2009

Dual Mode Scramjet: A Computational Investigation on Combustor Design and Operation

Ryan Timothy Milligan
Wright State University

Follow this and additional works at: http://corescholar.libraries.wright.edu/etd_all
Part of the Mechanical Engineering Commons

Repository Citation

This Thesis is brought to you for free and open access by the Theses and Dissertations at CORE Scholar. It has been accepted for inclusion in Browse all Theses and Dissertations by an authorized administrator of CORE Scholar. For more information, please contact corescholar@www.libraries.wright.edu.
DUAL MODE SCRAMJET:

A COMPUTATIONAL INVESTIGATION ON COMBUSTOR DESIGN AND OPERATION

A thesis submitted in partial fulfillment of the requirements for the degree of Master of Science in Engineering

By

RYAN TIMOTHY MILLIGAN
B.S., Wright State University, 2007

2009
Wright State University
I HEREBY RECOMMEND THAT THE THESIS PREPARED UNDER MY
SUPERVISION BY Ryan Timothy Milligan ENTITLED Dual Mode Scramjet: Design
and Operational Analysis BE ACCEPTED IN PARTIAL FULFILLMENT OF THE
REQUIREMENTS FOR THE DEGREE OF Master of Science in Engineering.

________________________
J. Mitch Wolff, Ph.D.
Thesis Director

________________________
George P.G. Huang, P.E., Ph.D.
Department Chair

Committee on
Final Examination

________________________
J. Mitch Wolff, Ph.D.

________________________
Dean Eklund, Ph.D.

________________________
Chung-Jen Tam, Ph.D.

________________________
Joseph F. Thomas, Jr., Ph.D.
Dean, School of Graduate Studies
ABSTRACT

Timothy, Ryan Milligan. M.S.Eng., Department of Mechanical and Materials Engineering, Wright State University, 2008.
Dual Mode Scramjet: A Computational Investigation on Combustor Design and Operation

Numerical analysis was performed on a Dual-Mode Scramjet isolator-combustor. Preliminary analysis was performed to form a baseline geometry. Another study validated the results of a 2D model compared to a 3D model. Stable combustion was shown at two different flight conditions, M=3.0 and M=2.5. A marginal 5% decrease in stream thrust was shown by introducing a 50/50 mix of methane and ethylene. Based on the results of the preliminary analysis, detailed geometry analysis was performed on the 3D baseline geometry. Adding a new set of cavity feeding injectors increased the overall stream thrust and the equivalence ratio in the cavity. Using less fuel than the baseline configuration, revealed a 6.4% increase in stream thrust and an 11% increase in combustion efficiency by placing the second stage injector further upstream. Future analysis includes combining the cavity feeding with closer injector placement, which is expected to yield even better results.
<table>
<thead>
<tr>
<th>Chapter</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>MOTIVATION</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>Author’s Note</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>Potential</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>Applications</td>
<td>3</td>
</tr>
<tr>
<td></td>
<td>Goals</td>
<td>5</td>
</tr>
<tr>
<td>2.</td>
<td>LITERATURE REVIEW</td>
<td>7</td>
</tr>
<tr>
<td></td>
<td>Ramjet</td>
<td>7</td>
</tr>
<tr>
<td></td>
<td>Scramjet</td>
<td>8</td>
</tr>
<tr>
<td></td>
<td>Dual Mode Scramjet</td>
<td>10</td>
</tr>
<tr>
<td></td>
<td>Previous Research</td>
<td>11</td>
</tr>
<tr>
<td>3.</td>
<td>Metacomp, CFD++</td>
<td>15</td>
</tr>
<tr>
<td></td>
<td>Introduction</td>
<td>15</td>
</tr>
<tr>
<td></td>
<td>Governing Equation Set</td>
<td>15</td>
</tr>
<tr>
<td></td>
<td>Turbulence Modeling</td>
<td>19</td>
</tr>
<tr>
<td></td>
<td>Wall Functions</td>
<td>22</td>
</tr>
<tr>
<td></td>
<td>Chemistry Modeling</td>
<td>23</td>
</tr>
<tr>
<td></td>
<td>Species Properties</td>
<td>25</td>
</tr>
<tr>
<td></td>
<td>Computational Methods</td>
<td>27</td>
</tr>
<tr>
<td></td>
<td>1-D Integration for Output</td>
<td>30</td>
</tr>
<tr>
<td>4.</td>
<td>CONVERGENCE STUDIES</td>
<td>31</td>
</tr>
<tr>
<td></td>
<td>Introduction</td>
<td>31</td>
</tr>
<tr>
<td>Grid and Boundary Conditions</td>
<td>31</td>
<td></td>
</tr>
<tr>
<td>Solution Methodology</td>
<td>33</td>
<td></td>
</tr>
<tr>
<td>Residual and Mass Conservation</td>
<td>36</td>
<td></td>
</tr>
<tr>
<td>Grid Convergence Study</td>
<td>37</td>
<td></td>
</tr>
<tr>
<td>CFL Study</td>
<td>45</td>
<td></td>
</tr>
<tr>
<td>5. PRELIMINARY DESIGN ANALYSIS</td>
<td>51</td>
<td></td>
</tr>
<tr>
<td>Introduction</td>
<td>51</td>
<td></td>
</tr>
<tr>
<td>Second Cavity Study</td>
<td>51</td>
<td></td>
</tr>
<tr>
<td>Axisymmetric vs. Sector Models</td>
<td>56</td>
<td></td>
</tr>
<tr>
<td>Reduced Flight Enthalpy (M=3.0 vs. M=2.5 flight conditions)</td>
<td>63</td>
<td></td>
</tr>
<tr>
<td>Fuel Mixture</td>
<td>67</td>
<td></td>
</tr>
<tr>
<td>6. DETAILED GEOMETRICAL DESIGN ANALYSIS</td>
<td>71</td>
<td></td>
</tr>
<tr>
<td>Introduction</td>
<td>71</td>
<td></td>
</tr>
<tr>
<td>Feeding the Cavity</td>
<td>71</td>
<td></td>
</tr>
<tr>
<td>Injector Placement</td>
<td>80</td>
<td></td>
</tr>
<tr>
<td>Baseline, Feeding and Placement</td>
<td>89</td>
<td></td>
</tr>
<tr>
<td>7. CONCLUSIONS</td>
<td>92</td>
<td></td>
</tr>
<tr>
<td>Future Research.</td>
<td>95</td>
<td></td>
</tr>
<tr>
<td>Appendix.</td>
<td>96</td>
<td></td>
</tr>
<tr>
<td>CFD++ Input File</td>
<td>96</td>
<td></td>
</tr>
<tr>
<td>REFERENCES</td>
<td>118</td>
<td></td>
</tr>
</tbody>
</table>
## LIST OF FIGURES

<table>
<thead>
<tr>
<th>Figure</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.1:</td>
<td>Specific Impulse vs. Mach Number for various engine types.</td>
</tr>
<tr>
<td>2.1:</td>
<td>Ramjet Engine.</td>
</tr>
<tr>
<td>2.2:</td>
<td>Scramjet Engine</td>
</tr>
<tr>
<td>2.3:</td>
<td>Dual Mode Scramjet Engine</td>
</tr>
<tr>
<td>4.1:</td>
<td>Original Grid Configuration</td>
</tr>
<tr>
<td>4.2:</td>
<td>Mixing Mass Flow, $\Phi_1=0.4, \Phi_2=0.4$</td>
</tr>
<tr>
<td>4.3:</td>
<td>Residual vs. Iteration</td>
</tr>
<tr>
<td>4.4:</td>
<td>Mass Conservation: Fine, Nominal and Coarse Configuration</td>
</tr>
<tr>
<td>4.5:</td>
<td>Stream Thrust</td>
</tr>
<tr>
<td>4.6:</td>
<td>Combustion Efficiency</td>
</tr>
<tr>
<td>4.7:</td>
<td>Mach Number</td>
</tr>
<tr>
<td>4.8:</td>
<td>Static Temperature</td>
</tr>
<tr>
<td>4.9:</td>
<td>Static Pressure</td>
</tr>
<tr>
<td>4.10:</td>
<td>Mass Conservation, Varying CFL Number</td>
</tr>
<tr>
<td>4.11:</td>
<td>Stream Thrust</td>
</tr>
<tr>
<td>4.12:</td>
<td>Mach Number</td>
</tr>
<tr>
<td>4.13:</td>
<td>Static Pressure</td>
</tr>
<tr>
<td>4.14:</td>
<td>Static Temperature</td>
</tr>
<tr>
<td>5.1:</td>
<td>Static Temperature (2D slice along injector centerline)</td>
</tr>
<tr>
<td>5.2:</td>
<td>Mass Fraction of Oxygen</td>
</tr>
<tr>
<td>5.3:</td>
<td>Fuel Distribution ($\Phi$ contours)</td>
</tr>
</tbody>
</table>
6.12: Mach Number . . . . . . . 85
6.13: Static Temperature (2D along injector centerline) . . 86
6.14: Static Temperature (3D off centerline). . . . 87
6.15: Stream Thrust and Combustion Efficiency . . . 88
6.16: Stream Thrust . . . . . . . 89
6.17: Combustion Efficiency . . . . . 90
6.18: Mach Number . . . . . . . 91

