Abstract

McDaniel, Keith S. Three Dimensional Simulation of Time-Dependent Scramjet Isolator / Combustor Flowfields Implemented on Parallel Architectures, (Under the directions of Dr. J. R. Edwards)

The development of a parallel Navier-Stokes solver for computing time-dependent, three-dimensional reacting flowfields within scramjet (supersonic combusting ramjet) engines is presented in this work. The algorithm combines low-diffusion upwinding methods, time accurate implicit integration techniques, and domain decomposition strategies to yield an effective approach for large-scale simulations. The algorithm is mapped to a distributed memory IBM SP-2 architecture and a shared memory Compaq ES-40 architecture using the MPI-1 message-passing standard. Two and three-dimensional simulations of time-dependent hydrogen fuel injection into a model scramjet isolator / combustor configuration at two equivalence ratios are performed. These simulations are used to gain knowledge of engine operability, inlet performance, isolator performance, fuel air mixing, flame holding, mode transition, and engine unstart. Results for an injection at a ratio of 0.29 show qualitative agreement with experiment for the two-dimensional case, but revealed a slow progression toward engine unstart for the three-dimensional case. Injection at an equivalence ratio of 0.61 resulted in engine unstart for both two-dimensional and three-dimensional cases. Engine unstart for the three-dimensional case occurs as a response to the formation and growth of large pockets of reversed flow along the combustor side wall. These structures develop at an incipient pressure above 154 kPa and result in significant blockage of the core flow, additional compression, and chemical reaction within the boundary layer. All of these factors promote a much more rapid unstart as compared with the two-dimensional case.
Three Dimensional Simulation of Time-Dependent Scramjet Isolator / Combustor Flowfields Implemented on Parallel Architectures

by

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I dedicate this thesis to my grandmother, Emily C. Dotson, and my brother, Don Mark McDaniels, who have stood behind me through many years of hard work. Their support of my goals and aspirations have kept me strong. Without them, my road would have contained many twisting turns, which I would have been unable to navigate.
Biography

Keith Scott McDaniel was born March 18, 1975 in Winston-Salem, North Carolina. He grew up near Liberty Airport in Winston-Salem where his fascination with aircraft and the driving forces behind them sprang from. After graduation from Carver High School, he began his collegiate activities at North Carolina State University. He received a Bachelor of Science in Aerospace Engineering in May of 1998 and is currently attaining a Master of Science in Aerospace Engineering from the same university. Keith will begin employment at the CFD Research Corporation in Huntsville, Alabama on January 2, 2001.
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List of Symbols

$A$ Pre-exponential factor
$\bar{A} - \tilde{G}$ Combined inviscid and viscous flux Jacobians
$\hat{A}$ System Jacobian matrix
$a$ Speed of sound
$b$ Reaction order
$C_p$ Coefficient of specific heats at constant pressure
$c_j$ Species Concentration
$D$ Diffusion coefficient
$e_t$ Total internal energy
$E, F, G$ Flux vectors ($x, y, z$, directions respectively)
$E$ Inviscid flux component ($x$-direction)
$E_p$ Parallel efficiency based on time
$E_v$ Viscous flux component ($x$-direction)
$F$ Inviscid flux component ($y$-direction)
$F_T$ Time averaged flow variable
$F_v$ Viscous flux component ($y$-direction)
$f$ Instantaneous flow variable
$G$ Inviscid flux component ($z$-direction)
$G_v$ Viscous flux component ($z$-direction)
$\bar{H}$ Combined Jacobian matrix at point $ijk$
$h$ Stagnation enthalpy per unit mass
$h_j^0$ Heat of formation for species $m$
$J$ Jacobian
$J_{mj}$ Diffusion Flux Tensor
$k, k_f, k_b$ Forward and backward reaction equilibrium constants
$k$ Turbulent kinetic energy (section 3)
$k$ Specific reaction rate (section 2.3.1)
$l_b$ Kolmogorov length scale
$l_{mfp}$ Mean free path length scale
$M$ Mach number (section 3)
$M$ Collision partner (section 2.3.1)
$M_j$ Molecular weight for species $j$
$Pr$ Prandtl number
$p$ Pressure
$q_j$ Heat flux vector
$q_{ij}$ Reynolds heat flux vector $-\rho u_i u_j r''$
$Re$ Reynolds number
$R$ Specific gas constant
\( R \)  \quad \text{Universal gas constant}

\( RR_f, RR_b \)  \quad \text{Forward and backward reaction rates}

\( S \)  \quad \text{Source vector}

\( S_p \)  \quad \text{Parallel speedup}

\( Sc \)  \quad \text{Schmidt number}

\( t \)  \quad \text{Time}

\( T \)  \quad \text{Temperature}

\( T_a \)  \quad \text{Activation Temperature}

\( T \)  \quad \text{Integral time scale}

\( TB \)  \quad \text{Third body efficiencies}

\( T_i \)  \quad \text{Turbulent integral time scale}

\( T_2 \)  \quad \text{Mean property variation time scale}

\( W \)  \quad \text{Primitive variable vector}

\( U \)  \quad \text{Conservative variable column vector}

\( u \)  \quad \text{Velocity component in streamwise direction}

\( u_j \)  \quad \text{Velocity vector with components } u, v, w

\( v \)  \quad \text{Velocity component in wall normal direction}

\( v_{m,n} \)  \quad \text{Stoichiometric coefficients for reactant } m \text{ in reaction } n

\( v_{m,n} \)  \quad \text{Stoichiometric coefficient for product } m \text{ in reaction } n

\( w \)  \quad \text{Velocity component in spanwise direction}

\( x \)  \quad \text{Cartesian coordinate (generally streamwise component)}

\( Y_m \)  \quad \text{Species mass fraction}

\( y \)  \quad \text{Cartesian coordinate (generally normal component)}

\( z \)  \quad \text{Cartesian coordinate (generally spanwise component)}

\( \dot{w}_m \)  \quad \text{Species production rate}

\( Q_j \)  \quad \text{Turbulent heat flux tensor}

\( \mathcal{T}_{ij} \)  \quad \text{Turbulent stress tensor}

\( \mathcal{U}, \mathcal{V}, \mathcal{W} \)  \quad \text{Contravariant velocity components}

\( V_j \)  \quad \text{Species diffusion velocity vector}

\( \mathcal{U}^m, \mathcal{V}^m, \mathcal{W}^m \)  \quad \text{Species contravariant diffusion velocity components}

\( \mathcal{Y}_{mj} \)  \quad \text{Turbulent species mass flux component}

**Greek Letters:**

\( \delta_{ij} \)  \quad \text{Kronecker Delta}

\( \rho \)  \quad \text{Density}

\( \xi, \eta, \zeta \)  \quad \text{Computational coordinate}

\( \psi, \phi \)  \quad \text{Arbitrary variables}

\( \gamma \)  \quad \text{Thermal conductivity}

\( \gamma_t \)  \quad \text{Turbulent thermal conductivity}

\( \mu \)  \quad \text{Molecular viscosity}

\( \mu_t \)  \quad \text{Apparent “eddy” viscosity}
\( \omega \) Specific dissipation rate
\( \tau_{ij} \) Laminar stress tensor
\( \nu \) kinematic viscosity

Subscripts:
\( \infty \) Freestream quantity
\( o \) Stagnation (total) quantity
\( i, j, k \) Spatial coordinates, cell indices
\( L, R \) Left and Right States
\( m \) Chemical species
\( n \) Time level or chemical reaction
\( t \) Total or turbulent quantity
\( mix \) Mixture quantity
\( v \) Viscous quantity
\( \frac{1}{2} \) Interface data

Superscripts:
\( ^r \) Reynolds fluctuating component
\( ^n \) Favre fluctuating component
\( c \) Convective component
\( p \) Pressure component

Accents:
\( \bar{\cdot} \) Averaged variable
\( \bar{\cdot} \) Favre-averaged component
\( \check{\cdot} \) Linear system flux Jacobian in computational space

Abbreviations:

- **CFD** Computational Fluid Dynamics
- **CS** Control Surface
- **CV** Control Volume
- **DNS** Direct Numerical Simulation
- **HXLV** Hyper-X Launch Vehicle
- **HXRV** Hyper-X Research Vehicle
- **LES** Large Eddy Simulation
- **RANS** Reynolds Averaged Navier Stokes Equations
- **NACA** National Aeronautics and Space Administration
- **NAL** National Aerospace Laboratory
- **NASA** National Aeronautics and Space Administration
- **NASP** National Aero Space Plane
- **NS** Number of species
- **NR** Number of reactions
- **PNS** Parabolized Navier-Stokes
- **SPGS** Symmetric planar Gauss-Seidel
- **VAG** Vitiated Air Generator
1 Introduction

The scramjet (supersonic combusting ramjet) engine is a key to air breathing hypersonic technology. This type of propulsion device has been studied by NACA/NASA for nearly 60 years [1]. A review of the scramjet technology in the 1980’s indicates a firm fundamental basis for the performance potential of dual mode scramjets. Dual mode scramjets are similar to conventional ramjets but do not contain a second minimal area. This allows both supersonic (scramjet) and subsonic (ramjet) combustion modes. For example, a tactical missile (an expendable, low cost, low weight, fixed geometry device) must operate as a ramjet at low flight Mach numbers and as a scramjet at high flight Mach numbers ($M > 6.5$). If adequate combustor-inlet isolation is provided, the scramjet will operate in a ramjet mode with slightly lower efficiencies than that of a conventional ramjet [2]. Knowledge of engine operability, inlet performance, isolator performance, fuel air mixing, flame holding, combustion efficiency, mode transition, and engine unstart is crucial for scramjet applications. A large amount of scramjet combustion experimental data was collected in ground based test facilities during the National Aero Space Plane (NASP) Program. After termination of NASP in 1995, the focus of NASA Langley shifted to the Hyper-X program. The Hyper-X program will demonstrate the free-flight operation of an airframe-integrated, hydrogen-fueled, scramjet flowpath in atmospheric flight at Mach 7 and 10 by 2002 [3]. “One shot” test experiments, such as Hyper - X, and scramjet experiments in ground-based facilities are limited in the amount of flowfield information which can be recorded.

When a stage in a development cycle is reached where wind tunnel or flight testing is required, computational techniques can be extremely useful as a diagnostic tool to explain certain unexplained flow phenomena observed in measured data. This is particular true for dynamic modes of operation, where test-to-test repeatability may not be easily attained. CFD simulations offer the potential to provide the necessary data for assessing scramjet
performance. The potential of CFD techniques as a diagnostic tool is directly related to the fact that computational solutions provide complete flow field data, whereas wind tunnel tests generally measure global characteristics and surface data. In the past, less general equation sets have been used for the simulation of scramjet flowfields. An example is the use of the Parabolized Navier-Stokes equations (PNS). For supersonic flow, the Navier-Stokes equations can be made parabolic in the streamwise directions by assuming that the streamwise viscous terms are negligible and by a special treatment of the pressure in the subsonic near wall region of the boundary later. The steady equations are then solved using a streamwise marching finite-difference scheme [4]. These schemes are efficient for a steady state solution but are only accurate if a supersonic core flow exits and are invalid for time dependent simulations. The solution of the complete Navier-Stokes equations is necessary to compute scramjet combustion flows were large subsonic or separated regions of flow may exist. These regions of flow may occur during a transition from scramjet to ramjet mode of operation and during unsteady modes of operation, such as time dependent fuel injection. Also, these subsonic regions as well as shock / boundary layer interactions play a major role in determining the inlet flow structure and the resulting inlet performance.

An understanding of dynamic modes of scramjet operation requires, at a minimum, time-dependent solutions of the Favre-Averaged Navier-Stokes equations, extended for chemically reacting flows. This equation system can capture complex flow structures such as expansion fans, boundary layers, shear layers, reaction fronts, subsonic separated-flow regions, and shock-boundary layer interactions. The use of Favre-Averaging for an unsteady mean flow implies the averaging of the Navier-Stokes equations over a time T much larger than the longest turbulent time scale but smaller than the time scale characteristic of the bulk fluid motion. This separates the turbulent fluctuating time scales from the bulk fluid motion time scale.

Numerical simulations are needed to obtain a better understanding of scramjet modes
of operation and to explain results obtained from ground-based experiments. One such mode of operation is the time dependent injection of fuel into the combustor. Time dependent fuel injection leads to concerns of flow path stability, scramjet / ramjet transition, flame stabilization, and engine unstart. This directly corresponds to the proposed Hyper-X Launch Vehicle (HXLV) flight test sequence. The HXLV will separate from a B-52 and will be boosted to the predetermined stage separation point. The Hyper-X Research Vehicle (HXRV) will then separate from the HXLV. After a 5 second unpowered controlled flight, sequenced fuel injection will commence [5]. Simulation of these dynamic modes of engine operation requires complete flowfield calculations of the combustor and inlet to capture the complex time dependent flow structures discussed previously. This requires of the order of $1.0 \times 10^6$ grid points for 3-D resolution of a model scramjet combustor, assuming that all effects of turbulence on the unsteady mean flow are modeled. Noting a solution of the reacting flowfield using a 7 species 7 reaction mechanism and the $k - \omega$ turbulence model will require the solution of 14 simultaneous equations at every grid point, a solution of roughly 14 million simultaneous equations is required at every time level. Obviously, a parallel algorithm is needed to solve a problem of this size. This work develops a parallel Navier-Stokes solver for conducting three-dimensional simulations of time-dependent scramjet flowfields.

Sections 2-3 present the governing Navier-Stokes equations, their closure using turbulence modeling concepts, their discretization using low-diffusion upwind methods, and their integration using time-accurate implicit methods. An approach for parallelizing the algorithm using a domain-decomposition / message-passing paradigm is discussed in section 4. The application of the algorithm to a model scramjet isolator / combustor configuration tested at the National Aerospace Lab, Japan [6] is discussed in Section 5, and results for stable and unstable modes of engine operation are discussed for both two and three dimensional cases.
2 Governing Equations

2.1 Reference Equations

This section will state the governing fluid dynamic equations for viscous, unsteady compressible flows. These equations are extended to account for finite rate chemical reactions. The extended equations are then Favre-Averaged to model the effects of all turbulent fluctuations on the mean flow.

