

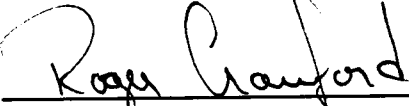
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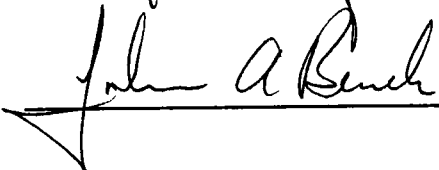
I am submitting herewith a thesis written by Mark C. Jechura entitled "Equilibrium Hydrogen-Oxygen Flow Field Calculations of a High Area Ratio Nozzle Using Full Navier-Stokes Code." I have examined the final copy of this thesis for form and content and recommend that it be accepted in partial fulfillment for the degree of Master of Science, with a major in Aerospace Engineering.



Frank G. Collins, Major Professor

We have read this thesis and
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EQUILIBRIUM HYDROGEN-OXYGEN FLOW FIELD CALCULATIONS
OF A
HIGH AREA RATIO NOZZLE
USING
FULL NAVIER-STOKES CODE

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

Mark C. Jechura

May, 1992

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ABSTRACT

The author modified a surface fit version of the PARCEQ implicit, Beam and Warming, real gas Navier-Stokes code to correct the calculation of the constant pressure specific heat and the compressibility parameter, to correct the surface fit model at low temperatures and to improve the computational speed of the calculation of gas properties using surface fits. The author then conducted a study of the NASA LeRC 1030:1 nozzle using the new version of the code. Based upon studies performed at NASA LeRC, the author assumed laminar flow in the nozzle for all calculations. The author presents calculated results of performance and compares them with published calculations performed with the Two-Dimensional Kinetics Program (TDK) and with published nozzle test data. The author also presents calculated results of nozzle wall heat flux and compares them with published nozzle test data. The performance results show agreement with TDK calculations and nozzle test data. The heat flux results indicate that the flow in the nozzle was not laminar, as claimed in the studies performed at NASA LeRC, but rather was transitional or fully turbulent.

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NOMENCLATURE

a	Speed of sound
A_T	Throat area
C_f	Skin friction coefficient
$C_{F,V,Th(TDK)}$	Theoretical two-dimensional kinetics vacuum thrust coefficient obtained from TDK program
C_h	Stanton number
C_p	Constant pressure specific heat
C^*	Experimentally measured characteristic exhaust velocity
C_{TH}^*	Theoretical characteristic exhaust velocity obtained from CEC program
e	Specific internal energy
F_v	Vacuum thrust
F_{scale}	Scaling factor
g	Gravitational constant, 9.807 m/s^2
h	Free convection coefficient, specific enthalpy
H	Enthalpy
I	Grid index, theoretical subsonic specific impulse inside the combustion chamber obtained from CEC program
k	Thermal conductivity
m	Mass
$\dot{m}$	Mass flow rate

M	Molecular weight, Mach number
n	Normal distance
P	Pressure
Pr	Prandtl number
q	Heat flux
$\mathbf{Q}$	Vector containing nondimensionalized flow properties
r	Recovery factor, radial direction
R	Radius
$\mathfrak{R}$	Universal gas constant
t	Time
T	Temperature
V_{av}	Mass-averaged injection velocity of propellants
x	Transformed specific internal energy
y	Transformed density
y^+	Y-plus
Z	Compressibility factor

Greek Symbols

α	Thermal diffusivity
β	Ratio of enthalpy to internal energy
Δ	Operator expressing a change in the value of a variable
ϵ_c	Combustor contraction area ratio

γ	Ratio of specific heats
η_c^*	Characteristic exhaust velocity efficiency
ρ	Density
τ	Shear stress
μ	Viscosity

Abbreviations

ANSI	American National Standards Institute
CEC	Chemical Equilibrium Composition program
cm	Centimeter
GL	Graphics Language
JANNAF	Joint Army, Navy, NASA, Air Force
kg	Kilogram
kN	Kilonewton
kPa	Kilopascal
K	Degrees Kelvin
LeRC	Lewis Research Center
m	Meter
MHz	Megahertz
MJ	Megajoule
N	Newton
NASA	National Aeronautics and Space Administration

O/F	Oxidant to fuel mixture ratio
PARC	Propulsion Ames Research Code
PARCEQ	Equilibrium Propulsion Ames Research Code
PHIGS	Programmers' Hierarchial Interactive Graphic Standard
RAM	Random Access Memory
RETF	Rocket Engine Test Facility
s	Second
TDK	Two Dimensional Kinetics Code
%	Percent

Subscripts

<i>a</i>	Ambient, static
<i>aw</i>	Adiabatic wall
<i>c</i>	Combustion chamber
<i>e</i>	Equilibrium, constant specific internal energy, effective
<i>i</i>	Inner
<i>ideal</i>	One-dimensional theory
<i>L</i>	Lower
<i>o</i>	Outer
<i>P</i>	Constant pressure, products
<i>r</i>	Reference
<i>R</i>	Reactants

T	Total
t	Total
U	Upper
w	Wall
ρ	Constant density
∞	Free stream

Superscripts

*	Nondimensionalized
°	Formation enthalpy, degree

CHAPTER I

INTRODUCTION

The design of rocket engines for space applications, ranging from the small thrusters needed for orbital maintenance and attitude adjustment on the Space Station Freedom to the large rocket engines needed for a lunar launched mission to Mars, will require low operating pressures and nozzles with high area ratios. These design conditions, in turn, will lead to thick boundary layers within the nozzle [1]¹. The Joint Army, Navy, NASA, Air Force (JANNAF) methodology [2], the current industry standard for the development of rocket engine designs, cannot simulate strong viscous/inviscid interactions. New design tools capable of simulating these effects within the nozzle, therefore, must be developed and validated before wall heat flux and nozzle performance predictions necessary for the design of rocket engines used for space applications can be made with confidence and accuracy.

One JANNAF rocket engine design tool used to predict wall heat flux and nozzle performance parameters is the Two-Dimensional Kinetics computer analysis program (TDK) [3]. TDK, which models kinetic equilibrium chemistry conditions within the nozzle, calculates the core flow separately from the boundary layer and then couples the two solutions to obtain the final flow field solution. The coupling technique for the solution of the flow field works quite well as long as the boundary layer is thin. However, under operating conditions which create thick boundary layers, such as those

¹Numbers in brackets refer to similarly numbered references in the List of References.

necessary for space application, it is uncertain how accurately TDK will make flow field predictions. It is believed that under such conditions that a full Navier-Stokes code which calculates the boundary layer and core flow field simultaneously will be necessary to make accurate flow field predictions.

The purpose of this research was to compare the TDK code with a full Navier-Stokes code to determine how accurately each code could predict the flow field within a high area ratio nozzle operating at low pressure conditions. The research, which was performed at The University of Tennessee - Calspan Center for Space Transportation and Applied Research (CSTAR), was funded under contract with NASA and Rocketdyne Division, Rockwell International Corporation.

For a comparison with TDK, the PARCEQ real gas full Navier-Stokes was used. PARCEQ was chosen because it had been previously validated for equilibrium chemistry calculations by Saladino [4] and Myruski [1] and also because its algorithm, which is based upon the original PARC2D algorithm [5], has been validated for many different flow field calculations, including high area ratio nozzles encountering strong viscous/inviscid interaction effects at the exit plane.

Gaseous hydrogen - gaseous oxygen test firings of a 1030:1 area ratio nozzle conducted at NASA LeRC (Lewis Research Center) by Pavli et al [6] were chosen to make an initial comparison between TDK, PARCEQ and test data. The wall heat flux and nozzle performance test data and TDK calculations simulating the test conditions have been extensively published [7], [8]. The large amount of easily accessible

information created a large data base from which to make a comparison between TDK, PARCEQ and the test data.

The 1030:1 area ratio nozzle was a good case for validation because the nozzle had a high area ratio and the operating pressures in the combustion chamber during test firing were low (2413 kPa). Although the test conditions did not totally simulate the conditions encountered by a rocket engine operating in the space environment (the boundary layer within the nozzle was still relatively thin), a failure under these conditions to make accurate predictions would be a good indication of failure under more extreme conditions.

The only chemistry options that were available in the original versions of PARCEQ were equilibrium air and equilibrium hydrogen-oxygen and the model used for the determination of equilibrium thermochemical and transport properties was very computationally intensive. Hence, prior to making any calculations on the 1030:1 nozzle, Klomfaß [9] removed the existing chemistry model within the code and replaced it with a model which incorporated surface fits of equilibrium thermochemical and transport properties. This author modified Klomfaß' model to correct the calculation of the constant pressure specific heat C_p and the compressibility parameter Z , corrected the model at low temperatures and improved the computational speed of the model. The combination of the modifications by Klomfaß and this author decreased the computational time needed for the determination of equilibrium thermochemical and transport properties and generalized the code so that any chemistry model could easily be incorporated into the code through the specification of the proper surface fits.

After these modifications were made, the data from the test firings of the 1030:1 nozzle were examined. Reading 112 was chosen for a comparison of the results from TDK, PARCEQ and the test data (see page 29). Next, surface fits of the equilibrium thermochemical and transport properties were generated and three sets of calculations simulating the test conditions of Reading 112 were performed with the modified version of PARCEQ. Nozzle performance parameters were calculated for two cases, one assuming complete combustion inside the nozzle using the adiabatic flame temperature for the combustion chamber conditions, the other assuming incomplete combustion. The combustion chamber temperature used for the incomplete combustion case was calculated using the characteristic exhaust velocity efficiency. This efficiency is the ratio of the measured characteristic exhaust velocity to the characteristic exhaust velocity predicted by one-dimensional theory.

$$\eta_{C^*} = \frac{C^*}{C_{TH}^*} \quad (1)$$

Using the equation for mass flow rate in the nozzle as predicted by one-dimensional theory,

$$\dot{m} = \sqrt{\frac{\gamma M}{\mathfrak{R}}} \left(\frac{\gamma + 1}{2} \right)^{\frac{-(\gamma + 1)}{2(\gamma - 1)}} \frac{p_c A_T}{\sqrt{T_t}} \quad (2)$$

the definition of the characteristic exhaust velocity,

$$C^* = \frac{p_c A_T}{\dot{m}} \quad (3)$$

and the definition for the characteristic exhaust velocity efficiency, a relation between the combustion chamber temperature for the test conditions and the adiabatic flame temperature was developed.

$$\eta_{C^*} = \left(\frac{T_t}{T_{t,ideal}} \right)^{\frac{1}{\gamma}} \quad (4)$$

The incomplete combustion chamber temperature was calculated using the above relation and was then used for the second set of performance calculations.

The third set of calculations were performed to determine the wall heat flux along the nozzle wall using the discretized form of the heat equation. This set of calculations was performed assuming complete combustion inside the combustion chamber.

The remainder of this thesis has been reserved for the purpose of providing a detailed account of the procedures undertaken to perform these calculations. In doing so, the following chapters provide a description of the computational tools used for the research effort (Chapter II), the modifications made to PARCEQ in order to incorporate the surface fits of equilibrium thermochemical and transport properties (Chapter III), a detailed description of the testing conditions and measurements made on the 1030:1 nozzle (Chapter IV), a presentation of the nozzle performance (Chapter IV) and wall heat flux (Chapter V) calculations, the assumptions used during these calculations, and finally

the conclusions reached by this student after an examination of all the results obtained from this study (Chapter VI).

CHAPTER II

COMPUTATIONAL TOOLS

PARCEQ Code

The PARCEQ code is a modified version of the PARC2D [5] code developed at Arnold Engineering Development Center, Arnold Air Force Base, Tennessee. A complete description of PARCEQ is included in [1] and [4]. The following paragraphs describe some of the major features of the code.

The PARCEQ code employs the Beam and Warming implicit approximate factorization [10] scheme to solve the complete Reynolds-averaged Navier-Stokes equations written in dimensionless conservative form. Jameson-type artificial viscosity formulation [11] exists in this scheme to ensure numerical stability and to dampen high frequency oscillations in the flow field solution.

The code assumes a chemically reacting mixture of thermally perfect gases in chemical and thermal equilibrium (real gas). The calculation of the equilibrium composition and transport properties is based upon statistical mechanics and kinetic theory. Two equilibrium chemistry models are presently available, one for equilibrium air chemistry and another for hydrogen-oxygen chemistry.

PARCEQ can simulate either viscous flows or inviscid flows. The viscous flux terms can be incorporated in only one direction for thin-layer simulations or in both directions to simulate fully viscous flow. For inviscid calculations, the viscous flux terms are dropped.

PARCEQ is designed so that general boundary conditions can be specified by the user. These boundary conditions as well as all other input parameters are specified directly in a FORTRAN namelist file.

The output from PARCEQ is contained in two files. One file contains the calculated values of flow properties at specified grid points within the flow field. The other file contains $\mathbf{Q} = [\rho^*, \rho^* u^*, \rho^* v^*, E_T^*]^2$, the dimensionless dependent variables, and the thermodynamic and transport properties at all grid points (see page 17). This file is used as an input file for the next group of iterations.

Two sets of calculations have been performed using PARCEQ. Saladino [4] has calculated the flow field about a hypersonic vehicle moving through the earth's atmosphere using the equilibrium air chemistry model. Myruski [1] has calculated the flow field inside the Space Shuttle Main Engine Nozzle using the hydrogen-oxygen equilibrium chemistry model. The results of both calculations agree with test data and calculations made by other flow field simulation codes.

EQGAS Software

EQGAS is a software package developed by Klomfaß [9] to create tables of equilibrium thermochemical and transport properties for an arbitrary chemical system. Equilibrium thermochemical properties are calculated on the basis of statistical mechanics. Transport properties are calculated using the elements of kinetic theory. The basic details regarding the algorithm and theory used in the software can be found in [9].

²The notation, $\mathbf{Q}$, will be used to refer to the vector, $\mathbf{Q} = [\rho^*, \rho^* u^*, \rho^* v^*, E_T^*]$, throughout the remainder of this text.

In order to use EQGAS to calculate transport properties, a set of data files containing the coefficients of the curve fits for the collision integrals of all component interactions is required. These data files can be generated from a supplied table of the collision integrals using the SURFIT software (described in the next section). Also, needed are data files containing the spectroscopic data of each of the chemical components occurring over the range of the calculations. All inputs concerning the execution of EQGAS are specified in a file named `exec.dat`³.

EQGAS generates the properties table over a specified temperature and density range or temperature and pressure range. The temperature progression can only be arithmetic, while the density/pressure progression can be either arithmetic or geometric. Different increments of temperature progression can be specified for each density/pressure point by specifying the respective increment in the input file, `temp.tab`. The properties table can also be normalized to a desired enthalpy or internal energy by adjusting the additive energy as discussed in [9]. This feature is attractive because it allows the user to choose a reference system or conform to JANNAF standards [2].

The versatility of EQGAS lies in its ability to create tables for an arbitrary chemical system. Specification of the chemical components, each of the chemical reactions and the initial mole or mass fractions of each component is made in `exec.dat`. With the spectroscopic data for each component and the collision integrals for all component interactions of the chemical system, EQGAS can create tables of properties

³UNIX filenames require specification of the correct case. All files in this paper represent the correct case needed for implementation on a UNIX system.

for reactions occurring from the combustion of fuels to reactions encountered by a vehicle entering the Martian atmosphere.