LIST OF TABLES

<table>
<thead>
<tr>
<th>Table</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.1 Transport Coefficients</td>
<td>26</td>
</tr>
<tr>
<td>4.1 Inlet Conditions</td>
<td>33</td>
</tr>
<tr>
<td>4.2 Summary of CFL Number</td>
<td>46</td>
</tr>
</tbody>
</table>
NOMENCLATURE

$I_{sp}$, specific impulse
$M$, Mach number
$F_{st}$, stream thrust
$e$, total energy
$\rho$, density
$q$, conservation variable
$f$, flux in x-dir
$g$, flux in y-dir
$h$, flux in z-dir
$S$, strain magnitude
$u$, velocity in x-dir
$v$, velocity in y-dir
$w$, velocity in z-dir
$\sigma$, turbulent transport quantity
$\gamma$, specific heat ratio
$N_s$, species
$T$, static temperature
$\tau$, viscous stress
$D$, coefficient of diffusion
$P$, static pressure
$R$ and $R_u$, universal gas constant
$g$, body force
$\Omega$, species production/dissipation
$\delta$, kronecker delta function
$\mu$, eddy viscosity
$K$, thermal conductivity
$\mu$, dynamic viscosity
$\kappa$, viscosity
$k$, turbulent kinetic energy
$\varepsilon$, rate of energy dissipation
$P_k$, ratio of turbulence energy
$T_t$, realizable turbulence timescale
$E$, dissipation rate
$f_r$, low-reynolds number function
$Y_i$, species mass fraction
$\nu_y$, diffusion velocity
$m$, mass flow rate
$k_{fi}$, forward reaction rate
$k_{ri}$, reverse reaction rate
$N_r$, number of reactions
$X_i$, species concentration
$C_p$, specific heat at constant pressure
$h$, enthalpy
$G$, Gibbs free energy

Pr, Prantle number
$\mathcal{D}$, multi-component diffusion
$\lambda$, mixture conductivity
$\eta_c$, combustion efficiency
$P_d$, pressure difference
$A_{th}$, throat area
$T_T$, total temperature
$P_T$, total pressure
Acknowledgements

The first author would like to thank the Dayton Area Graduate Studies Institute (DAGSI) for providing the resources necessary to accomplish this research at AFRL and Wright State University.

Special acknowledgements to those at the AFRL MSRC High Performance Computing facility who supplied access to the computer processing power necessary to run all of the models performed in this study. The personnel at the MSRC were very nice, professional, and helpful and responded quickly to whatever questions we may have had for them with regard to the computer systems.

Special thanks to all of those at AFRL RZAT, especially to Dr. Douglas Davis, who is the overseer for the account at the MSRC. Others of mention include the following: Dr. Daniel Risha, Lt. Matthew Satchel, Lt. Dell Olmstead and Mr. Christopher McGlown
CHAPTER 1

MOTIVATION

Author’s Note

I was probably ten years old when I looked through a World Encyclopedia. I began reading the section on propulsion systems for various aircraft. Already familiar with propeller driven aircraft, rockets and turbojet engines (my dad did some explaining on turbojets since he worked for General Electric Aviation at the time), I was rather intrigued by an engine with the funny name “scramjet.” This engine had no moving parts but could reach very high speeds. Not having any idea how this engine could do what it claims to do I put my interests aside and continued being a 10 year old. Never did I think I would one day be writing a thesis, especially on the “scramjet.” Knowing a little more now about the scramjet I have learned it is a ram air propulsion device utilizing a series of oblique shock waves through its inlet to provide a pressure rise suitable for a chemically reacting combustion process. Inside the combustor, gas velocities for combustion may be subsonic, supersonic or a transition between the two. This will be explained in greater detail in subsequent chapters. It is my personal belief the engine has the potential to revolutionize the way the world operates and be the backbone of a “Hypersonic Age.”
Potential

The potential gains of the scramjet seem unlimited, with new applications and uses popping up all the time. What makes the engine so appealing is its ability to operate at high Mach numbers, unlike turbojets which are limited to Mach numbers not much greater than Mach 3. The engine is capable of maintaining high efficiency over a large portion of its flight. To date the United States and most nations have relied upon rockets to achieve high Mach numbers. There are several reasons why scramjet power is more appealing than rocket power. First, the scramjet does not need to carry its own oxidizer for it draws oxygen from the atmosphere during flight much like any typical turbojet engine. Storing oxidizer is a complex, expensive and “heavy” process. Heavy meaning the launch vehicle itself becomes very heavy storing all the oxidizer. Granted during flight the oxidizer gets burned up making the launch vehicle lighter, but there is still a tremendous amount of bulk and material left over from the storage vessel itself. The scramjet has a longer powered range than a rocket which in turn yields much greater efficiency over a rocket during powered flight.¹ Unlike a rocket, a launch vehicle utilizing scramjet power is reusable not just refurbishable, which means a vehicle utilizing a scramjet simply needs to be refueled like one would refuel his car at a gas station. In perspective of the space shuttle, an expensive time consuming recovery of rocket material needs to be initiated, which ultimately leads to a time consuming inspection, rebuild and replenishment. Essentially, what is being discussed here is the potential of a scramjet powered vehicle doing the job of a rocket powered vehicle but with a cost reduction anywhere from 10-100 times per payload.¹ A scramjet powered launch vehicle would not only be cheaper and have a quick turnaround time but would
also perform its in-flight mission with a greater Isp (specific impulse) over a broader range of Mach numbers. In layman’s terms the Scramjet can get more “bang for its buck” except a buck in this case is a unit mass of fuel. Isp, is a measure of a change in exhaust gas momentum providing useful net thrust per some unit of propellant. This leads to greater efficiency and acceleration of a scramjet powered vehicle over a rocket powered vehicle. This can be seen in Figure 1.1.

![Figure 1.1: Specific Impulse vs. Mach Number for various engine types](image)

Applications

As mentioned in the previous section there are indeed many applications for this form of propulsion. A scramjet alone cannot however generate static thrust. What this means is the engine has to already be at a minimum flight Mach number before useful combustion can occur. Initially a scramjet would be reliant on a turbojet or rocket assist
propulsion. Ultimately, any kind of scramjet powered vehicle would be a combined-cycle vehicle utilizing a scramjet and some other form of propulsion.

For defense, a missile utilizing a scramjet is an attractive application. A missile with a scramjet would have a small amount of rocket propellant to aid in initially accelerating the missile up to speeds necessary for the scramjet to operate. Hydrocarbon fuels are a cheap common fuel that could propel such a missile. The high speed of such a missile would have a quicker response time and longer flight duration over a conventional missile\(^3\). The missile could be used to deal with on the ground threats where quick response turnaround is essential for success.