The compressible Navier-Stokes equations in Cartesian coordinates without body forces or external heat addition can be written as [7]:

\[
\frac{\partial}{\partial t} (\rho) + \frac{\partial}{\partial x_j} (\rho u_j) = 0
\]  \hspace{1cm} (2.1)

\[
\frac{\partial}{\partial t} (\rho Y_m) + \frac{\partial}{\partial x_j} (\rho Y_m u_j) = \frac{\partial}{\partial x_j} (J_{mj}) + \bar{w}_m
\]  \hspace{1cm} (2.2)

\[
\frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} (\rho u_i u_j) = -\frac{\partial}{\partial x_j} (p \delta_{ij}) + \frac{\partial}{\partial x_j} (\tau_{ij})
\]  \hspace{1cm} (2.3)

\[
\frac{\partial}{\partial t} (\rho e_t) + \frac{\partial}{\partial x_j} (\rho e_t u_j) = \frac{\partial}{\partial x_j} [q_j + \tau_{ij} u_i]
\]  \hspace{1cm} (2.4)

The diffusion flux tensor \(J_{mj}\), diffusion velocities \(V_j\), laminar stress tensor \(\tau_{ij}\), and the laminar heat flux vector \(q_j\) are given by:

\[
J_{mj} = -\rho_m V_j^{(m)}
\]  \hspace{1cm} (2.5)

\[
V_j^{(m)} = - \left( \frac{D}{Y_m} \right) \left( \frac{\partial (Y_m)}{\partial x_j} \right)
\]  \hspace{1cm} (2.6)

\[
\tau_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{1}{2} \delta_{ij} \mu \frac{\partial u_k}{\partial x_k}
\]  \hspace{1cm} (2.7)

where \(\mu\) is the laminar viscosity, \(\gamma\) is the thermal conductivity, \(D\) is the diffusion coefficient, and \(Y_m = \frac{\omega_m}{\rho}\) is the mass fraction for species \(m\).
The total enthalpy and energy are defined as [8]:

\[
\begin{align*}
h_t & = h_{mix} + \frac{u_i u_i}{2} \\
e_t & = h_t - \frac{p}{\rho}
\end{align*}
\]

(2.8)

where \( h_{mix} \) is the mixture static enthalpy.

The general effects of gravitational forces and radiative heat transfer are neglected in this formulation, and thermal equilibrium at a common temperature is assumed. The thermodynamic state of the gas mixture is specified by the following auxiliary relations [9]:

\[
\begin{align*}
\rho & = \sum_{m=1}^{NS} \rho_m \\
Y_m & = \frac{\rho_m}{\rho} \\
p & = \rho R_{mix} T \\
R_{mix} & = R \sum_{m=1}^{NS} \frac{Y_m}{M_m} \\
h_{mix} & = \sum_{m=1}^{NS} h_m Y_m \\
h_m & = h_{fm}^o + \int_{T_{ref}}^{T} C_{p_m} (T) \, dT \\
a^2 & = \left( \frac{C_{p_{mix}}}{C_{p_{mix}} - R_{mix}} \right) \left( \frac{p}{\rho} \right) \\
D & = \frac{1}{\overline{Sc} \rho} \\
C_{p_{mix}} & = \sum_{m=1}^{NS} Y_m C_{p_m} (T)
\end{align*}
\]

(2.9) \hspace{1cm} (2.10) \hspace{1cm} (2.11) \hspace{1cm} (2.12) \hspace{1cm} (2.13) \hspace{1cm} (2.14) \hspace{1cm} (2.15) \hspace{1cm} (2.16) \hspace{1cm} (2.17)

Mixture values for the specific gas constant \( R_{mix} \) are defined in equation 2.12, where \( R \) is the universal gas constant, \( M_m \) is the molecular weight of species \( m \). The specific heat at constant pressure for species \( m \) is \( C_{p_m} \). Equation 2.11 defines the state equation for a mixture of ideal gases. The species enthalpy \( h_{m}^o \) is equal to the species enthalpy of formation \( h_{m}^o \) plus the integral of \( C_{p_m} \) from \( T_{ref} \) to \( T \) (equation 2.14). Equation 2.13 defines
the mixture enthalpy. Curve-fit polynomials from McBride et al [10] are used for obtaining 
\( C_{p,m} \) as a function of temperature. The molecular viscosity \( \mu \) and thermal conductivity \( \gamma \) are determined from Sutherland’s viscosity law while Wilke’s law [11] is used to determine mixture values. The molecular diffusion coefficient \( D \) is modeled using Fick’s law. By assuming a constant Schmidt number of 0.5 for all species, one diffusion coefficient can be defined as in equation 2.16.

The four governing equations represented (equations 2.1-2.4) in vector form are the Conservation of Mass, Conservation of Momentum (Newton’s 2nd Law), and the Conservation of Energy (1st Law of Thermodynamics) laws applied to an arbitrary control volume (CV). They are referred to as the Continuity, Momentum, and Energy equations respectively. The first term in the continuity equation is the rate of increase of the mass per unit volume in the CV, and the second term represents the rate of mass flux per unit volume passing through the control surface (CS). The first term in the momentum equation is the rate of increase of momentum per unit volume in the CV and the second term represents the rate of momentum loss per unit volume through the CS due to convection and stress on the fluid internal to the CV. The first term in the energy equation is the rate of increase of total energy per unit volume in the CV and the second term represents the rate of energy lost to convection, conduction, and dissipation through the CS. The equations formulated above can be written in Cartesian vector form as

\[
\frac{\partial U}{\partial t} + \frac{\partial (E)}{\partial x} + \frac{\partial (F)}{\partial y} + \frac{\partial (G)}{\partial z} = S \tag{2.18}
\]

If equation 2.1 is replaced by the auxiliary equation 2.9, then solution of the species conservation, momentum, and energy equations is needed. The flux vectors \( E, F, G \) can be split into inviscid and viscous components. For example, the x-direction flux vector can be
written as

\[
E = E - E_v = \begin{pmatrix}
\rho_1 u \\
\vdots \\
\rho_N S u \\
\rho u^2 + p \\
\rho u w \\
\rho w u \\
\hat{h} u
\end{pmatrix} - \begin{pmatrix}
\rho_1 U^{(1)} \\
\vdots \\
\rho_N S U^{(NS)} \\
\tau_{xx} \\
\tau_{yx} \\
\tau_{zx} \\
\mu \tau_{xx} + \nu \tau_{xy} + \nu \tau_{xx} + \nu
\end{pmatrix}
\]

(2.19)

2.2 Averaging

Turbulent reacting flow fields at large Reynolds numbers are inherently three dimensional and cover a large spectrum of turbulent length and time scales [12]. The smallest of these scales are the Kolmogorov scales. One of the premises of Kolmogorov’s equilibrium theory is that the smaller eddies are in a state at which the rate of their receiving energy from the larger eddies is nearly equal to the rate at which the smallest eddies dissipate energy to heat. The smallest turbulent scales can be shown to be a continuum phenomenon. For example, the ratio of the Kolmogorov length scale to the mean free path of air moving 65 MPH over a driver’s window at 68° F is approximately 72.

\[
\frac{\eta}{l_{mfp}} \approx \frac{1.8 \cdot 10^{-4} \text{inch}}{2.5 \cdot 10^{-6} \text{inch}} \approx 72
\]

(2.20)

Therefore the Kolmogorov length scale is much bigger than the mean free path of air, which in turn, is typically 10 times the molecular diameter.

To resolve all the turbulent length scales of a high Reynolds number flow using the discretized Navier-Stokes equations would require extremely small spatial grid spacing. In addition, large integration times are needed to resolve the average flow field over the time scales. There have been several approaches used for solving the turbulent Navier-Stokes equations. One method, known as Direct Numerical Simulation (DNS), is to solve the governing equations directly. DNS attempts to resolve all important scales down to the Kolmogorov scales. This method is useful in observing flow field characteristics but is very costly for high Reynolds number flows.
Another method is Large Eddy Simulation (LES), which attempts to resolve only the larger eddies in the flowfield while modeling the effects of unresolved (subgrid) eddies. LES is also quite expensive for high Reynolds number flows.

Another method is to model the effects of all turbulent fluctuations on the mean flow properties. In this the governing equations are averaged over a time $T$ that is much larger than all the turbulent fluctuating time scales $T_1$. For unsteady flows, such as those investigated in this work, the averaged time $T$ must be smaller than the time scale of the slow mean property variations $T_2$. Therefore, the turbulent fluctuations are averaged over time $T$, while maintaining the time dependent mean property variations in the flow field. This implies that a large separation of time scales between the mean property variations and the turbulent fluctuations must exist in the flow field for this approach to be valid.

2.2.1 Reynolds Averaging

The following sections present Reynolds and Favre-averaging techniques as applied to the Navier-Stokes equations. The averaging concepts introduced by Reynolds [13] generally assume a wide variety of forms. The type most often used in CFD is time averaging. The following is a derivation of the Reynolds Averaged Navier-Stokes (RANS) equations. Although the RANS equations are derived from time averaging, the form of the equations generalizes to time, spatial, and ensemble averaging. The time averaged flow variables can be expressed as:

$$\overline{f}(x_i) = \lim_{T \to \infty} \frac{1}{T} \int_t^{t+T} f_i(x_i, t) \, dt$$

(2.21)

where $f$ is the instantaneous flow variable. This variable can be decomposed into mean and fluctuating components,

$$f = \overline{f} + f'$$

(2.22)

where the over-bar indicates time averaging. In practice an infinite $T$ cannot be realized; instead the equations are integrated over a time $T$ that is much larger than the time scales
of turbulent fluctuations but smaller than the smallest period of slow property variations in the mean flow field. This type of decomposition results in the time average of a fluctuating component being equal to zero. It also results in the time average of the products of mean components to be equal to the products themselves.

\[
\overline{\Phi \Psi} = \overline{\Phi \Psi},
\]

\[
\overline{\Phi \psi'} = \overline{\Psi \phi'} = 0
\]

Equations 2.23-2.24 are known as the Reynolds postulates. They do not imply however, that the time average of the products of fluctuating components are equal to zero [14]. The average of the product of two fluctuating properties is:

\[
\overline{\phi \psi} = (\overline{\Phi + \phi'}) (\overline{\Psi + \psi'}) = \overline{\Phi \Psi + \Phi \psi' + \Psi \phi' + \phi' \psi'} = \overline{\Phi \Psi + \phi' \psi'}
\]

### 2.2.2 Favre Averaging

Density and temperature fluctuations must be taken into account for compressible flow fields. A density weighting procedure (Favre Averaging) is used to simplify the derivation of the time averaged equations [13]. The Favre (mass) averaged component is defined as

\[
\bar{f} (x_i) = \frac{1}{\rho} \lim_{\Delta t \to \infty} \frac{1}{\Delta t} \int_t^{t+\Delta t} \rho f (x_i, t) \, dt = \frac{\rho \bar{f}}{\rho}
\]

The instantaneous function \( f \) can now be decomposed into Favre mean and Favre fluctuating components as:

\[
f = \bar{f} + f''
\]
Favre averaging is employed by decomposing $p$, $\rho$, $q_j$ in the normal Reynolds averaging fashion and decomposing the remaining variables using the Favre decomposition.

$$\begin{align*}
\rho &= \overline{\rho} + \rho' \quad u_j = \bar{u}_j + u''_j \quad u^{(m)}_j = \bar{u}^{(m)}_j + u''^{(m)}_j \\
p &= \overline{p} + p' \quad \tau_{ij} = \bar{\tau}_{ij} + \tau''_{ij} \quad T = \bar{T} + T'' \\
q_j &= \bar{q}_j + q'_j \quad Y_m = \bar{Y}_m + Y''_m \quad \bar{w}_m + \bar{w}'_m \\
\epsilon_t &= \bar{\epsilon}_t + \epsilon''_t \quad h_t = \bar{h}_t + h''_t
\end{align*}$$

(2.28)

The equations are then mass-averaged using the definition of the Favre averaged component in equation 2.26. Using this type of decomposition, the compressible Favre-Averaged Navier-Stokes Equations (RANS) extended for species mass transport can be written as

$$\begin{align*}
\frac{\partial}{\partial t} (\overline{\rho}) + \frac{\partial}{\partial x_j} (\overline{\rho u_j}) &= 0 \\
\frac{\partial}{\partial t} (\overline{\rho Y_m}) + \frac{\partial}{\partial x_j} (\overline{\rho Y_m u_j}) &= \frac{\partial}{\partial x_j} \left[ \overline{\rho Y^{(m)}_m + Y_{mj}} \right] + \overline{w_m} \\
\frac{\partial}{\partial t} (\overline{\rho u_i}) + \frac{\partial}{\partial x_j} (\overline{\rho u_i u_j}) &= -\frac{\partial}{\partial x_j} (\overline{p \delta_{ij}}) + \frac{\partial}{\partial x_j} (\overline{\tau_{ij} + T_{ij}}) \\
\frac{\partial}{\partial t} (\overline{\rho \epsilon_t}) + \frac{\partial}{\partial x_j} (\overline{\rho \epsilon_t u_j}) &= \frac{\partial}{\partial x_j} \left[ \overline{\rho Y^{''}_m u''_j} + Q_j \right] \\
Y^{''}_{mj} &= \overline{\rho Y^{''}_m u''_j} \\
T_{ij} &= -\rho u''_i u''_j \\
Q_j &= -\rho u''_i \bar{h}_t - \bar{u}_i T_{ji} = \bar{q}_j - u_i T_{ji} \\
\overline{\rho \epsilon_t} &= \overline{\rho \epsilon_t} + \overline{\rho} \\
\overline{\rho \bar{h}_t} &= \overline{\rho \epsilon_t} + \overline{\rho}
\end{align*}$$

(2.29) - (2.37)
The averaged laminar stress tensor, heat flux, and diffusion velocities are given by:

\[
\bar{\tau}_{ij} = \mu \left( \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) - \frac{1}{2} \delta_{ij} \mu \frac{\partial \tilde{u}_k}{\partial x_k}
\]

\[
\bar{q}_j = \lambda \frac{\partial \tilde{T}}{\partial x_j} - \sum_{m=1}^{N_S} \tilde{p} \bar{h}_m \bar{Y}_m \tilde{V}_j^{(m)}
\]

\[
\tilde{V}_j^{(m)} = \frac{1}{\bar{Y}_m} \frac{\partial \bar{Y}_m}{\partial x_j}
\]

(2.38)

2.3 Chemically Reacting Equation Set

The Favre averaged equation set described above is transformed into curvilinear coordinates by the steady transformation[12]:

\[
\xi = \xi (x, y, z)
\]

\[
\eta = \eta (x, y, z)
\]

(2.39)

\[
\zeta = \zeta (x, y, z)
\]

to yield the following equation set:

\[
\frac{\partial U}{\partial t} + \frac{\partial \left( \tilde{E} - \bar{E}_v \right)}{\partial \xi} + \frac{\partial \left( \tilde{F} - \bar{F}_v \right)}{\partial \eta} + \frac{\partial \left( \tilde{G} - \bar{G}_v \right)}{\partial \zeta} = S
\]

(2.40)

The conservative variable vector \( U \) and the source term vector \( S \) are:

\[
U = \frac{1}{J} \begin{pmatrix}
\tilde{p}_1 \\
\vdots \\
\tilde{p}_{NS} \\
\tilde{\rho} \bar{u} \\
\tilde{\rho} \bar{v} \\
\tilde{p} \bar{w} \\
\tilde{p} \bar{\varepsilon}_t
\end{pmatrix}, \quad S = \begin{pmatrix}
\bar{w}_1 \\
\vdots \\
\bar{w}_{NS}
\end{pmatrix}
\]