Klomfaß has conducted several tests to determine how accurately EQGAS computes the thermochemical and transport properties of hydrogen-oxygen equilibrium mixture [9]. His calculations when compared with those performed by Svehla [12] were in good agreement. The two calculations varied slightly because Svehla's method of determining the equilibrium composition was different than Klomfaß.

This author also conducted a test with EQGAS for hydrogen-oxygen with a mixture ratio of 5~~2~~3. Comparisons made with Svehla were in good agreement for the entire range of temperatures and pressures, Table 1 through Table 4. The conclusion of this test was that EQGAS is an acceptable tool for generating a table of equilibrium thermochemical and transport properties for an arbitrary chemical system.

SURFIT Software

SURFIT is a software package designed by Klomfaß [9] to surface fit equilibrium thermochemical and transport properties calculated using EQGAS. SURFIT uses the method of undetermined multipliers to determine the least squares coefficients for a spline-type approximation. The details of the algorithm and the theory behind it can be found in [9]. Since all thermodynamic and transport properties are a function of two variables, SURFIT was designed for the surface fitting of a property in terms of two variables. However, SURFIT can also be used for curve fitting a property in one variable.

TABLE 1

Comparison of Svehla and EQGAS at P = 3040 kPa, O/F = 5%

	Svehla				EQGAS			
T K	C _p J/kg/K	γ _e	M	μ kg/m/s 10 ⁻⁷	C _p J/kg/K	γ _e	M	μ kg/m/s 10 ⁻⁷
600	2553	1.320	13.44	221	2544	1.321	13.44	219
1100	2914	1.270	13.44	387	2881	1.273	13.44	388
1600	3250	1.235	13.44	531	3192	1.240	13.44	554
2100	3541	1.213	13.44	658	3452	1.220	13.44	657
2600	4200	1.187	13.40	772	4060	1.194	13.40	770
3100	6614	1.151	13.16	876	6436	1.157	13.16	877

TABLE 2

Comparison of Svehla and EQGAS at P = 304.0 kPa, O/F = 5%

	Svehla				EQGAS			
T K	C _p J/kg/K	γ _e	M	μ kg/m/s 10 ⁻⁷	C _p J/kg/K	γ _e	M	μ kg/m/s 10 ⁻⁷
600	2553	1.320	13.44	221	2544	1.321	13.44	219
1100	2914	1.270	13.44	387	2881	1.273	13.44	388
1600	3253	1.235	13.44	531	3194	1.240	13.44	554
2100	3644	1.209	13.43	658	3558	1.215	13.43	657
2600	5384	1.162	13.31	772	5265	1.167	13.31	769
3100	14126	1.124	12.49	872	14010	1.126	12.49	873

TABLE 3

Comparison of Svehla and EQGAS at $P = 30.40 \text{ kPa}$, $O/F = 5\%$

T K	Svehla				EQGAS			
	C_p J/kg/K	γ_e	M	μ kg/m/s 10^{-7}	C_p J/kg/K	γ_e	M	μ kg/m/s 10^{-7}
600	2553	1.320	13.44	221	2544	1.321	13.44	219
1100	2914	1.270	13.44	387	2881	1.273	13.44	388
1600	3260	1.235	13.44	531	3202	1.240	13.44	534
2100	3975	1.196	13.41	658	3896	1.210	13.41	656
2600	9875	1.126	13.01	770	9766	1.128	13.00	768
3100	39374	1.113	10.50	853	40200	1.114	10.46	853

TABLE 4

Comparison of Svehla and EQGAS at $P = 3.040 \text{ kPa}$, $O/F = 5\%$

T K	Svehla				EQGAS			
	C_p J/kg/K	γ_e	M	μ kg/m/s 10^{-7}	C_p J/kg/K	γ_e	M	μ kg/m/s 10^{-7}
600	2553	1.320	13.44	221	2544	1.321	13.44	219
1100	2914	1.270	13.44	387	2881	1.273	13.44	388
1600	3284	1.233	13.44	531	3227	1.238	13.44	534
2100	5067	1.167	13.36	658	5011	1.170	13.35	656
2600	27985	1.100	11.94	763	28130	1.102	11.93	761
3100	81954	1.120	7.08	778	83600	1.118	7.00	775

A unique feature of SURFIT is that it allows the user to break the abscissa into separate intervals, each with a different spline condition. This feature allows the surface fits to be optimized over the entire domain for the highest accuracy. Continuity of the zeroth, first or second derivative can be maintained at the transition point between intervals through proper specification.

The input files needed for SURFIT are the *exec.dat* file and *filename.dat* file. The *exec.dat* file contains the input specifications for optimizing the surface fits. The *filename.dat* file contains the data to be surface fit. Upon execution, EQGAS generates an output file named *filename.pol* containing the polynomial coefficients for the surface fit.

SURFIT has been tested for several applications for curve and surface fits (see Klotz [9] and Chapter IV of this paper). The results show that SURFIT is an acceptable tool for generating spline approximations for two or three dimensional data sets.

GRIDGEN Code

The GRIDGEN code was obtained from the Flight Dynamics Laboratory at Wright Patterson Air Force Base, Ohio. GRIDGEN is a multiple block interactive grid generation code developed by General Dynamics Fort Worth Division under contract by the Air Force. A version modified by Brigham Young University was used because of its compatibility with the GL (Graphics Language) library on IBM RISC/6000 POWERstations. A detailed description of the GRIDGEN code can be found in [13] and [14]. The following is a brief description of some of the code's features.

GRIDGEN is composed of three codes GRIDBLOCK, GRIDGEN2D and GRIDGEN3D. GRIDBLOCK defines the blocking structure of the grid through specification of the physical shape and computational size of each block. GRIDGEN2D develops the surface grids on each face of each block. GRIDGEN3D performs the volume generation for a three dimensional grid. Since two dimensional grids only require a single face of a block, they can be generated without GRIDBLOCK or GRIDGEN3D.

The code contains numerous features and options all of which are designed to give the user maximum flexibility in the design and construction of computational grids. Among these are several grid packing and edge definition options, various grid solvers, an adaptive grid generation option and a grid viewing option. The two features which this user found to be particularly invaluable were the specification of break points along edge definitions and the grid viewing option. Break point specification allows the user to specify a point at a particular location within a subface or specify the number of points within a portion of a subface. The viewing option of the code allows the user to translate or enlarge all or a portion of the grid. This feature enables the user to generate and modify grids interactively.

Because of the simplicity of the grids constructed for this work, the author only needed the most basic features of GRIDGEN. However, even in simplicity the power of GRIDGEN as a computational grid generation device was clearly evident.

PLOT3D Code

PLOT3D [15] is a flow field visualization code used to generate flow field parameter contour plots. The code was developed by P. Buning at NASA Ames Research

Center, Moffet Field, California [8]. PLOT3D is designed for visualization of flow fields calculated with the calorically perfect gas assumption. Inputs to the code include the computational grid and Q at each grid point. With these inputs, PLOT3D can produce plots of seventy-four different functions. Four of these functions are used for the direct plotting of Q .

Since the computations performed in this thesis assume real gas behavior, all seventy-four functions available could not be used. Plots had to be made by precalculating four flow field parameters such as Mach number, equilibrium ratio of specific heats, molecular weight and temperature. These values were then input into PLOT3D in place of Q . Plots could then be made by using the functions designated for Q .

IBM RISC/6000 POWERstation

An IBM RISC/6000 POWERstation 320H was used for all the computational work performed in this thesis. The work station is located on the computer system network at the University of Tennessee - Calspan Center for Space Transportation and Applied Research, Tullahoma, Tennessee. It has been fitted with a 640 megabyte hard disk, has 64 megabytes RAM and a clock speed of 25 MHz. The work station is equipped with a UNIX operating system, the graPHIGS graphics library and the AIX XL FORTRAN Compiler [16]. The machine allowed for efficient code development and minimal turn around time for computations.

CHAPTER III

MODIFICATIONS TO PARCEQ

Prior to making the calculations on the 1030:1 nozzle, several modifications were made to the PARCEQ code. These modifications included the incorporation of surface fits of the equilibrium thermochemical and transport properties by Klomfaß [9], modifications to the calculation of the reference properties needed for the dimensionless parameters and changes to the restart and output files, the namelist input file, data blocks and the input of the wall temperature boundary condition.

Incorporation of Surface Fits

Because the calculation of properties by statistical mechanics and kinetic theory is time consuming, the previous version of PARCEQ updated properties infrequently and required a temperature relaxation scheme to maintain a stable solution [1]. To increase computational speed, Klomfaß removed the routines containing the statistical mechanics and kinetic theory from PARCEQ and replaced them with a single routine which calculates the properties using multiple interval surface fits. This author modified the routine to incorporate single interval surface fits. Single interval surface fits were chosen to further increase computational speed. With multiple interval surface fits, the code cannot vectorize because it must choose the correct interval at each point in the flow field for each property at every iteration [17]. The incorporation of single interval surface fits enabled the code to vectorize, allowed the relaxation scheme to be removed and therefore allowed properties to be updated at each iteration.

Klomfaß [9] found that the equilibrium thermochemical and transport properties needed by PARCEQ can be determined with surface fits of $T(\rho, e)$, $p/\rho(\rho, e)$, $C_p(\rho, e)$, $\mu(\rho, e)$ and $k(\rho, e)$. The surface fits are in terms of ρ and e to avoid the peaks in k and C_p which occur when they are expressed in terms of T and ρ , Figure 1 and Figure 2. When the properties are expressed in terms of ρ and e , they exhibit monotonic behavior and therefore can be fitted with the highest accuracy, Figure 3 and Figure 4.

The remaining equilibrium properties needed by the code are β , the ratio of enthalpy to internal energy, M , the molecular weight, Z , the compressibility, a_e , the equilibrium speed of sound and γ_e , the equilibrium ratio of specific heats. Klomfaß [9] found that these properties can be determined from the following formulations:

$$\begin{aligned}
 \beta &= \frac{e + p/\rho}{e} \\
 M &= \frac{p/\rho}{\Re T} \\
 Z &= \frac{M}{M_r \gamma_r} \\
 a_e^2 &= \left(\frac{\partial p}{\partial \rho} \right)_e + \frac{p}{\rho^2} \left(\frac{\partial p}{\partial e} \right)_\rho \\
 \gamma_e &= \frac{a_e^2}{p/\rho}
 \end{aligned} \tag{5}$$

The equilibrium speed of sound is determined through numerical differentiation of the surface fit, $p/\rho(\rho, e)$. The rest of the properties, β , M , Z and γ_e , are computed using the surface fits for $T(\rho, e)$ and $p/\rho(\rho, e)$. Thus, all of the equilibrium thermochemical and transport properties needed by PARCEQ can be determined with five surface fits. As

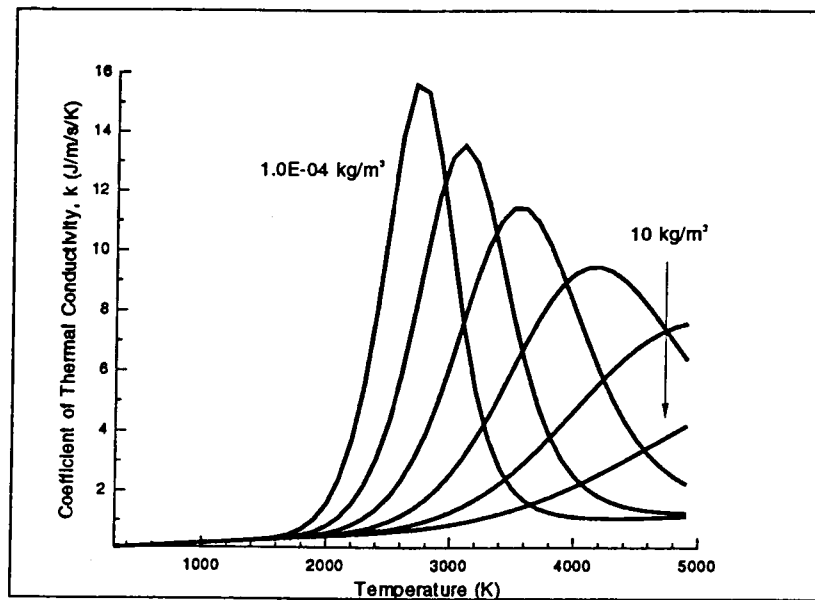


Figure 1 - Surface plot for coefficient of thermal conductivity, $k(T, \rho)$, $O/F = 3.84$.

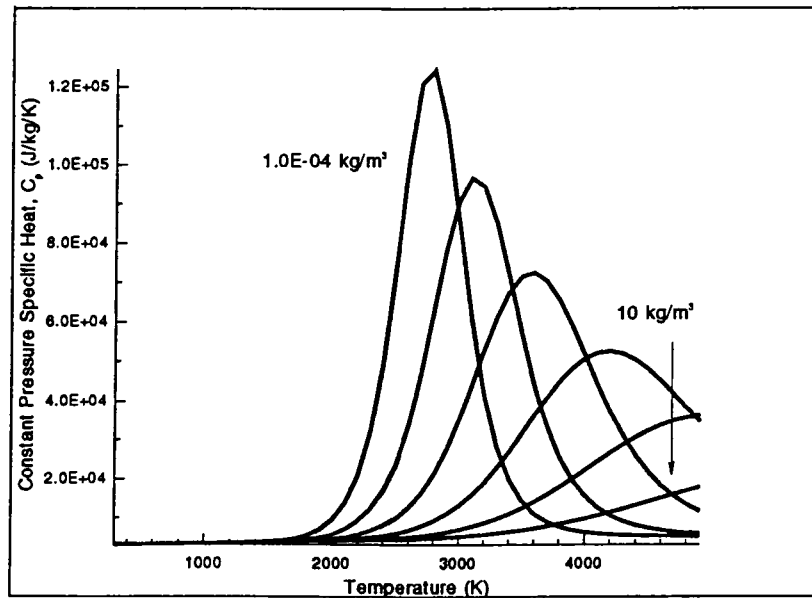


Figure 2 - Surface plot for constant pressure specific heat, $C_p(T, \rho)$, $O/F = 3.84$.

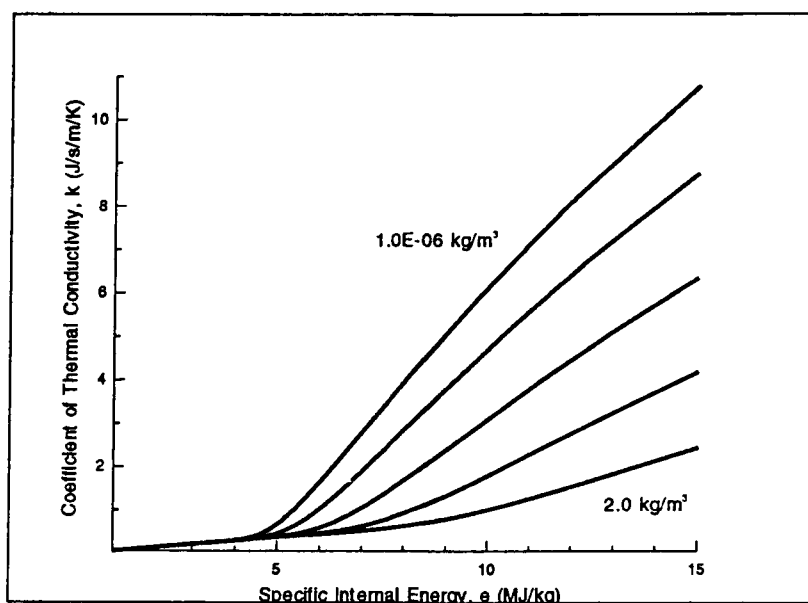


Figure 3 - Surface plot for coefficient of thermal conductivity, $k(\rho, e)$, $O/F = 3.84$.