For the commercial industry an airliner using a turbofan-scramjet combined-cycle would be attractive in greatly reducing intercontinental flight time duration. A flight from California to Australia typically can take 18-20 hours using turbofan propulsion alone. With a scramjet added to the equation the flight time can be reduced to 2 hours during hypersonic flight.\(^4\)

With the ever aging space shuttle being retired due to its high turnaround costs and complexity a replacement would once again be some combined-cycle scramjet powered vehicle. This vehicle could use a turbojet-scramjet setup. The scramjet would have to be hydrogen fueled to achieve Mach numbers necessary to skip out of earth’s atmosphere into orbit. This would be a two-stage to orbit reusable launch vehicle\(^5\).

Obviously, there are many applications for this type of propulsion and its potential is high. The scramjet from an academic viewpoint is also very exciting. There are a tremendous amount of physical phenomena that occur at hypersonic speeds. The scientific community has for years been limited in collecting data to better understand
hypersonic flight. This is in large part due to the high cost of doing high speed high altitude testing using conventional rockets. A scramjet powered experimental vehicle could make studying hypersonic flight more cost effective.

Goals

By this time the reader can see the scramjet has a great deal of potential over other forms of propulsion and has several applications. However, there are new challenges. One of the unappealing attributes is the need for having a combined cycle launch vehicle. The scramjet is not capable of being at rest and producing thrust so it relies on other forms of propulsion to accelerate the scramjet up to speeds necessary to produce stream thrust (stream thrust: the net momentum carried by a uniform dynamic flow, which can be expressed as a unit force). This makes one of the goals of this investigation to extend the range of the scramjet down to lower Mach numbers so the launch vehicle itself becomes less reliant on other forms of propulsion. Coupled with this goal is the desire to burn efficiently and mix fuel inside the combustion chamber without inducing blowout or unstart. Another objective is to study different hydrocarbon fuels for the scramjet. To date hydrocarbon fuels such as ethylene and JP7 have been analyzed as fuel types to be used by a scramjet engine, however, some rockets use methane as one of its propellants. Methane is a “mild cryogenic” that can be kept on the vehicle for significantly longer time than cryogenic hydrogen. It has good energy density and heat capacity. It is desirable to observe a scramjet’s response to methane as a possible fuel or as a mixture. From a kinetics point of view there are some very well established kinetics models using methane and ethylene as species types. Mixing the two in a computational model could
help mimic a JP fuel such as cracked JP7. This could be useful since JP fuels are very complex hydrocarbons and are difficult to model. 6

Historically, there are two types of scramjets. First, is a subsonic combustion ramjet usually called a “Ramjet.” The second is a supersonic combustion ramjet typically called a “Scramjet.” Up to this point for simplicity, each has been referred to as scramjet. Now that the distinction has been made the appropriate names will be used from this point on.

A ramjet allows only subsonic combustion velocities in its combustion chamber making its operability range anywhere between Mach 2.5 and Mach 6. Anything beyond Mach 6 the engine loses performance and will ultimately blowout. A Scramjet will only operate with supersonic combustion velocities inside its combustion chamber so it operating range is anything Mach 6+. In the 1960’s a hybrid of the two was conceived and the dawn of the Dual Mode Scramjet (DMSJ) came into being. The DMSJ is capable of having both subsonic and supersonic combustion velocities inside its combustion chamber. Operability of the DMSJ is between Mach 3.0 and Mach 15+, however as is the goal of this thesis, the lower limit is continually being extended to lower Mach numbers. Details of the three engine types will be discussed extensively in the following chapters.
CHAPTER 2

LITERATURE REVIEW

Ramjet

As mentioned previously, a ramjet engine allows only subsonic combustion velocities inside its combustion chamber. There are a few design features about the engine that cause this. The inlet to the ramjet is typically very aggressive taking full advantage of the high dynamic pressure and converts most of the dynamic pressure into a total pressure rise. This means most of the compression occurs on the external portion of the inlet with little internal contraction. These inlets require a large amount of turning to achieve the desired compression ratio. The inlets use boundary-layer bleed to increase pressure recovery, stabilize shock boundary layer interactions, and serve as a trap for the terminal shock system. The inlet at fairly low Mach numbers will efficiently recover its total pressure. The most efficient operating range for the Ramjet is typically between Mach 2.5-6. The pressure rise occurs in the inlet duct across a normal shock or a few very strong oblique shocks. At that point fuel is added to the airstream at a subsonic velocity which further gives pressure rise due to combustion. The hot exhaust gases then travel through a physical throat at the end of the combustion chamber, typically a converging-diverging nozzle. This accelerates the subsonic combustion gases to supersonic speeds to provide the exhaust momentum necessary to accelerate the vehicle. Observe the aggressive inlet design and the physical throat at the combustor exit in Figure 2.1.
The low velocities inside the ramjet combustor allow for efficient mixing and combustion near stoichiometric where exhaust gas temperatures for a kerosene based fuel will reach upwards $T=2400\text{K}$. At Mach numbers below Mach=2.5, there is simply not enough dynamic pressure to give stagnation pressure rise. This leads to inefficient combustion and low thrust making the engine less efficient than a jet engine or a rocket. At velocities higher than Mach 6 a normal shock will begin to form at the lip of the inlet; this yields poor total pressure recovery through the inlet and efficiency drops off.\textsuperscript{7}

**Scramjet**

A Scramjet has a new set of design features to allow for a different operating range. The inlet is less aggressive meaning some of the total pressure is recovered but the inlet also maintains a portion of its dynamic pressure. The inlet utilizes less turning to reduce cowl drag. The compression process is split between the external and internal portions of the inlet; therefore, high internal contraction ratios are common. During the compression process a series of oblique shocks provide a suitable total pressure recovery for combustion. What this means is at higher Mach numbers the engine is not as prone to normal shock losses that occur as a result of an aggressive cowling. When fuel is added
to the supersonic freestream a pressure rise occurs pushing the oblique shock system/train forward, this shock train can vary rapidly change in strength and position. High dynamic pressure will keep this shock train from protruding through the inlet causing unstart. Unstart occurs because of too much heat release, if the pre-combustion shock train exists it may be pushed too far forward, through the isolator, into the inlet. Unstart would choke off the flow and result in a thermal blockage. The low drag inlet takes advantage of the high dynamic pressure to keep the shock train isolated in the inlet. This means the engine will typically only operate at Mach>6. During combustion a physical throat does not exist as it does for a ramjet because inflow Mach numbers to the combustor are already M>1. Figure 2.2 shows a generic scramjet design. Observe the lack of a physical throat at the combustor exit and the oblique shock system in the inlet.

![Scramjet Engine](image)

Figure 2.2: Scramjet Engine²
Dual Mode Scramjet

Now that the ramjet and scramjet have been explained, it is time to look at the dual mode scramjet. There are several design aspects to the dual mode which are familiar. There are more similarities between the dual mode scramjet and the scramjet than with the ramjet. However, there are some clear differences.

![Dual Mode Scramjet Engine](http://www.aip.org-tip/INPHFA/vol-10/iss-4/images/24-2.jpg)

In Figure 2.3, like the scramjet, the dual mode scramjet has a series of oblique shocks in the inlet to promote pressure rise. However, there is now a section called an isolator that did not exist previously as well as a staged combustor. Both these new features are slightly diverging. The dual mode scramjet has no physical throat much like the scramjet. A Dual Mode Scramjet, however, takes advantage of a thermal throat which is a two-fold development. First, combustion or heat release inside a supersonic flow field will slow the flow down to subsonic velocities, which corresponds to a static pressure rise in the combustor. Second, the hot combustion products will propagate through a slightly diverging combustor section which accelerates the flow back to M=1. A delicate balance between heat release and the diverging area change of the combustor
is important to the development of the thermal throat.\textsuperscript{7} Another feature not actually shown in the figure is the utilization of a cavity for flame holding. The cavity is a cut out in the wall shortly after fuel injection. The key design features for the dual mode scramjet are the isolator and the diverging duct combustor, which takes advantage of the thermal throat. Staging fuel injection, cavity based injection and diverging the isolator are all “upgrades” to the dual mode scramjet.

