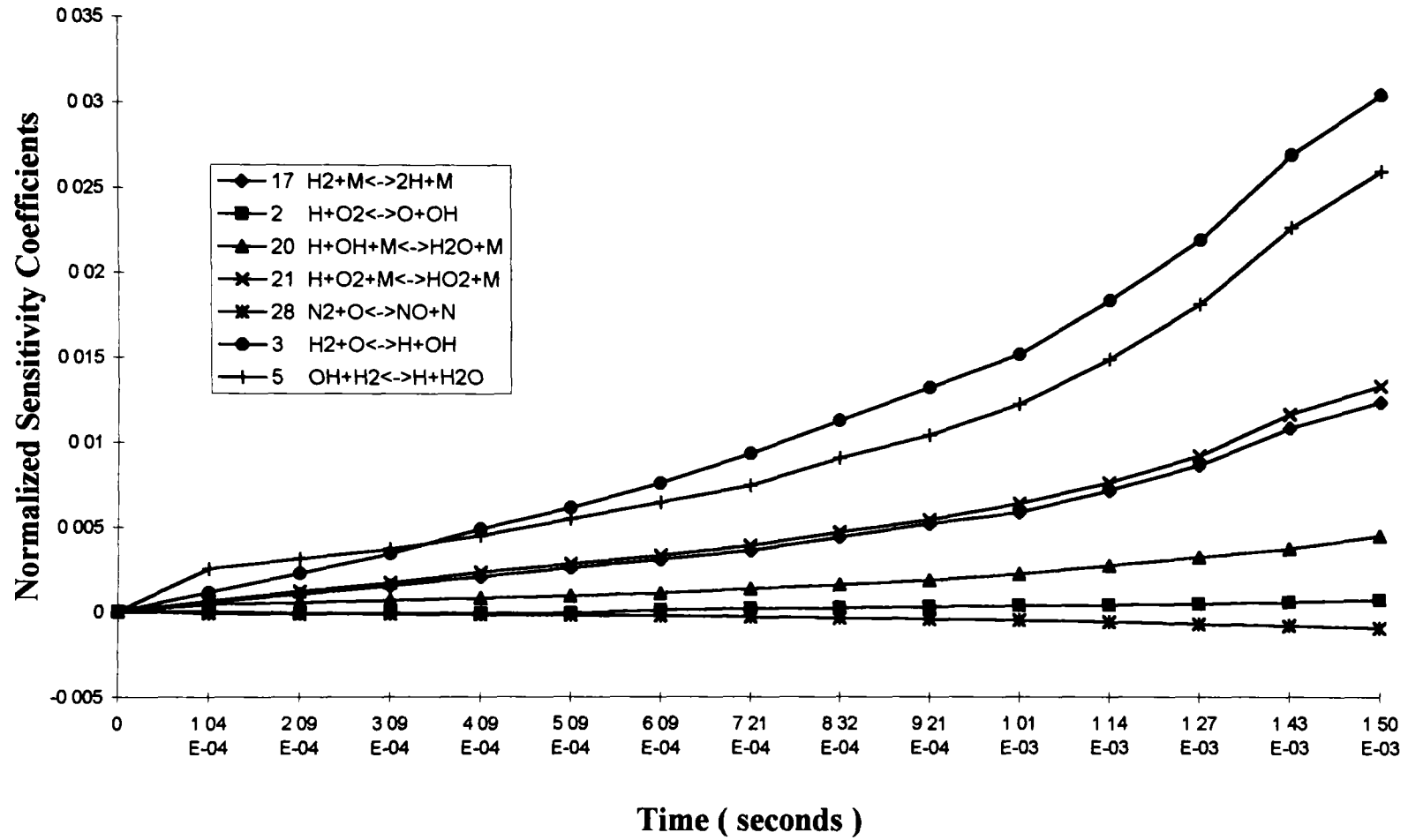
Figure 11.0. Normalized sensitivity coefficients against time for constant nozzle outlet conditions.

meters. Figure 11.0 shows that chemical reaction 3 predominates; its sensitivity coefficient values increases in time. Chemical reaction 5 is the second most important as it exhibits the second highest sensitivity coefficient value. Chemical reactions 17 and 21 are also of importance because of the increase of sensitivity coefficient values, although at a lower rate. The sensitivity coefficient values of reactions 20 and 2 increase at a slow rate, and reaction 28 sensitivity coefficient value decreases at a nearly constant rate.

CHAPTER 6

6.0 RECOMMENDATIONS

This chapter describes the future recommendations to be made as a complement to this investigation. The following recommendations are made; investigation of changes in nozzle geometry, investigation of ionization effects, investigation of nozzle thermal effects in nozzle design, and investigation of effects of nitrogen species.

In this investigation only one geometry was considered which was a conical shape nozzle. Results for pressure, density, temperature, velocity and specific impulse may change by considering different geometry's for nozzles.

Ionization effects become evident at very high temperatures. Under these conditions new chemical species must be considered in the chemical reaction mechanism. This will change the results for pressure, density, velocity, temperature and specific impulse. Also sensitivity analysis results will change due to the newly introduced chemical species.

In this investigation thermal effects such as heat conduction or heat radiation were neglected. If these effects were to be considered, the result will be of contribution of extra terms to the energy equation, ultimately results will change for pressure, density, temperature, velocity and specific impulse by the addition of extra terms.

Clearly this investigation shows what effects different nitrogen species will have on nozzle performance (I_{sp}). Further investigation is recommended for these chemical species, specially if the chemical reaction mechanism differs from the one used in this investigation, i.e., if there are more chemical reactions to be considered with other NO_x species not used in this study.

APPENDIX A

GOVERNING FLOW EQUATIONS

Mass Conservation Equation.

$$\frac{\partial \rho}{\partial t} + \frac{1}{g_2 g_3} \frac{\partial}{\partial x}\left(\rho v g_2 g_3\right) = 0 \quad . \tag{2-1}$$

Knowing that $g_2{}^*g_3 = A$ and $\dfrac{\partial \rho}{\partial t}$

$$\frac{1}{A} \frac{d}{dx}\left(\rho vA\right) = 0 .$$

After integration is performed :

$$\rho \, v \, A = \text{constant} .$$

Multiplying both sides by In and deriving by x :

$$\frac{d}{dx}\left(\text{In}\rho\right) + \frac{d}{dx}\left(\text{In}v\right) + \frac{d}{dx}\left(\text{In}A\right) = \frac{d}{dx}\left(\text{In constant}\right),$$

$$\boxed{\frac{1}{\rho} \frac{d\rho}{dx} + \frac{1}{v} \frac{dv}{dx} + \frac{1}{A} \frac{dA}{dx} = 0 .} \tag{2-6}$$

Momentum Equation.

$$\frac{\partial v}{\partial t} + v\frac{\partial v}{\partial x} = -\frac{1}{\rho}\frac{\partial P_{11}}{\partial x} + \frac{(P_{22}-P_{11})}{\rho}\frac{1}{g_2}\frac{\partial g_2}{\partial x} + \frac{(P_{33}-P_{11})}{g_3}\frac{1}{g_3}\frac{\partial g_3}{\partial x} + \sum_{i=1}^{N} Y_i f_i \quad . \qquad (2\text{-}2)$$