(2.41)
The inviscid flux vectors are given by:

\[
\hat{E} = \frac{1}{J} \begin{pmatrix}
\bar{\rho} \mathbf{U} \\
\vdots \\
\bar{\rho}_{NS} \mathbf{U} \\
\bar{\rho} \mathbf{U} + \xi_x \bar{p} \\
\bar{\rho} \mathbf{U} + \xi_y \bar{p} \\
\bar{\rho} \mathbf{U} + \xi_z \bar{p} \\
\bar{\rho} \bar{h} \mathbf{U}
\end{pmatrix}, \quad \hat{F} = \frac{1}{J} \begin{pmatrix}
\bar{\rho} \mathbf{V} \\
\vdots \\
\bar{\rho}_{NS} \mathbf{V} \\
\bar{\rho} \mathbf{V} + \eta_x \bar{p} \\
\bar{\rho} \mathbf{V} + \eta_y \bar{p} \\
\bar{\rho} \mathbf{V} + \eta_z \bar{p} \\
\bar{\rho} \bar{h} \mathbf{V}
\end{pmatrix}, \quad \hat{G} = \frac{1}{J} \begin{pmatrix}
\bar{\rho} \mathbf{W} \\
\vdots \\
\bar{\rho}_{NS} \mathbf{W} \\
\bar{\rho} \mathbf{W} + \zeta_x \bar{p} \\
\bar{\rho} \mathbf{W} + \zeta_y \bar{p} \\
\bar{\rho} \mathbf{W} + \zeta_z \bar{p} \\
\bar{\rho} \bar{h} \mathbf{W}
\end{pmatrix}
\]

(2.42)

The viscous flux vectors are given by:

\[
\hat{E}_v = \frac{1}{J} \begin{pmatrix}
-\bar{\rho}_1 \mathbf{U}^{(1)} \\
\vdots \\
-\bar{\rho}_{NS} \mathbf{U}^{(NS)} \\
\xi_x (\mathbf{T}_{xx} + \mathbf{T}_{xx}) + \xi_y (\mathbf{T}_{xy} + \mathbf{T}_{xy}) + \xi_z (\mathbf{T}_{xz} + \mathbf{T}_{xz}) \\
\xi_x (\mathbf{T}_{yx} + \mathbf{T}_{yx}) + \xi_y (\mathbf{T}_{yy} + \mathbf{T}_{yy}) + \xi_z (\mathbf{T}_{yz} + \mathbf{T}_{yz}) \\
\xi_x (\mathbf{T}_{zx} + \mathbf{T}_{zx}) + \xi_y (\mathbf{T}_{zy} + \mathbf{T}_{zy}) + \xi_z (\mathbf{T}_{zz} + \mathbf{T}_{zz}) \\
\xi_x (\bar{u} \mathbf{T}_{xx} + \bar{v} \mathbf{T}_{xy} + \bar{w} \mathbf{T}_{xx}) + \xi_y (\bar{u} \mathbf{T}_{yx} + \bar{v} \mathbf{T}_{yy}) + \xi_z (\bar{u} \mathbf{T}_{xz} + \bar{v} \mathbf{T}_{yy}) + \bar{q}_x + \bar{q}_y + \bar{Q}_x \\
+\xi_x (\bar{u} \mathbf{T}_{zx} + \bar{v} \mathbf{T}_{zy}) + \bar{q}_x + \bar{q}_y + \bar{Q}_x
\end{pmatrix}
\]

(2.43)

\[
\hat{F}_v = \frac{1}{J} \begin{pmatrix}
-\bar{\rho}_1 \mathbf{V}^{(1)} \\
\vdots \\
-\bar{\rho}_{NS} \mathbf{V}^{(NS)} \\
\eta_x (\mathbf{T}_{xx} + \mathbf{T}_{xx}) + \eta_y (\mathbf{T}_{xy} + \mathbf{T}_{xy}) + \eta_z (\mathbf{T}_{xz} + \mathbf{T}_{xz}) \\
\eta_x (\mathbf{T}_{yx} + \mathbf{T}_{yx}) + \eta_y (\mathbf{T}_{yy} + \mathbf{T}_{yy}) + \eta_z (\mathbf{T}_{yz} + \mathbf{T}_{yz}) \\
\eta_x (\mathbf{T}_{zx} + \mathbf{T}_{zx}) + \eta_y (\mathbf{T}_{zy} + \mathbf{T}_{zy}) + \eta_z (\mathbf{T}_{zz} + \mathbf{T}_{zz}) \\
\eta_x (\bar{u} \mathbf{T}_{xx} + \bar{v} \mathbf{T}_{xy} + \bar{w} \mathbf{T}_{xx}) + \eta_y (\bar{u} \mathbf{T}_{yx} + \bar{v} \mathbf{T}_{yy}) + \eta_z (\bar{u} \mathbf{T}_{xz} + \bar{v} \mathbf{T}_{yy}) + \bar{q}_x + \bar{q}_y + \bar{Q}_x \\
+\eta_x (\bar{u} \mathbf{T}_{zx} + \bar{v} \mathbf{T}_{zy}) + \bar{q}_x + \bar{q}_y + \bar{Q}_x
\end{pmatrix}
\]

(2.44)

\[
\hat{Q}_v = \frac{1}{J} \begin{pmatrix}
-\bar{\rho}_1 \mathbf{W}^{(1)} \\
\vdots \\
-\bar{\rho}_{NS} \mathbf{W}^{(NS)} \\
\zeta_x (\mathbf{T}_{xx} + \mathbf{T}_{xx}) + \zeta_y (\mathbf{T}_{xy} + \mathbf{T}_{xy}) + \zeta_z (\mathbf{T}_{xz} + \mathbf{T}_{xz}) \\
\zeta_x (\mathbf{T}_{yx} + \mathbf{T}_{yx}) + \zeta_y (\mathbf{T}_{yy} + \mathbf{T}_{yy}) + \zeta_z (\mathbf{T}_{yz} + \mathbf{T}_{yz}) \\
\zeta_x (\mathbf{T}_{zx} + \mathbf{T}_{zx}) + \zeta_y (\mathbf{T}_{zy} + \mathbf{T}_{zy}) + \zeta_z (\mathbf{T}_{zz} + \mathbf{T}_{zz}) \\
\zeta_x (\bar{u} \mathbf{T}_{xx} + \bar{v} \mathbf{T}_{xy} + \bar{w} \mathbf{T}_{xx}) + \zeta_y (\bar{u} \mathbf{T}_{yx} + \bar{v} \mathbf{T}_{yy}) + \zeta_z (\bar{u} \mathbf{T}_{xz} + \bar{v} \mathbf{T}_{yy}) + \bar{q}_x + \bar{q}_y + \bar{Q}_x \\
+\zeta_x (\bar{u} \mathbf{T}_{zx} + \bar{v} \mathbf{T}_{zy}) + \bar{q}_x + \bar{q}_y + \bar{Q}_x
\end{pmatrix}
\]

(2.45)
where \( \overline{w}_m \) is the averaged species production rate for species \( m \), \( \mathcal{U}, \mathcal{V}, \mathcal{W} \) are the contravariant velocity components and \( \mathcal{U}^m, \mathcal{V}^m, \mathcal{W}^m \) are the contravariant diffusion velocities for species \( m \) defined by:

\[
\begin{align*}
\mathcal{U} & \equiv \xi_x \ddot{u} + \xi_y \ddot{v} + \xi_z \ddot{w} \\
\mathcal{V} & \equiv \eta_x \ddot{u} + \eta_y \ddot{v} + \eta_z \ddot{w} \\
\mathcal{W} & \equiv \zeta_x \ddot{u} + \zeta_y \ddot{v} + \zeta_z \ddot{w}
\end{align*}
\]

\[
\begin{align*}
\mathcal{U}^m & \equiv \xi_x \ddot{V}_1^m + \xi_y \ddot{V}_2^m + \xi_z \ddot{V}_3^m \\
\mathcal{V}^m & \equiv \eta_x \ddot{V}_1^m + \eta_y \ddot{V}_2^m + \eta_z \ddot{V}_3^m \\
\mathcal{W}^m & \equiv \zeta_x \ddot{V}_1^m + \zeta_y \ddot{V}_2^m + \zeta_z \ddot{V}_3^m
\end{align*}
\]

(2.46)

(2.47)

and \( J \) is the Jacobian of the coordinate transformation.

### 2.3.1 Chemical Kinetics

The chemical mass production rate per unit volume \( \overline{w}_m \) for species \( m \) is given by the law of mass action:

\[
\overline{w}_m = \sum_{n=1}^{NR} \left[ \left( v''_{nn} - v'_{nn} \right) \left( RR_{f_n} - RR_{b_n} \right) \right]
\]

\[
= \sum_{n=1}^{NR} \left[ \left( v''_{mm} - v'_{mm} \right) \left( k_{f_n} \prod_{j=1}^{NS} \left( \tilde{c}_j \right)^{v'_j} - k_{b_n} \prod_{j=1}^{NS} \left( \tilde{c}_j \right)^{v''_j} \right) \right]
\]

(2.48)

and \( v'_j \) is the stoichiometric coefficient of the reactants, \( v''_j \) is the stoichiometric coefficient of the products, \( NR \) is the total number of reactions involved, \( NS \) is the total number of species involved, \( RR_{f_n} \) and \( RR_{b_n} \) are the forward and backward reaction rates respectively for reaction \( n \), where \( \tilde{c}_j = \frac{n}{M_j} \) is the molar density for species \( j \). The specific reaction rate \( k \) is written below in Arrhenius form:

\[
k(T) = AT^{\alpha}e^{\left( \frac{-E}{RT} \right)}
\]

(2.49)
where $A$ is the pre-exponential constant, and $T_a$ is the activation temperature [15]. The variables $A$, $b$, and $T_a$ are found in Tables 1 and 2 for the two reaction mechanisms considered in this study. The reaction mechanisms are composed of two types of reactions, exchange and third body. The exchange reaction describes the interdependent forward and backward reactions between products and reactants. For the following exchange reaction:

$$A + B \rightleftharpoons C + D \quad (2.50)$$

The forward and backward reaction rates are given by the law of mass action as:

$$RR_f = k_f (T) \tilde{c}_A^{v_A} \tilde{c}_B^{v_B}$$

$$RR_b = k_b (T) \tilde{c}_C^{v_C} \tilde{c}_D^{v_D} \quad (2.51)$$

Third body reactions occur when two species react in the presence of a collision partner $M$. The law of mass action can be rewritten for a third body reaction by considering that a third body reaction is actually $NS$ reactions where the reaction rate depend on the collision partner $M$.

$$\bar{w}_m = \sum_{n}^{NR} \left( v_m - v_m' \right) \sum_{i=1}^{NS} (RR_{fni} - RR_{bni} \right) \quad (2.52)$$

For the following third body reaction

$$AB + M \rightleftharpoons A + B + M \quad (2.53)$$

the third body reaction rate $R_n$ for reaction $n$ is

$$R_n = \sum_{i=1}^{NS} (RR_{fni} - RR_{bni}) \quad (2.54)$$

and the forward and backward reaction rate in equation 2.54 are

$$RR_{fni} = k_{fni} \tilde{c}_A^{v_A} \tilde{c}_B^{v_B} \tilde{c}_M^{v_M} \quad (2.55)$$

$$RR_{bni} = k_{bni} \tilde{c}_A^{v_A} \tilde{c}_B^{v_B} \tilde{c}_M^{v_M} \quad (2.56)$$
If one of the specific reaction rate coefficients is chosen as a reference value, denoted by \( k_{f_n}^' \), then the third body efficiency can be written as the ratio of the particular species coefficient \( A_{f_n,i} \) to the reference coefficient \( A_{f_n}^' \):

\[
(T_B)_i = \frac{A_{f_n,i}}{A_{f_n}^'}
\]  

(2.57)

Using this relation, the forward and backward specific reaction rates can be written as

\[
k_{f_n,i} = k_{f_n}^' (T_B)_i
\]

\[
k_{b_n,i} = k_{b_n}^' (T_B)_i
\]

(2.58)

Using equation 2.58 in equation 2.55 and 2.56, then the third body reaction efficiency can be written in terms of the third body efficiencies as

\[
R_n = \left[ k_{f_n}^' \frac{x_{AB}^i}{c_{AB}} - k_{b_n}^' \frac{x_{A}^i}{c_{A}} \frac{x_{B}^i}{c_{B}} \right] \sum_{i=1}^{N_S} (T_B)_i \frac{x_{M_i}^i}{c_{M_i}}
\]

(2.59)

The 7 species 7 hydrogen-oxidation reaction mechanism by Eklund [16] is used for the chemistry modeling in the 3-D scramjet combustor simulations. This involves six reacting species, \( \text{H}_2, \text{O}_2, \text{H}_2\text{O}, \text{OH}, \text{H}, \text{O} \), plus inert \( \text{N}_2 \), that interact through a seven-step reaction mechanism. This reaction mechanism was chosen for the 3-D scramjet simulation to maintain a minimal problem size. Also as indicated by the 2-D results, the flame is stabilized at the fuel injector exit and therefore the inclusion of ignition chemistry should provide little variation in the flame downstream of the nozzle exit. This should have little effect on the thermal choking of the combustor.