\textbf{Previous Research}

Isolator-combustor interaction and overall performance is being studied in this investigation. Therefore, the focus in this section will be on the isolator-combustor, performance and engine operability. Design features will be covered first, starting with the isolator and moving back through the combustor. Later, fuel types will be discussed along with some numerical considerations.

In order for the dual mode scramjet to be successful, an isolator is placed between the inlet and the combustion chamber itself, which aids in preventing unstart. A constant area isolator captures the pressure rise due to combustion in the form of oblique shock waves during scramjet operation; this generates a separated free stream flow and produces a minimal entropy rise. During ramjet operation a normal shock exists at the end of the isolator before the combustor, this means flow separation does not occur and the entropy rise is significant inside the isolator. Any small perturbations generated by the combustion process can drastically change the location of this normal shock inside a constant area isolator, this can cause unstart. It was shown by replacing the constant area
isolator with a diverging isolator aided in stabilizing the normal shock produced during ramjet operation without upsetting scramjet operation.  

Cavity based fuel injection for the dual mode scramjet was proven experimentally to capture a small amount of air/fuel and circulate this mixture at low Mach numbers. This mixture would then be ignited and the flame sustained. This flame proved useful in igniting and stabilizing the free stream flow. It was shown by Mathur et. al. for a dynamic pressure of 1000psf (simulating Mach 4-5 flight) that once the fuel-air mixture was ignited in the cavity that a wide range of equivalence ratios (Φ=0.25 to 0.75) yielded stable flames and sustainable combustion without the need of further ignition efforts. Low angle flush wall injection aided in flame stability. It was also shown there is a limitation on cavity size. For flush wall injection of 45 degrees the cavity length over diameter ratios should be between 0.5 and 5 to maintain a stable flame. Cavities that are too short could not capture enough air-fuel to sustain a flame and cavities that are too long yield vortex shedding and unstable flames. For this investigation the cavity configuration has a length over diameter of 3.88.

In this investigation wall injection was utilized for fueling the combustor. Wall injectors are attractive because they penetrate the freestream efficiently with little effect on total pressure recovery. This is unlike intrusive fuel injection such as ramp or strut injections which have higher pressure recovery losses and usually require cooling.

A study using both strut and wall injection was performed at flight Mach numbers from 4 to 6. For the Mach 4 case, only wall injectors were used. For the Mach 4 case the study showed maximum combustion efficiency around 0.75 for a fuel-air equivalence ratio of about 0.2-0.6. Later, studies performed by Ogorodnikov et. al. on a round
combustor, using hydrogen fuel, at $M=3.5$ flight conditions showed the combustion efficiency was slightly higher than for the rectangular geometry at a Mach 4 flight condition. This study also showed a maximum fuel-air equivalence ratio of 0.75 for the Mach 3.5 case before the combustor inlet became affected.\textsuperscript{11}

Staging fuel injection in a diverging duct combustor was proven experimentally to greatly enhance stream thrust by not upsetting combustor isolator interaction by only producing a pressure rise at the second stage.\textsuperscript{12-15} Experimentally, for Mach 4 flight condition it was shown the total injected equivalence ratio of fuel could be doubled and the thrust could be increased to 2230 N from 1380N due to the addition of a second stage fuel injector.\textsuperscript{12} In addition, another experiment showed similar results at Mach 2.5 flight conditions for the same equivalence ratio.\textsuperscript{13}

A diverging combustor is a very important feature for the dual mode scramjet. The implementation of a diverging duct combustor develops the “thermal throat.” The expanding combustion products will accelerate to Mach=1 or choked flow prior to the nozzle.\textsuperscript{16}

Significant computational and experimental research has been accomplished on rectangular combustors. Round flow paths for the isolator combustor have shown to decrease structural weight for a rectangular flow path of the same area. In addition, heat load is reduced on the combustor when utilizing a round geometry. Numerically, a round flow path makes modeling a 2D geometry as axisymmetric more attractive and less computationally expensive.\textsuperscript{17}

Fuel types are important for high speed operation of an air breathing engine. Hydrocarbon fuel has been and still is an attractive fuel to use for operation of a dual
mode scramjet from low Mach numbers up to about $M=8$. Hydrocarbon fuel can be stored easily at room temperatures and provides higher fuel density than alternative fuels such as hydrogen. Ethylene, for research purposes, is a very reactive hydrocarbon fuel, since air-fuel mixing and duration time in the combustor is very small (sometimes less than 1ms) having a highly reactive fuel is useful to achieve timely efficient combustion. Lately, methane has been investigated as a possible fuel type. Methane is less reactive but is used as a fuel for some rocket combined-cycle assisted scramjets. Mixing different amounts of a less reactive fuel such as methane with a more reactive fuel such as ethylene is a method used in the mimicking of different JP fuels.\(^6\) This method could be used because ethylene and methane are simple hydrocarbons that have well developed kinetic mechanisms for computational analysis.

A previous study performed by Corbin\(^{18}\) using a computational solver called VULCAN formed the basis for this investigation. The study showed comparable results between cases run in 2D axisymmetric and 3D for the same equivalence ratio. An increase in thrust of 11.6\% was shown in this study by injecting a fuel equivalence ratio of 0.437 upstream and a fuel equivalence ratio of 0.369 at a location 0.8 meters downstream of the first injector. This was equivalent to a total equivalence ratio of 0.8. The 11.6\% increase in thrust was an increase compared to a nominal case.\(^{18}\) The nominal case for this study was a single stage combustor that injected a maximum equivalence ratio of 0.488 at the injector location before unstart occurred. The geometry and injector locations for this previous study were determined by a one-dimensional cycle code, SRGULL, developed by NASA Langley. The geometry determined in this study became the original geometry for the new studies performed in this investigation.
CHAPTER 3

METACOMP, CFD++

Introduction

As mentioned in chapter 2, the original geometry used in this investigation was supplied to us by Corbin. All the studies performed stemmed from this original geometry. The studies were performed using MetaComp’s CFD++ instead of VULCAN. CFD++ is a versatile code capable of solving structured and unstructured grids in both 2D and 3D by converting different cell shapes, overset, and non-aligned meshes into a unified grid transparency framework capable of being computationally analyzed. Unified treatment of the grid for cell generation includes hexahedral, tetrahedral, pyramid and triangular prism cells for 3D analysis and quadrilateral and triangular for 2D analysis. In this particular analysis hexahedral elements and quadrilateral elements were used for the 3D sector and 2D axisymmetric models, respectively. A review of the physics and the numerics will be presented next. It is important to understand the code’s structure and methodology for achieving solutions.

Governing Equation Set

In this investigation, steady state solutions are defined by mechanical and thermal equilibrium. The pressure and temperature of each cell is not changing as the solution marches in time and space. The equation set type utilized was MetaComp’s Reynold’s
averaged Navier-Stokes equations. These equations are recommended for variable density, multi-species flows or flows in which the ideal gas law is not an adequate assumption. This (non-preconditioned) form is recommended for flows in which the global Mach number is generally higher than about 0.2. The conservation form of the governing equations is as follows:

\[
\frac{\partial q}{\partial t} + \frac{\partial (f_i - f_v)}{\partial x} + \frac{\partial (g_i - g_v)}{\partial y} + \frac{\partial (h_i - h_v)}{\partial z} = S
\]