Body forces and viscosity neglected :

$$P_{11} = P + \left(\frac{2}{3}\mu - \kappa\right)\frac{1}{g_2 g_3}\frac{\partial}{\partial x}(vg2g3) - 2\mu\frac{\partial v}{\partial x}, \qquad\qquad P_{11} = P,$$

$$P_{22} = P_{11} + 2\mu\left(\frac{\partial v}{\partial x} - \frac{v}{g_2}\frac{\partial g_2}{\partial x}\right), \qquad\qquad P_{22} = P_{11} = P,$$

$$P_{33} = P_{11} + 2\mu\left(\frac{\partial v}{\partial x} - \frac{v}{g_3}\frac{\partial g_3}{\partial x}\right), \qquad\qquad P_{33} = P_{11} = P,$$

After substitution ·

$$\boxed{\rho v\,\frac{d v}{d x} + \frac{d P}{d x} = 0 \quad .}\qquad\qquad (2\text{-}7)$$

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Energy Equation.

$$\frac{\partial}{\partial t}\left(h+\frac{v^2}{2}\right)+\frac{\partial}{\partial x}\left(h+\frac{v^2}{2}\right)=-\frac{1}{\rho\,g_2 g_3}\frac{\partial}{\partial x}(q g_2 g_3)+\frac{1}{\rho}\frac{\partial \rho}{\partial t}+$$

$$+\frac{1}{\rho\,g_2 g_3}\frac{\partial}{\partial x}\left[(P-P_{11})\,v g_2 g_3\right]+\sum_{i=1}^{N}Y_i f_i(v+V_i). \qquad (2\text{-}3)$$

Making use of assumptions a) through i) and :

$$v\frac{d}{dx}\left(h+\frac{v^2}{2}\right)=0\;, \qquad\text{or}\qquad v\frac{dh}{dx}+v^2\frac{dv}{dx}=0\,.$$

Knowing that :

$$h=\sum_{i=1}^{N}h_i Y_i\,, \qquad \frac{dh}{dx}=C_{pi}\frac{dT}{dx}\,, \qquad\text{and}\qquad \frac{dY_i}{dx}=\frac{\omega_i W_i}{\rho v}$$

Substituting the equations from before :

$$\rho\,v\overline{C}_p\frac{dT}{dx}+\sum_{i=1}^{N}h_i\omega_i W_i+\rho v^2\frac{dv}{dx}=0\;, \qquad (2\text{-}8)$$

Species Equation.

$$\frac{\partial Y_i}{\partial t} + v\frac{\partial Y_i}{\partial x} = \frac{\omega_i}{\rho} - \frac{1}{\rho g_2 g_3}\frac{\partial}{\partial x}\left(\rho Y_i V_i g_2 g_3\right), \qquad (2\text{-}4)$$

$$i=1,2,3...,N.$$

Making use of assumption a) through i) and knowing that :

$$w_i = \omega_i W_i \ ,$$

$$\boxed{\rho v \frac{d Y_i}{d x} = \omega_i W_i \ , \qquad\qquad i=1,2,3...,N.} \qquad (2\text{-}9)$$

State Equation.

$$P = \rho R^0 T \sum_{i=1}^{N} \frac{Y_i}{W_i} \qquad (2\text{-}5)$$

Where :

$$W = \frac{1}{\sum_{i=1}^{N} \frac{Y_i}{W_i}} \ .$$

Multiplying by ln and deriving by d/dx :

$$\frac{1}{P}\frac{dP}{dx} + \frac{1}{W}\frac{dW}{dx} = \frac{1}{\rho}\frac{d\rho}{dx} + \frac{1}{R^0}\frac{dR^0}{dx} + \frac{1}{T}\frac{dT}{dx} \; ,$$

$$\boxed{\frac{1}{P}\frac{dP}{dx} + \frac{1}{W}\frac{dW}{dx} = \frac{1}{\rho}\frac{d\rho}{dx} + \frac{1}{T}\frac{dT}{dx}}$$

(2-10)

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APPENDIX B

FLOW EQUATIONS SUMMARIES

Mass Conservation Equation.

Will be the same for frozen flow and detailed chemistry flow :

$$\frac{1}{\rho}\frac{d\rho}{dx} + \frac{1}{v}\frac{dv}{dx} + \frac{1}{A}\frac{dA}{dx} = 0$$

For equilibrium flow the equation is as follows :

$$\dot{m} = \rho\, v\, A = constant$$

Momentum Equation.

Will be the same for frozen flow and detailed chemistry flow :

$$\rho\, v\, \frac{d\,v}{d\,x} + \frac{d\,P}{d\,x} = 0 \quad .$$

For equilibrium flow the momentum equation is used in combination to obtain other equations.

Energy Equation.

$$\rho \, v\overline{Cp}\frac{dT}{dx} + \rho \, v^2 \frac{dv}{dx} = 0 \, . \qquad\qquad \text{Frozen flow,}$$

$$h_o = h + \frac{v^2}{2} = \text{constant} \quad . \qquad\qquad \text{Equilibrium flow,}$$

$$\rho \, v\overline{C}_p\frac{dT}{dx} + \sum_{i=1}^{N} h_i \omega_i W_i + \rho \, v^2 \frac{dv}{dx} = 0 \, . \qquad \text{Detailed Chemistry flow,}$$

Species Equation.

Will be the same for frozen flow and detailed chemistry flow :

$$\rho \, v \, \frac{d Y_i}{d x} = \omega_i W_i \quad . \qquad \text{Frozen flow, Detailed Chemistry flow,}$$

$$i = 1,2,3...,N.$$

For equilibrium flow, the species equation can be replaced by atom conservation and chemical equilibrium equations.

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State Equation.

$$\frac{1}{P}\frac{dP}{dx} = \frac{1}{\rho}\frac{d\rho}{dx} + \frac{1}{T}\frac{dT}{dx}$$

Frozen flow,

$$P = \rho R^0 T \sum_{i=1}^{N} \frac{Y_i}{W_i}.$$

Equilibrium flow,

$$\frac{1}{P}\frac{dP}{dx} + \frac{1}{W}\frac{dW}{dx} = \frac{1}{\rho}\frac{d\rho}{dx} + \frac{1}{T}\frac{dT}{dx} .$$

Detailed Chemistry flow.