The 9 species 21 reaction mechanism proposed by Balakrishnan, et al. [17] is used to model the hydrogen oxidation for the 2-D scramjet combustor simulations. This involves the same reaction species as in the reaction mechanism by Eklund plus \( \text{H}_2\text{O}_2 \) and \( \text{HO}_2 \). These radicals have been shown to important during ignition of the hydrogen-oxygen reaction and may be significant for lifted flame calculations where flame propagation and stabilization is important.
Table 1: Abridged Jachimowski Chemistry Model

<table>
<thead>
<tr>
<th>#</th>
<th>Reaction</th>
<th>A</th>
<th>b</th>
<th>$T_a$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$\text{H} + \text{OH} + \text{M} \rightleftharpoons \text{H}_2\text{O} + \text{M}$</td>
<td>$221E + 23$</td>
<td>-2.0</td>
<td>0.0</td>
</tr>
<tr>
<td>2</td>
<td>$\text{H} + \text{H} + \text{M} \rightleftharpoons \text{H}_2 + \text{M}$</td>
<td>$730E + 18$</td>
<td>-1.0</td>
<td>0.0</td>
</tr>
<tr>
<td>3</td>
<td>$\text{H}_2 + \text{O}_2 \rightleftharpoons \text{OH} + \text{OH}$</td>
<td>$170E + 14$</td>
<td>0.0</td>
<td>24157.0</td>
</tr>
<tr>
<td>4</td>
<td>$\text{H} + \text{O}_2 \rightleftharpoons \text{OH} + \text{O}$</td>
<td>$120E + 18$</td>
<td>-0.91</td>
<td>8310.5</td>
</tr>
<tr>
<td>5</td>
<td>$\text{OH} + \text{H}_2 \rightleftharpoons \text{H}_2\text{O} + \text{H}$</td>
<td>$220E + 14$</td>
<td>0.0</td>
<td>2591.8</td>
</tr>
<tr>
<td>6</td>
<td>$\text{O} + \text{H}_2 \rightleftharpoons \text{OH} + \text{H}$</td>
<td>$506E + 05$</td>
<td>2.67</td>
<td>3165.6</td>
</tr>
<tr>
<td>7</td>
<td>$\text{OH} + \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{O}$</td>
<td>$630E + 13$</td>
<td>0.0</td>
<td>548.6</td>
</tr>
</tbody>
</table>

TBEs: H$_2$ O 16.0, H$_2$ 2.5, and 1.0 for all other species
A, b, and $T_a$ are given in units of moles cm$^3$s$^1$K, and cal/mole,

$k = AT^b e^{(\frac{-A}{RT})}$

Modeling procedures that account for the effects of turbulent fluctuations on chemical reaction rates are difficult to develop due to the large number of unclosed correlations which arise. Two alternative methods discussed by Roy [12], the probability density formulation (PDF) and Eddy Dissipation Concept (EDC), were shown to have deficiencies in calculating supersonic combustion flames. The more attractive (PDF) method also had negligible effects for calculating attached supersonic flames. Therefore, the above formulation for the species production rates is evaluated using mean quantities. The effects of turbulent fluctuations on rate coefficients and on molar density are neglected, thus

$k_f (T) \rightarrow k_f (\overline{T})$ \hspace{1cm} (2.60)

$c_j (\rho_j) \rightarrow c_j (\overline{\rho_j})$ \hspace{1cm} (2.61)

While this approach is questionable, no clearly better alternative has emerged for high-speed combustion flames such as those present in the current work.
Table 2: Balakrishnan et al. Chemistry Model

<table>
<thead>
<tr>
<th>#</th>
<th>Reaction</th>
<th>A</th>
<th>b</th>
<th>E</th>
</tr>
</thead>
<tbody>
<tr>
<td>1&lt;sup&gt;a&lt;/sup&gt;</td>
<td>H + OH + M ⇌ H₂O + M</td>
<td>2.2e22</td>
<td>-2.0</td>
<td>0.0</td>
</tr>
<tr>
<td>2&lt;sup&gt;b&lt;/sup&gt;</td>
<td>H + H + M ⇌ H₂ + M</td>
<td>1.e18</td>
<td>-1.0</td>
<td>0.0</td>
</tr>
<tr>
<td>3&lt;sup&gt;a&lt;/sup&gt;</td>
<td>H + O + M ⇌ OH + M</td>
<td>6.2e16</td>
<td>-0.6</td>
<td>0.0</td>
</tr>
<tr>
<td>4&lt;sup&gt;a&lt;/sup&gt;</td>
<td>O + O + M ⇌ O₂ + M</td>
<td>6.17e15</td>
<td>-0.5</td>
<td>0.0</td>
</tr>
<tr>
<td>5&lt;sup&gt;a&lt;/sup&gt;</td>
<td>H₂O₂ + M ⇌ HO₂ + M</td>
<td>6.76e19</td>
<td>-1.42</td>
<td>0.0</td>
</tr>
<tr>
<td>6&lt;sup&gt;c&lt;/sup&gt;</td>
<td>H₂O₂ + M ⇌ OH + OH + M</td>
<td>1.2e17</td>
<td>0.0</td>
<td>45500.0</td>
</tr>
<tr>
<td>7</td>
<td>O + OH + M ⇌ HO₂ + M</td>
<td>1.0e16</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>8</td>
<td>H + O₂ ⇌ OH + O</td>
<td>3.52e16</td>
<td>-0.7</td>
<td>17070</td>
</tr>
<tr>
<td>9</td>
<td>OH + H₂ ⇌ H₂O + H</td>
<td>1.17e9</td>
<td>1.3</td>
<td>3626</td>
</tr>
<tr>
<td>10</td>
<td>O + H₂ ⇌ OH + H</td>
<td>5.06e4</td>
<td>2.67</td>
<td>6290</td>
</tr>
<tr>
<td>11</td>
<td>OH + OH ⇌ H₂O + O</td>
<td>7.0e14</td>
<td>0.0</td>
<td>56767</td>
</tr>
<tr>
<td>12</td>
<td>HO₂ + H ⇌ H₂ + O₂</td>
<td>4.28e13</td>
<td>0.0</td>
<td>1411.0</td>
</tr>
<tr>
<td>13</td>
<td>HO₂ + H ⇌ OH + OH</td>
<td>1.70e14</td>
<td>0.0</td>
<td>874.0</td>
</tr>
<tr>
<td>14</td>
<td>HO₂ + O ⇌ O₂ + OH</td>
<td>2.00e13</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>15</td>
<td>HO₂ + OH ⇌ H₂O + O₂</td>
<td>2.89e13</td>
<td>0.0</td>
<td>-497.0</td>
</tr>
<tr>
<td>16</td>
<td>HO₂ + HO₂ ⇌ H₂O₂ + O₂</td>
<td>3.02e12</td>
<td>0.0</td>
<td>1390.0</td>
</tr>
<tr>
<td>17</td>
<td>H + H₂O₂ ⇌ H₂ + HO₂</td>
<td>4.79e13</td>
<td>0.0</td>
<td>7950.0</td>
</tr>
<tr>
<td>18</td>
<td>H + H₂O₂ ⇌ OH + H₂O</td>
<td>1.00e13</td>
<td>0.0</td>
<td>3590.0</td>
</tr>
<tr>
<td>19</td>
<td>H₂O₂ + H ⇌ H₂O + OH</td>
<td>7.08e12</td>
<td>0.0</td>
<td>1430.0</td>
</tr>
<tr>
<td>20</td>
<td>H + HO₂ ⇌ O + H₂O</td>
<td>3.10e13</td>
<td>0.0</td>
<td>1720.0</td>
</tr>
<tr>
<td>21</td>
<td>H₂ + O₂ ⇌ OH + OH</td>
<td>1.70e13</td>
<td>0.0</td>
<td>44780.0</td>
</tr>
</tbody>
</table>

<sup>a</sup> TBEs: H₂ O 12.0, H₂ 2.5  
<sup>b</sup> TBEs: H₂ O 6.5, O₂ 0.5, N₂ 0.4  
<sup>c</sup> TBEs: H₂ O 15.0, H₂ 2.5  

A, b, and E are given in units of moles, cm, s, K, and cal/mole,  

\[ k = AT^b e^{\left(\frac{E}{RT}\right)} \]
3 Numerical Formulation

3.1 Turbulent Closure

The process of averaging the Navier-Stokes equations results in extra terms that must be modeled. These terms arise because of the nonlinearity of the equations. By investigation of equations 2.33-2.35, three unknown terms appear due to the averaging. These include the Reynolds shear stress $T_{ij}$, Reynolds heat flux $q_{ht}$, and the turbulent species diffusion $\mathcal{Y}_{mj}$. In order to obtain turbulent closure, models for each of the terms must be developed.

Most turbulence models in use today employ the Boussinesq eddy-viscosity approximation for the Reynolds stress tensor, which assumes that the Reynolds stress behaves in a manner similar to the laminar stress tensor [18]:

$$T_{ij} = \mu_T \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \frac{\partial \bar{u}_k}{\partial x_k} \quad (3.3.1)$$

The Reynolds heat flux is modeled using a gradient-diffusion approximation, yielding an expression similar to Fourier’s law:

$$q_{ht} = \gamma_t \frac{\partial \tilde{T}}{\partial x_j} - \sum_{m=1}^{NS} P \tilde{h}_m \tilde{Y}_m \tilde{V}^{(m)}_{t_j} \quad (3.3.2)$$

$$\gamma_t = \frac{\mu_T C_p}{P_r_t} \quad (3.3.3)$$

$$\tilde{V}^{(m)}_{t_j} = -\frac{1}{\tilde{Y}_m} D_t \frac{\partial \tilde{Y}_m}{\partial x_j} \quad (3.3.4)$$

$$D_t = \frac{\mu_t}{S_{ct} \bar{p}} \quad (3.3.5)$$

The turbulent species diffusion is modeled by a gradient diffusion model as

$$\mathcal{Y}_{mj} = \rho \tilde{Y}_m u_j^m = -\frac{\mu_T}{S_{ct}} \frac{\partial \tilde{Y}_m}{\partial x_j} \quad (3.3.6)$$

The closure problem is reduced to specification of the eddy viscosity. If we assume that the eddy viscosity can be computed in a similar fashion as the molecular viscosity, then the eddy viscosity is also dependent on a velocity scale and length scale.

$$\mu_T = \rho u_{mix}^l_{mix} \quad (3.3.7)$$
where \( u_{mix} \) and \( l_{mix} \) denote velocity and length scales, respectively, that are associated with the mixing of turbulent eddies. These scales must be provided by the turbulence model. The turbulence model used in this work is the zonal two equation \( k-\omega \) model developed by Menter [19]. This model is a combination of the Wilcox \( k-\omega \) and the standard \( k-\epsilon \) models. The \( k-\omega \) model is used in the laminar sublayer of the boundary layer and logarithmic region of the boundary layer. This model has been shown to be superior to the \( k-\epsilon \) model in adverse pressure gradient flows and in compressible flows. The zonal model approaches a \( k-\epsilon \) model in the outer parts of the boundary layer and in free-shear regions. This reduces the sensitivity of the calculation to free-stream turbulence quantities and allows reasonable predictions of free-shear flows. The transition from \( k-\omega \) to \( k-\epsilon \) is facilitated by a blending function \( F_1 \), which is zero in the wake region and free-shear layer and one in the wall region. This model is written below as:

\[
\nu_t = \frac{a_1 k}{\max (a_1 \omega; \Omega F_2)}
\]

(3.3.8)

\[
\frac{\partial}{\partial t} (\rho k) + \frac{\partial}{\partial x_j} (\rho k u_j) = \frac{\partial}{\partial x_j} \left( u_i \frac{\partial u_i}{\partial x_j} - \beta^* \rho \omega k + \frac{\partial}{\partial x_j} \left[ (\mu + \sigma_k \mu_k) \frac{\partial k}{\partial x_j} \right] \right)
\]

(3.3.9)

\[
\frac{\partial}{\partial t} (\rho \omega) + \frac{\partial}{\partial x_j} (\rho \omega u_j) = \frac{\gamma}{\nu_t} \frac{\partial u_i}{\partial x_j} - \beta^* \rho \omega^2 + \frac{\partial}{\partial x_j} \left[ (\mu + \sigma_\omega \mu_k) \frac{\partial \omega}{\partial x_j} \right] + 2 \rho (1 - F_1) \sigma_2 \frac{1}{\omega} \frac{\partial k}{\partial x_j} \frac{\partial \omega}{\partial x_j}
\]

(3.3.10)

Let \( \phi_1 \) represent any constant in the original \( k-\omega \) and \( \phi_2 \) any constant in the transformed \( k-\epsilon \) model. Then \( \phi \) is defined by the blending function:

\[
\phi = F_1 \phi_1 + (1 - F_1) \phi_2
\]

(3.3.11)

The \( \phi_1 \) constants of the (Wilcox) \( k-\omega \) model are:

\[
\sigma_{k1} = 0.85, \quad \sigma_{\omega 1} = 0.5, \quad \beta_1 = -0.0750, \quad a_1 = 0.31
\]

(3.3.12)

\[
\beta^* = 0.09, \quad \kappa = 0.41, \quad \gamma_1 = \frac{\beta_1}{\beta^*} - \sigma_{\omega 1} \frac{\kappa^2}{\sqrt{\beta^*}}
\]

(3.3.13)
The constants \( \phi_2 \) of the standard \( (k - \epsilon) \) are:

\[
\sigma_{k2} = 1.0, \quad \sigma_{\omega} = 0.856, \quad \beta_2 = 0.0828, \quad a_1 = 0.31 \quad (3.3.14)
\]

\[
\beta^* = 0.09, \quad \kappa = 0.41, \quad \gamma = \frac{\beta_2}{\beta^*} - \sigma_{\omega} \frac{\kappa^2}{\beta^*} \quad (3.3.15)
\]

The blending functions are defined by Menter as:

\[
F_1 = \tanh(\arg_1^1), \quad \text{where} \quad \arg_1 = \min \left[ \max \left( \frac{\sqrt{k}}{0.09\omega y}, \frac{500\nu}{y^2\omega} \right); \frac{4\rho\sigma_{\omega} k}{C D_{kw} y^2} \right], \quad \text{and} \quad (3.3.16)
\]

\[
F_2 = \tanh(\arg_2^2), \quad \text{where} \quad \arg_2 = \max \left( \frac{2\sqrt{k}}{0.09\omega y}, \frac{500\nu}{y^2\omega} \right) \quad (3.3.17)
\]

\[
\text{where, } C D_{kw} = \max \left( \frac{2\rho\sigma_{\omega} \frac{1}{\omega} \frac{\partial k}{\partial x_j} \frac{\partial \omega}{\partial x_j}}{\partial x_j} \right) \quad (3.3.18)
\]

Equation 3.3.8 satisfies Bradshaw’s assumption [19] that the shear stress is proportional to the turbulent kinetic energy in the boundary layer, while preserving the original formulation that \( \nu_t = k/\omega \) for the rest of the flow.