Where \( q \) represents the conservation dependant variables \( f, g, h \) represent fluxes in the three spatial directions and \( S \) represents the source terms. The subscript \( i \), and \( v \), denote the inviscid and viscous flow terms, respectively. For dependant quantities the inviscid flux terms can be written as:

\[
q = \begin{pmatrix}
e \\
\rho \\
\rho u \\
\rho v \\
\rho w \\
\rho \sigma_1 \\
\vdots \\
\rho \sigma_n
\end{pmatrix}, \quad f_i = \begin{pmatrix}
(e + p)u \\
\rho u \\
\rho u^2 + p \\
\rho u v \\
\rho u w \\
\rho u \sigma_1 \\
\vdots \\
\rho u \sigma_n
\end{pmatrix}, \quad g_i = \begin{pmatrix}
(e + p)v \\
\rho v \\
\rho v^2 + p \\
\rho v w \\
\rho v \sigma_1 \\
\vdots \\
\rho v \sigma_n
\end{pmatrix}, \quad h_i = \begin{pmatrix}
(e + p)w \\
\rho w \\
\rho w u \\
\rho w v \\
\rho w w \\
\rho w \sigma_1 \\
\vdots \\
\rho w \sigma_n
\end{pmatrix}
\]

where \( e \) is the total energy per unit cell volume and \( \rho \) is the density. The \( u, v \) and \( w \) represent the velocities in the \( x, y, \) and \( z \) directions, respectively. The \( \sigma \)'s represent color tracers or turbulence transport quantities such as turbulence kinetic energy and “undamped” eddy viscosity in the pointwise turbulence models. The first five rows represent the standard Euler equations, which are energy, continuity, \( x \)-momentum, \( y \)-momentum, and \( z \)-momentum.
momentum and z-momentum, respectively. The equation of state that couples the pressure to density and temperature using the perfect gas equation of state can be written:

\[
p = \left(\gamma(N_s, T) - 1\right) \left(e - \frac{1}{2\rho} \left(\left(\rho u\right)^2 + \left(\rho v\right)^2 + \left(\rho w\right)^2\right)\right)
\]

\(\gamma\) is the ratio of specific heats which is a function of species type, \(N_s\) and temperature, \(T\). The viscous terms are as follows:

\[
f_v = \begin{bmatrix}
& K \frac{\partial T}{\partial x} + u \tau_{xx} + v \tau_{xy} + w \tau_{xz} \\
& \tau_{xx} \\
& \tau_{xy} \\
& \rho D \frac{\partial \sigma_1}{\partial x} \\
& \rho D \frac{\partial \sigma_n}{\partial x} \\
0 & \tau_{xz}
\end{bmatrix}, \quad \quad g_v = \begin{bmatrix}
& K \frac{\partial T}{\partial y} + u \tau_{yx} + v \tau_{yy} + w \tau_{yz} \\
& \tau_{xy} \\
& \tau_{yy} \\
& \rho D \frac{\partial \sigma_1}{\partial y} \\
& \rho D \frac{\partial \sigma_n}{\partial y} \\
0 & \tau_{yz}
\end{bmatrix}, \quad \quad h_v = \begin{bmatrix}
& K \frac{\partial T}{\partial z} + u \tau_{xz} + v \tau_{yz} + w \tau_{zz} \\
& \tau_{xz} \\
& \tau_{yz} \\
& \rho D \frac{\partial \sigma_1}{\partial z} \\
& \rho D \frac{\partial \sigma_n}{\partial z} \\
0 & \tau_{zz}
\end{bmatrix}
\]
T is temperature, K is the coefficient of thermal conductivity, D is the coefficient of diffusivity and $\tau_{ij}$ are the viscous stresses defined subsequently as:

$$
\tau_{xx} = 2\mu \frac{\partial u}{\partial x} - \frac{2}{3} \mu \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right)
$$

$$
\tau_{yy} = 2\mu \frac{\partial v}{\partial y} - \frac{2}{3} \mu \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right)
$$

$$
\tau_{zz} = 2\mu \frac{\partial w}{\partial z} - \frac{2}{3} \mu \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right)
$$

$$
\tau_{xy} = \mu \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right)
$$

$$
\tau_{xz} = \mu \left( \frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \right)
$$

$$
\tau_{yz} = \mu \left( \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right)
$$

where the 2/3 comes from Stokes theorem for gases, relating the second coefficient of viscosity, $\kappa$, to the dynamic viscosity, $\mu$, such that $\kappa=2/3\mu$. Temperature is related to the gas constant $R$ through the perfect gas equation of state.

$$
T = \frac{p}{\rho R} = \left( e - \frac{(\rho u)^2 + (\rho v)^2 + (\rho w)^2}{2\rho^2} \right) \frac{\gamma(N_s, T) - 1}{R}
$$
The source terms are:

$$S = \begin{pmatrix}
0 \\
0 \\
g_x \\
g_y \\
g_z \\
\Omega_1 \\
. \\
\Omega_n
\end{pmatrix}$$

where \(g_x\), \(g_y\), and \(g_z\) are body forces and \(\Omega_i\)’s are the production and dissipation of turbulence and chemical species.

**Turbulence Modeling**

The most commonly used turbulence model for the Reynolds averaged Navier-Stokes equations is the k-\(\varepsilon\) model. Various modifications have been made to improve the accuracy and stability of the model. A realizable k-\(\varepsilon\) model was used. The realizable variant accounts for certain known physical properties of the stress tensor by introducing a bound on the magnitude of the predicted tensor components, which improves predictive accuracy and has a beneficial effect on stability. The Boussinesq relation is used to obtain Reynold’s stresses (algebraically) from the modeled eddy viscosity, \(\mu_t\) and available mean-strain tensor:

$$\rho u_v = \frac{2}{3} \delta_{xy} \rho k - \mu_t S_{xy}$$
where

\[
S_{xy} = \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} + \frac{2}{3} \frac{\partial w}{\partial z} \delta_{xy} \right)
\]

The Kronecker delta function, \( \delta_{xy} \), is defined as,

\[
\delta_{xy} = \begin{cases} 
1, & x = y \\
0, & x \neq y
\end{cases}
\]

The following transport equations for \( k \) and \( \varepsilon \) are as follows:

\[
\frac{\rho k}{\partial t} + \frac{\partial}{\partial y} \left( v \rho k \right) = \frac{\partial}{\partial y} \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial y} \right] + P_k - \rho \varepsilon,
\]

\[
\frac{\rho \varepsilon}{\partial t} + \frac{\partial}{\partial y} \left( v \rho \varepsilon \right) = \frac{\partial}{\partial y} \left[ \left( \mu + \frac{\mu_t}{\sigma_{\varepsilon}} \right) \frac{\partial \varepsilon}{\partial y} \right] + \left( C_{\varepsilon 1} P_k - C_{\varepsilon 2} \rho \varepsilon + E \right) T_t^{-1},
\]

and the rate of production of turbulence energy is:

\[
P_k = -\rho uv \frac{\partial u}{\partial y}
\]

\( T_t \) is a realizable estimate of the turbulence timescale:

\[
T_t = \frac{k}{\varepsilon} \max \left\{ 1, \frac{1}{\varepsilon^2} \right\} \quad \varepsilon = \sqrt{\frac{R_t}{2}}
\]

and the turbulence Reynolds number:
\[ R_t = \frac{\rho k^2}{\mu \varepsilon} \]

The \( E \), term in the dissipation-rate equation is to improve the model response to adverse pressure-gradient flows and has the form:

\[
E = A_E \rho \sqrt{\varepsilon T_t} \psi \max \left\{ \frac{1}{k^2}, (\nu \varepsilon)^\frac{1}{4} \right\}
\]

\[
\psi = \max \left\{ \frac{\partial k}{\partial \tau}, \frac{\partial \tau}{\partial y}, 0 \right\}, \quad \tau = k / \varepsilon
\]

The model constants are:

\[ C_\mu = 0.09, \quad C_{\varepsilon 1} = 1.44, \quad C_{\varepsilon 2} = 1.92, \quad \sigma_k = 1.0, \quad \sigma_{\varepsilon} = 1.3, \quad A_E = 0.3 \]

eddy viscosity, \( \mu_t \), is:

\[
\mu_t = \min \left\{ \frac{C_\mu f_\mu \rho k^2}{\varepsilon}, \frac{2 \rho k}{3S} \right\}
\]

where

\[
S = \frac{S_{kl}}{\sqrt{2}}
\]

is the dimensional strain magnitude and \( f_\mu \) is a low-Reynolds number function, designed to account for viscous and inviscid damping of turbulent fluctuations in the proximity of solid surfaces:
This model can be integrated directly to walls or used in conjunction with wall functions as in this investigation.