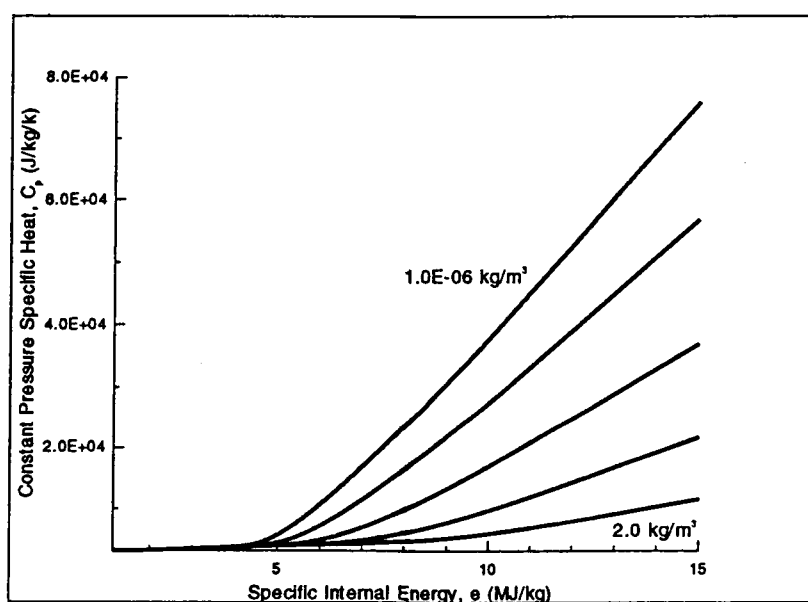


Figure 4 - Surface plot for constant pressure specific heat, $C_p(\rho, e)$, $O/F = 3.84$.

mentioned previously, this author made modifications to the above formulations to correct the calculation of C_p and Z .

Calculation of Reference Properties

PARCEQ contains a routine which calculates the reference properties needed for the dimensionless parameters [1]. These reference properties are based upon adiabatic flame conditions. Inputs for the routine include the combustion chamber pressure, the oxidizer to fuel mixture ratio and the enthalpies of the oxidizer and the fuel before injection to the combustion chamber. The routine iterates using the Method of Bisection [18] until the adiabatic flame temperature is determined. Using the adiabatic flame temperature and the combustion chamber pressure, the reference properties are calculated using the statistical mechanics and kinetic theory routines. This method is not implemented very easily with the surface fits because the needed variables are p and e , not T and p . A different method is now used. The adiabatic flame temperature is determined using the EQGAS software. The p and e are then calculated at the adiabatic flame temperature and combustion chamber pressure. They are specified in INPUT.DAT and the reference properties are computed by the routine containing the surface fits.

Porting Modifications

Several changes to the CRAY X-MP version of PARCEQ were made when it was ported to the IBM POWERstation. The major modifications involved were changes to the restart and output files, the namelist input file, data blocks and the input of the wall temperature boundary condition.

The CRAY restart file was a single file containing the grid, Q and the equilibrium and transport properties at each grid point. To conserve memory, this single file was replaced with two files. These files are GRID.DAT, a file containing the computational grid and QIN.DAT, a file containing Q at each grid point. The incorporation of the surface fits eliminated the need to save the equilibrium and transport property data. This information is now calculated very quickly with surface fits upon restart of the code.

The code still produces a single output file. The name has been changed to QOUT.DAT and only contains the newly calculated values of Q at each grid point. To restart the code, the QIN.DAT file needs to be replaced with the QOUT.DAT file. The changes in the restart and output files resulted in the savings of over two and a half megabytes storage space for each set of iterations.

Because the namelist format in PARCEQ was not totally compatible with the AIX XL FORTRAN Compiler/6000, the namelist input file was replaced with a formatted data input file, INPUT.DAT. INPUT.DAT contains all necessary parameters and boundary specifications needed for the execution of PARCEQ. Unfortunately, INPUT.DAT limits the ease with which the user can change many of the default values within the code. However, these values can still be changed in the BLOCK DATA routine but the code must then be recompiled before execution.

The last two changes were made to the data blocks and the input of the wall temperature boundary condition. Because the AIX XL FORTRAN Compiler/6000 only supports the ANSI standard, all data blocks for default parameters were moved to a BLOCK DATA routine. Previously, the wall temperature profile was specified in

PARCEQ through the use of data blocks. These data blocks and the routine containing them have been removed from the code. Now, the wall temperature boundary condition is input into PARCEQ using the data file temp.vec. The data file temp.vec contains the specified values of the temperature at each grid point along the boundary [19].

Calculations have been conducted on the Space Shuttle Main Engine to validate the surface fit model incorporated into PARCEQ [20]. The performance results show excellent agreement with test data taken from [21] and previous calculations performed with PARCEQ by Myruski [1], Table 5. In comparison with PARCEQ, the surface fits

Table 5

SSME Performance Computations Assuming Laminar Adiabatic Flow

Case	Mass Flow Rate (kg/s)	Thrust (kN)	Specific Impulse (s)
PARCEQ [1]	467.65	2164.94	471.9
PARCEQ using surface fits [20]	472.16	2213.87	461.2
Test data [21]	472.16	2089.76	452.0

decreased computation time by a factor of 10^4 , achieved a higher level of convergence by a factor of ten and decreased the total number of iterations needed for convergence from 12,000 to 9000 total iterations. The results of this test increased confidence in the

⁴ Direct comparison made between the computational time for 1000 iterations using PARCEQ on a CRAY X-MP and 1000 iterations using PARCEQ with surface fits on the IBM RISC/6000 POWERstation 320H. Calculations performed were with the same grid and same initial and boundary conditions.

accuracy of the surface fit model and a decision was made to conduct calculations on the NASA LeRC 1030:1 nozzle using this new version of the code.

CHAPTER IV

PERFORMANCE COMPUTATIONS

Test Conditions

The basis for these calculations are gaseous hydrogen - gaseous oxygen experimental test firings of a 1030:1 area ratio nozzle at a nominal chamber pressure of 2413 kPa. The tests were conducted in an altitude test capsule at the NASA Lewis Rocket Engine Test Facility (RETF), Cleveland, Ohio. A photograph of the nozzle and testing apparatus, as taken from [6], is shown in Figure 5. Each of the test firings was

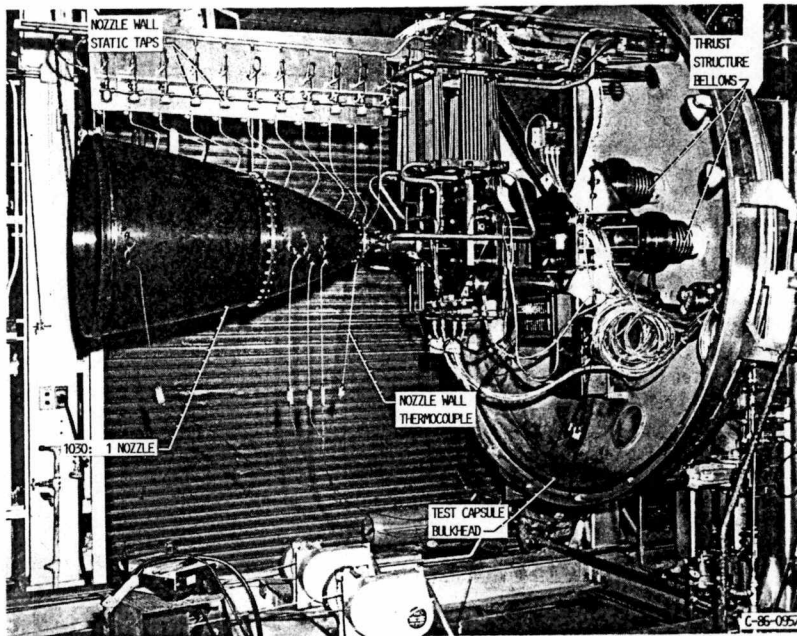


Figure 5 - 1030:1 NASA LeRC nozzle and testing apparatus in test capsule [6].

conducted at a different oxidant to fuel mixture ratio. All tests were performed for three second durations because the pressure measurements indicated that the nozzle flow was fully developed after this period of time. The following paragraphs are a brief description of the test conditions as taken from references [6], [7] and [8].

The 1030:1 nozzle was made of three sections. The first section was connected to the combustion chamber, converged to the 2.54 cm diameter throat and then diverged to an area ratio of 29.9. This section, made of nickel with a ceramic coating on the inner wall, was water cooled from the throat to an area ratio of five. The second and third sections extended from area ratios of 29.9 to 427.5 and 427.5 to 1030, respectively. Each of these sections was made from 0.625 cm thick carbon steel with no ceramic coatings or cooling. The axial distance from the combustion chamber to the throat was 3.5499 cm, and from the throat to the nozzle exit plane was 128.5725 cm.

The combustion chamber pressure for each test firing was not measured directly because circumferential and radial pressure distributions often exist at the injector face. Instead, an integrated mean pressure distribution across the injector face was calculated by Pavli et al [6]. This mean pressure, the effective chamber pressure $p_{c,e}$, was calculated with the ratio $p_{c,e}/p_{c,T}$, where $p_{c,T}$ is the total pressure in the chamber after combustion. This ratio was determined for the combustor at each oxidant to fuel mixture ratio using data taken from atmospheric tests of the combustor fired with a 1.4:1 area ratio copper nozzle. During these atmospheric tests, the vacuum thrust F_v and the injector-end static pressure $p_{c,a}$ were measured. The effective chamber pressure $p_{c,e}$ was then calculated

using F_v , the predicted vacuum thrust coefficient for the nozzle using TDK, $C_{F,v,Th(TDK)}$, the throat area A_t and the following equation:

$$p_{c,e} = \frac{F_v}{C_{F,v,Th(TDK)} A_t} \quad (6)$$

Next, $p_{c,T}$ was calculated using the momentum pressure loss equation.

$$p_{c,T} = p_{c,a} \left[\frac{p_s}{p_T} + \frac{I g - V_{av}}{C_{TH}^* \epsilon_c} \right]^{-1} \quad (7)$$

The injector-end static pressure, $p_{c,a}$, was measured during the low area ratio tests, "the mass-averaged velocity V_{av} was calculated by measuring the injector pressure drops and assuming an effective fuel and oxygen injection area" [13], and the remaining terms in the equation were determined using the Chemical Equilibrium Composition (CEC) program.

After $p_{c,e}/p_{c,T}$ was determined for the combustor at each oxidant to fuel mixture ratio, the 1030:1 nozzle was test fired, the value of $p_{c,a}$ was measured and the effective chamber pressure for each test firing was calculated by adjusting $p_{c,a}$ for momentum pressure loss to obtain $p_{c,T}$ and multiplying it by $p_{c,e}/p_{c,T}$. Using these calculations as a basis, effective chamber pressure was used for the combustion chamber pressure for all calculations with PARCEQ.

A schematic of the nozzle instrumentation system is shown in Figure 6, as taken from [6]. The nozzle wall static pressure was measured at eleven axial locations using

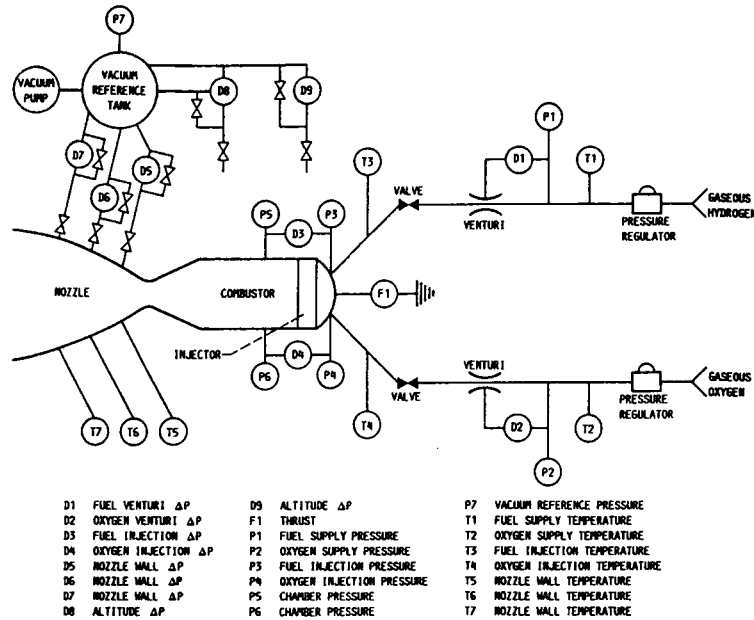


Figure 6 - Schematic of 1030:1 NASA LeRC nozzle instrumentation system [6].

different pressure transducers referenced to the vacuum reference pressure tank. The first measurement was made at an axial distance 3.8882 cm downstream of the throat and the eleventh measurement made was at an axial distance 121.6284 cm downstream of the throat. The nozzle outer wall temperatures were measured at twelve axial locations using thermocouples placed on the nozzle outer wall. The first measurement was made at an axial distance 2.1925 cm downstream of the throat. The remaining measurements were made at the same axial locations as the pressure measurements but were displaced 90° in the circumferential direction from the pressure transducers.

The mass flow rate of the propellants was measured using venturis calibrated for the test conditions. Accurate thrust measurements in the test capsule were made by adding an aneroid corrective term to account for the transient pressure conditions inside

the test capsule. The vacuum thrust was then determined from these measurements by adding the product of the nozzle exit area and the test cell ambient pressure to the measured thrust.

Studies conducted by Smith [22] concluded that the flow in the nozzle is completely laminar at a chamber pressure of 2482 kPa. Smith's conclusion was based upon a comparison of laminar heat flux calculations performed using TDK and the wall heat flux determined from the test data. Using these studies as a basis, laminar flow was assumed in both the axial and radial directions for all computations with PARCEQ.