APPENDIX C

FROZEN FLOW RESULTS TABLE

x-distance	I_sp	Temp	Velocity	Density	Pressure
m	sec	K	m/sec	Kg/m3	atm
0	600.58	3072	5634	0.07144	1
0.1	604.31	3015.5	5683.07	0.061	0.68
0.2	607.62	2965.5	5726.47	0.0527	0.5717
0.3	610.57	2919	5765.18	0.046	0.4859
0.4	613.23	2876	5799.99	0.0405	0.4169
0.5	615.64	2850.5	5831.5	0.0405	0.3607
0.6	617.83	2797	5860.18	0.0359	0.3145
0.7	619.84	2761	5886.42	0.0288	0.276
0.8	621.69	2726.5	5910.55	0.026	0.2437
0.7	619.84	2693.5	5932.83	0.0236	0.2164
0.8	621.69	2662	5910.55	0.0215	0.1932
0.9	623.39	2631.5	5932.83	0.0197	0.1864
1	624.98	2602	5953.47	0.0181	0.1832
1.1	626.45	2573.5	5972.67	0.0167	0.1732
1.2	627.82	2546	5990.57	0.0154	0.156
1.3	629.1	2573.5	6007.32	0.0143	0.1411
1.4	630.31	2546	6023.03	0.0133	0.128
1.5	631.44	2519	6037.8	0.0124	0.1166
1.6	632.5	2493	6051.72	0.0116	0.1065
1.7	633.51	2467.5	6064.86	0.0108	0.09755
1.8	634.46	2442.5	16077.29	0.0102	0.08962
1.9	635.36	2418	6089.08	0.00957	0.08254
2	636.22	2394	6100.27	0.0102	0.07621
2.1	637.04	2370	6110.91	0.00957	0.07053
2.2	637.81	2347	6121.04	0.00902	0.06541
2.3	638.55	2324	6130.7	0.00851	0.06079
2.4	639.25	2302	6139.93	0.00804	0.0566
2.5	639.93	2279.5	6148.75	0.00761	0.0528
2.4	639.25	2257.5	6157.2	0.00722	0.04934
2.5	639.93	2236	6148.75	0.00685	0.04618
2.6	640.57	2215	6157.2	0.00651	0.04934
2.7	641.19	2194	6165.29	0.0062	0.04618
2.8	641.78	2173	6173.06	0.0059	0.0433
2.9	642.35	2153	6180.51	0.00563	0.04065
3	642.9	2173	6187.68	0.00538	0.03822
3.1	643.42	2153	6194.58	0.00514	0.03598
3.2	643.93	2132.5	6201.22	0.00492	0.03392
3.3	644.42	2112	6207.62	0.00471	0.03202
3.4	644.89	2093	6213.79	0.00452	0.03026

Table 4.0. Frozen flow results for a hypersonic nozzle .

x-distance	I$_{sp}$	Temp	Velocity	Density	Pressure
m	sec	K	m/sec	Kg/m3	atm
3.5	645.34	2073	6219.75	0.00433	0.02863
3.6	645.78	2054	6225.5	0.00416	0.02711
3.7	646.2	2035	6231.06	0.00433	0.02571
3.8	646.61	2016	6236.44	0.00416	0.0244
3.9	647.01	1998	6246.69	0.004	0.02318
4	647.39	1980	6251.58	0.00385	0.02204
4.1	647.76	1962	6256.32	0.0037	0.02098
4.2	648.12	1944	6259.23	0.00357	0.01998
4.3	648.47	1925	6260.92	0.00344	0.01905
4.4	648.81	1910	6265.38	0.00332	0.01818
4.5	649.13	1893	6269.71	0.0032	0.01905
4.6	649.45	1876	6273.92	0.00309	0.01818
4.7	649.76	1859.5	6278.01	0.00299	0.01736
4.8	650.06	1843.5	6281.99	0.00289	0.01659
4.9	650.36	1859.5	6285.86	0.00279	0.01587
5	650.64	1843.5	6289.63	0.0027	0.01518
5.1	650.92	1827.5	6293.3	0.00262	0.01454
5.2	651.19	1812	6296.88	0.00254	0.01393
5.3	651.45	1781	6300.36	0.00246	0.01336
5.4	651.71	1766.5	6303.76	0.00238	0.01282
5.5	651.96	1752	6307.07	0.00231	0.01231
5.6	652.2	1737.5	6310.31	0.00238	0.01182
5.7	652.44	1723.5	6313.46	0.00231	0.01137
5.8	652.67	1710	6316.54	0.00225	0.01093
5.9	652.9	1696	6319.55	0.00218	0.01052
5.8	652.67	1682	6322.49	0.00212	0.01013
5.9	652.9	1669	6325.36	0.00206	0.009754
6	653.12	1656	6322.49	0.002	0.009064
6.1	653.33	1643.5	6325.36	0.00195	0.0094
6.2	653.54	1631	6328.16	0.0019	0.009064
6.3	653.75	1618.5	6330.91	0.00185	0.008743
6.4	653.95	1606.5	6333.59	0.0018	0.008438
6.5	654.15	1594.5	6336.22	0.00175	0.008146
6.6	654.34	1606.5	6338.79	0.00171	0.007869
6.7	654.53	1594.5	6341.3	0.00166	0.007604
6.8	654.71	1583	6343.76	0.00162	0.007351
6.9	654.9	1571	6346.18	0.00158	0.007109
7	655.07	1560	6348.54	0.00154	0.006878

Table 4.0. Frozen flow results for a hypersonic nozzle

x-distance	I_sp	Temp	Velocity	Density	Pressure
m	sec	K	m/sec	Kg/m3	atm
7.2	655.42	1558.64	6353.12	0.00147	0.006445
7.3	655.58	1550.52	6355.35	0.00151	0.006243
7.4	655.74	1542.54	6357.53	0.00147	0.006049
7.5	655.9	1534.71	6359.67	0.00144	0.005863
7.6	656.06	1527.01	6361.76	0.0014	0.005684
7.5	655.9	1519.45	6363.82	0.00137	0.005513
7.6	656.06	1492.01	6365.84	0.00134	0.005349
7.7	656.21	1484.71	6363.82	0.00131	0.005191
7.8	656.37	1477.53	6365.84	0.00128	0.005349
7.9	656.51	1460.46	6367.82	0.00125	0.005191
8	656.66	1453.52	6369.77	0.00122	0.00504
8.1	656.8	1446.69	6371.68	0.0012	0.004895
8.2	656.94	1439.96	6373.56	0.00117	0.004755
8.3	657.08	1423.35	6375.4	0.00115	0.00462
8.4	657.21	1396.84	6377.21	0.00112	0.004491
8.5	657.35	1380.44	6378.99	0.0011	0.004366