**Wall Functions**

Practical predictions of 3D turbulent flows involve regions of coarse mesh which preclude the application of low-Reynolds number turbulence models for solving the RANS equations directly to walls. It is common practice, therefore, to use wall functions to return acceptable wall fluxes for momentum and energy even though the first centroids away from walls are located deep into the so-called logarithmic overlap region of the boundary layer (say $y^+ > 50$). The wall functions implemented in CFD++ work reliably on fine grids as well as on coarse ones ($300 > y^+ > 0.1$) and they take into account effects of compressibility, heat transfer and pressure gradient. It is important to keep in mind the fact that wall functions work best on geometries which do not grossly deviate from a flat plate and for flows subject to mild pressure gradients. There is no general rule as to when to avoid using wall functions and experience indicates reasonable results even in cases which sharply deviate from the above guidelines. In this investigation the recommended advanced two-layer wall function was used. CFD++ incorporates elements from the formulation suggested by Launder and Spalding and is based on a velocity scale of $(k)^{0.5}$, where $k$ is the turbulence kinetic energy (predicted by any $k$-ε closure). Three advantages of using turbulence kinetic energy are:
1. Immunity to reversed flow regions, including separation and reattachment points where $\tau_w = 0$, 

2. Avoidance of iterative solutions for $u_\epsilon$ since $k$ is directly available from the turbulence model, 

3. Readily extendable to rough walls. 

**Chemistry Modeling**

In addition to the RANS equations there is a conservation of species equation for each of the chemical species included. 

$$
\frac{\partial}{\partial t} \left( \rho Y_i \right) + \frac{\partial}{\partial y} \left( \rho Y_i \nu + \bar{\rho} Y_i \nu^* + \rho Y_i \nu_y \right) = \dot{m}_i^{in}
$$

where $Y_i$ is the mass fraction of each species, $\nu_y$ is the diffusion velocity defined by Fick’s law as, 

$$
\nu_y = \frac{\mathcal{D}}{Y_i} \frac{\partial Y_i}{\partial y}
$$

where $\mathcal{D}$ is the multi-component diffusion coefficient for each species and, 

$$
\rho Y_i \nu_y \approx -\frac{\mu}{Sc} \frac{\partial Y_i}{\partial y}
$$
The term \( \overline{\rho Y_i' v''} \) is the Reynolds mass flux and is defined as,

\[
\overline{\rho Y_i' v''} = -\frac{\mu_T}{Sc_T} \frac{\partial \overline{Y_i}}{\partial y}.
\]

\( \dot{m}_i''' \) is the production of species \( i \) on a mass basis defined by,

\[
\dot{m}_i''' = \dot{\omega}_i MW_i,
\]

where \( \dot{\omega}_i \) is the species production term defined by,

\[
\dot{\omega}_i = \sum_{j=1}^{N_r} \left( v''_{ji} - v'_{ji} \right) \left( k_{fi} \prod_{k=1}^{N_s} [X_k]^{v'_k} - k_{ri} \prod_{l=1}^{N_s} [X_l]^{v'_l} \right),
\]

where \( v''_{ji} \) is the stoichiometric coefficient of the \( i \)-th species in the \( j \)-th chemical reaction on the RHS, \( v'_{ji} \), the stoichiometric coefficient of the \( i \)-th species in the \( j \)-th chemical reaction on the LHS, \( k_{fi} \) is the forward reaction rate of the \( i \)-th species, \( k_{ri} \) is the reverse reaction rate of the \( i \)-th species, \( N_r \) is the number of reactions, \( N_s \) is the number of species, and \([X_i]\) is the species concentration defined by,

\[
[X_i] = \chi_i \frac{P}{R_a T}.
\]

This study uses a 22 species reduced kinetics model (UD_RED1), which uses the Princeton methodology for its reduction.\(^{23}\) The detailed mechanism comes from the
University of Delaware and consisted of 75 species and 529 elementary reactions. Species are: \( H_2, H, O, O_2, OH, H_2O, HO_2, H_2O_2, CH_3, CH_4, CO, CO_2, CH_2O, C_2H_2, C_2H_4, C_2H_6, HCCO, CH_2CO, CH_3CHO, C_3H_5, C_3H_6, \) and \( N_2 \).

**Species Properties**

For the compressible real gas assumptions being implemented for the equation set in this investigation the species for the reacting flow are specified through the species selection command. Using this command, the dimensional molecular weight, species symbol, Sutherland viscosity parameters (always dimensional), and thermodynamic properties can be set. The entries for these quantities are those commonly found in thermodynamics property tables, this investigation used the McBride et. al.\textsuperscript{25} thermodynamic properties. Properties are needed, however, for all species. The thermodynamic properties used in this mode depend on the following set of equations:

\[
\frac{C_{P_i}}{R_i} = a_i + b_i T + c_i T^2 + d_i T^3 + e_i T^4
\]

\[
h_i = R_i \left( a_i + \frac{b_i T}{2} + \frac{c_i T^2}{3} + \frac{d_i T^3}{4} + \frac{e_i T^4}{5} \right) T + \Delta H f_i
\]

\[
\frac{G_i}{R_i} = a_i \left( T - T \ln T \right) - \frac{b_i T^2}{2} - \frac{c_i T^3}{6} - \frac{d_i T^4}{12} - \frac{e_i T^5}{20} T + \frac{\Delta H f_i}{R_i} - g_i T
\]
Cp\(_i\) is the specific heat at constant pressure for the i-th species and is a fourth order polynomial fit in temperature with coefficients \(a_i, b_i, c_i, d_i\) and \(e_i\). The enthalpy, \(h_i\), of the i-th species, is the integral of \(Cp_i\) with respect to temperature. \(\Delta Hf_i\) is the enthalpy of formation of the i-th species. Finally, \(G_i\) is the Gibbs free energy of the i-th species. The constants \(a_i, b_i, c_i, d_i, e_i, G_i\) and \(\Delta Hf_i\) are tabulated in the literature for various temperature ranges. Typically a two or three temperature range fit to \(Cp_i, h_i\) and \(G_i\) is used. The Prandtl number, \(Pr\), is used to relate conductivity to viscosity by,

\[
Pr = \frac{Cp \mu}{\lambda}.
\]

In order to relate, \(D\), to known quantities the Schmidt number, \(Sc\), is used which is defined by,

\[
Sc = \frac{\mu}{\rho D}.
\]

Values for laminar and turbulent Prandtl and Schmidt numbers that are used in CFD++ for this investigation are given in Table 3.1.

<table>
<thead>
<tr>
<th>TABLE 3.1: TRANSPORT COEFFICIENTS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number</td>
</tr>
<tr>
<td>---------</td>
</tr>
<tr>
<td>(Pr_T/Pr_L)</td>
</tr>
<tr>
<td>(Sc_L)</td>
</tr>
<tr>
<td>(Sc_T)</td>
</tr>
</tbody>
</table>
These values for turbulent Prandtl and Schmidt number are consistent with values from Baurle and Eklund.\textsuperscript{26}

**Computational Methods**

CFD++ has methods for accurately computing time-dependent problems. Usually methods that are attempting to accurately compute time-dependant problems are inefficient when used to solve steady-state problems. Therefore, the fastest methods for computing steady state problems are usually inaccurate or non-physical when applied directly to transient flows. CFD++ has several numerical schemes and various auxiliary options for controlling the time-advancement of the solution. In this investigation the backward Euler implicit scheme with multi-grid acceleration was used. The implicit scheme implies a discretization of the RHS based on the time-advanced of unknown quantities, \( U^{n+1} \):

\[
\frac{U^{n+1} - U^n}{\Delta t} = RHS^{n+1}
\]

\( RHS^{n+1} \) may be linearized about the current (known) time level, resulting in a linear system of equations for \( U \), or rather its increment:

\[
\frac{U^{n+1} - U^n}{\Delta t} = RHS^n + \left( \frac{\partial RHS}{\partial U} \right)^n \left( U^{n+1} - U^n \right)
\]
\[
\frac{\partial U}{\partial t} = RHS^n + \left( \frac{\partial RHS}{\partial U} \right)^n \delta U
\]

\[
\delta U = U^{n+1} - U^n
\]