The chemical components used for the hydrogen-oxygen equilibrium chemistry model were H , O , H_2 , O_2 , OH and H_2O . Myruski [1] and Klomfaß [9] showed that other components such as H_2O_2 and HO_2 have mole fractions less than 0.00001 over the range of conditions in the nozzle and can be ignored for an equilibrium calculation. Figure 7 shows each of the five chemical components used and their mole fractions at an oxidant to fuel mixture ratio of 3.84 and a density of 0.001 kg/m^3 for various temperatures. Considering the five chemical components, four chemical reactions were considered. Each of these chemical reactions is shown below:



After examining the data from the test firings, Reading 112 was chosen for an initial comparison between the experimental data and calculations, Table 6. Reading 112 was chosen to make a comparison because the oxidant to fuel mixture ratio used during

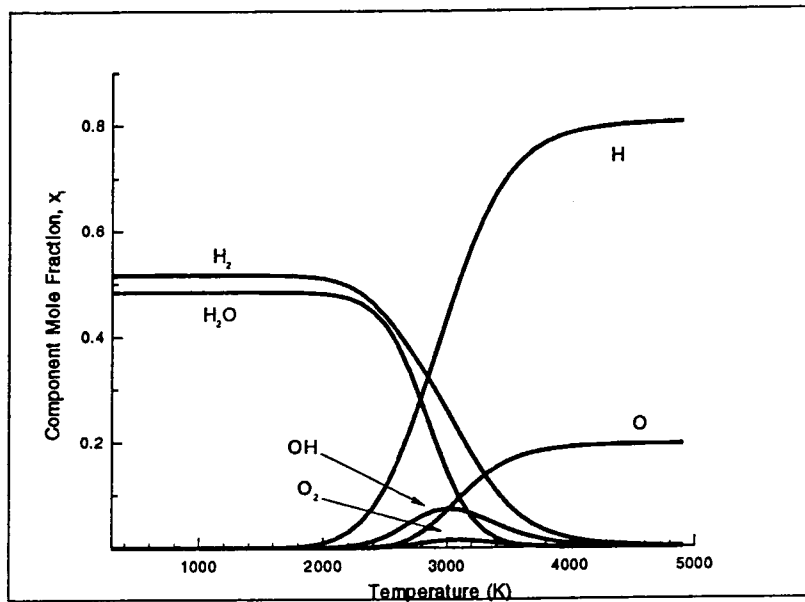


Figure 7 - Equilibrium composition at $\rho = 0.001 \text{ kg/m}^3$, $O/F = 3.84$.

Table 6

Experimental Test Conditions Reading 112

Condition	Value
Effective chamber pressure (kN/m^2)	2482
Oxidant to fuel mixture ratio	3.84
Fuel injection pressure (kN/m^2)	3061
Fuel injection temperature (K)	285.6
Oxidizer injection pressure (kN/m^2)	2809
Oxidizer injection temperature (K)	279.2
Ambient pressure around the nozzle (kN/m^2)	0.2682

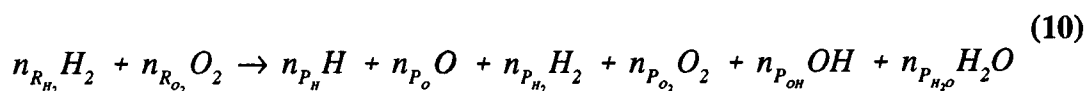
this test firing was at the limit for which TDK could be run. TDK could not run for oxidant to fuel mixture ratios below 3.84 because the program cannot handle the low pressure/low temperature flow conditions which occur when the flow expands to high area ratios. Thus, it was assumed that a comparison of the Reading 112 data would show how well PARCEQ and TDK perform at TDK's lower limit for calculations.

Adiabatic Flame Temperature

The first law of thermodynamics for steady-state steady-flow with no work or heat transfer applied to an open system, neglecting changes in kinetic and potential energy, states that for a combustion process the enthalpy of the products must equal the enthalpy of the reactants [23].

$$H_R = H_P \quad (9)$$

Thus, for the chemical reaction



the first law of thermodynamics becomes

$$\sum_R m_{R_i} (h_R - h_R^o)_i = \sum_P m_{P_i} (h_P - h_P^o)_i + \Delta H^o \quad (11)$$

Given the enthalpy of the reactants and the pressure of the equilibrium mixture of the products, the above equation is satisfied for only one temperature, the adiabatic flame temperature.

The EQGAS software was used to calculate the adiabatic flame temperature for Reading 112 test conditions. The enthalpy of the fuel and the oxidizer at the injector temperature and pressure were calculated using EQGAS. Using the two enthalpies, the total enthalpy of the reactants was calculated. Using the effective chamber pressure and the enthalpy of the reactants, the adiabatic flame temperature was calculated with EQGAS using an iterative technique. An adiabatic flame temperature of 3059 K was calculated with this technique. For comparison, the adiabatic flame temperature was calculated with TDK and the adiabatic flame routine in PARCEQ. The results of these calculations are shown in Table 7. The differences between EQGAS, PARCEQ and TDK are caused by

Table 7
Adiabatic Flame Temperature
Reading 112 Conditions

Computer Program	Adiabatic Flame Temperature (K)
EQGAS	3059
PARCEQ	3027
TDK	3034

small differences in the method used for each calculation. However, despite these differences, the temperature determined using EQGAS was used for the adiabatic flame temperature because the equilibrium thermochemical and transport properties were calculated with EQGAS. Using the calculated value of the adiabatic flame temperature,

ρ and e were computed for use as inputs in the data file, INPUT.DAT. Using ρ and e , the reference properties needed for the dimensionless parameters were calculated using the surface fits.

Surface Fits

A table of the equilibrium thermochemical and transport properties was calculated at an oxidant to fuel mixture ratio of 3.84 using the temperature and density range option available with EQGAS. The specific internal energy, e , was referenced to 1 MJ/kg at 100 K and 1.25 kg/m³ in order to ensure that β was always positive. Since β is part of the equation of state for a real gas, $p = (\beta - 1)\rho e$ [4], it must always have a value greater than unity to maintain the physical consistency of the real gas equation of state. The temperature, T , of the properties table ranged from 100 K to 3600 K and ρ ranged from 10⁻⁶ kg/m³ to 2 kg/m³. These ranges corresponded to an e range of 1 MJ/kg to 15 MJ/kg. This range was chosen based upon an analysis of the conditions in the combustion chamber using the adiabatic flame properties and the conditions at the exit plane of the nozzle using one-dimensional theory [25].

Using the calculated table of properties, surface fits for $T(\rho, e)$, $p/\rho(\rho, e)$, $k(\rho, e)$, $\mu(\rho, e)$ and $C_p(\rho, e)$ were generated using SURFIT. The most accurate surface fits were obtained using the following transformation [9]:

$$\begin{aligned} x &= \frac{e}{10^6} \\ y &= \log_{10} \rho \end{aligned} \tag{12}$$

The plots of the five surface fits are shown in Figure 8 through Figure 12.

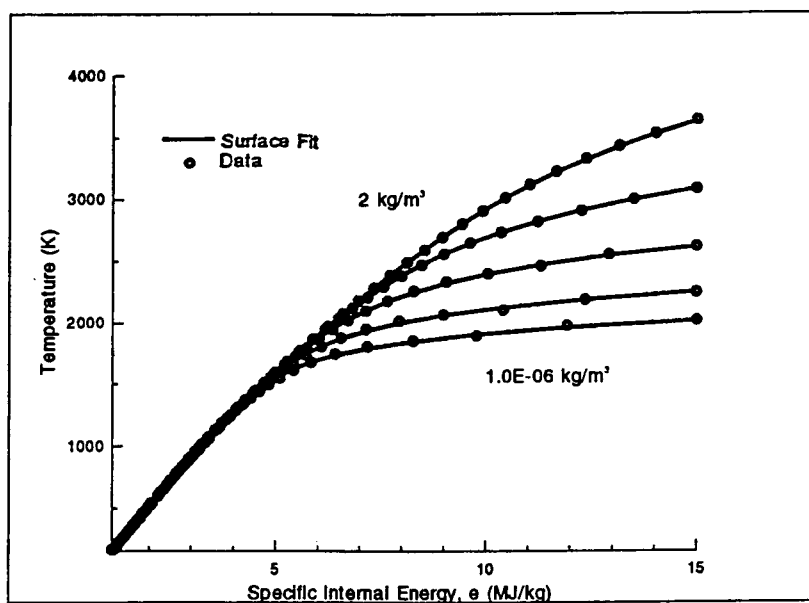


Figure 8 - Surface fit for temperature, $T(\rho, e)$, $O/F = 3.84$.

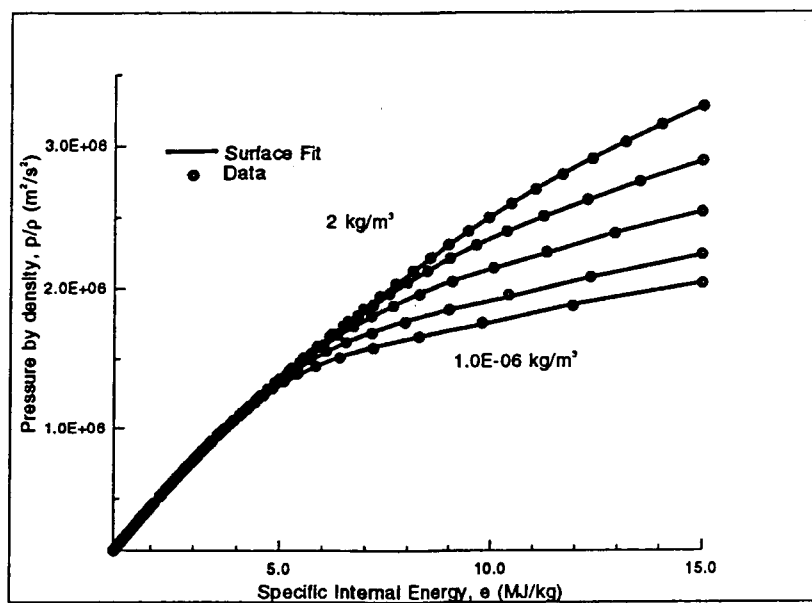


Figure 9 - Surface fit for pressure by density, $p/\rho(\rho, e)$, $O/F = 3.84$.

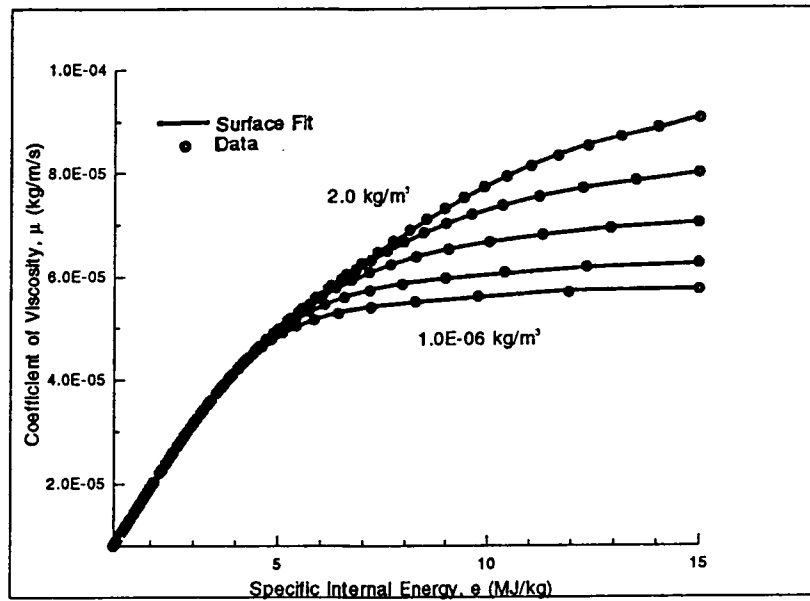


Figure 10 - Surface fit for coefficient of viscosity, $\mu(\rho, e)$, O/F = 3.84.

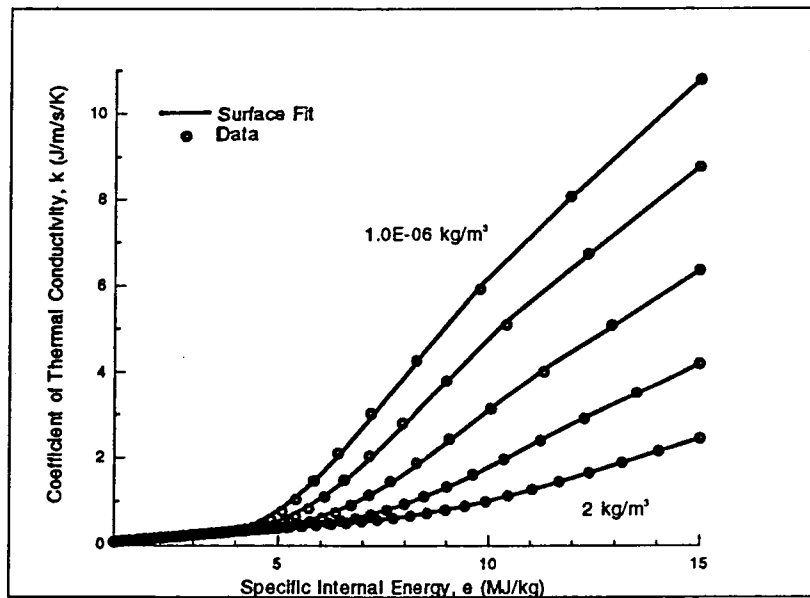


Figure 11 - Surface fit for coefficient of thermal conductivity, $k(\rho, e)$, O/F = 3.84.

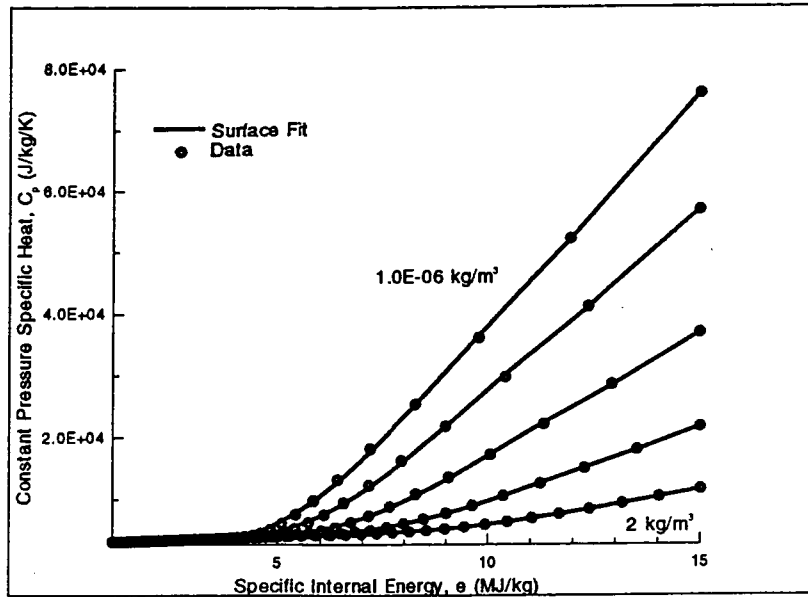


Figure 12 - Surface fit for constant pressure specific heat, $C_p(\rho, e)$, $O/F = 3.84$.

All of the fits agreed very well with the calculated table of properties except for k and C_p in the low energy range, Figure 13 and Figure 15. Since both k and C_p were independent of ρ in the low energy range, they were fitted as a function of temperature from 100 K to 1000 K, Figure 14 and Figure 16. These fits were then incorporated into the code and were called when the temperature went below 1000 K.