### 3.2 Upwinding

The inviscid fluxes in the Navier-Stokes equations are discretized using the Low Diffusion Flux Splitting Scheme (LDFSS) of Edwards [20]. This scheme attempts to combine the accuracy of flux difference splitting methods with the numerical efficiency of flux vector splitting methods. The LDFSS algorithm provides accurate resolution of stationary and moving contact discontinuities while preserving solution monotonicity and entropy satisfaction. The LDFSS algorithm requires \( O(N) \) operations for \( N \) equations compared with \( O(N^2) \) operations of flux difference schemes. [21] For clarity, the algorithm is applied to the three dimensional instantaneous equations in the \( \xi \) direction. Similar results are obtained for the remaining directions. The inviscid \( \xi \)-direction flux \( \hat{E} \) can be split into
advection and pressure components, as

$$\hat{E} = \hat{E}^c + \hat{E}^p = \frac{\nabla \xi}{J} \left( \rho \mathcal{U} \bar{E}^c + p \bar{E}^p \right), \quad \mathcal{U} = \frac{1}{|\nabla \xi|} (\xi_x u + \xi_y v + \xi_z w)$$ (3.3.21)

is the normalized contravariant velocity in the $\xi$ direction,

$$\bar{E}^c = \begin{bmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_{NS} \\ u \\ v \\ w \\ h_t \\ k \\ \omega \end{bmatrix}, \quad \bar{E}^p = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ \bar{\xi}_x \\ \bar{\xi}_y \\ \bar{\xi}_z \\ 0 \\ 0 \end{bmatrix}$$ (3.3.22)

$$\bar{\xi}_x = \frac{\xi_x}{|\nabla \xi|}, \quad \bar{\xi}_y = \frac{\xi_y}{|\nabla \xi|} \quad \bar{\xi}_z = \frac{\xi_z}{|\nabla \xi|}$$ (3.3.23)

The upwinding is performed at the cell interfaces, denoted by $\frac{1}{2}$ in Figure 1, using the properties at the the left (L) and the right (R) states. The discretization stores information at the node cell vertex, with the mesh cells denoted by dashed lines. The metric derivatives are evaluated at the cell interfaces. The LDFSS scheme applied to the cell interfaces results in the inviscid flux being split into convective and pressure components, with the convective flux written as

$$E_{1+\frac{1}{2}}^c = \frac{\nabla \xi}{J} \left( \rho_L a_{\frac{1}{2}} c^+ E_{1+\frac{1}{2}}^c + \rho_R a_{-\frac{1}{2}} c^- E_{R}^c \right)$$ (3.3.24)

and the pressure flux defined by

$$\hat{E}_{\frac{1}{2}}^p = \frac{\nabla \xi}{J} \hat{E}_{\frac{1}{2}}^p \left[ D_{L}^+ p_L + D_{R}^- p_R \right]$$ (3.3.25)

where $a_{\frac{1}{2}}$ is the interface sound speed, written as

$$a_{\frac{1}{2}} = \frac{a_L + a_R}{2}$$ (3.3.26)
and $C^\pm$ and $D^\pm$ are functions of the Mach number, defined as

\[
D^+ = \alpha_L^+ (1 + \beta_L) - \beta_L P_L^+ \\
D^- = \alpha_R^- (1 + \beta_R) - \beta_R P_R^-
\]

(3.3.27) (3.3.28)

\[
C^+ = \alpha_L^+ (1 + \beta_L) M_L - \beta_L M_L^+ + \beta_L \beta_R \overline{M}^+ \\
C^- = \alpha_R^+ (1 + \beta_R) M_R - \beta_R M_R^- + \beta_L \beta_R \overline{M}^-
\]

(3.3.29) (3.3.30)

where

\[
\alpha_L^+ = \frac{1}{2} [1 + \text{sign} (1.0, \ M_L)] \quad (3.3.31)
\]

\[
\alpha_R^+ = \frac{1}{2} [1 - \text{sign} (1.0, \ M_R)] \quad (3.3.32)
\]

\[
\beta_L = -\max [0.0, \ 1.0 - \text{int} (|M_L|)] \quad (3.3.33)
\]

\[
\beta_R = -\max [0.0, \ 1.0 - \text{int} (|M_R|)] \quad (3.3.34)
\]

\[
M_L^+ = \frac{1}{4} (M_L + 1)^2 \\
M_R^- = -\frac{1}{4} (M_R - 1)^2 \\
\overline{P}_L^+ = \frac{1}{4} (M_L + 1)^2 (2 - M_L) \\
\overline{P}_R^- = \frac{1}{4} (M_R^2 - 1)^2 (2 - M_R) \\
\overline{M}^+ = \left[ 1 - \left( \frac{p_L - p_R}{p_L + p_R} + 2 \frac{|p_L - p_R|}{p_L} \right) \right] \mathcal{M}^{L+} \\
\overline{M}^- = \left[ 1 + \left( \frac{p_L - p_R}{p_L + p_R} - 2 \frac{|p_L - p_R|}{p_L} \right) \right] \mathcal{M}^{L-} \\
\mathcal{M}^{L\pm} = \frac{1}{4} \left( \sqrt{\frac{1}{2} (M_L^2 + M_R^2) - 1} \right)^2
\]

(3.3.35) (3.3.36) (3.3.37) (3.3.38) (3.3.39) (3.3.40) (3.3.41)

and the left and right state Mach numbers are defined according to the interface sound speed

\[
M_{L,R} = \frac{1}{a^{\pm}} (\xi_x u + \xi_y v + \xi_z w)_{L, R}
\]

(3.3.42)
In the definitions of $\tilde{M}^+$ and $\tilde{M}^-$ (Equations 3.3.39-3.3.40), the first term involving the pressures provides monotone capturing of discontinuities [12], while the second term counteracts the “carbuncle”-type odd-even decoupling discussed in Reference [22].

### 3.3 Time Advancement

The 3-D code uses a three-point backward Euler time advancement procedure that results in a large sparse linear system, formulated for a particular grid point as:

\[
\left[ \frac{3 \, M}{2 \, \Delta t} + \tilde{A} - \frac{\partial \tilde{S}}{\partial \tilde{W}} \right]_{ij, k}^{n} \Delta \tilde{W}_{i, j, k} = \frac{\tilde{B}}{\tilde{W}_{i, j, k}} + \frac{\tilde{B}}{\tilde{W}_{i, j, k-1}} + \frac{\tilde{B}}{\tilde{W}_{i, j, k+1}} + \frac{\tilde{C}}{\tilde{W}_{i, j, k}} + \frac{\tilde{C}}{\tilde{W}_{i, j+1, k}} + \frac{\tilde{E}}{\tilde{W}_{i, j, k-1}} + \frac{\tilde{E}}{\tilde{W}_{i, j+1, k}} + \frac{\tilde{G}}{\tilde{W}_{i, j, k+1}} + \frac{\tilde{G}}{\tilde{W}_{i, j, k+1}} + \frac{\tilde{G}}{\tilde{W}_{i, j+1, k}} + \frac{\tilde{G}}{\tilde{W}_{i, j+1, k}} \]

\[
= -\tilde{R}_{ij, k} + \frac{1}{2} \left( \frac{\tilde{U}}{\tilde{W}_{ij, k}} - \frac{\tilde{U}_{ij, k-1}}{\Delta t} \right) \]  

(3.3.43)

where $\tilde{A} - \tilde{G}$ are function of the inviscid and viscous flux Jacobians, as outlined in Reference [23]. $M$ is the transformation matrix $\frac{\partial \tilde{U}}{\partial \tilde{W}}$, $\frac{\partial \tilde{S}}{\partial \tilde{W}}$ is the Jacobian of the source term vector, and $\Delta t$ is the physical time step.

The basic implicit operator is formed by ordering equation 3.3.43 over the grid nodes and incorporating implicit representations for the boundary conditions [12]. The resulting system Jacobian matrix is denoted as $\hat{A}$. This system is approximately solved using a symmetric planar Gauss-Seidel (SPGS) algorithm. Denoting $\left[ \frac{3 \, M}{2 \, \Delta t} + \hat{A} - \frac{\partial \tilde{S}}{\partial \tilde{W}} \right]$ as $\hat{H}$, a planar Gauss-Seidel partitioning [12, 20, 24, 25] is defined by first grouping matrix elements corresponding to an $i = \text{constant}$ plane as $D$

\[
D = \left[ \hat{H} + \hat{B} + \hat{C} + \hat{D} + \hat{E} \right] \quad \text{(3.3.44)}
\]

and grouping off-plane elements into $L$ and $U$ respectively, where

\[
L = \hat{F} \quad \text{(3.3.45)}
\]

\[
U = \hat{G} \quad \text{(3.3.46)}
\]
In this formulation all matrix elements composing of $D$, $L$, and $U$ are stored over the entire mesh. The partitioning is then defined by

$$
(D + L)^n \left( D^{n-1} \right) (D + U)^n \Delta \tilde{W}^{n+1} = -\tilde{R}^n + \frac{1}{2} \left( \tilde{U}^n - \tilde{U}^{n-1} \right) \Delta t \tag{3.3.47}
$$

This Gauss-Seidel partitioning is an approximation to the matrix $\hat{A}$, with factorization error $LD^{-1}U\delta W$. The factorization is nearly exact for streamwise supersonic flows, but the factorization error increases as the the number of nonzero elements in $U$ increases [25]. This means that as the amount of streamwise subsonic flow increases, the performance of the algorithm will degrade. The SPGS algorithm is implemented in two steps, a forward and backward step in the $\xi$ direction:

forward sweep:  $\Delta \tilde{W}_{i+\frac{1}{2}}^{n+1} = (D_i^n)^{-1} \left[ -\tilde{R}_i^n - L_{i-1}^n \Delta \tilde{W}_{i-\frac{1}{2}}^{n+1} \right] \tag{3.3.48}$

backward sweep:  $\Delta \tilde{W}_{i+1}^{n+1} = \Delta \tilde{W}_{i+\frac{1}{2}}^{n+1} - (D_i^n)^{-1} U_{i+1}^n \Delta \tilde{W}_{i+1}^{n+1} \tag{3.3.49}$

The approximate inversion of the block pentadiagonal matrix $D_i$ at each $i$ index is accomplished using an Alternating Direction-Implicit algorithm developed in earlier works [12, 20, 24, 25].
4 Multiblock Parallel Implementation

The calculation of flows within complex domains using structured grids usually requires some type of domain-decomposition strategy. Domain decomposition involves the partitioning of a complex domain into simpler subdomains, which may be solved in sequence or in parallel. The following subsections discuss the domain decomposition strategy used for time-dependent, 3-D scramjet calculations. The parallel implementation of the solution algorithm is also discussed. A combined decomposition is used over the three dimensional domain. The combined decomposition contains a primary decomposition in the $\xi$ and $\eta$ directions and a secondary decomposition in the $\zeta$ direction. The Multiplicative Schwarz method[26] is used to solve the primary decompositions. Multiplicative Schwarz methods solve each subdomain problem in sequence by using the most recent artificial boundary data from the adjacent blocks. The Additive Schwarz method is used to solve the secondary decompositions. Additive Schwarz methods solve each subdomain problem using the last artificial boundary data from the adjacent blocks. Parallelism can be achieved in the secondary direction because of the use of the Additive Schwarz algorithm, where no dependence on updated data from adjacent domains exists. Therefore, the primary decomposition is calculated in a serial fashion, while the secondary decomposition is calculated in parallel. The 2-D calculations use only the primary decomposition and were run on the Cray T-90, a vector architecture. The 3-D calculations were run in parallel on the IBM-SP at the North Carolina Super Computing Center (NCSC) and on a Compaq ES-40 at North Carolina State University (NCSU).

4.1 Algorithm

The development of this algorithm was governed by the flow model being used. The time advancement scheme discussed earlier may be written for the entire domain $\Omega$ as the linear system $\hat{A}_\Omega^n \Delta W_{\Omega}^{n+1} = -\mathcal{R}_\Omega^n$, where $\hat{A}$ is Jacobian matrix of the nonlinear system, $\Delta \hat{W}$ is
the correction vector, and $\mathcal{R}$ is the residual vector. The system can be decomposed over a set of subdomains as follows.

$$\hat{A}_\Omega = \begin{pmatrix} \hat{A}_{\Omega_1} & \hat{A}_{\Omega_1|\Omega_1} \\ \vdots & \vdots \\ \hat{A}_{\Omega_{m-1}|\Omega_{m-1}} & \hat{A}_{\Omega_{m-1}|\Omega_m} \\ \hat{A}_{\Omega_m|\Omega_m_1} & \hat{A}_{\Omega_m|\Omega_m} \end{pmatrix}$$ (4.4.1)

where $\hat{A}_{\Omega_k}$ denotes elements of the Jacobian corresponding strictly to subdomain $k$ and $\hat{A}_{\Omega_k|\Omega_k}$ denotes elements that connect the solution within block $k$ to that within other blocks. By removing the explicit dependence on the $\hat{A}_{\Omega_k|\Omega_k}$ elements, a successive iteration procedure for solving the system can be used, with the boundary data updated through the calculation of the residual vector $\mathcal{R}$ on $\Omega_k$. Considering a two block decomposition the Multiplicative Schwarz algorithm can be written as a two step process.

$$\Delta W^{n+\frac{1}{2}} \leftarrow \Delta W^n + \begin{pmatrix} \hat{A}_{\Omega_1}^{-1} \\ 0 \\ 0 \\ 0 \end{pmatrix} \mathcal{R}^n$$ (4.4.2)

$$\Delta W^{n+1} \leftarrow \Delta W^{n+\frac{1}{2}} + \begin{pmatrix} 0 \\ 0 \\ 0 \\ \hat{A}_{\Omega_2}^{-1} \end{pmatrix} \mathcal{R}^{n+\frac{1}{2}}$$ (4.4.3)

The $n + \frac{1}{2}$ notation denotes the updating of information from adjacent to subdomain interfaces. This updated information is incorporated into the calculation of the residual operator as soon as it becomes available. The matrix inverse indicated in 4.4.2 and 4.4.3 actually represents the application of the planar Gauss-Seidel procedure 3.3.47 on each subdomain. If an Additive Schwarz type decomposition is also applied in the block then the result is a four block decomposition with a hybrid Multiplicative and Additive Schwarz scheme. Equation 4.4.2-4.4.3 becomes:

$$\Delta W^{n+\frac{1}{2}} \leftarrow \Delta W^n + \begin{pmatrix} \hat{A}_{\Omega_{1,1}}^{-1} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & \hat{A}_{\Omega_{1,2}}^{-1} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \mathcal{R}^n$$ (4.4.4)

$$\Delta W^{n+1} \leftarrow \Delta W^{n+\frac{1}{2}} + \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & \hat{A}_{\Omega_{2,1}}^{-1} & 0 \\ 0 & 0 & 0 & \hat{A}_{\Omega_{2,2}}^{-1} \end{pmatrix} \mathcal{R}^{n+\frac{1}{2}}$$ (4.4.5)
This is a two step Multiplicative Schwarz method with Additive Schwarz sub-steps. This requires the update of the residual vector after each Multiplicative step for the primary decomposition while only updating the residual vector for the secondary decomposition after all the Multiplicative Schwarz steps are complete. This allows each Multiplicative step to be solved in parallel. For nominally two dimensional problems with a uniform mesh in the third dimension, it is convenient to apply Additive Schwarz in the uniform direction and to apply Multiplicative Schwarz decomposition in the non-uniform directions. The above method can generalized for the actual Scramjet combuster geometry decomposition as shown in Figure 2. The primary decomposition is in the $\xi$ and $\eta$ directions while the secondary decomposition is in the $\zeta$ direction. Figure 3 illustrates the solution procedure for the combined Multiplicative and Additive Schwarz methods for two processors. Consider the $\xi$, $\eta$, $\zeta$ decomposition of blocks 1 through 5 in Figure 2, with reference to the flowchart in Figure 3. Each processor receives an $\zeta$ decomposition for blocks 1 - 5, where these blocks are decomposed in the $\xi$ and $\eta$ directions. Then each inner loop on the flow chart begins on block 1 and sequences through to block 5 i.e. $(m=1...mb)$. First, each processor allocates the primitive vector $W_{\Omega_m}$ over the subdomain for the current block, including the artificial boundaries. Then the residual vector $R_{\Omega_m}$ is formed for the subdomain. The system of linear equations $A_{\Omega_m}\Delta W_{\Omega_m}^{m+1} = R_{\Omega_m}$ is then approximately solved for the update vector $\Delta W_{\Omega_m}^{m+1}$. After the interior points are updated, a serial transfer of the artificial boundary information to adjacent blocks in the $\xi$ and $\eta$ directions satisfying $[W_{\Omega_m} \cap W_{\Omega_m}]_{\xi,\eta}$ takes place. After all the blocks are sequenced through, a parallel data transfer updates the solution variables on the artificial boundaries in the $\zeta$ direction, satisfying $[W_{\Omega_m}^{\zeta} \cap W_{\Omega_m}^{\zeta}]_{\zeta}$ takes place. Therefore, the parallel algorithm is independent of the time integration method used to solve the system. The equation set in 4.4.2-4.4.3 is dependent on the proper update of the residual vector $R$ at each Schwarz step. Therefore synchronization of the parallel algorithm after each sub-step is necessary to maintain the proper update of the residual
vector $\mathcal{R}$

The parallel transfers were carried out by using the Message Passing Interface [27] (MPI-1) standard. A sample program of the MPI block transfer is given in the Appendix. A buffer is used to store the data being transferred for the secondary decomposition. This buffer is sent using blocking, combined send-receive commands in the $\zeta$ direction in the appendix. Two waves of send-receive are performed to transfer data for the two artificial faces at each interface. This type of message passing only completes when all the processors involved in the transfer have posted their individual send-receive calls. This ensures that data is transferred at the right time level of the integration and also prevents system buffering that could lead to slow performance as the system could be overloaded with buffered data. This type of message passing also prevents deadlock as waves of data are transferred for each face.