The solution of this linear system results in a numerical scheme with enhanced stability properties. Theoretically implicit schemes are stable for any size of time step, although in practice, non-linear effects (such as signals which want to change direction within a single time-step) often prevent the use of infinite time steps, at least in the early stages of a calculation. Once most transients have settled down, it becomes possible to significantly increase the size of the time step. CFD++ accounts for this by providing a ramping schedule, which attempts to increase the CFL gradually over a number of steps. In this investigation a fixed CFL (Courant-Friedrichs-Lewy) number was used:

\[
CFL = a \frac{\Delta t}{\Delta x}
\]

where a, is the max signal speed. The option to fix the time step is available. The CFL number in CFD++ can be determined globally (over all cells) or locally, so that each cell operates at some factor multiplied by its maximum (explicitly determined) stable time step. If the time-step is specified in terms of a CFL number, this can also be ramped gradually over a number of steps. The conservative recommendation for CFL number as recommended by Metacomp is a CFL of 20 ramped over the first 200 iterations.\textsuperscript{21} This recommendation was used for the results in this investigation. Total Variation Diminishing (TVD) discretization is available for all grid topologies, 1\textsuperscript{st} and 2\textsuperscript{nd} order
blending is also an option to help reduce strong gradients produced by oblique shocks. CFD++ has a finite-volume numerical framework with Riemann solvers for accurate representation of supersonic flows. Several types of Riemann solvers are available; the HLLC Riemann solver\textsuperscript{27} with the Van Leer continuous flux limiting was used in this investigation. RHS dissipation is not recommended for final steady state convergence of solutions. Dissipation on the RHS is artificial and can change the solution and should only be implemented during early stages of a solution such as the ignition process. All studies performed in this investigation were run with RHS dissipation control set equal to zero during the entire solution process. A "Pressure Switch" determines where CFD++ will add extra dissipation. CFD++ does this by examining a cell and its neighbors and comparing the selected "Pressure Switch" threshold level with the normalized pressure difference, $P_d$, in the cell locality:

$$P_d = \frac{P_{\text{max}} - P_{\text{min}}}{P_{\text{max}} - P_{\text{min}}}$$

In regions where $P_d$ is larger than the selected threshold, the pressure dissipation becomes active. CFD++ also adjusts this dissipation so that it increases linearly from the set (Pressure Dissipation) level to a maximum of 1.0 (full dissipation) according to the magnitude of $P_d$. 
1-D Integration for Output

To make case by case comparisons and comparisons between 2D and 3D, the data gets dimensionalized to evaluate performance. All results are one-dimensionalized using a mass-averaging technique. This is determined by a mass flux through a cell as defined by the following equation.

\[
f_{1D} = \frac{\int \rho uy dy}{\int \rho u dy}
\]

The one-dimensionalization tool calculates combustion efficiency. The method used in this investigation is:

\[
\eta_c = \frac{h(T_{REF}, Y_i) - h(T_{REF}, Y_{REF})}{h(T_{REF}, Y_{IDEAL}) - h(T_{REF}, Y_{REF})}
\]

This is a measure of combustion efficiency based on how much heat is released versus an ideal heat release. \(Y_{IDEAL}\) is determined from the local static pressure and enthalpy. \(T_{REF}\) and \(Y_{REF}\) are reference values from the inlet throat. Stream thrust, \(F_{ST}\) was determined by the following:

\[
F_{ST} = \int (\rho u^2 + p) dA
\]

which can be determined by subtracting the stream thrust at the exit to the combustor from the stream thrust at the inlet.
CHAPTER 4
CONVERGENCE STUDIES

Introduction

The original grid with two cavities came from the study performed by Corbin. The 3D sector geometry was approximately 3,000,000 cells and the 2D axisymmetric was approximately 90,000 cells. Currently, a similar geometry from Research Cell 22 (RC22) at the Air Force Research Laboratory’s Aerospace Propulsion Division (AFRL/RZA) is being investigated. The general procedure was to run 2D simulations, observe the results and decide which 2D simulations would be attractive to run in 3D. To do this a detailed grid convergence study was performed as well as a detailed CFL study. A review of the original geometry and its boundary conditions will be discussed.

Grid and Boundary Conditions

Figure 4.1: Original Grid Cconfiguration
The original 3D sector grid consists of an isolator-combustor length of 2.438 meters with 2 sets of 8 equally spaced round flush wall fuel injectors with the first and second stages located 1.067 and 1.867 meters, respectively, downstream of the entrance to the isolator. The injectors in the combustor have a flame holding cavity (Length/Diameter=3.88) located behind them in the flow path, which can be seen in Figure 5. The injector diameters are 3.175 mm and the average radius of the isolator 7.75 cm. The isolator entrance is at 0.0.

Initially, the new studies were performed as 2D axisymmetric with 2D grids. This was helpful in reducing computational time and making it possible to run only the best 2D simulations as 3D, because 3D sector grids take significantly longer computationally to run. In order to run in 2D, the 3D sector had to be mimicked to maintain consistency. The 2D grid consists of two continuous injectors which wrap around the combustor like a donut. In 2D the injector cannot be individualized as a single injector penetrating the combustion chamber like it can in 3D. In order for fuel to be injected into supersonic flow the fuel has to be choked at the sonic velocity, where Mach number is approximately equal to 1. The present 3D sector geometry achieves this condition; however, the 2D geometry needed modified. The inflow area of 8 equally spaced injectors at each injection stage for the 3D sector was computed in order to appropriately size the width of the donut slit for the 2D geometry. This made it possible to match injector inflow areas and maintain the appropriate mass flow and sonic fuel injection for the 2D axisymmetric model. The total conditions to the inlet are summarized in Table 4.1. This summary of conditions is for all simulations performed in this investigation.
The total conditions were meant to match the static throat conditions which were from a
generic inlet suggested by Billig.\textsuperscript{28}

\begin{table}[h]
\begin{center}
\begin{tabular}{|c|c|c|c|}
\hline
\textbf{Parameter:} & Mach 3.0 flight & Mach 3.0 flight & Mach 2.5 flight \\
 & 58960ft & 60720ft & 51450ft \\
\hline
$T_T$ (K) & 688 & 667 & 600 \\
$P_T$ (kPa) & 379 & 337 & 300 \\
$T_{throat}$ (K) & 414.7 & 398.7 & 356.7 \\
$P_{throat}$ (kPa) & 59.05 & 55.07 & 46.60 \\
\hline
\end{tabular}
\end{center}
\caption{INLET CONDITIONS}
\end{table}

\textbf{Solution Methodology}

Initially the air mass flow rate and fuel mass flow rate were analytically
determined using the following equations. For air mass flow, the equation is as follows.

$$\dot{m}_{air} = \frac{P_T}{\sqrt{T_T}} A_{th} \left( \frac{\gamma}{R} \left( \frac{2}{\gamma + 1} \right) \right)^{\gamma - 1}$$

$P_T$ and $T_T$ are the total conditions at the inlet from Table 2. $A_{th}$ is the minimum area of the
inlet throat. $R$ is the ordinary gas constant for air and $\gamma$ is the specific heat ratio for air
under the perfect gas assumption. The mass flow of fuel was determined using the
following:

$$\dot{m}_f = \Phi \left( \frac{\dot{m}_f}{m_{O2}} \right) \left( Y_{O2} \ast \dot{m}_{air} \right)$$

$\Phi$ is the equivalence ratio; multiplied by the stoichiometric ratio of the fuel type to
oxygen; multiplied by the mass fraction of oxygen in standard air. These equations are
very good approximations for determining the appropriate mass flow rates, however they are not exact because they do not take into account boundary layer development through the inlet throat which will affect, to a small degree, the mass flow rate. These equations will allow for comparison between analytical mass flows with computational mass flows, which will be beneficial in determining mass conservation.