Wall Temperature Profile

The wall temperature profile used as the wall temperature boundary condition input was determined from a curve fit of estimated wall temperature in the region where wall temperature was not measured and experimentally determined inner wall temperature in the region where the nozzle outer wall temperature was measured [7]. During the test firing, the outer wall temperatures of the nozzle were measured at 12 area ratio locations.

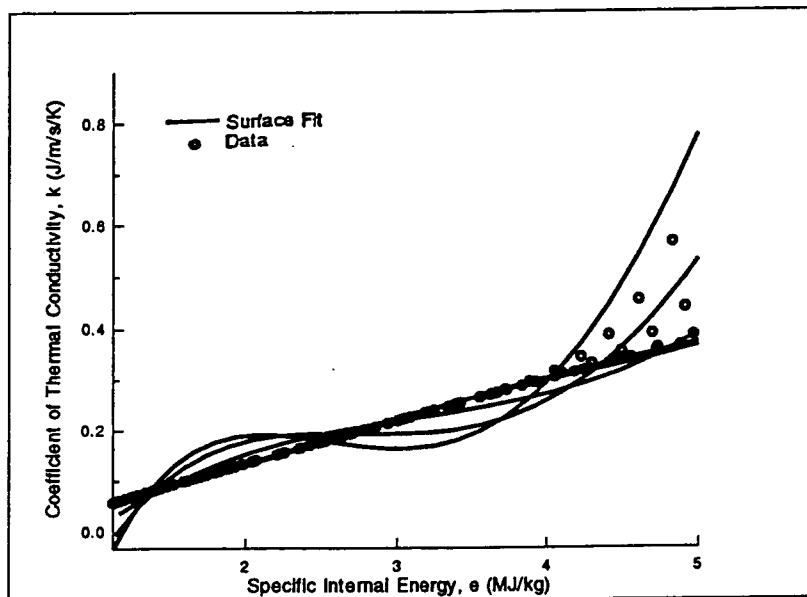


Figure 13 - Surface fit for $k(\rho, e)$ in the low e range, $O/F = 3.84$.

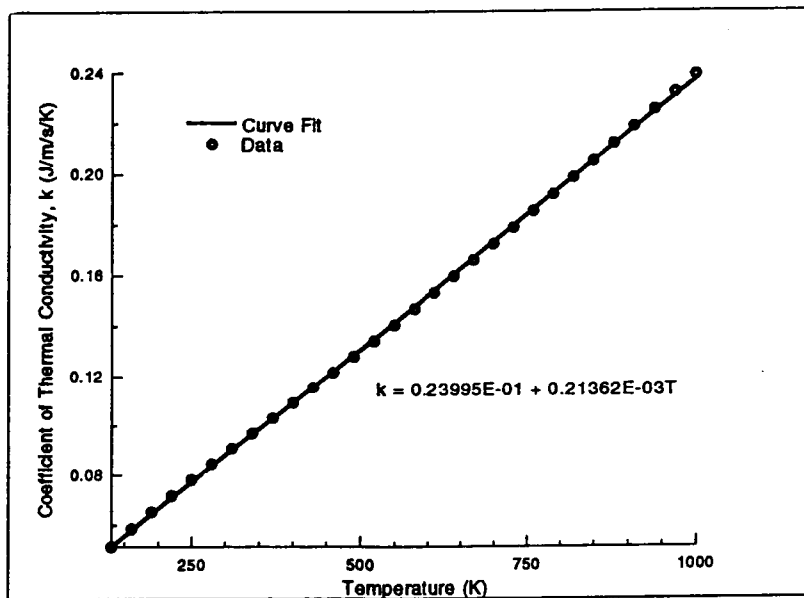


Figure 14 - Curve fit of $k(T)$ for $100\text{ K} < T < 1000\text{ K}$, $O/F = 3.84$.

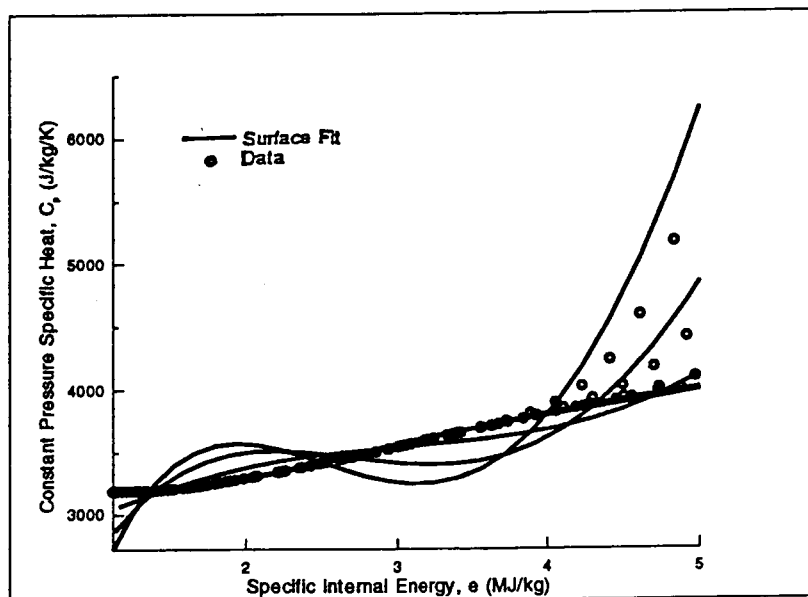


Figure 15 - Surface fit for $C_p(\rho, e)$ in the low e range, $O/F = 3.84$.

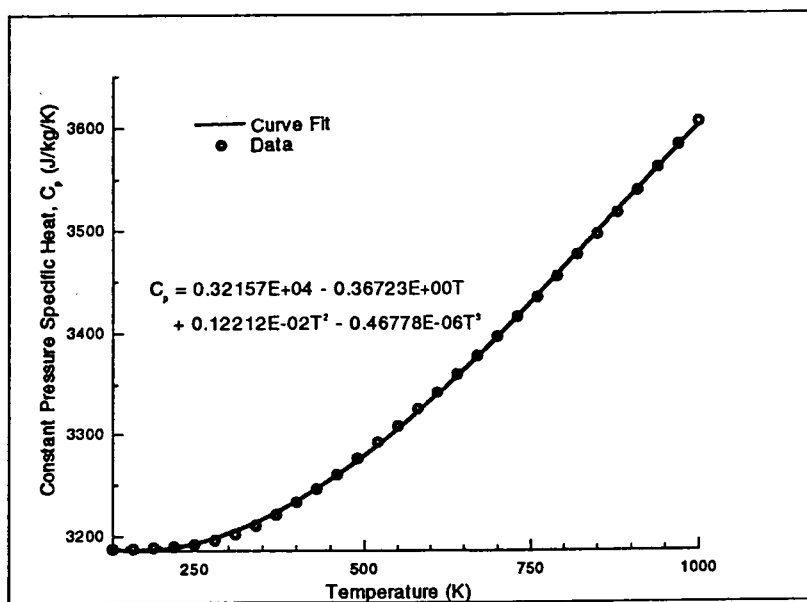


Figure 16 - Curve fit of $C_p(T)$ for $100 \text{ K} < T < 1000 \text{ K}$, $O/F = 3.84$.

The nozzle inner wall temperatures were then determined by Kacynski et al [7] using the energy equation.

$$\rho C_p \left(\frac{\partial T}{\partial t} \right) = \frac{1}{r} \frac{\partial}{\partial r} \left[(kr) \frac{\partial T}{\partial r} \right] \quad (13)$$

The solution of the energy equation for the inner wall temperature assuming constant properties, no axial or circumferential conduction, adiabatic outer wall and a linear rate of temperature rise is [22]

$$T_i = T_o - \frac{R_o^2}{4\alpha} \frac{\partial T}{\partial t} \left[1 - \left(\frac{R_i}{R_o} \right)^2 + \ln \left(\frac{R_i}{R_o} \right)^2 \right] \quad (14)$$

Using the above equation, the outer wall temperature, the rate of outer wall temperature increase, the nozzle wall thickness and the diffusivity of carbon steel, the nozzle inner wall temperature was calculated.

Examination of the experimentally determined inner wall temperatures revealed a slight scatter of the data. The temperatures followed a zig-zag pattern alternating from 6 - 8 K increase in wall temperature to a 6 - 10 K decrease in wall temperature from point to point along the last 80 cm of the nozzle. Although some data scatter is expected, the fluctuations in temperature along the nozzle wall seem to indicate the outer wall was not adiabatic as assumed and quite possibly the measurements were in error as well.

Since the first thermocouple for wall temperature measurement was located 2.193 cm downstream of the throat, nozzle wall temperatures upstream of this point had to be

estimated. The inputs for TDK from [7] were initially used to estimate the wall temperatures in this region. However, using these temperatures, flow heating by the nozzle wall in the throat region was observed. The inputs to TDK were then thoroughly examined to determine if they were a reasonable estimation. Examination determined that the temperatures used were high, particularly in the water cooled throat region where a wall temperature of 2250 K was estimated. The TDK wall temperature estimation was then abandoned for a more reasonable temperature estimation in the throat region. Since there was a copper insert in the throat during the test firing [26], a temperature of 1100 K was used at the throat (information was later obtained that the throat was actually made of nickel as previously mentioned, however, the temperature estimation was still not a bad approximation). This temperature, which is 258 K lower than the melting point of copper [27], seemed to be a reasonable estimation because the temperature in the throat region should have been high but not high enough to melt the copper insert. A nozzle wall temperature of 800 K was estimated upstream of the throat near the first point of the computational grid. This temperature was estimated because upstream of the throat the wall temperature must remain high since it is not far downstream from the combustion chamber, but it still must remain low enough to allow the wall temperature to peak at the throat. Both estimations of wall temperature were further justified after computations were performed and observation of the flow field showed that the flow heating by the wall was eliminated.

Having established a temperature distribution along the wall using the experimentally determined wall temperatures and the estimated wall temperatures, the data

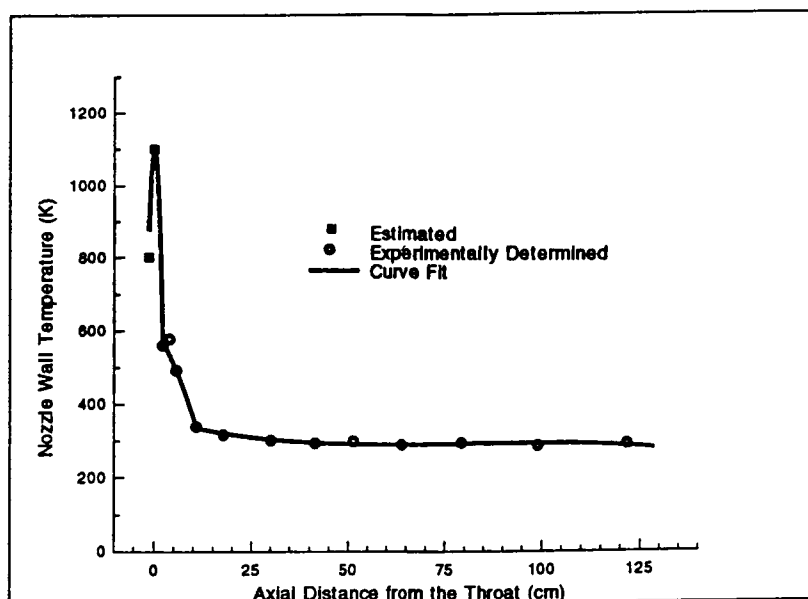


Figure 17 - Plot comparing the estimated and experimentally determined temperatures with those input for the constant wall temperature boundary condition, Reading 112, 1030:1 NASA LeRC nozzle.

points were curve fit. Lagrange second and third order polynomials [18] were used to approximate the first six points and a cubic polynomial generated with SURFIT was used to approximate the remaining eight points, Figure 17. The cubic polynomial for the last eight points was fitted through the data to remove the scatter occurring over the last 80 cm of the nozzle. Using these polynomials and the computational grid, the wall temperature at each grid point was calculated for input as the wall temperature boundary condition.

Computational Grid

GRIDGEN was used to construct a 195 by 80 grid for the prediction of the nozzle performance parameters. The grid was constructed to simulate both the nozzle and the

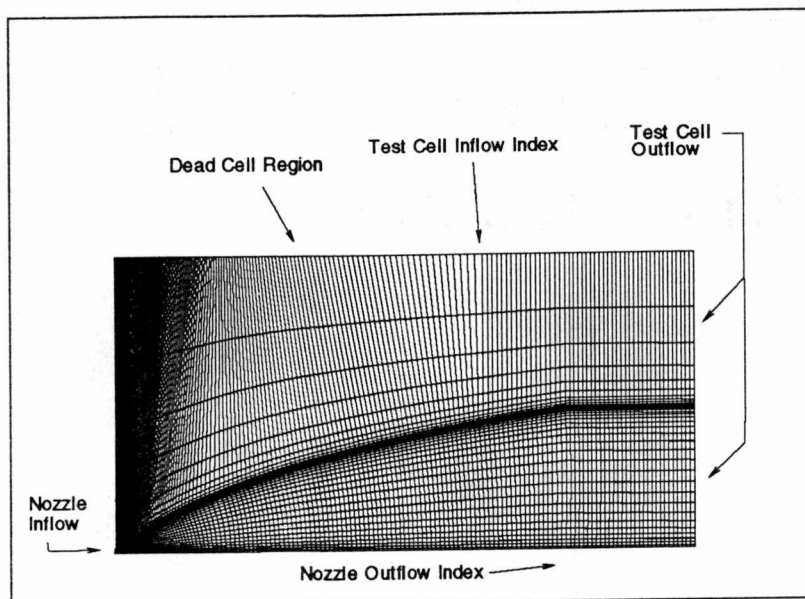


Figure 18 - Computational grid used for the performance calculations, 1030:1 NASA LeRC nozzle (every other point plotted in the radial direction).

test cell, Figure 18. The nozzle coordinates came from shop measurements and were supplied by Albert J. Pavli [28]. By including the test cell as part of the grid, specification of the subsonic outflow pressure boundary condition was avoided. This gives a more realistic calculation, improves exit plane accuracy and eliminates the need for a nozzle extension as was previously used by Orr [29]. However, because PARCEQ is not a blocked computer code, 2940 dead cells had to be generated in the region above the nozzle and to the left of the test cell inflow index.

The first points of the grid start at the area ratio where $M \approx 0.3$, as determined using one-dimensional isentropic theory. Starting the grid at this location instead of inside the combustion chamber increased convergence rates by eliminating the subsonic

local time-step limiting cells located in the combustion chamber region [19]. The grid extended above the nozzle wall and downstream of the exit plane of the nozzle by the length of the exit plane nozzle radius. The grid was constructed this way to capture any expansion or compression shocks that may occur at the nozzle lip.

Because fine resolution of the boundary layer is not necessary for performance prediction, the grid packing toward the nozzle wall was only tight enough to maintain at least three points inside the subsonic portion of the boundary layer. Three subsonic points were chosen so that information could propagate upstream through the subsonic portion of the boundary layer. To maintain accuracy for the axisymmetric calculation, the grid was mildly packed to the axis.

Distribution of points in the axial direction was controlled by using three subfaces within the nozzle, Figure 19. The highest concentration of points was placed in the throat region because the gradients in that region are usually the strongest. The remaining points were distributed by gradually reducing the number of points in each region until the axial spacing was uniform at the nozzle exit.