Table 4.0. Frozen flow results for a hypersonic nozzle

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APPENDIX D

EQUILIBRIUM FLOW RESULTS TABLE

x-distance	I_{sp}	Temp	Velocity	Density	Pressure
m	sec	K	m/sec	Kg/m3	atm
0	600.58	3072	5634	0.07144	1
0.112737	604.79	2944.59	5714.79	0.05959	0.8187
0.226852	608.59	2830.48	5788.96	0.050327	0.6799
0.341778	612.08	2727.48	5858.4	0.042986	0.5717
0.457952	615.23	2633.88	5921.06	0.037076	0.4858
0.529574	617.09	2548.33	5957.63	0.03401	0.4417
0.692114	620.88	2469.71	6034.41	0.028305	0.3607
0.810803	623.36	2397.15	6084.64	0.024994	0.3144
0.929682	625.69	2329.88	6131.87	0.02222	0.276
1.04942	627.87	2397.15	6176.27	0.024994	0.2437
1.1702	629.9	2329.88	6217.53	0.02222	0.2164
1.29071	631.82	2267.29	6257.09	0.019863	0.1932
1.41271	633.63	2208.86	6293.82	0.017844	0.1732
1.53433	635.34	2154.14	6327.07	0.016116	0.156
1.65739	636.94	2102.75	6361.39	0.01461	0.141
1.53433	635.34	2054.36	6327.07	0.01331	0.156
1.65739	636.94	2008.7	6361.39	0.012157	0.141
1.7799	638.48	1965.5	6392.85	0.011152	0.128
1.90327	639.92	1924.56	6422.67	0.01026	0.1166
2.02667	641.29	1885.69	6449.25	0.009472	0.1065
2.15085	642.6	1848.71	6476.17	0.008765	0.09755
2.27509	643.85	1813.48	6501.11	0.008134	0.08961
2.39954	645.05	1779.85	6524.59	0.007568	0.08254
2.52392	646.21	1747.72	6548.24	0.007057	0.07621
2.64872	647.29	1716.98	6569.56	0.006596	0.07054
2.7737	648.34	1687.52	6590.04	0.006177	0.06541
2.89931	649.32	1659.26	6609.04	0.005796	0.06079
3.02444	650.3	1632.12	6627.75	0.00545	0.0566
3.14958	651.23	1659.26	6645.77	0.005796	0.0528
3.27471	652.11	1632.12	6662.43	0.00545	0.04935
3.40054	652.95	1606.03	6678.03	0.005133	0.04618
3.52624	653.77	1580.93	6693.29	0.004844	0.04329
3.65126	654.57	1556.74	6708.2	0.004577	0.04065
3.77714	655.31	1533.42	6722.63	0.004331	0.03822
3.65126	654.57	1510.92	6708.2	0.004106	0.04065
3.77714	655.31	1489.19	6722.63	0.003896	0.03822
3.90249	656.06	1468.19	6735.15	0.003703	0.03598
4.02884	656.78	1447.87	6748.06	0.003523	0.0339
4.15384	657.44	1428.2	6760.26	0.003357	0.03201

Table 5.0. Equilibrium flow results for a hypersonic nozzle .

x-distance	I_{sp}	Temp	Velocity	Density	Pressure
m	sec	K	m/sec	Kg/m3	atm
4.278	658.12	1409.16	6771.96	0.003204	0.03025
4.40334	658.75	1390.69	6783.23	0.003059	0.02863
4.52921	659.37	1372.79	6792.92	0.002924	0.02711
4.65442	659.97	1355.41	6803.32	0.002798	0.0257
4.77964	660.54	1338.54	6812.99	0.00268	0.02439
4.90434	661.09	1322.15	6822.14	0.00257	0.02318
5.03023	661.64	1306.21	6831.02	0.002465	0.02204
5.15352	662.17	1290.71	6839.69	0.002369	0.02098
5.28972	662.73	1306.21	6848.74	0.002465	0.0199
5.40414	663.16	1290.71	6855.45	0.002369	0.01906
5.52958	663.65	1275.63	6863	0.002269	0.01817
5.65369	664.12	1260.95	6869.97	0.00219	0.01736
5.77785	664.58	1246.66	6878.06	0.002108	0.01659
5.90204	665.02	1232.73	6885.33	0.002031	0.01587
5.77785	664.58	1219.15	6878.06	0.001958	0.01659
5.90204	665.02	1205.9	6885.33	0.001889	0.01587
6.02827	665.45	1192.98	6891.11	0.001823	0.01518
6.15298	665.87	1180.37	6897.58	0.001761	0.01454
6.39991	666.69	1168.06	6909.68	0.001647	0.01336
6.52563	667.07	1156.04	6915.2	0.001593	0.01282
6.65092	667.44	1144.29	6920.84	0.001542	0.01231
6.77514	667.82	1132.81	6926.38	0.001493	0.01182
6.89832	668.17	1121.59	6931.77	0.001448	0.01137
7.02358	668.52	1110.61	6936.81	0.001403	0.01094
7.14773	668.87	1099.87	6941.52	0.001362	0.01052
7.27211	669.22	1089.36	6946.48	0.001321	0.01013
7.39688	669.54	1079.07	6951.53	0.001283	0.009084
7.52188	669.86	1089.36	6955.89	0.001321	0.009074
7.64707	670.17	1079.07	6962.52	0.001283	0.009064
7.77206	670.48	1069	6964.69	0.001246	0.008743
7.89669	670.78	1059.14	6968.99	0.00121	0.008437
8.02136	671.07	1049.47	6973.25	0.001177	0.008147
8.14921	671.36	1040	6973.67	0.001144	0.007869
8.02136	671.07	1030.72	6973.25	0.001113	0.007604
8.14921	671.36	1021.62	6973.67	0.001083	0.007351
8.27192	671.64	1012.69	6982.87	0.001054	0.007604
8.39572	671.92	1003.94	6985.16	0.001027	0.007351
8.52199	672.19	995.35	6989.71	0.001	0.007109

Table 5.0. Equilibrium flow results for a hypersonic nozzle .

APPENDIX E

DETAILED CHEMISTRY FLOW RESULTS TABLE

x-distance	I_{sp}	Temp	Velocity	Density	Pressure
m	sec	K	m/sec	Kg/m3	atm
0	600.58	3072	5634	0.07144	1
0.1	604.32	2964.74	5681.74	0.061	0.8236
0.2	607.66	2883.16	5723.26	0.0527	0.6908
0.3	610.68	2811.34	5760.49	0.046	0.5867
0.4	613.42	2744.84	5794.32	0.0405	0.5033
0.5	615.92	2682.07	5825.29	0.0405	0.4355
0.6	618.22	2622.35	5853.79	0.0359	0.3796
0.7	620.34	2565.36	5880.15	0.0288	0.3332
0.8	622.31	2510.91	5904.61	0.026	0.2942
0.7	624.13	2458.87	5927.39	0.0236	0.2612
0.8	625.83	2409.15	5948.65	0.0215	0.2331
0.9	627.42	2361.63	5968.56	0.0197	0.209
1	625.83	2409.15	5948.65	0.0181	0.1882
1.1	627.42	2361.63	5968.56	0.0167	0.1701
1.2	628.91	2316.21	5987.24	0.0154	0.1882
1.3	630.3	2272.78	6004.81	0.0143	0.1701
1.4	631.62	2231.23	6021.38	0.0133	0.1544
1.5	632.86	2191.45	6037.02	0.0124	0.1405
1.6	634.03	2153.36	6051.82	0.0116	0.1284
1.7	635.14	2116.84	6065.85	0.0108	0.1176
1.8	636.19	2081.8	6079.17	0.0102	0.108
1.9	637.19	2048.17	6091.83	0.00957	0.0995
2	638.15	2015.85	6103.9	0.0102	0.09187
2.1	639.05	1984.77	6115.4	0.00957	0.08503
2.2	639.92	1954.86	6126.39	0.00902	0.07887
2.3	640.75	1926.04	6136.89	0.00851	0.0733
2.4	641.54	1898.27	6146.95	0.00804	0.06827
2.5	642.29	1871.47	6156.59	0.00761	0.06369
2.4	643.02	1845.59	6165.83	0.00722	0.05953
2.5	643.72	1820.59	6174.71	0.00685	0.05574
2.6	644.39	1796.41	6183.25	0.00651	0.05227
2.7	643.72	1820.59	6174.71	0.0062	0.04908
2.8	644.39	1796.41	6183.25	0.0059	0.04616
2.9	645.03	1773.02	6191.46	0.00563	0.04908
3	645.65	1750.37	6199.37	0.00538	0.04616
3.1	646.25	1728.43	6206.99	0.00514	0.04348
3.2	646.83	1707.15	6214.35	0.00492	0.041
3.3	647.38	1686.51	6221.45	0.00471	0.03871
3.4	647.92	1666.47	6228.31	0.00452	0.0366