The artificial boundary information on each $\zeta$ plane is mapped into an one dimensional array before the parallel transfer to adjacent blocks. This allows an explicit packing and unpacking of the buffer, instead of using implicit derived data types generated by MPI. Derived data types may be dependent on the system being used, as different systems use different memory layouts and sizes. The explicit buffering is system-independent, but requires $(\xi_{\text{max}} + 6)(\eta_{\text{max}} + 6)6$ operations to pack and unpack the buffer. The time to perform these operations is negligible compared with the time required to perform one iteration of the flow solver.

4.2 Parallel Performance

Computational performance of the parallel algorithm is measured by speedup and efficiency of the algorithm compared to its serial counterpart. These quantities are defined below as:
\[ S(1, p) = \frac{t_1}{t_p} \quad (4.4.6) \]
\[ E(1, p) = \frac{t_1}{pt_p} \quad (4.4.7) \]

The speedup \( S \) in equation 4.4.6 will not exceed the number of processors \( p \) used in a particular calculation, as indicated by the Speedup Folklore Theorem [28]. If the speedup \( S \) is greater than the number of processes, then a faster serial algorithm can be made be simulating the parallel one, provided that it can be simulated. In the case where cache performance gets better with smaller subdomains via domain decomposition, the serial program can not simulate the parallel program and therefore super-linear speedup is observed. The efficiency \( E \) in equation 4.4.7 is simply a measure of the time cost optimization, described below as:

If \( E(1, p) < 1 \) then the parallel algorithm is not time cost optimal

If \( E(1, p) = 1 \) then the parallel algorithm is time cost optimal, provided that the sequential algorithm is time optimal \((4.4.9)\)

If \( E(1, p) > 1 \) then a faster sequential algorithm can be obtained by simulating the parallel one

Tables 3 through 4 provide the time data for the parallel algorithm applied to a Large Eddy Simulation (LES) calculation on a 4-processor Compaq ES-40 shared memory architecture and an IBM-SP distributed memory architecture. The LES calculation on 33x65x65 and 65x65x65 grids is that of a plane Poiseuille channel flow. This was used to validate the parallel interface boundary transfers and to gain knowledge of parallel performance. The times T1, T2, T3, are real, cpu, and system times in units of seconds. The 33x65x65 node case solved for twenty iterations is shown in Table 3. The expected trend that increasing the number of processors results in the speedup being less than the number of processors was observed. The performance of this algorithm degrades as the level of compiler optimization
is increased, as the compiler only optimizes the serial portion of the algorithm. The time to perform twenty iterations using four processors took 343 seconds with no optimization. A 71 percent decrease in time was accomplished by using a level four compiler optimization, but this only resulted in a 25 percent decrease in the efficiency of the algorithm as compared to the efficiency of the case without optimization. Using the Speedup Folklore theorem of 4.4.9, the most optimal condition for the current algorithm is with four processes and full optimization, with a speedup of 3.04. This algorithm did not have the highest speedup for the four processor cases, but had the highest speedup for the most time optimal serial program.

Most of the performance loss is direct result of the parallel algorithm requiring an order of \(O\left((\xi_{\text{max}}\eta_{\text{max}}(\xi_{\text{max}} + p - 1))^2\right)\) operations. As the domain is broken into up smaller segments, then the overall domain size increases by \(p - 1\) \(\zeta\) planes of data. With an overlap of 6 planes of data between \(\zeta\) domains, each iteration requires \(6p\) planes of data transfer and an additional computation of \(p - 1\) planes of data.

<table>
<thead>
<tr>
<th>T1</th>
<th>T2</th>
<th>T3</th>
<th>node %</th>
<th>n</th>
<th>options</th>
<th>speedup</th>
<th>efficiency</th>
</tr>
</thead>
<tbody>
<tr>
<td>1250.0</td>
<td>1249.75</td>
<td>.37</td>
<td>99</td>
<td>1</td>
<td>-O0</td>
<td>1.0</td>
<td>1.00</td>
</tr>
<tr>
<td>623.0</td>
<td>622.41</td>
<td>1.31</td>
<td>199</td>
<td>2</td>
<td>-O0</td>
<td>2.01</td>
<td>1.01</td>
</tr>
<tr>
<td>343.0</td>
<td>341.92</td>
<td>2.25</td>
<td>399</td>
<td>4</td>
<td>-O0</td>
<td>3.64</td>
<td>0.91</td>
</tr>
<tr>
<td>750.0</td>
<td>749.61</td>
<td>.77</td>
<td>99</td>
<td>1</td>
<td>-O1</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>400.0</td>
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<td>6.58</td>
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<td>0.94</td>
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<tr>
<td>215.0</td>
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<td>399</td>
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<td>342.0</td>
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<td>-O2</td>
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<td>1.00</td>
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<tr>
<td>309.0</td>
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<td>1.00</td>
<td>1.00</td>
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<td>193.0</td>
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<td>101.0</td>
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<tr>
<td>295.0</td>
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<td>4</td>
<td>-O4-fast</td>
<td>3.04</td>
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</tr>
</tbody>
</table>

Table 3: Execution Times on Scramjet

Table 4 shows the time for 1, 2, 4, 8, and 16 processors for the 65x65x65 grid on the
IBM SP at the North Carolina Supercomputing center for 1000 iteration runs. These runs were calculated using level 3 optimization on IBM SP, which is comparable to the level 4 optimization on the Compaq ES40. The speedup and efficiency results here demonstrate that increases in the number of subdomains and the attendant communication and execution costs degrade the program performance for processor numbers larger than eight. This can be explained by the fact that the ratio of the number of computational ζ planes to communication planes is \( \frac{5}{6} \), and the problem size has increased by 21 percent. The extra iteration work can be avoided by using a cell-centered finite volume discretization, but the communication costs do not disappear.

<table>
<thead>
<tr>
<th>T1</th>
<th>T2</th>
<th>T3</th>
<th>n</th>
<th>speedup</th>
<th>efficiency</th>
<th>comment</th>
</tr>
</thead>
<tbody>
<tr>
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<td>21222.52</td>
<td>24.30</td>
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<td>1.0</td>
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<td>13129.44</td>
<td>15.43</td>
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<td>.808</td>
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<td>5690.53</td>
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<td>3.7357</td>
<td>.934</td>
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<td>3091.07</td>
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<td>8</td>
<td>6.8774</td>
<td>.860</td>
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<td>1792.48</td>
<td>3.44</td>
<td>16</td>
<td>11.198</td>
<td>.700</td>
<td>LES (274625 nodes)</td>
</tr>
</tbody>
</table>

Table 4: Execution Times on IBM SP
5 Application

5.1 Flow Model

The National Aerospace Lab (NAL) nominally two-dimensional scramjet isolator / combustor configuration is simulated in this work [29]. This configuration as shown in Figure 4 consists of a wedge shaped fuel strut on the centerline of the combustor. The strut wedge angle is 5° and the isolator length is 0.140 m. The total length of the combustor is 0.540 m with the strut placed 0.043 m behind the inflow plane. Pressure taps were placed 10 mm apart on the centerline of the top wall for the first 0.340 m and 0.020 m apart for the rest of the combustor. The fuel strut shown in Figure 5 is 94.3 mm wide in the spanwise direction. The injector throat was designed to maintain supersonic injection of the fuel stream. The 5 degree wedge angle was determined by Masuya[30] to not induce boundary layer separation on the duct wall due to the impinging shock from the fuel strut. The fuel strut is preceded by the inlet section that receives vitiated air from the upstream combustor. The inflow conditions are shown in Table 5. The scramjet combustor inlet

<table>
<thead>
<tr>
<th>Flow Property</th>
<th>Experiment</th>
<th>Simulation</th>
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<tr>
<td>$T_o$</td>
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<td>2214</td>
</tr>
<tr>
<td>$h_o$</td>
<td>2.79</td>
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<tr>
<td>$p_o$ (kPa)</td>
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<td>1012</td>
</tr>
<tr>
<td>$M_\infty$</td>
<td>2.44</td>
<td>2.43</td>
</tr>
<tr>
<td>$p_\infty$</td>
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<tr>
<td>$m_{O_2}$</td>
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<tr>
<td>$\gamma_\infty$</td>
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<tr>
<td>$R_\infty$</td>
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</tr>
<tr>
<td>$Y_{O_2}$</td>
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<tr>
<td>$Y_{H_2O}$</td>
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</tr>
<tr>
<td>$\delta$(mm)</td>
<td>5.5</td>
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</tr>
</tbody>
</table>

Table 5: Flow Conditions (vitiated air stream)
conditions were obtained from the exhaust gas of a Vitiated Air Generator (VAG). This type of test gas contains a large water mass fraction of 0.2097 as seen in Table 5. The nominal Mach number and stagnation temperature are 2.45 and 2214 respectively, leading to a static temperature that is well above the auto-ignition temperature for hydrogen combustion. The three-dimensional block decomposition is shown in Figure 2-6. The nominally two-dimensional geometry of the NAL combustor is modeled precisely in the $\xi$ and $\eta$ directions and is extended in the $\zeta$ direction. Block 1 contains 17x41x33 points, block 2 contains 17x9x33 points, block 3 contains 49x41x33 points, block 4 contains 61x33x33 points, and block 5 contains 133x73x33 points, for a total of 481,173 points. Due to computer memory restrictions, the resolution in the $\xi$ and $\eta$ directions is a fourth of that used in the 2-D simulations of Reference [6]. The two-dimensional grid is shown in Figure 6 with every other grid point shown. Mesh clustering to all solid surfaces is used to capture viscous layer gradients. Also the grid was stretched in the $\xi$ direction to resolve the shock structure around the wedge leading edge, the Prandtl-Meyer expansion near the centerline strut, the recirculation region behind the fuel strut, and the free shear layer that develops aft of the fuel strut.

5.2 Boundary Conditions

Both two and three dimensional turbulent channel flow calculations were performed to obtain the inflow data for the simulations. All flow variables are extrapolated from the interior of the combustor section to the outflow plane of the combustor using second order extrapolation. This method of extrapolation is questionable where thermal choking results and the combustor is subsonic, but without a knowledge of the back pressure, no better method can be found. No-slip and adiabatic wall conditions were applied to all solid boundaries on the fuel strut and the scramjet combustor. This assumes that the there is no heat transfer through solid surfaces during the short test run of the NAL tunnel. The
decomposition discussed in section 4.3 introduces interface boundaries between adjacent blocks. The flow variables along interface boundaries in the $\zeta$ direction are not updated during the Multiplicative Schwarz solution steps, while the interface boundaries in the $\xi$ and $\eta$ directions are updated from data contained on adjacent blocks. The $\zeta$ interface boundaries are updated using adjacent interface data during the parallel transfer.

5.3 Fuel Injection

All cases were initialized with a converged solution of the baseline case in which the equivalence ratio ($\phi$) is set 0.0. This corresponds to no hydrogen fuel injection. The fuel flow rate was ramped over time to match the equivalence ratio for each case, then maintained for the duration of the simulation. The fuel flow rate through the geometric throat $A_t$ was calculated from:

$$\frac{\dot{m}_{H_2}}{A_t} = \frac{\phi \dot{m}_{O_2}}{A_t} \frac{M_{H_2}}{M_{O_2}} = 51.388 \phi$$

(5.5.1)

The fuel flow rate was ramped using the following procedure:

$$\frac{\dot{m}_{H_2}}{A_t} = \min \left(1.0, \frac{t}{t_c} \right) \frac{\dot{m}_{H_2}}{A_t}$$

(5.5.2)

where $t_c$ is the flow-through time based on the free-stream velocity. The fuel is ramped over one half of a flow-through time (approximately 0.00015 seconds). After this time, the fuel flow rate is held constant. The conditions at the subsonic inflow boundary of the fuel injector are set by the known fuel mass flow rate per unit area, pressure extrapolation from the interior, a constant stagnation temperature, and the gas composition (pure hydrogen).
6 Results and Discussion

6.1 Two Dimensional Results

Three fuel equivalence ratio cases of 0.0 (no fuel injection), 0.29, and 0.61 were simulated in two dimensions. The \( \phi = 0.0 \) and \( \phi = 0.29 \) cases are nominally steady, while the \( \phi = 0.61 \) case resulted in a unsteady unstart. All reactive flow simulations were initialized from a converged \( \phi = 0.0 \) solution.

The Mach number, temperature, and pressure contours are shown in Figure 8 for the \( \phi = 0.0 \) case. This case is useful in as a reference point for describing changes due to mass injection and combustion of fuel for the higher equivalence ratio cases. The boundary layer thickness is approximately 5.5 mm thick and increases through the duct due to friction and shock boundary layer interactions to about 12 mm at the end of the combustor section. A small separation region results from the interaction of the bow shock formed ahead of the fuel strut with the top wall boundary layer, and a second separation zone results from the recompression shock that forms behind the expansion fan aft of the fuel strut. A large recirculation region exists behind the fuel strut. In this symmetric case, upper and lower supersonic cores result in the combustor section, with a subsonic mixing layer between them. Temperature increases can be observed near the adiabatic walls, behind the recompression shocks, and in the separation zones. A maximum static temperature of 2250 K is observed in the stagnation region at the bow of the fuel strut. The pressure contours illustrate the complex shock system in the isolator and combustor regions. The oblique shock system / expansion fan interactions continue throughout the combustor with a total of six shock reflections in the combustor. The total pressure ratio \( \frac{P}{P_{\infty}} \) along the centerline is .4635. This ratio is slightly less than the .47911 total pressure ratio that would result from a normal shock in the duct at the free-stream Mach number of 2.44. The static pressure increases toward the exit as a result of the effects of friction and shock interactions. The recirculation region behind the fuel injector and the temperature
rise across the recompression shock promote flame stabilization for the higher equivalence ratios. This flow solution and its 3-D analogue is used as the initial condition for the higher equivalence ratio cases.