All subface edges in the radial direction were specified with circular arcs so that the intersection of grid lines at the axis and the nozzle wall would be nearly orthogonal. An orthogonal grid was desired because more accurate results are obtained with PARCEQ if the grid lines are parallel and perpendicular to the local streamline. Orthogonality also reduces the truncation error caused by non-orthogonality and decreases the computational time needed for the solution of the off-diagonal metric tensor terms needed for the Jacobian transformation from physical space to computational space [29]. Using the

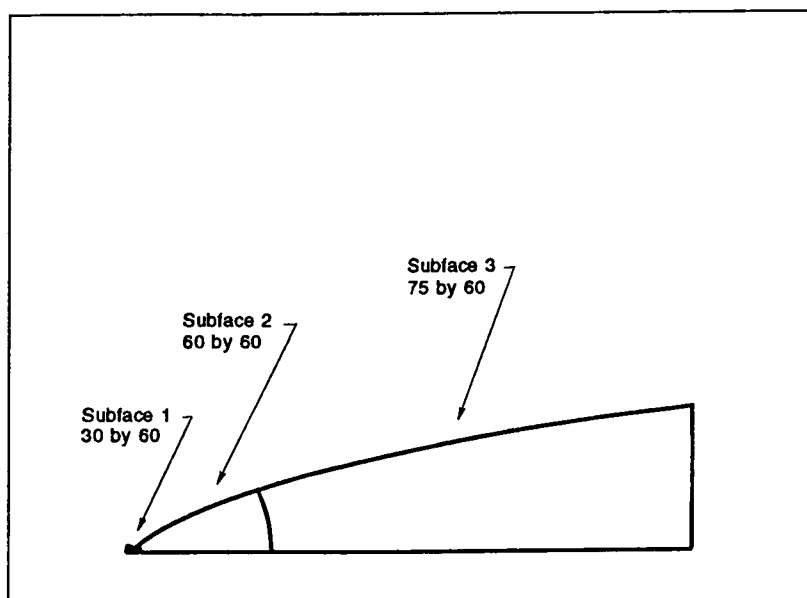


Figure 19 - Subface layout used for the construction of the computational grid used for performance calculations, 1030:1 NASA LeRC nozzle.

viewing feature of GRIDGEN as a check, very good orthogonality between the intersection of grid lines and the nozzle wall was observed.

Boundary Conditions

To simulate conditions inside the nozzle and the test cell, seven boundary conditions had to be specified. The nozzle conditions were specified using the stagnation pressure and total energy at the inflow boundary, the no-slip constant wall temperature condition along the nozzle wall and the symmetric boundary condition along the axis. The test cell conditions were specified using the test cell static pressure and the total energy assuming a gas velocity of 300 m/s for the inflow boundary, a pressure 6% below the test cell static pressure for the outflow boundary and adiabatic slip conditions along

the test cell wall and the nozzle outer wall. A velocity of 300 m/s was chosen to realistically approximate the flow of ambient gases which were pumped out of the test cell with the exhaust gases during test firing. A 6% pressure gradient was determined after trial and error to be low enough to prevent any inflow from occurring at the test cell outflow boundary. A gradient of this magnitude is realistic because at the very least a minimal pressure gradient must have existed in order to remove exhaust gases from the test cell. Adiabatic slip conditions were specified on the test cell wall and the outer nozzle wall to simplify the calculation and to avoid calculation of the interaction at the nozzle lip between the boundary layers of flow along the nozzle outer wall and the flow along the nozzle inner wall. The boundary conditions for both the nozzle and test cell are summarized in Table 8.

Initial Conditions

Specification of initial conditions is arbitrary if only a steady-state solution is required. However, good initial conditions can significantly decrease the computational time to achieve convergence. Typically, one dimensional isentropic theory [30], a bursting diaphragm approach [19] or combustion chamber conditions [1] are used as initial conditions in nozzle computations. One dimensional theory typically results in the fastest convergence times as long as velocity gradients in the radial direction are not large. Using combustion chamber conditions throughout the nozzle results in the slowest convergence because of the large differences between initial and final conditions near the nozzle exit. The bursting diaphragm approach with a high temperature, high pressure gas upstream of the throat and a low pressure, low temperature gas downstream of the throat

Table 8
Nozzle and Test Cell Boundary Conditions

Boundary	Boundary Specification
Nozzle Inflow	stagnation pressure total energy
Axis	axisymmetric
Nozzle inner wall	no-slip constant wall temperature
Test cell inflow	stagnation pressure total energy
Nozzle outer wall	slip adiabatic wall
Test cell wall	slip adiabatic wall
Test cell outflow	static pressure

is not as fast as one dimensional theory but is generally the best initialization technique when one dimensional theory cannot be applied.

One dimensional theory, itself, would not have worked very well in the 1030:1 nozzle because in the throat region there are very strong velocity gradients in the radial direction. The bursting diaphragm technique was not chosen because the small pressure gradient across the test cell was not enough to prevent outflow from occurring at the inflow boundary of the test cell. To initialize the flow field in the 1030:1 nozzle, a combination of both techniques was used. One dimensional theory was used upstream of the throat and a low velocity, low temperature, low pressure condition was specified

in the test cell and the nozzle downstream of the throat. This technique achieved very good initial conditions and avoided the problems associated with the one dimensional theory and bursting diaphragm initialization techniques alone.

Solution Convergence

Two computations were run to predict the performance of the 1030:1 nozzle. One computation was performed with the adiabatic flame temperature assuming 100% combustion. The other computation was performed assuming incomplete combustion. The combustion chamber temperature for the incomplete combustion calculation was determined to be 2790 K using a characteristic exhaust velocity efficiency, η_c , of 95.5%. The two computations were labeled Case I and Case II for the complete combustion calculation and the incomplete combustion calculation, respectively.

Using the initial conditions described above, each case was run for 5000 iterations to allow the flow to transition from the non-physical initial conditions to near steady-state conditions. After 5000 iterations, both flow fields were investigated to determine how close the solution was to steady-state. A small region of separation was observed at the nozzle lip of each flow field. The separation was caused by some inflow into the nozzle from the test cell at the nozzle lip.

The test cell ambient pressure was then reduced to 10% below the last test data point taken on the nozzle wall and then gradually increased back up to the measured test cell ambient pressure over 1000 iterations. This technique eliminated the inflow into the nozzle.

At this point, an additional 1000 iterations was run for Case I. The additional 1000 iterations had no effect upon decreasing the residual. The local time step was then limited to bring the solution to convergence. Over the next 3000 iterations, the residual seemed to oscillate. Investigations revealed that disturbances in the flow field along the mixing region of the subsonic stream of the test cell and the supersonic stream of the nozzle were causing the residual to oscillate. The 3000 iterations were run again without limiting the time-step and the residual did not oscillate.

The convergence history for both runs are shown in Figure 20. Case Ia is with the time-step limited for the last 3000 iterations. Case Ib is without the time step limited for the last 3000 iterations. It is believed that the oscillations in the residual that occurred with the time-step limited were caused by vortices being shed at the nozzle lip. The oscillations show the natural frequencies of the vortices as they are being shed. The oscillations did not show up in the runs without the time step limited because they were time-averaged.

Because of the oscillations in the residual, other parameters were investigated to assure that flow field inside the nozzle was steady-state. Over the last 3000 iterations, plots of mass flow rate throughout the nozzle, nozzle wall pressure, nozzle wall heat flux and the performance parameters were examined for changes. All changes in these plots were minimal. Therefore, there was high confidence that a converged steady-state solution inside the nozzle was achieved after 10,000 total iterations.

A similar method was used to converge the Case II calculation, however, the time step was limited after 6000 iterations instead of 7000 iterations as was done in Case I.

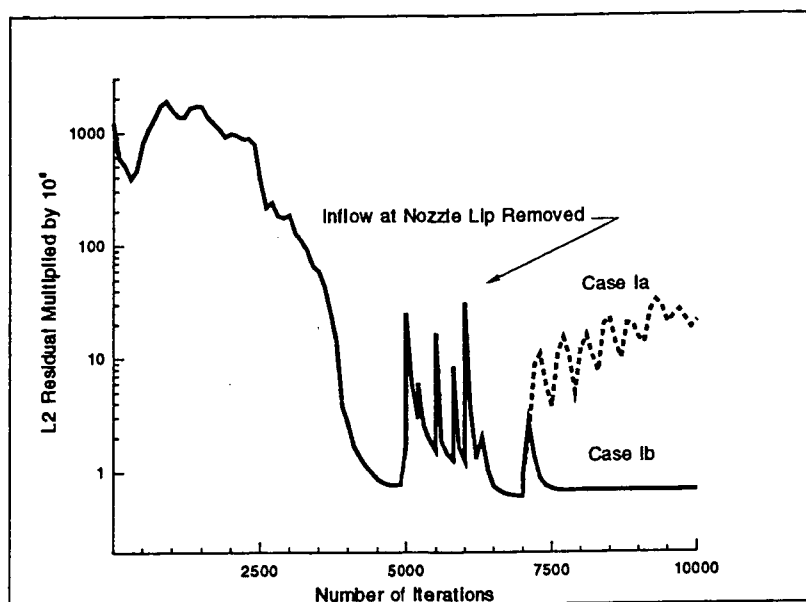


Figure 20 - Convergence history for Case I calculations, Reading 112 1030:1 NASA LeRC nozzle.

The convergence history for the runs with the time-step limited and unlimited over the last 3000 iterations are shown in Figure 21 as Case IIa and Case IIb, respectively. Similar phenomenon with the residual occurred as in Case I. To check for convergence, the same criteria were applied as in Case I. After the last 3000 iterations, no changes in the observed parameters were noticed, therefore convergence was achieved after 9000 total iterations for Case II.

Results and Comparisons

The performance parameters calculated for Case I and Case II are compared in Table 9 with the test measurements and the calculated results with TDK. Case I and II

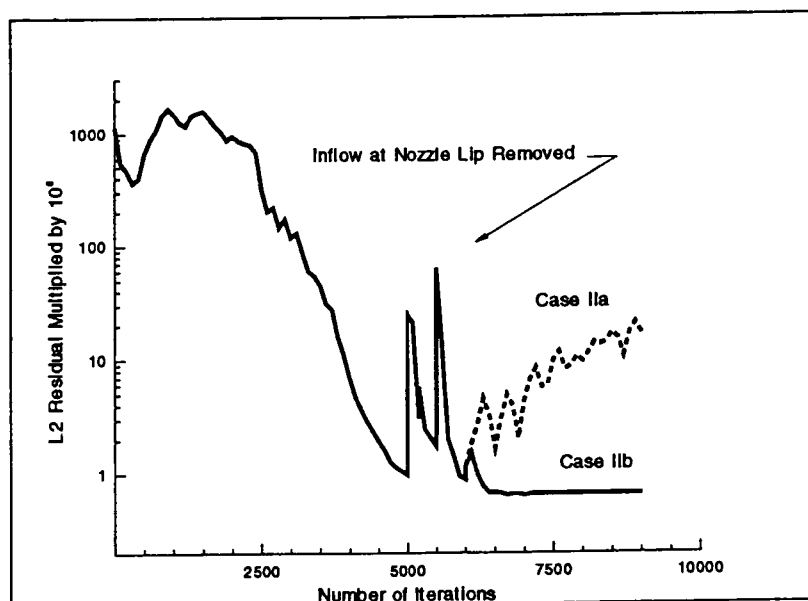


Figure 21 - Convergence history for Case II calculations, Reading 112 1030:1 NASA LeRC nozzle.

Table 9

**1030:1 Nozzle Performance Computations
Reading 112 Conditions**

Case	Mass Flow Rate (kg/s)	Vacuum Thrust (N)	Vacuum Specific Impulse (s)
PARCEQ with $T_c = 3059$ K	0.5026	2427	492.9
PARCEQ with $T_c = 2790$ K	0.5312	2389	459.1
TDK	0.5034	2383	482.7
Test Data	0.5266	2422	468.9

bracket the test measurements. This seems to indicate that there probably is incomplete combustion occurring in the combustion chamber.

The Mach number contours for Cases I and II are shown in Figures 22 and 23, respectively. The contours show that a weak shock emanates from the throat region and a compression shock emanates from the nozzle lip. The internal shock is caused by the second derivative discontinuity near the throat. The external shock occurs because the flow leaving the nozzle is at a lower pressure than the flow in the test cell. The observance of the external shock was very satisfying because this shock was expected.

The mass flow rate throughout the nozzle for both cases is shown in Figure 24. Less than 1% deviation in mass flow rate across the nozzle is observed. This agreement is as good as can be obtained with any numerical scheme in use [19]. Better agreement could have been obtained through increased packing in the areas of deviation, but the effect on the final results would have been minimal and did not warrant the effort.

Boundary layer profiles for velocity and temperature near the exit plane for both cases are shown in Figure 25, Figure 26 and Figure 27. The viscous boundary layer profiles were as expected for two dimensional nozzle flow. The thermal boundary layer profiles show that the temperature of the flow increases away from the wall, reaches a peak and then decreases from the peak to the axis of the nozzle. This profile is as expected for cold wall nozzle flow.

Plots of calculated wall pressure compared to measured wall pressure are shown for both cases in Figure 28. The calculations are slightly lower than test data which seems to indicate that γ_e or T did not quite match the test conditions.

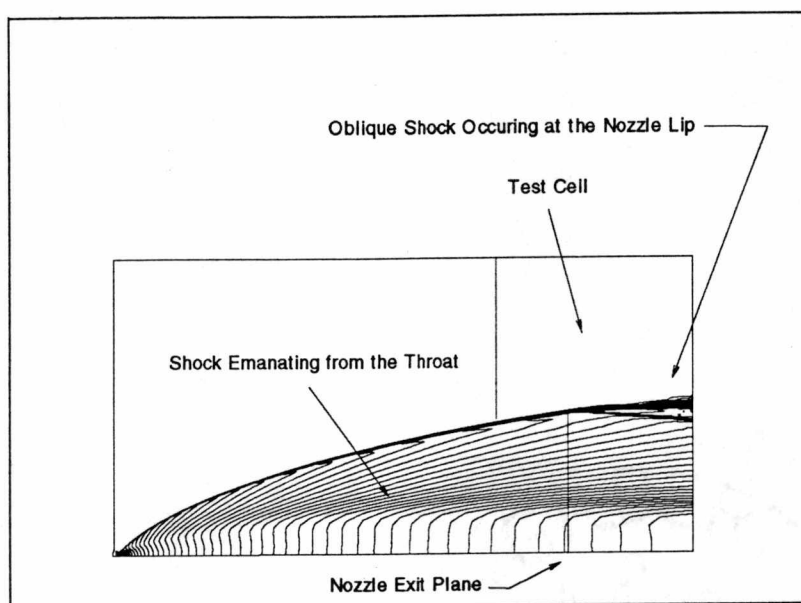


Figure 22 - Mach number contours for Case I, Reading 112 1030:1 NASA LeRC nozzle.