Table 6.0. Detailed chemistry flow results for a hypersonic nozzle .

x-distance	I_{sp}	Temp	Velocity	Density	Pressure
m	sec	K	m/sec	Kg/m3	atm
3.5	648.44	1647	6234.94	0.00433	0.03464
3.6	648.94	1628.09	6241.36	0.00416	0.03282
3.7	649.42	1609.7	6247.57	0.00433	0.03113
3.8	649.89	1591.81	6253.59	0.00416	0.02956
3.9	650.35	1574.4	6259.42	0.004	0.02809
4	650.79	1557.44	6265.08	0.00385	0.02672
4.1	651.22	1540.91	6270.57	0.0037	0.02545
4.2	651.63	1524.81	6275.9	0.00357	0.02425
4.3	652.03	1509.11	6281.07	0.00344	0.02313
4.4	652.43	1493.79	6286.11	0.00332	0.02208
4.5	652.81	1478.83	6291	0.0032	0.02109
4.6	653.18	1464.24	6292.3	0.00309	0.02017
4.7	653.54	1449.98	6295.76	0.00299	0.01929
4.8	653.89	1436.05	6300.39	0.00289	0.01847
4.9	654.23	1422.43	6304.9	0.00279	0.0177
5	654.56	1409.11	6309.3	0.0027	0.01697
5.1	654.88	1396.09	6313.58	0.00262	0.01628
5.2	655.2	1383.35	6321.83	0.00254	0.01563
5.3	655.51	1370.87	6325.8	0.00246	0.01501
5.4	655.81	1358.66	6329.68	0.00238	0.01442
5.5	656.1	1346.7	6333.47	0.00231	0.01387
5.6	656.39	1334.99	6337.17	0.00238	0.01335
5.7	656.66	1323.51	6340.78	0.00231	0.01285
5.8	656.94	1312.26	6344.31	0.00225	0.01238
5.9	657.2	1301.22	6347.76	0.00218	0.01193
5.8	657.46	1290.41	6351.14	0.00212	0.0115
5.9	657.72	1279.79	6354.44	0.00206	0.01109
6	657.97	1269.38	6357.67	0.002	0.0107
6.1	657.72	1279.79	6360.83	0.00195	0.01033
6.2	657.97	1269.38	6357.67	0.0019	0.009982
6.3	658.21	1259.16	6360.83	0.00185	0.01033
6.4	658.45	1249.13	6363.92	0.0018	0.009982
6.5	658.68	1239.28	6366.95	0.00175	0.009646
6.6	658.91	1229.61	6369.92	0.00171	0.009325
6.7	659.14	1220.11	6372.83	0.00166	0.009019
6.8	659.35	1210.77	6375.68	0.00162	0.008726
6.9	659.57	1201.6	6378.48	0.00158	0.008446
7	659.78	1192.59	6381.22	0.00154	0.008178

Table 6.0. Detailed chemistry flow results for a hypersonic nozzle .

x-distance	I_sp	Temp	Velocity	Density	Pressure
m	sec	K	m/sec	Kg/m3	atm
7.1	659.99	1183.72	6383.9	0.00151	0.007921
7.2	660.19	1175.01	6386.54	0.00147	0.007675
7.3	660.39	1166.44	6389.12	0.00151	0.00744
7.4	660.58	1158.02	6391.66	0.00147	0.007214
7.5	660.77	1149.72	6394.15	0.00144	0.006998
7.6	660.96	1141.57	6396.59	0.0014	0.00679
7.5	661.14	1133.54	6398.99	0.00137	0.00659
7.6	661.32	1125.64	6401.35	0.00134	0.006399
7.7	661.5	1117.86	6403.67	0.00131	0.006215
7.8	661.32	1125.64	6405.94	0.00128	0.006038
7.9	661.5	1117.86	6403.67	0.00125	0.005868
8	661.67	1110.21	6405.94	0.00122	0.006038
8.1	661.84	1102.67	6408.18	0.0012	0.005868
8.2	662.01	1095.24	6410.37	0.00117	0.005704
8.3	662.18	1087.93	6412.53	0.00115	0.005546
8.4	662.34	1080.73	6414.65	0.00112	0.005395
8.5	662.5	1073.63	6416.74	0.0011	0.005248

Table 6.0. Detailed chemistry flow results for a hypersonic nozzle

APPENDIX F

SENSITIVITY RESULTS TABLES

Time	Reactions numbers						
millisec	17	2	20	21	28	3	5
0	0	0	0	0	0	0	0
1.04E-04	8.84E-04	4.68E-04	-1.15E-03	9.30E-04	2.30E-04	-2.06E-03	-3.79E-03
2.09E-04	1.44E-03	9.63E-04	-1.89E-03	1.62E-03	2.89E-04	-3.20E-03	-5.37E-03
3.09E-04	2.04E-03	1.23E-03	-2.72E-03	2.34E-03	3.60E-04	-3.75E-03	-6.47E-03
4.09E-04	2.55E-03	1.49E-03	-3.23E-03	2.86E-03	4.26E-04	-4.63E-03	-7.50E-03
5.09E-04	3.15E-03	1.74E-03	-3.73E-03	3.38E-03	4.90E-04	-5.64E-03	-9.20E-03
6.09E-04	3.77E-03	2.02E-03	-4.55E-03	3.88E-03	6.14E-04	-6.64E-03	-1.08E-02
7.21E-04	4.61E-03	2.52E-03	-5.54E-03	4.90E-03	7.37E-04	-7.63E-03	-1.32E-02
8.32E-04	5.59E-03	3.01E-03	-6.52E-03	5.87E-03	8.59E-04	-9.40E-03	-1.58E-02
9.21E-04	6.57E-03	3.50E-03	-7.50E-03	6.80E-03	9.87E-04	-1.11E-02	-1.84E-02
1.01E-03	7.55E-03	4.06E-03	-8.45E-03	7.78E-03	1.23E-03	-1.26E-02	-2.13E-02
1.14E-03	9.24E-03	4.85E-03	-1.04E-02	9.70E-03	1.48E-03	-1.53E-02	-2.58E-02
1.27E-03	1.09E-02	5.78E-03	-1.23E-02	1.15E-02	1.71E-03	-1.83E-02	-3.03E-02
1.43E-03	1.35E-02	7.25E-03	-1.55E-02	1.39E-02	2.13E-03	-2.32E-02	-3.87E-02
1.50E-03	1.51E-02	8.13E-03	-1.83E-02	1.56E-02	2.45E-03	-2.66E-02	-4.49E-02

Table 7.0. Sensitivity results for a hypersonic nozzle at inlet conditions P=1atm and Temperature 3072 K.