Figure 9 displays surface pressure distribution for the $\phi = 0.0$ and $\phi = 0.29$ cases at several characteristic time levels. A steady scramjet mode of combustion is obtained after $22.66t_c$ characteristic times ($t_c = .314$ ms). For the $\phi = 0.0$ cases, reasonably good agreement with experimental data is found throughout the combustor except near the impingement point of the bow shock on the upper boundary layer. The peak pressure rise is significantly underpredicted, and the subsequent wave interactions are less pronounced than shown in the experimental data. These discrepancies may result from several numerical factors, such as insufficient grid resolution in the impingement region, the discretization scheme’s relatively low order of accuracy near discontinuities, and the possible tendency of the turbulence model to “over-separate” the boundary layer in response to the adverse pressure gradient. The experimental data shows that the actual combustion process in the combustor influences the flow in the isolator section to a large extent, indicating that the shock train established to contain the combustion-induced pressure rise propagates into the isolator region and is stabilized there. This is not seen here in the two dimensional results, but is observed for the three dimensional case as discussed later. The two dimensional results also show a transition to subsonic flow through a successive weakening of the oblique shock structure at after $x = 200mm$, rather than a continuing oblique shock pattern throughout the nozzle as observed in the experiment. The hydroxyl mass fraction (OH), Mach number, temperature, and pressure contours are shown in Figure 10 for the $\phi = 0.29$ case. Contour levels for Mach number and temperature are restricted to $|M| < 1$ and $T > 2000$ respectively to better distinguish regions of subsonic flow and regions of strong heat release. The free-stream temperature entering the combustor is near 1500 degrees, well above the autoignition limits of hydrogen. This leads to immediate ignition of the flame
that is stabilized in the recirculation region discussed earlier. The gradual pressure rise in the combustor is due to the outward deflection of the reactive shear layer, which decreases the effective flow area occupied by the core fluid. Small regions of high-temperature, low-momentum fluid occur on the upper boundary layer due to shock / boundary layer interactions. The temperature in the mixing region reaches a maximum value of around 2800 Kelvin. A comparison of the hydroxyl contours and the Mach number contours shows that chemical reactions occur in the supersonic region of the flow. The majority of the combustion occurs between the fuel strut and $x = 200mm$ meters plane, as indicated by the large levels of hydroxyl in that region. This region is also the expansion region, which will become a more significant part of the flow for the higher equivalence ratio cases. The flame structure shown is typical of diffusion flames, where the maximum concentrations of hydroxyl radical delineate the flame front and correspond to the regions of highest temperature.

Figures 11 - 15 illustrate the response of the isolator / combustor flowfield to time-dependent injection of hydrogen at $\phi = 0.61$. In Figure 11 wall pressure distributions along the top wall of the scramjet combustor at several time levels are compared with experimental pressure data time averaged over 40 ms. Three stages of the unsteady response are observed for this case. The initial stage occurs before $t < 4.63t_c$, where the injection process raises the static pressure of the fluid within the injector from around 50 kPa to nearly 300 kPa, resulting in choked flow at the nozzle throat. The expansion behind the fuel strut is nearly eliminated while the recompression shock is strengthened due to the displacement effect of the hydrogen fuel mass injection ($t = 1.54t_c$). OH contours shown in the close up view of the injector region (Figure 14) reveal that the initial stages of fuel-air mixing occur through the growth of the vortical structures generated through Kelvin-Helmholtz mechanisms. This results in the intermittent pulsing of the fuel flow rate before stabilization occurs at $t = 1t_c$. As in the previous case ignition occurs almost immediately
and the flame is stabilized in the recirculation regions located behind the injector lip. By $t = 4.63t_e$, the reactive shear layer has propagated through the entire combustor section. As in the $\phi = 0.29$, case peak temperatures are approximately 2800 Kelvin.

In the intermediate stages ($4.63t_e < t < 15.88t_e$), the initial injection of hydrogen results in a decreased velocity core as a result of the displacement effect of the reactive shear layer and the associated increase in oblique shock strength. This in turn increases the residence time of the hydrogen in the combustor and allows for stronger mixing, combustion, and heat release. Figure 12 shows the steady growth of the subsonic shear layer until $t = 15.88t_e$, where it contacts the bottom and top wall boundary layers. As a result, an oblique shock train forms in the isolator/combustor region. This compressive system connects the combustor conditions to the upstream isolator conditions, as seen in Figure 13. The boundary layer thickens due to the stronger oblique reflections on the wall and the increase in back pressure in the combustor. At $t = 15.88t_e$, hydrogen fuel is able to diffuse into the boundary layer around the fuel strut, moving the ignition points backward along the upper and lower surfaces of the fuel strut, as seen in Figure 14. Figure 15 shows that the increase in combustor pressure decreases the the velocity and momentum flux of the hydrogen fuel. This shortens the fuel rich core and allows for more complete combustion. In the last stage, $t > 15.88t_e$, increasing combustor pressure levels result from the local thickening of the boundary layer and thermal expansion of the reactive shear layer. The established shock system now moves forward into the isolator region, and the scramjet transitions to a ramjet mode of operation. As time progress, the oblique shock system is disgorged from the inlet. The experimental data indicates a standing normal shock at the bow of the fuel strut after unstart, and the pressure levels in the remaining sections are indicative of subsonic flow in the combustor. This condition was not obtained here, as the solution during the latter stages of unstart is corrupted due to the fixed boundary conditions at the inflow.
6.2 Three Dimensional Results

The three dimensional results are discussed using plots of x-y cross-sections at several z locations and time levels to show both three dimensional and time dependent effects. The following properties were chosen to illustrate the flow features: static pressure, u-velocity, temperature, density, hydrogen mass fraction, water mass fraction, hydroxyl mass fraction, and turbulent kinetic energy. Three dimensional plots are used to illustrate the unstart condition at the final time level. Similar unstart structures can be identified for both equivalence ratio cases. Three stages of operation are discussed for the equivalence ratio of 0.29 case while only two stages of operation are discussed for the equivalence ratio of 0.61 case. In both cases, the unstart mechanism results from the growth and upstream propagation of sidewall separation zones, formed due to shock interactions and heat release. Side wall boundary layer separation occurs at an incipient pressure of approximately 154 kPa for both cases, initiating the process of flowpath destabilization and eventual engine unstart.

6.2.1 Equivalence Ratio 0.29

Figure 16 shows a three dimensional view of u velocity contours at \( t = 13.25 \) milliseconds for \( \phi = 0.29 \). The increased flow blockage in the streamwise direction is illustrated in the figure. The supersonic boundary layer at \( x = 0.4467m \) encompasses 83 percent of the area at this X location. Figures 17-21 illustrate the flowfield properties for the \( \phi = 0.29 \) case at \( t = 6.88, 11.88, \) and \( 13.38 \) milliseconds and at \( z = 0.0471, 0.0236, \) and \( 0.009 \) m planes at each time level. The \( z_c \) plane is in the boundary layer of the sidewall; \( z_b \) is midway between the centerline plane of the combustor and the wall; and \( z_a \) is the X-Y symmetry plane of the combustor.

Referring to Figure 17 at \( t = 6.88ms \), the reactive shear layer has fully developed at this time level. The flow structure outside of the sidewall boundary layer is similar to
two-dimensional results at this time level. At this time level and subsequent time levels, the facility is operating as a scramjet, with combustion primarily occurring at supersonic speeds. The $z_a$ and $z_b$ planes have similar flowfield properties indicating that the flow is nominally two dimensional. The bow shock and subsequent oblique shock reflections have risen the free-stream temperature above 1400 K, which aids in stabilizing the diffusion flame. The oblique shock system deflects the reactive shear layer outward and enhances mixing of fuel and oxidizer in the shear layer. The hydrogen injection velocity is subsonic at this time level and remains subsonic for the rest of the simulation. This is due to the increased back pressure in the combustor. The slower injection speed allows more time for mixing and combustion in the combustor. At $t = 11.88ms$ the combustor is operating as a high-efficiency scramjet, where the heat release is complete at the combustor exit and the Mach number is nearly one. A recompression shock emanating from the trailing edge of the fuel injector separates the top and bottom boundary layers while thickening the sidewall boundary layer at $t = 11.88ms$. The recirculation region just behind the fuel strut has grown to 0.13 m in length. At $t = 13.88ms$ the reactive front in the boundary layer has propagated forward and separated a large portion of the boundary layer. The pressure rise in the combustor due to shear layer and boundary layer growth has formed a strong oblique shock, illustrated in Figure 18 at $t = 11.88ms$ on planes $z_b$ and $z_c$. The oblique shock is formed as the reactive shear layer deflects outward into the supersonic core near the fuel strut. The impingement of the oblique shock on the sidewall boundary layer at $x = .244m$ creates a large separation bubble, entraining fuel in the normal direction through the sidewall boundary layer. This formation of the sidewall separation zone occurs at an incipient pressure of 154 kPa. This pressure occurs at the impingement location of the oblique shock emanating from the injector trailing edge. The reactive shear layer then moves parallel to the sidewall through the boundary layer and downstream of the separation bubble. The supersonic boundary layer then expands in the spanwise direction
due to heat release, illustrated from $t = 11.88\,ms$ to $t = 13.88\,ms$ in Figure 19. The maximum temperature at $t = 13.38\,ms$ is approximately 3400 Kelvin. At this time level the reactive shear layer has also propagated upstream in the near wall region as shown by the temperature at the $z_e$ location.

Hydrogen fuel mass fraction contours are shown in Figure 20. At $t = 6.88\,ms$ the hydrogen injection is nearly uniform through the combustor. The hydrogen then begins to flow into the sidewall recirculation zones after $t = 11.88\,ms$ (shown here at $z_e$). After unstart the mass fraction of hydrogen near the wall indicates that the hydrogen is moving upstream of the fuel strut. This leads to combustion and subsequent heat release in the boundary layer forward of the isolator section. The movement of the flame front from a diffusion flame at $t = 6.88\,ms$ to a more premixed flame in the reactive boundary at $t = 13.38\,ms$ is shown in the hydroxyl contours in Figure 21.

Without the extra compression due to the formation of sidewall separation regions, the strong oblique system would simply move into the isolator region over the fuel strut. The flowpath may or may not stabilize at this juncture, depending on whether the isolator is long enough to contain the pressure rise in the combustor. But three-dimensional effects lead to the faster side wall compression mechanism, which results in significant flow blockage and chemical reactions within the sidewall boundary layer. The fast unstart mechanism can occur even before actual choking occurs in the combustor, which is seen in the $\phi = 0.61$ case.

The experiment conducted in the VAG did not show the unstart for the $\phi = 0.29$ case but indicated that the second oblique shock in the isolator has increased in strength in response to the increased pressure in the combustor. Figure 22 illustrates six time levels of wall pressure data along the top wall x centerline. At $t = 6.88$, the incipient pressure of 154.0 kPa is reached in the adverse pressure gradient region, leading to separation and local thickening of the boundary layer. The corresponding back pressure is 210 kPa. The
unstart of the inlet takes approximately 2.0 ms after the reactive shear layer merges with
the sidewall boundary layer. The time-averaged pressure along the top wall is shown in
Figure 23. The pressure at the nozzle exit agrees well with the VAG experiment but
is higher in the combustor section than observed in experiment. The shock reflection
pressure is still underpredicted as in the two-dimensional cases. Discrepancies between
the simulation results and the experimental trends may relate to the relative coarseness of
the computational mesh, the inadequacy of the turbulence model in predicting separated
flow, the lack of a proper exit boundary condition when thermal choking results, and a
general overprediction of heat release due to over-simplified chemical kinetics. Future work
will attempt to resolve these discrepancies.

6.2.2 Equivalence Ratio 0.61

Figures 24-29 show the effects of time-dependent injection of fuel on the flow structure for
the $\phi = 0.61$ case. The complete unstart is shown in Figure 24, where the reactive shear
layer encompasses nearly the entire domain. The large separation region induced by the
oblique shock is shown in Figure 25 where a large region of reversed flow near the trailing
edge of the fuel strut is seen at $t = 2.75ms$ and at the $z_c$ plane location. At the end of
the simulation the centerline plane is still mostly supersonic, while the flow at the wall
has reversed and has a peak velocity of ~420.0 m/s in the streamwise direction. The inlet
unstart in the $\phi = 0.61$ case is about 3 times as fast as in the $\phi = 0.29$ case. The reactive
shear layer is fully developed after $t = 1.25ms$, shown in Figure 26 by the temperature
contours. The heat release in the supersonic boundary layer raises the temperature above
3400 Kelvin. This is in indication of strong combustion occurring in this region. The peak
temperature in the reactive shear layer outside the boundary layer is approximately 2400
Kelvin at $t = 1.25 ms$. A reservoir of cold hydrogen fuel builds up at $t = 2.75ms$ just aft
the fuel strut near the sidewall, which aids in increasing the flow blockage in the combustor
(shown in Figure 28).
Animations show that the pressure in the expansion region behind the strut rises above the aforementioned incipient pressure of 154 kPa at \( t = 0.55ms \). The reactive shear layer movement into the sidewall boundary layer is controlled by the back pressure of 94867.1 kPa at this time level. Referring to Figure 27 at \( t = 2.75ms \), the incipient pressure at \( x = 161mm \) is 165.0 kPa at the near wall \( z_c \) plane, which is higher than the incipient pressure of 154 kPa required to separate the flow. This leads to onset of the sidewall compression mechanism discussed for the \( \phi = 0.29 \) case, beginning the unstart.

The combustor is operating at a low - efficiency scramjet mode for this case when the unstart begins, showing the importance of sidewall combustion for the stability of the combustor, rather than thermal choking alone. The combustion in the sidewall boundary layer can be visualized in the temperature (Figure 26) and mass fraction contour plots (Figure 28- 29). As seen in Figure 26, the reactive shear layer has moved up the wall directly behind the impinging shock at \( t = 2.75ms \). This intense heat release drives the shock system out of the inlet in about 1.5 ms. A much stronger oblique shock system forms in this case to compensate for the pressure rise in the combustor, as shown in Figure 27 at \( t = 4.25ms \). After the passage of the normal shock out of the inlet at \( t = 4.25 \) ms, the reactive sidewall boundary layer continues to grow into the reactive shear layer, completely choking about half of the flowfield. The unstart at the end of the simulation results in a small supersonic layer existing at the centerline of the inlet. The bow shock in front of the fuel strut is nearly a standing normal shock. Figure 28, plane \( z_c \), shows that enough hydrogen fuel entrains through the sidewall boundary layer to cause combustion to occur within the sidewall boundary layer upstream of the fuel injection trailing edge at \( t = 4.25ms \).