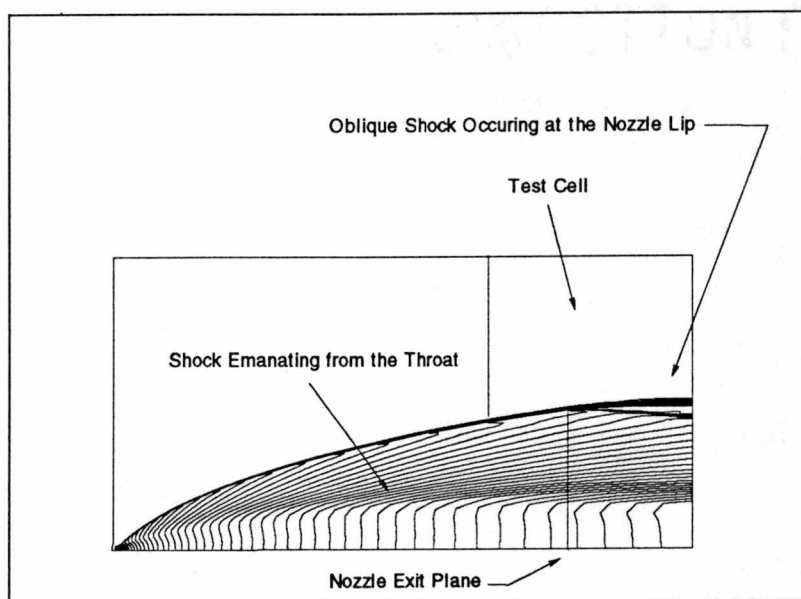


Figure 23 - Mach number contours for Case II, Reading 112 1030:1 NASA LeRC nozzle.

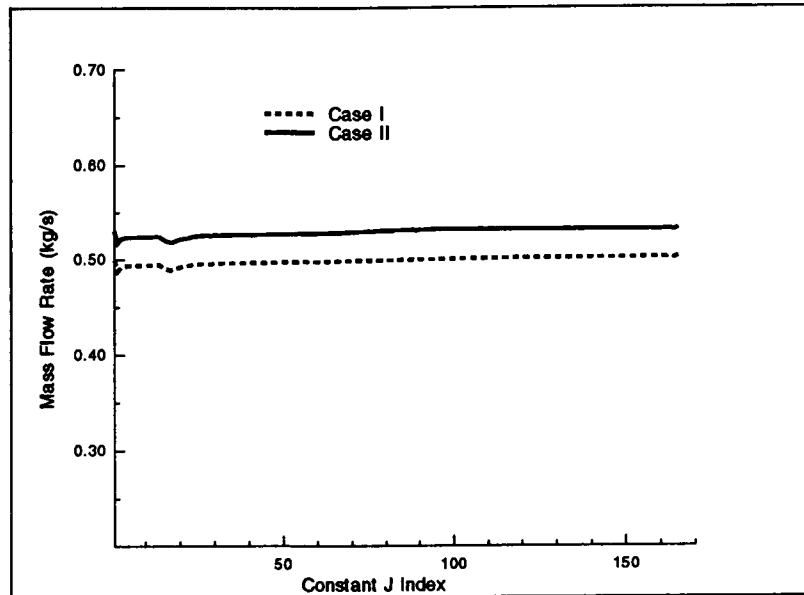


Figure 24 - Mass flow rate through the nozzle for Case I and Case II, Reading 112 1030:1 NASA LeRC nozzle.

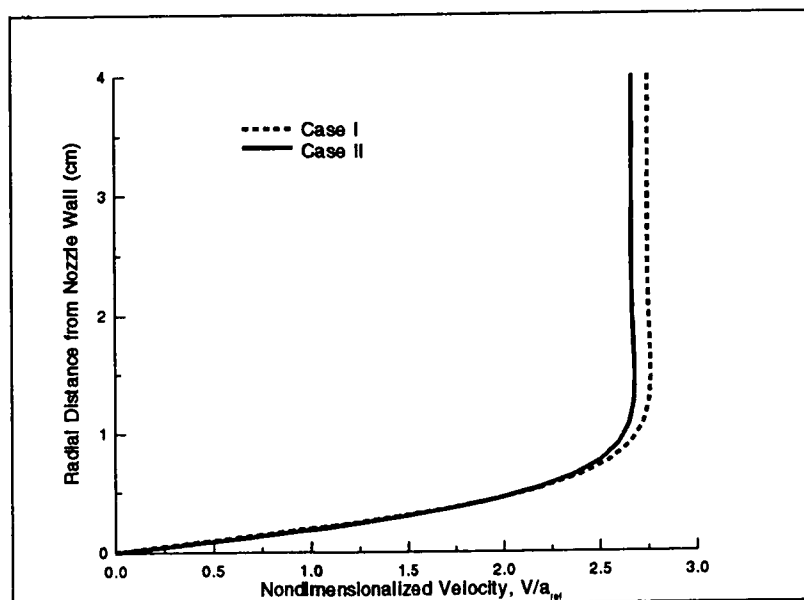


Figure 25 - Viscous boundary layer profile for Case I and Case II, 6.6525 cm upstream from the nozzle exit plane, Reading 112 1030:1 NASA LeRC nozzle.

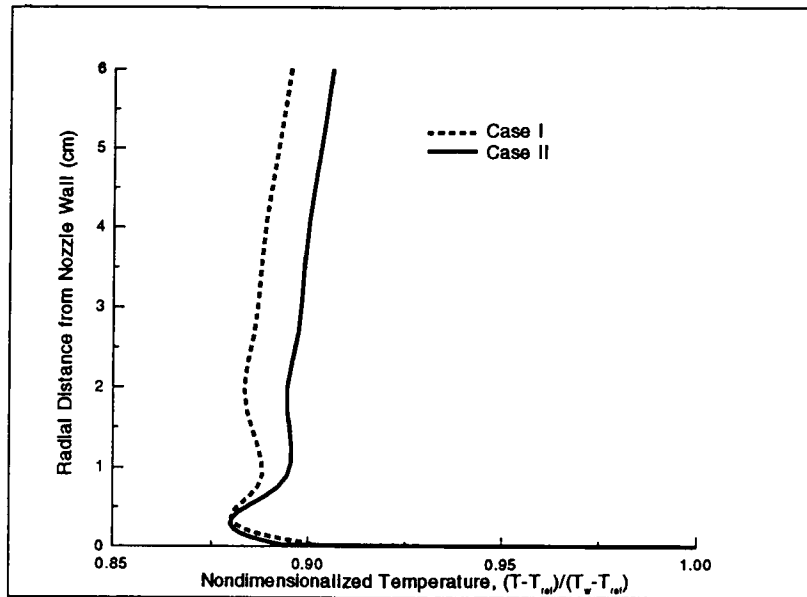


Figure 26 - Thermal boundary layer profile for Case I and Case II, 6.6525 cm upstream from the nozzle exit plane, Reading 112 1030:1 NASA LeRC nozzle.

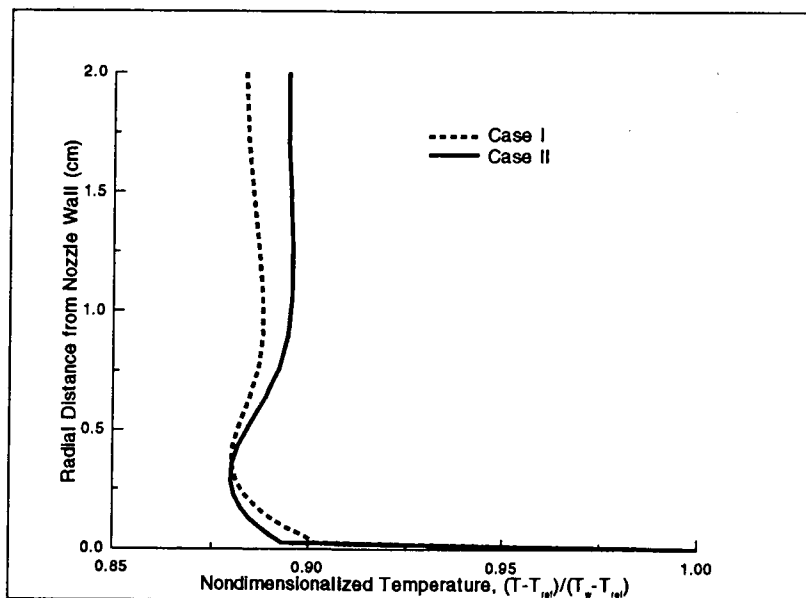


Figure 27 - Close up of thermal boundary layer profile for Case I and Case II, 6.6525 cm upstream from the nozzle exit plane, Reading 112 1030:1 NASA LeRC nozzle.

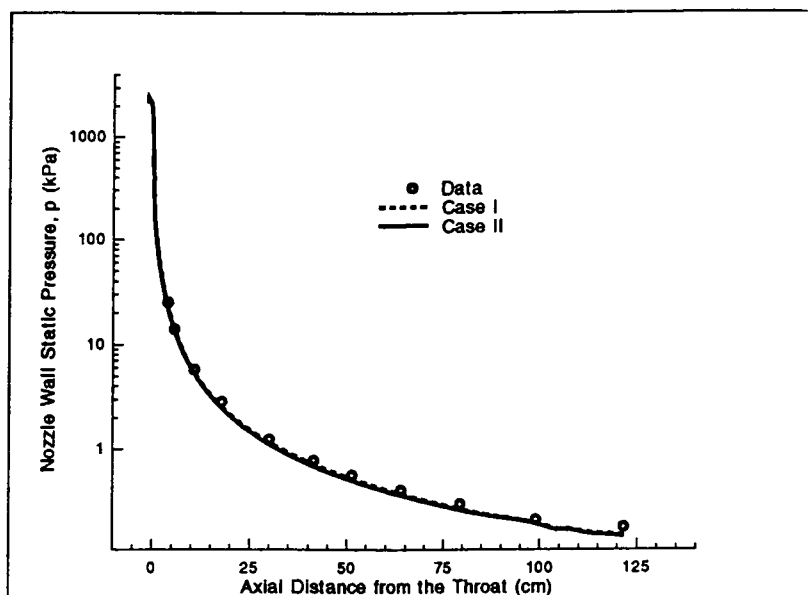


Figure 28 - Comparison of experimentally measured wall static pressure with calculated wall static pressure for Case I and Case II, Reading 112 1030:1 NASA LeRC nozzle.

Plots of calculated wall heat flux and experimentally determined wall heat flux (to be discussed in Chapter V) are shown for both cases in Figure 29. As expected, the impact of a decrease in combustion chamber temperature (Case II) on the wall heat flux is minimal beyond the throat region. The wall heat flux calculations for both cases are lower than the experimentally determined heat flux. Artificial dissipation inside the boundary layer was not removed for either calculation. As to be discussed in Chapter V, removal of the artificial dissipation inside the boundary layer increases the accuracy of the wall heat flux calculation.

Plots of y^+ for the first point off the nozzle wall are shown in Figure 30. The plots reveal that for better resolution of the boundary layer tighter grid packing near the

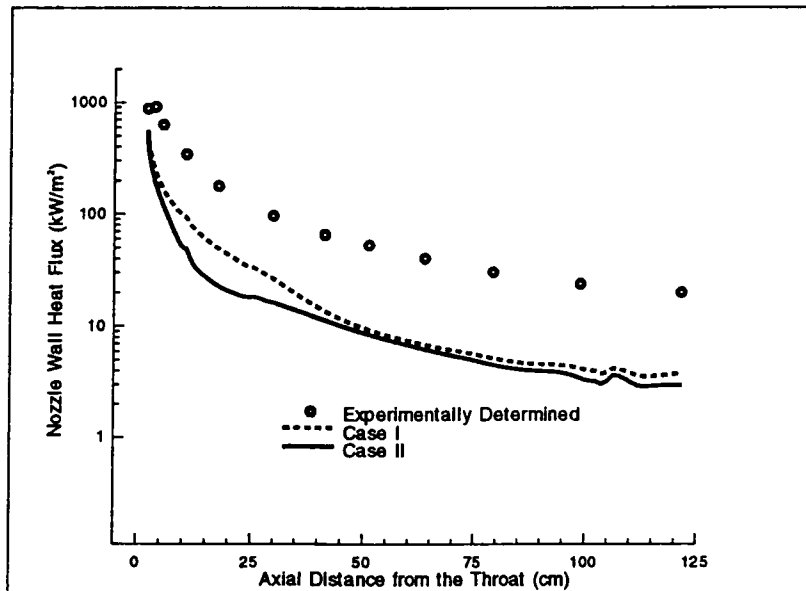


Figure 29 - Comparison of experimentally determined wall heat flux with calculated wall heat flux for Case I and Case II, Reading 112 1030:1 NASA LeRC nozzle.

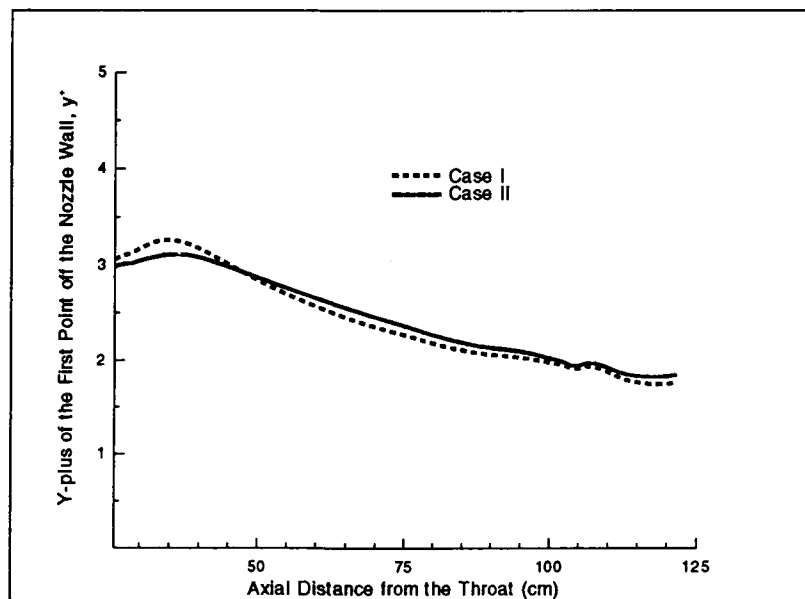


Figure 30 - Plot of y^+ of the first point off the nozzle wall for Case I and Case II, Reading 112 1030:1 NASA LeRC nozzle.

wall is needed. However, a well resolved boundary layer was not the objective of this calculation, therefore, this information was recorded and used to construct the grid for determination of wall heat flux.

Over all, the calculations for nozzle performance were satisfying. The bracket approach with Case I and Case II reveals that most probably incomplete combustion is occurring in the combustion chamber. The shock structure observed in the Mach number contours for both internal and external shocks were as expected. The results of y^+ plots and boundary layer profiles indicate that a more tightly packed grid would give better resolution of the boundary layer.

CHAPTER V

WALL HEAT FLUX COMPUTATIONS

A new grid was constructed after examining the boundary layer predictions that were made during the performance computations, Chapter IV. The grid was then used to simulate the nozzle flow, assuming 100% combustion in the combustion chamber. After sufficient iterations were run to fully develop the boundary layer, the wall heat flux was calculated by three different methods and compared to the experimentally determined wall heat flux for Reading 112.