Time	Reactions numbers						
millisec	17	2	20	21	28	3	5
0	0	0	0	0	0	0	0
1.04E-04	5.59E-04	0.00E+00	4.33E-04	5.92E-04	-9.49E-05	1.15E-03	2.52E-03
2.09E-04	1.04E-03	-8.26E-05	5.24E-04	1.19E-03	-1.14E-04	2.25E-03	3.11E-03
3.09E-04	1.53E-03	-9.73E-05	6.70E-04	1.70E-03	-1.39E-04	3.41E-03	3.68E-03
4.09E-04	2.08E-03	-1.08E-04	7.98E-04	2.32E-03	-1.72E-04	4.89E-03	4.48E-03
5.09E-04	2.58E-03	-1.07E-04	9.23E-04	2.83E-03	-2.04E-04	6.13E-03	5.49E-03
6.09E-04	3.08E-03	1.18E-04	1.12E-03	3.32E-03	-2.35E-04	7.60E-03	6.48E-03
7.21E-04	3.64E-03	2.04E-04	1.36E-03	3.92E-03	-2.90E-04	9.36E-03	7.47E-03
8.32E-04	4.44E-03	2.42E-04	1.61E-03	4.71E-03	-3.52E-04	1.13E-02	9.08E-03
9.21E-04	5.21E-03	3.10E-04	1.85E-03	5.44E-03	-4.15E-04	1.33E-02	1.04E-02
1.01E-03	5.89E-03	3.63E-04	2.24E-03	6.41E-03	-4.75E-04	1.52E-02	1.23E-02
1.14E-03	7.17E-03	4.11E-04	2.73E-03	7.65E-03	-5.86E-04	1.84E-02	1.49E-02
1.27E-03	8.66E-03	4.76E-04	3.22E-03	9.22E-03	-7.06E-04	2.20E-02	1.82E-02
1.43E-03	1.08E-02	5.62E-04	3.71E-03	1.17E-02	-8.30E-04	2.69E-02	2.27E-02
1.50E-03	1.24E-02	7.04E-04	4.49E-03	1.33E-02	-9.52E-04	3.05E-02	2.60E-02

Table 8.0. Sensitivity results for a hypersonic nozzle at outlet conditions P=0.005248atm and Temperature 1073.63 K.

Time millisec	Reaction 20	Time millisec	Reaction 17	Time millisec	Reaction 2	Reaction 21
0.00E+00	0	0	0	0	0	0
1.40E-05	2.36E-03	2.27E-05	4.50E-04	1.04E-04	1.00E-05	2.60E-04
2.27E-05	3.18E-03	4.55E-05	7.30E-04	2.09E-04	2.00E-05	2.10E-04
4.55E-05	3.69E-03	6.82E-05	9.10E-04	3.09E-04	8.00E-05	1.80E-04
6.82E-05	4.33E-03	1.04E-04	1.00E-03	4.09E-04	1.06E-04	1.70E-04
1.04E-04	4.40E-03	2.09E-04	9.50E-04	5.09E-04	1.70E-04	1.20E-04
2.09E-04	3.91E-03	3.09E-04	8.20E-04	6.09E-04	2.09E-04	1.00E-04
3.09E-04	3.27E-03	4.09E-04	6.40E-04	7.21E-04	2.90E-04	9.10E-05
4.09E-04	2.63E-03	5.09E-04	5.09E-04	8.32E-04	3.70E-04	8.10E-05
5.09E-04	2.18E-03	6.09E-04	3.83E-04	9.21E-04	4.60E-04	7.20E-05
6.09E-04	1.92E-03	7.21E-04	2.67E-04	1.01E-03	5.50E-04	7.10E-05
7.21E-04	1.71E-03	8.32E-04	1.98E-04	1.14E-03	6.50E-04	6.80E-05
8.32E-04	1.55E-03	9.21E-04	1.90E-04	1.27E-03	7.63E-04	6.70E-05
9.21E-04	1.45E-03	1.01E-03	1.86E-04	1.35E-03	8.10E-04	6.60E-05
1.01E-03	1.33E-03	1.14E-03	1.52E-04	1.43E-03	8.90E-04	6.50E-05
1.14E-03	1.18E-03	1.27E-03	1.17E-04	1.46E-03	9.30E-04	6.40E-05
1.27E-03	1.12E-03	1.35E-03	9.54E-05	1.50E-03	1.00E-03	6.30E-05
1.35E-03	1.09E-03	1.43E-03	9.60E-05			
1.43E-03	1.05E-03	1.46E-03	9.20E-05			
1.35E-03	1.09E-03	1.43E-03	9.60E-05			
1.43E-03	1.05E-03	1.46E-03	9.20E-05			
1.46E-03	1.02E-03	1.50E-03	9.00E-05			
1.50E-03	1.00E-03					

Table 9.0. Sensitivity results through out a hypersonic nozzle

Time	Reaction	Reaction	Reaction
millisec	28	3	5
0	0	0	0
1.04E-04	2.50E-04	2.00E-05	1.17E-04
2.09E-04	3.70E-04	4.00E-05	2.33E-04
3.09E-04	4.30E-04	8.10E-05	3.13E-04
4.09E-04	4.86E-04	1.00E-04	4.06E-04
5.09E-04	5.40E-04	1.30E-04	4.86E-04
6.09E-04	5.50E-04	1.80E-04	5.56E-04
7.21E-04	5.70E-04	2.20E-04	6.48E-04
8.32E-04	6.10E-04	2.80E-04	7.86E-04
9.21E-04	6.20E-04	3.40E-04	8.44E-04
1.01E-03	6.30E-04	3.94E-04	9.48E-04
1.14E-03	6.40E-04	4.52E-04	1.05E-03
1.27E-03	6.50E-04	5.09E-04	1.12E-03
1.35E-03	6.60E-04	5.56E-04	1.13E-03
1.43E-03	6.80E-04	6.02E-04	1.14E-03
1.46E-03	7.10E-04	6.20E-04	1.17E-03
1.50E-03	7.20E-04	6.50E-04	1.18E-03

Table 9.0. Sensitivity results through out a hypersonic nozzle .