Figure 30 shows the wall pressure at several characteristic time levels for the \( \phi = 0.61 \) case. At the time level of 5.5 ms, the standing normal shock seen in the experiment is captured in front of the fuel strut. Unlike the experiment, the simulation still shows a
pressure increase throughout the entire combustor. This again is due to the supersonic exit flow boundary conditions, which do not allow the back pressure to influence the flow. Figure 31 shows the time averaged wall pressure for the $\phi = 0.61$ case. The average window for the numerical simulation was 5.5 ms, where each pressure data point in the VAG experiment was averaged over 40 ms. This is a much larger window and indicates that the flow remains choked with a normal shock in the inlet and subsonic combustion in the combustor. The averaged pressure in the simulation is much lower for this equivalence ratio due to the small average window allowed by the simulation. Better inflow boundary conditions are needed to allow for longer compute times to gain meaningful averaged data.
7 Conclusions

A parallel Navier-Stokes solver for computing time-dependent, three-dimensional reacting flowfields within scramjet engines was developed in this work. Parallelization was accomplished using the MPI-I message passing standard and was validated using a Large Eddy Simulation, which showed that the parallel algorithm’s transfer of interface data was spatially and temporally accurate. Scramjet dynamic modes of operation have been investigated for the time-dependent injection of hydrogen fuel into a model scramjet isolator / combustor geometry at the equivalence ratios of 0.0, 0.29 and 0.61.

The two-dimensional results show a steady combustion process for the $\phi = 0.29$ case, and an unsteady inlet unstart for the $\phi = 0.61$ case. This unstart is characterized by a slow pressure growth period that leads to boundary layer and shear layer thickening, thermal expansion, oblique shock system movement into isolation section, and regions of separated flow on the isolator top and bottom walls. Qualitative agreement with experiment is made for the centerline wall pressure data, but the results lack three dimensional blockage effects.

Three-dimensional time-dependent fuel injection results in an engine unstart for both the equivalence ratio of $\phi = 0.29$ and $\phi = 0.61$ cases, the former being contradictory to experimental data. These unstarts are characterized by the formation of a large pocket of separated flow in the side wall boundary layer. This region develops from the impingement of an oblique shock emanating from the reactive shear layer, which deflects upward in response to the pressure rise induced by heat release. The unstart is initiated by the entrainment of hydrogen fuel into the side wall recirculation zones of the combustor. This results in combustion within the sidewall boundary layer and further growth of the separated regions due to thermal expansion with both effects leading to the unstart of the engine. These results have shown that the inlet unstart is controlled by thermal expansion, boundary layer growth, shear layer growth, and side wall separation region growth due to shock interactions and combustion.
While reasonable agreement with the experimentally observed process is obtained for the $\phi = 0.61$ case, the $\phi = 0.29$ results indicate that an unstart occurs, while experimental measurements indicate that a stable burning process is achieved. This major discrepancy could be a result of insufficient mesh resolution, the use of an over-simplified combustion model without ignition chemistry, and the inability of the two equation model to predict the growth of sidewall separation regions accurately. The effects of heat-transfer away from the combustor also remain to be accounted for.
8 Figures

Figure 1: Upwinding stencil (\(\xi\) - direction)
Figure 2: Block decomposition of domain

Figure 3: Parallel algorithm flow chart
Figure 4: NAL isolator / combustor configuration

Figure 5: NAL fuel strut
Figure 6: NAL isolator / combustor configuration grid, (every second point shown)

Figure 7: Hydrogen mass flow rate normalized by equivalence ratio versus time
Flow structure: $\phi = 0$ (no fuel injection)

Figure 8: Flowfield contour plots, $\phi = 0.0$
Figure 9: Wall pressure at several characteristic times $\phi = 0.29$
Figure 10: Flowfield contour plots, $\phi = 0.29$
Figure 11: Wall pressure at several characteristic times, $\phi = 0.61$
regions of separated flow near injector \((t = 20 \, t_c)\)

Figure 12: Mach number contour plot at several time levels, \(\phi = 0.61\)
Figure 13: Static pressure at several time levels, $\phi = 0.61$
Figure 14: OH contours at several time levels, $\phi = 0.61$
Figure 15: Centerline Mach number versus X, $\phi = 0.61$
Figure 10: Velocity contours. 

Velocity contours near fuel strut: 

- At time $t = 1.25$ ms, $\phi = 0.29$ ms. 

Flow direction: 

- Centerline $xy$-plane: $z = 47.15$ mm. 

Central fuel strut: 

- Near-wall $xy$-plane: $z = 0.914$ mm. 

Velocity range: 

- $-400.000$ to $1700.000$ m/s.

Legend: 

- Blue: $-400.000$. 
- Green: $1466.667$. 
- Orange: $1700.000$. 
- Red: $0.000$. 
- Brown: $766.667$. 
- Gray: $300.000$. 
- Olive: $1233.333$. 
- Brown: $533.333$. 
- Black: $1000.000$. 

Flow direction and velocity contours.
\( t = 6.88 \text{ ms} \)

\( t = 11.88 \text{ ms} \)

\( t = 13.38 \text{ ms} \)

\( z_a = 0.0471, \ z_b = 0.0236, \ z_c = 0.0009 \)

Figure 17: U-velocity contours \( \left( \frac{u}{v} \right) \), \( \phi = 0.29 \)
\( t = 6.88 \text{ ms} \)

\( t = 11.88 \text{ ms} \)

\( t = 13.38 \text{ ms} \)

\( (z_a = 0.0471, z_b = 0.0236, z_c = 0.0009) \)

Figure 18: Static pressure (Pa) contours, \( \phi = 0.29 \)
\( z_a = 0.0471, z_b = 0.0236, z_c = 0.0009 \)

Figure 19: Temperature contours (K), \( \phi = 0.29 \)
(z_a = 0.0471, z_b = 0.0236, z_c = 0.0009)

Figure 20: Hydrogen mass fraction, $\phi = 0.29$)
$t = 6.88 \text{ ms}$

$z_a$

$z_b$

$z_c$

$2.00E-04  4.62E-03  9.04E-03  1.35E-02  1.79E-02  2.23E-02  2.67E-02  3.12E-02  3.56E-02  4.00E-02$

$z_a$

$z_b$

$z_c$

$t = 11.88 \text{ ms}$

$z_a$

$z_b$

$z_c$

$2.00E-04  4.62E-03  9.04E-03  1.35E-02  1.79E-02  2.23E-02  2.67E-02  3.12E-02  3.56E-02  4.00E-02$

$z_a$

$z_b$

$z_c$

$t = 13.88 \text{ ms}$

$z_a$

$z_b$

$z_c$

$\left( z_a = 0.0471, \quad z_b = 0.0236, \quad z_c = 0.0009 \right)$

Figure 21: Hydroxyl mass fraction contours, $\phi = 0.29$
Figure 23: Time-averaged wall pressure, $\phi = 0.29$.

![Graph showing time-averaged wall pressure plotted against distance (x) for phi = 0.29.](image1)

Figure 24: Wall pressure at several characteristic times, $\phi = 0.29$.

![Graph showing wall pressure at different characteristic times for phi = 0.29.](image2)
Figure 24: U-velocity contours ($u$) near fuel strut ($t = 0.25$ ms, $\phi = 0.61$)
(z_a = 0.0471, z_b = 0.0119, z_c = 4.04e-5)

Figure 25: U-velocity contours ($\frac{m}{s}$), $\phi = 0.61$
\[ t = 1.25 \text{ ms} \]

\[ t = 2.75 \text{ ms} \]

\[ t = 4.25 \text{ ms} \]

\[ (z_a = 0.0471, \ z_b = 0.0119, \ z_c = 4.04e-5) \]

Figure 26: Temperature contours (K), \( \phi = 0.61 \)
\( t = 2.75 \text{ ms} \)

\( z_a \)
\( z_b \)
\( z_c \)

\( 2.97 \times 10^4 \ 7.23 \times 10^4 \ 1.15 \times 10^5 \ 1.57 \times 10^5 \ 2.00 \times 10^5 \ 2.42 \times 10^5 \ 2.85 \times 10^5 \ 3.28 \times 10^5 \ 3.70 \times 10^5 \ 4.13 \times 10^5 \ 4.55 \times 10^5 \)

\( t = 4.25 \text{ ms} \)

\( z_a \)
\( z_b \)
\( z_c \)

\( (z_a = 0.0471, \ z_b = 0.0119, \ z_c = 4.04 \times 10^{-5}) \)

Figure 27: Static pressure (Pa) contours, \( \phi = 0.61 \)
(z_a = 0.0471, z_b = 0.0119, z_c = 4.04e-5)

Figure 28: Hydrogen mass fraction, ϕ = 0.61
\( t = 1.25 \text{ ms} \)

\( t = 2.75 \text{ ms} \)

\( t = 4.25 \text{ ms} \)

\( z_a = 0.0471, \ z_b = 0.0119, \ z_c = 4.04 \times 10^{-5} \)

Figure 29: Hydroxyl mass fraction contours, \( \phi = 0.61 \)
Figure 31: Time-averaged wall pressure, $\phi = 0.61$

Figure 32: Wall pressure at several time levels, $\phi = 0.61$
References


Appendix: A Sample Parallel Transfer

!*---------------------------------------------------------------------------------------*
!*---------------------------------------------------------------------------------------*
!* subroutine interface(q,irank,ISIZE,MYCOMM,II,JJ,KK,NVAR) *
!*---------------------------------------------------------------------------------------*
!* The MPI Communication Library *
!* include "mpif.h" *
!* **Rank of the processor to send buffered data *
!* integer dest *
!* **Rank of the processor buffered data is originating *
!* integer source *
!* **Rank of each individual processor *
!* integer irank *
!* **Communication domain in which all processor exist *
!* integer mycomm *
!* **Number of processes in the communication domain *
!* integer isize *
!* **Status of of the sendrecv command *
!* integer status(MPI_STATUS_SIZE) *
!* **Determines if an error has occurred in communication *
!* integer ierr *
!* **Number of primitive variables to transfer *
!* integer nvar *
!* **Send and receive buffer counter *
!* integer lc *
!* **Subdomain size in the xi, eta, and zeta directions *
!* integer ii,jj,kk *
!* **Dimension the primitive array *
!* dimension q(-1:ii+2,-1:jj+2,-1:kk+2,nvar) *
!* **Dimension the receive buffer array *
!* dimension buf((ii+4)*(jj+4)*3) *
!* **Dimension the send buffer array *
!* dimension bufs((ii+4)*(jj+4)*3) *
!*---------------------------------------------------------------------------------------*
!* This subroutine transfer artificial data for overlapping domains in *
!* the zeta direction, where the overlap is 3. Dirichlet Boundary *
!* conditions are imposed on the interface of the left adjacent domain. *
!* Additional compute time is used to pack and unpack buffers *
!* explicitly to ensure machine independence. Blocking Sendrecv commands *
!* are used to avoid the use of system buffers and possible deadlock. *
!* This program is not scalable to highly parallel architectures, *
!* but is very safe and is machine independent. *
!*---------------------------------------------------------------------------------------*
!* **Loop over the number of primitive variables**---------------------------------------------------------------------------------------*
do var=1,nvar

**Synchronize before the transfer of each primitive variable**
call MPI_BARRIER(mycomm,ierror)

!********************************************************************!
**Send buffered data from the left domain to the right domain’s******!
!********************************************************************!
!********************************************************************

!**********Define destination and source for right wave*************
  if( irank .eq. isize-1) then
    dest=MPI_PROC_NULL !no processor to right
    source=irank-1     !left domain
  elseif( irank .eq. 0) then
    dest=irank+1       !right domain
    source=MPI_PROC_NULL !no processor to left
  else
    dest=irank+1       !right domain
    source=irank-1     !left domain
  endif

  if( isize .eq. 1) then
    dest=MPI_PROC_NULL !no artificial boundaries
    source=dest       !for one processor
  endif

!****Pack send buffer into one dimensional array**********************
lc=0.0
  do ii=1,ii+2
    do jj=1,jj+2
      do kk=1,kk+1
        lc=lc+1
        bufs(lc)=q(i,j,k,var)
      enddo
    enddo
  enddo
enddo
enddo

!**********Do blocking sendrecv communication************************
call MPI_SENDRECV(bufs,lc,MPI_REAL8,dest,
          c var, bufr,lc,MPI_REAL8,source,var,
          c mycomm,status,ierror)

!**Check for communication error**************************************
  if( ierror /= MPI_SUCCESS) then
    print*, 'SENDRECV error',irank
    stop
endif

call MPI_BARRIER(mycomm,ierror)

!**Decompose receive buffer into left domain artificial boundaries******
if (irank .gt. 0) then
  lc=0.0
  do i=-1,ii+2
    do j=-1,jj+2
      do k= -1,1,1
        lc=lc+1
        q(i,j,k,var)=bufr(lc)
      enddo
    enddo
  enddo
endif

!******************************************************************************
!**Send buffered data from the right domain to the left domain’s***********
!******************************************************************************

!******************************************************************************
!******Define destination and source for left wave**************
if( irank .eq. isize-1) then
  dest=irank-1 !
  source=MPI_PROC_NULL ! no processor to right
elseif(irank .eq. 0) then
  dest=MPI_PROC_NULL      ! no processor to left
  source=irank+1
else
  dest=irank-1
  source=irank+1
endif
if (isize .eq. 1) then
  dest=MPI_PROC_NULL
  source=dest
endif

!******************************************************************************
!****Pack send buffer into one dimensional array******************************
lc=0.0
  do i=-1,ii+2
    do j=-1,jj+2
      do k= 2,3
        lc=lc+1
        bufs(lc)=q(i,j,k,var)
      enddo
    enddo
  enddo
enddo
enddo

!**************************Perform blocking sendrecv communication**************************
call MPI_SENDRECV(bufs,lc,MPI_REAL8,dest,
c  var+20,bufr,lc,MPI_REAL8,source,var+20,
c  mycomm,status,ierror)

!**Check for communication error******************************
if( ierror /= MPI_SUCCESS) then
  print*, 'SENDRECV error',irank
  stop
endif
  call MPI_BARRIER(mycomm,ierror)

!**Decompose receive buffer into right domain artificial boundaries*****
if (irank .ne. isize -1) then
  lc=0.0
  do i=-1,ii+2
    do j=-1,jj+2
      do k=kk+1,kk+2
        lc=lc+1
        q(i,j,k,var)=bufr(lc)
      enddo
    enddo
  enddo
endif
enddo
enddo
return
end