Computational Grid

To obtain higher resolution of the boundary layer, a new grid with the packing ten times closer to the wall was constructed. For simplicity, the test cell cavity was removed from the grid and replaced with a 19 cm nozzle extension. The nozzle extension was simulated with a 16 by 60 mesh. The resulting computational grid simulating both the nozzle and the nozzle extension was a 180 by 60 mesh, Figure 31.

Boundary Conditions

To simulate the flow inside the nozzle, four boundary specifications were necessary. At the inflow and along the axis, the same conditions that were used for the performance computations were specified. Along the wall, the no slip constant wall temperature boundary condition was used. For this condition, the temperature profile along the nozzle wall was the same as used in the performance computations. The temperature profile used for the wall along the nozzle extension assumed a constant value

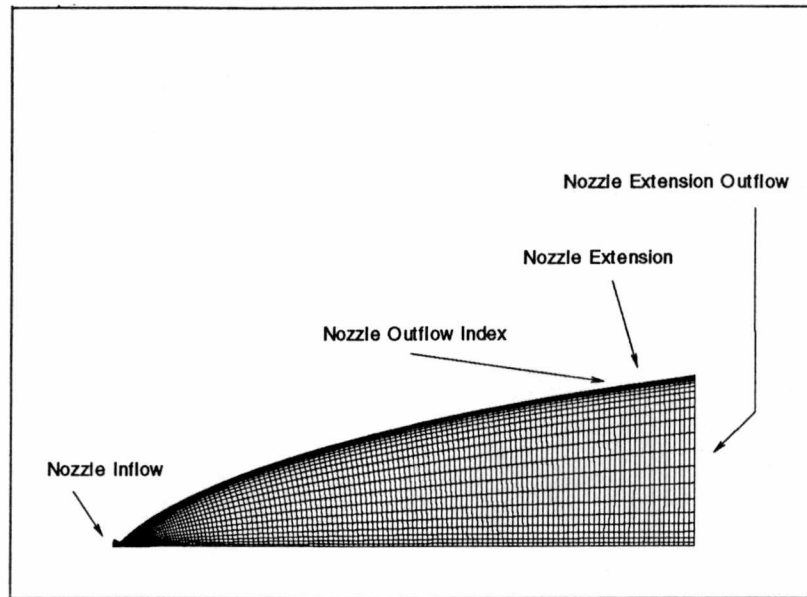


Figure 31 - Computational grid used for the wall heat flux calculation, 1030:1 NASA LeRC nozzle (every other point plotted in the radial direction).

equal to the wall temperature used at the nozzle exit plane. A static pressure equal to 68.4 kPa was used for the outflow boundary condition. After trial and error, this pressure was determined to be low enough to prevent inflow at the lip of the nozzle extension.

Boundary Layer Development

The flow field for the boundary layer development was initialized using the one dimensional theory and the bursting diaphragm technique discussed previously. After initializing the flow field, 5000 iterations were run to progress the solution past the non-physical stages of convergence. Examination of the flow field revealed that the solution was progressing normally. Additional iterations were then run to allow the boundary layer to fully converge. The boundary layer was examined every 1000 iterations for

changes in thickness and pressure. Approximately 10 points inside the subsonic boundary layer were observed along the entire nozzle wall. After 10,000 total iterations, no changes in boundary layer thickness or pressure inside the boundary layer were observed. Using this information, the boundary layer was assumed to be fully developed. Also, computed were the nozzle performance parameters. These parameters were compared to those calculated in Chapter IV, see Table 10. The performance parameters calculated with the heat flux grid agree with those calculated with the test cell grid.

Table 10
Comparison of Performance Computations
with Test Cell Grid and Heat Flux Grid

Case	Mass Flow Rate (kg/s)	Vacuum Thrust (N)	Vacuum Specific Impulse (s)
Test Cell Grid $T_c = 3059 \text{ K}$	0.5026	2427	492.9
Heat Flux Grid $T_c = 3059 \text{ K}$	0.5008	2418	492.9

Heat Flux Computations

Heat flux calculations were made with artificial dissipation inside the boundary layer, with artificial dissipation removed inside the boundary layer and using Reynold's Analogy. The results of these calculations were then compared to the experimentally determined heat flux.

The experimentally determined heat flux for Reading 112 was obtained through a solution of the energy equation.

$$\rho C_p \left(\frac{\partial T}{\partial t} \right) = \frac{1}{r} \frac{\partial}{\partial r} \left[(kr) \frac{\partial T}{\partial r} \right] \quad (15)$$

The solution of the energy equation for the nozzle wall heat flux assuming constant properties, no axial or circumferential conduction, adiabatic outer wall and a linear rate of temperature rise is [22]

$$q = \frac{kR_i}{2\alpha} \frac{\partial T}{\partial t} \left[\left(\frac{R_o}{R_i} \right)^2 - 1 \right] \quad (16)$$

Using the above equation, the rate of outer wall temperature increase, the nozzle wall thickness and the diffusivity of carbon steel, the inner nozzle wall heat fluxes were calculated by Kacynski et al [7].

Initially, the nozzle wall heat flux was computed with full dissipation inside the boundary layer. The heat flux was calculated by discretizing the heat equation.

$$q_w = -k \left(\frac{\partial T}{\partial n} \right)_w \quad (17)$$

Next, the artificial dissipation inside the boundary layer was removed using a hyperbolic scaling factor [29].

$$F_{scale} = \frac{1}{2} \left(1 + \frac{\tanh \left(I - \frac{(I_L + I_U)}{2} \right)}{\tanh \left(\frac{(I_U - I_L)}{2} \right)} \right) \quad (18)$$

From the wall to I_L , all artificial dissipation is removed. From I_L to I_U , the artificial dissipation is ramped back into the solution using the scaling factor F_{scale} . For the present computation, I_L was set to the fourth grid point off the wall and I_U was set to the fifteenth grid point off the wall. An additional 17,000 iterations were run using this scaling factor and the wall heat flux was calculated using the discretized form of the heat equation shown above.

Finally, the wall heat flux was calculated by applying Reynold's Analogy to the flow field that had artificial dissipation removed inside the boundary layer. Reynold's Analogy is used quite frequently to predict wall heat flux and the method has been corroborated through many experiments. The analogy states that for fully turbulent boundary layer flows over a flat plate with $Pr = 1$ and constant ρ , μ and k that $C_f \approx 2C_h$ [31]. Combining the forced convection equation for wall heat flux

$$q_w = h(T_{aw} - T_w) \quad (19)$$

the equation for the adiabatic wall temperature

$$T_{aw} = T_\infty + \frac{r U_\infty^2}{2 C_p} \quad (20)$$

and Reynold's Analogy

$$C_f = \frac{2\tau_w}{\rho U_\infty^2} \approx C_h = \frac{h}{C_p \rho U_\infty} \quad (21)$$

an equation for wall heat flux can be developed

$$q_w = \frac{\tau_w C_p}{U_\infty} (T_\infty - T_w) + \frac{1}{2} r \tau_w U_\infty \quad (22)$$

For laminar flows with $0.1 \leq Pr \leq 3.0$, the recovery factor, r , can be approximated by $Pr^{1/2}$ [31]. Thus, using the above developed equation for the calculation of heat flux and the assumption for recovery factor, the wall heat flux was calculated at three locations along the nozzle wall.

The results of the three methods for the prediction of wall heat flux are compared with the experimentally determined wall heat flux in Figure 32. Note that the computational predictions of wall heat flux are significantly lower than the experimentally determined wall heat flux, where as, the predictions by Reynold's Analogy are higher than the experimentally determined heat flux.

The results with full dissipation inside the boundary layer were expected to predict a lower heat flux. Artificial dissipation helps maintain stability by smoothing gradients in the solution. Large temperature gradients which should naturally occur near the nozzle wall are thus reduced significantly. Since the temperature gradient at the nozzle wall is the dominant term in the heat equation, a decreased temperature gradient results in lower

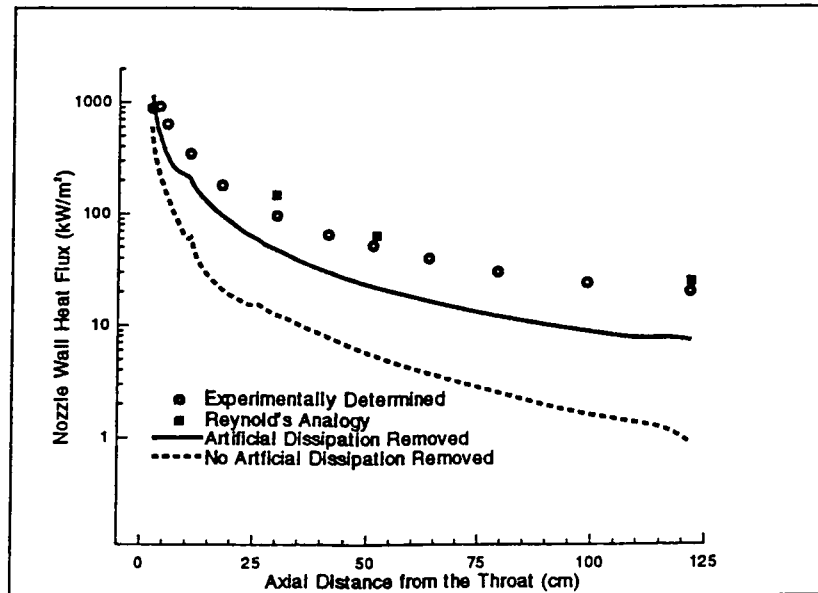


Figure 32 - Comparison of experimentally determined heat flux and calculated wall heat flux.

heat flux predictions. This effect was evident when heat flux predictions without artificial dissipation removed inside the boundary layer were compared with those made with artificial dissipation removed inside the boundary layer.

The heat flux predictions with artificial dissipation removed from inside the boundary layer using F_{scale} were also lower than the experimentally determined wall heat flux. This indicates that the artificial dissipation inside the boundary layer must be removed in a more physically meaningful manner before accurate wall heat fluxes can be predicted. However, this problem is very difficult to solve because a reduction in the dissipation often leads to instabilities and difficulty in achieving convergence.

The assumption of a laminar boundary layer within the nozzle could be another reason why the wall heat flux predictions using the discretized form of the energy equation were low. If the boundary layer inside the nozzle during the test firing were transitional or fully turbulent, the assumption of laminar flow would result in low heat flux predictions.

The predictions of heat flux using Reynold's Analogy are closer to the experimentally determined heat flux than those predicted with the discretized form of the heat equation (only slightly higher). However, Reynold's Analogy was theoretically derived as a predictor of wall heat flux for *turbulent* boundary layer flows over a flat plate with $Pr = 1$ and assuming constant ρ , μ and k . Since these conditions are not the conditions inside the nozzle, the heat flux predictions made using the analogy cannot be substantiated. Instead, it seems more coincidental that the heat flux prediction using Reynold's Analogy is closer to the experimentally determined wall heat flux than the results using the discretized form of the heat equation.

CHAPTER VI

CONCLUSIONS AND RECOMMENDATIONS

Modifications to the PARCEQ real gas Navier-Stokes code to incorporate single interval surface fits of equilibrium thermochemical and transport properties were completed. Surface fits for equilibrium hydrogen-oxygen chemistry with an oxidant to fuel mixture ratio of 3.84 were accurately generated using the EQGAS and SURFIT software. Calculations of a 1030:1 area ratio nozzle were conducted with the modified version of PARCEQ. Performance predictions made by PARCEQ and TDK and wall heat flux predictions made by PARCEQ were compared with the Reading 112 test data to evaluate the validity of PARCEQ and TDK as design tools to be used for the development of rocket engines for space applications. Wall heat flux comparisons with TDK were not made because published wall heat flux predictions for the Reading 112 conditions were not found.

The results of a performance analysis indicate that both PARCEQ and TDK made accurate vacuum thrust predictions. However, since the boundary layer along the nozzle wall was relatively thin, little difference between the vacuum thrust predictions made by TDK and PARCEQ and the test data was expected.

Comparison of mass flow rate predictions by TDK and PARCEQ with test data show that the assumption of complete combustion in the combustion chamber resulted in lower mass flow rate predictions. However, the calculation with PARCEQ assuming incomplete combustion resulted in a very accurate mass flow rate prediction. The

conclusions drawn were that most probably there was incomplete combustion occurring in the combustion chamber during the Reading 112 test firings.

The nozzle wall heat flux predicted by PARCEQ was low in comparison with test data. One possible reason for the low prediction of wall heat flux might be that the nozzle wall did not reach thermal equilibrium during the test firing. This conclusion is not entirely unlikely, since the duration of the test firing was only three seconds and the thickness of the carbon steel nozzle wall was 0.625 cm. Since the calculations made with PARCEQ were for thermal equilibrium conditions and if thermal equilibrium during the test firing was not reached, a comparison between the test data and the wall heat flux prediction is not meaningful.

Another possible source of the discrepancy could be the inaccuracy of the test data itself. As mentioned previously, there was a lot of data scatter in the wall temperature data over the last 80 cm of the nozzle. The inaccuracy in the wall temperature data and the fact that the inner wall temperature was estimated from an outer wall temperature measurement could account for some of the deviation between the prediction between PARCEQ and the test data. It is also possible that the artificial dissipation was not removed in a physically meaningful manner in the near wall region. A better algorithm for the removal of artificial dissipation inside the boundary layer perhaps would lead to different predictions of the wall heat flux.

In summary, the results of this study were meaningful. Further confidence in the accuracy of the newly modified version of PARCEQ was gained. The technique of simulating the test cell conditions was successfully implemented. Investigation of the

nozzle wall heat flux revealed that a better algorithm for the removal of artificial dissipation inside the boundary layer must be implemented in the PARCEQ code. However, the main objective of the research to compare TDK and PARCEQ as design tools for the development of rocket engines for space applications was not reached. Mainly this objective was not reached because the boundary layer inside the nozzle for the Reading 112 conditions was too thin to accurately simulate the thick boundary layer conditions which will be encountered in the space environment. Tests must be developed which more closely simulate these thick boundary layer conditions in order to create a data base for the comparison of predictions made by design tools. Likewise, these tests must be conducted reliably so that the data from the tests can be confidently used for the validation of design tools.

It is recommended that continued research be planned to further explore the usage of TDK and PARCEQ as design tools for the development of rocket engines for space applications. A calculation should be performed for the Reading 112 conditions with a recently obtained version of TDK and the nozzle wall heat flux extracted for a comparison with PARCEQ and the test data. The Baldwin-Lomax turbulence model, which has recently been successfully incorporated into the PARCEQ code, should be run to make a comparison of the turbulent wall heat flux with the laminar wall heat flux predictions and test data. Calculations should be run with TDK and PARCEQ on the 1030:1 area ratio nozzle using a reduced chamber pressure and an increased wall temperature. The objective of these calculations would be to thicken the boundary layer inside the nozzle to determine if any deviation between the results predicted by TDK and

PARCEQ occurs. Finally, data taken from test firings of the thrusters developed for the Space Station Freedom should be examined to determine if the data can be used for the validation of TDK and PARCEQ.

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