APPENDIX G

FROZEN FLOW PROGRAM

```fortran
PROGRAM FROZEN
C
C*******double precision
IMPLICIT DOUBLE PRECISION (A-H,O-Z), INTEGER (I-N)
C*******END double precision
C*******single precision
C      IMPLICIT REAL (A-H,O-Z), INTEGER (I-N)
C*******END single precision
C
PARAMETER(LENIWK=4000, LENRWK=4000, LENCWK=500,
+ NK=5, NLMAX=55, LRW=1000, LIW=100, LIN=5, LOUT=6,
+ LINCK=25, KMAX=50)
 DIMENSION X(KMAX), Y(KMAX), Z(KMAX), ELWRK(LRW), IELWRK(LIW)

 INTEGER
C
COMMON /PARAM/ ICKWRK(4000), RCKWRK(4000), Y, KK
COMMON /ALG/ ALFA, A, PI, RO
COMMON /ALG/ ALFA, A, PI, RO


C
CHARACTER CCKWRK(LENCWK)*16,KSYM(KMAX)*16
LOGICAL KERR,IERR

EXTERNAL FUN

DATA KERR/.FALSE./,X/KMAX*0.0/,KSYM/KMAX*' '/
C
C     Open the Chemkin II LINK file
open (linck, form = 'unformatted', file = 'cklink')
C     Initialize Chemkin II
C
CALL CKINIT (LENIWK,LENRWK,LENCWK,LINCK,
+ LOUT,ICKWRK,RCKWRK,CCKWRK)
CALL CKINDX (ICKWRK,RCKWRK,MM,KK,II,NFIT)

CALL CKSYMS (CCKWRK,LOUT,KSYM,IERR)
CALL CKSYMS (CCKWRK,LOUT,KSYM,IERR)

DO 100 I=1,14
X(I)=0.0
100    CONTINUE

DO 200 I=1,14
PRINT 202, KSYM(I)
202     FORMAT(/,3X,'ENTER THE VALUE OF X(',A4,'):')
READ*,X(I)
200    CONTINUE

CALL CKXTY (X,ICKWRK,RCKWRK,Y)
```

```
PRINT 400
400 FORMAT(/,/,3X,'ENTER INITIAL PRESSURE (atm):')
READ*,PE
P = PE*1013250
READ*,PE
P = PE*1013250

PRINT 450
450 FORMAT(/,3X,'ENTER INITIAL TEMPERATURE (K):')
READ*,T

PRINT 500
500 FORMAT(/,3X,'ENTER INITIAL VELOCITY (m/s):')
READ*,VE
V = VE*100

PRINT 550
550 FORMAT(/,3X,'ENTER INITIAL AREA (m^2):')
READ*,AE
A = AE*10000

PRINT 600
600  FORMAT(/,3X,'ENTER INITIAL DISTANCE (cm):')
PRINT 600
600  FORMAT(/,3X,'ENTER INITIAL DISTANCE (cm):')
READ*,XO

PRINT 650
650 FORMAT(/,3X,'ENTER SPACE STEP (cm):')
READ*,XT

PRINT 700
700 FORMAT(/,3X,'ENTER NUMBER OF STEPS:')
READ*,NT

ALFA = 12.431/57.3

Q = -1.0
PI = ACOS(Q)
RO = SQRT(A/PI)
C
C     INITIAL CONDITIONS
C
C     INITIAL CONDITIONS
C
Z(1) = P
Z(2) = T
Z(3) = V
CALL CKRHOY (Z(1),Z(2),Y,ICKWRK,RCKWRK,Z(4))
C
```

```fortran
C     INTEGRATION CONTROL PARAMETERS
C
NEQ = 4
MF  = 10
ITOL= 1
IOPT= 0
RTOL= 1.0d-6
ITASK= 1
ATOL = 1.0d-9
ISTATE= 1
ATOL = 1.0d-9
ISTATE= 1

C
DO 40 I=1,NT
XEND = XO + XT

CALL LSODE (FUN, NEQ, Z, XO, XEND, ITOL, RTOL, ATOL,
+ ITASK, ISTATE, IOPT, ELWRK, LRW, IELWRK, LIW, JAC, MF)
C

P = Z(1)
T = Z(2)
V = Z(3)
RHO = Z(4)
C
SPI = V / 980 + P/(RHO*V*980)

PRINT 1001,XO,P,T,SPI,RHO
PRINT 1001,XO,P,T,SPI,RHO
1001   FORMAT(/2X,F10.2,2X,E14.4,2X,F10.2,2X,F10.2,2X,E14.3)

C      PRINT 50, XO, P, T, SPI, RHO
C50    FORMAT(/,2X,'X= ',F10.2,2X,'P= ',E14.4,2X,'T= ',F10.2,2X,
C      + 'ISP= ',F10.2,2X,'RHO= ',E14.3)

40    CONTINUE
STOP
END
C
SUBROUTINE FUN(NEQ,XO,Z,ZDOT)
C
C******double precision
IMPLICIT DOUBLE PRECISION (A-H,O-Z), INTEGER(I-N)
C******END double precision
C******single precision
C      IMPLICIT REAL (A-H,O-Z), INTEGER (I-N)
C******single precision
C      IMPLICIT REAL (A-H,O-Z), INTEGER (I-N)
C******END single precision
```

```
DIMENSION Z(4),ZDOT(4),Y(50)
COMMON /PARAM/ ICKWRK(4000), RCKWRK(4000), Y, KK
COMMON /ALG/ ALFA, A, PI, RO

C
C     FORM GOVERNING EQUATIONS
C


C*****************************************************************
C     Z(1) = P   ;   ZDOT(1) = DP/DX
C     Z(2) = T   ;   ZDOT(2) = DT/DX
C     Z(3) = V   ;   ZDOT(3) = DV/DX
C     Z(4) = RHO ;   ZDOT(4) = DRHO/DX
C     CPBML = CP MEAN
C     AF = CHANGE OF AREA WITH XO
C     CPBML = CP MEAN
C     AF = CHANGE OF AREA WITH XO
C     DADX = DAF/DX
C     A = INITIAL AREA
C     XO = DIRECTION IN X OF NOZZLE
C*****************************************************************


CALL CKCPBS (Z(2),Y,ICKWRK,RCKWRK,CPBML)

AF = A + 2*PI*RO*XO*DTAN(ALFA) + PI*(XO**2)*(DTAN(ALFA))**2

DADX = 2*PI*(RO + XO*DTAN(ALFA))*DTAN(ALFA)

D1 = -(DADX)/AF

R1 = -(Z(4)*Z(3))/Z(1)

R2 = 1/Z(3)
R2 = 1/Z(3)

R3 = (Z(3))/(CPBML*Z(2))

ZDOT(3) = D1/(R1+R2+R3)

ZDOT(1) = -Z(4)*Z(3)*ZDOT(3)

ZDOT(4) = -(Z(4)*ZDOT(3))/Z(3)-(DADX*Z(4))/AF

ZDOT(2) = -(Z(3)*ZDOT(3))/CPBML

C
RETURN

END
```

APPENDIX H

DETAILED CHEMISTRY FLOW PROGRAM

```fortran
PROGRAM KINETICS
C
C*******double precision
IMPLICIT DOUBLE PRECISION (A-H,O-Z), INTEGER (I-N)
C*******END double precision
C*******single precision
C      IMPLICIT REAL (A-H,O-Z), INTEGER (I-N)
C*******END single precision
C
PARAMETER(LENIWK=4000, LENRWK=4000, LENCWK=500,
+ NK=5, NLMAX=55, LRW=1000, LIW=100, LIN=5, LOUT=6,
+ LINCK=25, KMAX=50)
DIMENSION X(KMAX),Y(KMAX),Z(KMAX),ELWRK(LRW),IELWRK(LIW)

INTEGER I
C
COMMON /PARAM/ ICKWRK(4000),RCKWRK(4000),WT(50),WDOT(50),
+         HMS(50),Y(50),KK
COMMON /PARAM/ ICKWRK(4000),RCKWRK(4000),WT(50),WDOT(50),
+         HMS(50),Y(50),KK
COMMON /ALG/ ALFA, A, PI, RO, RU

C
CHARACTER CCKWRK(LENCWK)*16,KSYM(KMAX)*16
LOGICAL KERR,IERR

EXTERNAL FUN

DATA KERR/.FALSE./,X/KMAX*0.0/,KSYM/KMAX*' '/
C
C      Open the Chemkin II LINK file
open (linck, form = 'unformatted', file = 'cklink')
C      Initialize Chemkin II
C
CALL CKINIT (LENIWK,LENRWK,LENCWK,LINCK,
+ LOUT,ICKWRK,RCKWRK,CCKWRK)
CALL CKINDX (ICKWRK,RCKWRK,MM,KK,II,NFIT)
+ LOUT,ICKWRK,RCKWRK,CCKWRK)
CALL CKINDX (ICKWRK,RCKWRK,MM,KK,II,NFIT)

CALL CKSYMS (CCKWRK,LOUT,KSYM,IERR)

DO 100 I=1,14
X(I)=0.0
100    CONTINUE

DO 200 I=1,14
PRINT 202, KSYM(I)
202    FORMAT(/,3X,'ENTER THE VALUE OF X(',A4,'):')
READ*,X(I)
```

```
200    CONTINUE
CALL CKXTY (X,ICKWRK,RCKWRK,Z(5))

PRINT 400
400    FORMAT(/,/,3X,'ENTER INITIAL PRESSURE (atm):')
PRINT 400
400    FORMAT(/,/,3X,'ENTER INITIAL PRESSURE (atm):')
READ*,PE
P = PE*1013250

PRINT 450
450    FORMAT(/,3X,'ENTER INITIAL TEMPERATURE (K):')
READ*,T

PRINT 500
500    FORMAT(/,3X,'ENTER INITIAL VELOCITY (m/s):')
READ*,VE
V = VE*100

PRINT 550
550    FORMAT(/,3X,'ENTER INITIAL AREA (m^2):')
READ*,AE
A = AE*10000
A = AE*10000

PRINT 600
600    FORMAT(/,3X,'ENTER INITIAL DISTANCE (cm):')
READ*,XO

PRINT 650
650    FORMAT(/,3X,'ENTER SPACE STEP (cm):')
READ*,XT

PRINT 700
700    FORMAT(/,3X,'ENTER NUMBER OF STEPS:')
READ*,NT

ALFA = 12.431/57.3

Q = -1.0
PI = ACOS(Q)
RO = SQRT(A/PI)
PI = ACOS(Q)
RO = SQRT(A/PI)
C
C      INITIAL CONDITIONS
C
Z(1) = P
Z(2) = T
Z(3) = V
```

```
      CALL CKRHOY (Z(1),Z(2),Z(5),ICKWRK,RCKWRK,Z(4))

      CALL CKWT (ICKWRK,RCKWRK,WT)

      CALL CKRP (ICKWRK,RCKWRK,RU,RUC,PATM)

C
C      INTEGRATION CONTROL PARAMETERS
C

      NEQ = 18
      NEQ = 18
      MF  = 22
      ITOL= 1
      IOPT= 0
      RTOL= 1.0d-6
      ITASK= 1
      ATOL = 1.0d-9
      ISTATE= 1

C
      DO 40 I=1,NT
      XEND = XO + XT

      CALL LSODE (FUN, NEQ, Z, XO, XEND, ITOL, RTOL, ATOL,
     + ITASK, ISTATE, IOPT, ELWRK, LRW, IELWRK, LIW, JAC, MF)
C

      P = Z(1)
      P = Z(1)
      T = Z(2)
      V = Z(3)
      RHO = Z(4)

C
      SPI = V / 980 + P/(RHO*V*980)

      PRINT 1001,XO,SPI
 1001 FORMAT(/2X,F10.2,2X,E14.4,2X,F10.2,2X,F10.2,2X,E14.3)

C      PRINT 50, XO, P, T, SPI, RHO
C50   FORMAT(/,2X,'X= ',F10.2,2X,'P= ',E14.4,2X,'T= ',F10.2,2X,
C     + 'ISP= ',F10.2,2X,'RHO= ',E14.3)

 40   CONTINUE
      STOP
      END
      STOP
      END
C
```

```fortran
      SUBROUTINE FUN(NEQ,XO,Z,ZDOT)
C
C*******double precision
      IMPLICIT DOUBLE PRECISION (A-H,O-Z), INTEGER(I-N)
C*******END double precision
C*******single precision
C     IMPLICIT REAL (A-H,O-Z), INTEGER (I-N)
C*******END single precision
C
      DIMENSION Z(NEQ),ZDOT(NEQ),WT(50),WDOT(50),HMS(50),Y(50)
      COMMON /PARAM/ ICKWRK(4000),RCKWRK(4000),WT,WDOT,HMS,Y,KK
      COMMON /ALG/ ALFA, A, PI, RO, RU


C
C
C     FORM GOVERNING EQUATIONS
C

      CALL CKHMS (Z(2),ICKWRK,RCKWRK,HMS)
      CALL CKWYP (Z(1),Z(2),Z(5),ICKWRK,RCKWRK,WDOT)
      CALL CKCPBS (Z(2),Z(5),ICKWRK,RCKWRK,CPB)
      CALL CKMMWY (Z(5),ICKWRK,RCKWRK,WTM)


      AF = A + 2*PI*RO*XO*DTAN(ALFA) + PI*(XO**2)*(DTAN(ALFA))**2

      DADX = 2*PI*(RO + XO*DTAN(ALFA))*DTAN(ALFA)

      SUM = 0.0

      SUM1 = 0.0
      SUM1 = 0.0

      SUM2 = 0.0

      DO 800  K = 1,14

      ZDOT(K+4) = (WDOT(K)*WT(K))/(Z(4)*Z(3))

      SUM = SUM + ZDOT(K+4)/WT(K)

800      CONTINUE

      DO 801  K = 1,14

      SUM1 = SUM1 + HMS(K)*WDOT(K)*WT(K)

801      CONTINUE
```

```
DO 802  K = 1,14
DO 802  K = 1,14

SUM2 = SUM2 + Z(K+4)/WT(K)

802      CONTINUE

R1 = SUM

R11 = SUM2

R2 = (Z(4)*Z(2)*R1)/R11

R3 = SUM1

R4 = R3/(Z(3)*CPB)

R5 = (Z(2)*Z(4)*DADX)/AF
R5 = (Z(2)*Z(4)*DADX)/AF

R6 = 1/(RU*R11)-(1/CPB)-Z(2)/(Z(3)**2)

ZDOT(1) = (R2-R4-R5)/R6

ZDOT(3) = -ZDOT(1)/(Z(4)*Z(3))

R41 = ZDOT(3)/Z(3) + DADX/AF

ZDOT(4) = -Z(4)*R41

R7 = -RU*Z(2)*R11*ZDOT(4)

R8 = -Z(4)*RU*Z(2)*R1

R31 = R7+R8+ZDOT(1)

R32 = Z(4)*RU*R11
R32 = Z(4)*RU*R11

ZDOT(2) = R31/R32

C

RETURN

END
```

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