A “cold flow” mixing solution was executed at a total $\Phi$ of 0.8. With $\Phi$ being distributed equally between the first stage and second stage fuel injectors at $\Phi_{1,2}=0.4$. It was shown by Corbin\textsuperscript{18} that an equivalence ratio much greater than 0.8 yielded unsteady solutions, therefore, an equivalence ratio of 0.8 became the baseline equivalence ratio. The “cold flow” solution was a non-reacting solution whose sole purpose was to compare analytical mass flow to computational mass flow. The mixing solution was then used to compare computational mass flow when the kinetics model was implemented. An example of a steady state converged mixing solution using the 1D utility can be seen in Figure 4.2.
Once the mixing solution was finished the flow would be ignited at a lower equivalence ratio, $\Phi_{1,2}=0.3$, using an ethylene 3 step ignition model with artificially high reaction rates. The 3 step model utilized 7 basic species $H_2$, $N_2$, $O_2$, $C_2H_4$, $CO_2$, $H_2O$ and $CO$. Once cavity temperatures were elevated to approximately 2000K the 22 species kinetics model was initialized. For axisymmetric cases it was observed initially that by lowering the total equivalence ratio to $\Phi=0.6$, once reactions were implemented, aided in achieving
steady state solutions faster. Once the steady state solution was achieved at Φ=0.6 the equivalence ratio could be ramped up to the desired total Φ=0.8. Since Φ=0.6 converged very quickly, this was the equivalence ratio used to perform the grid and CFL convergence studies.

Residual and Mass Conservation

Convergence for a steady state solution means the solution is not changing with time or is changing within acceptable limits. Therefore, the solution is changing very little if at all over an infinite period of iterations. The criterion in this investigation for a steady solution was less than 1% change in mass conservation and performance over a period of solution captures. In these combustion simulations, several different species are being introduced into the flow field. The best indicator of steadiness was to observe mass conservation. The 1D utility for mass conservation was the most sensitive utility used when checking mass conservation. Residual level was also used to estimate steadiness and to observe any solution instabilities if they occurred. Residual is based upon average cell values and was computed on an absolute log scale for mass, momentum and energy.

\[
RES = \frac{1}{N_{cells}} \sum_{i=1}^{N_{cells}} |RHS_i|
\]

A mass conservation utility in CFD++ was also used as an indicator of mass conservation during the solution process. Figure 4.3 shows residual vs. iteration number plot where a steady state solution was achieved.
Figure 4.3: Residual vs. Iteration

Grid Convergence Study

The grid convergence study had a nominal fueling of $\Phi_t = 0.6$ using the baseline axisymmetric grid. The baseline grid was slightly different from the original grid supplied by Corbin. The second cavity was removed. The baseline grid consisted of 82,620 cells. A fine grid consisting of 174,100 cells was investigated as well as a coarse grid of 49,440 cells. The solutions of each were compared to the baseline grid with the nominal fueling. The grid convergence study focused on adding or subtracting cells in the y-direction thus adding cells or removing cells perpendicular to the wall of the combustor. This was done to observe the accuracy of our solutions near the combustor wall. Once a steady solution was obtained for each grid type it became possible to interrogate the solution and the effect the grid has on engine performance. Figure 4.4
shows the steady state mass conservation utility for the three different grid types at a CFL=10.

![Figure 4.4: Mass Conservation; Fine, Nominal and Coarse Configuration](image)

All three yielded nicely converged solutions for mass conservation. It is important to note the spikes seen in the conservation utility are a result of the way data is averaged and interpolated across strong gradients such as shocks and rapidly accelerated
flow regions in calculating one-dimensional properties. These spikes are artificial to the solution. All three grids agreed in terms of performance with negligible differences.

The net thrust is the difference between the outflow stream thrust minus the stream thrust at the isolator entrance as shown in Figure 4.5.

![Figure 4.5: Stream Thrust](image)

Stream thrust was determined by the following equation.
\[ F_{st\text{net}} = \left[ \int_{\text{exit}} (\rho u^2 + P) dA \right] - \left[ \int_{\text{inlet}} (\rho u^2 + P) dA \right] \]

No significant difference in combustion efficiency was observed as seen in Figure 4.6. Once again, combustion efficiency was determined by the following equation.

\[ \eta_c = \frac{h(T_{\text{REF}}, Y_i) - h(T_{\text{REF}}, Y_{\text{REF}})}{h(T_{\text{REF}}, Y_{\text{i, IDEAL}}) - h(T_{\text{REF}}, Y_{\text{REF}})} \]

The efficiency was determined by a mass weighted enthalpy based equation. \( Y_{\text{i, IDEAL}} \) (species mass fraction) was determined from the local static pressure and \( h \) (enthalpy). \( T_{\text{REF}} \) (temperature) and \( Y_{\text{REF}} \) are reference values from the inlet throat. \( Y_i \) was the computational result for mass fraction.
The solution was further interrogated by looking at certain solution parameters such as Mach number, temperature and pressure (Figures 4.7, 4.8 and 4.9). When looking at the following figures, the 1D utility for a particular parameter is on top with corresponding contour maps of that parameter on the bottom, all of which correspond to the same location in the scramjet.
Figure 4.7: Mach Number
Figure 4.8: Static Temperature
When interrogating these parameters, they showed good agreement between the three grid types. A small 1.5 cm difference in shock position was observed between the fine and the nominal, Figure 4.7 and 4.9. It seems the finer grid resolves the shock structure in more detail. The difference in shock location can be largely explained by the shock-boundary layer interaction. The fine grid yielded average $Y^+$ values near the wall of the isolator of approximately 60. $Y^+_{ave}=90$ for the nominal grid and $Y^+_{ave}=130$ for the coarse grid. When looking at differences in temperature and Mach number, it could...
be seen by adding points near the wall region refined the grid in the shear layer between the cavity and the freestream of the combustor. This is marked by small dips in Mach number and temperature on the fine grid compared to the nominal, Figures 4.7 and 4.8. Despite these marginal differences in the solution parameters there effect on the overall performance was negligible and since this is a performance based analysis it was concluded the nominal grid used in this investigation was a valid accurate grid to achieve solutions and perform analysis.

**CFL Study**

Adjusting the CFL number in CFD++ can have an impact on the solution. In the CFL convergence study the same grid was used and the relative timestep was changed by adjusting CFL number. CFD++ has an internal mechanism which detects solution instabilities due to too large of a timestep. This mechanism is known as the Automatic CFL Adjustment Procedure (ACAP), which will continually reduce and ramp the CFL number until solution instabilities are overcome. For this investigation, a CFL value for reacting high speed flows as recommended by the CFD++ user’s manual was 20. Further interrogation of CFL number was performed to justify the use of this recommended value in correspondence with the 22 species reacting kinetics model. A wide range of user specified CFL numbers were selected for reacting solutions on the fine axisymmetric grid. The total equivalence ratio, \( \Phi_t = 0.6 \) was used. Table 4.2 summarizes the user specified CFL number, the number of times the ACAP became activated and the final steady state CFL number. Figure 4.10 shows mass conservation, which means all solutions in the CFL study were run to converged steady state solutions.
TABLE 4.2: SUMMARY OF CFL NUMBER

<table>
<thead>
<tr>
<th>CFL (user specified)</th>
<th>Number of ACAP</th>
<th>CFL (final)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>0</td>
<td>5</td>
</tr>
<tr>
<td>10</td>
<td>0</td>
<td>10</td>
</tr>
<tr>
<td>20</td>
<td>0</td>
<td>20</td>
</tr>
<tr>
<td>40</td>
<td>10</td>
<td>23.95</td>
</tr>
<tr>
<td>60</td>
<td>7</td>
<td>44.10</td>
</tr>
</tbody>
</table>

Observe Table 4.2 and Figure 4.10 they provide an opportunity for further clarification of the CFL and the ACAP. CFL=5, 10, 20, 40, 60 were selected by the user which is shown
in Table 4.2 and the legend in Figure 4.10. CFL=5, 10, 20, 23.95, 44.1 as seen in Table 4.2 correspond to the final CFL number. The numbers 0, 0, 0, 10 and 7 from Table 4.2 correspond to the number of times the ACAP ramping procedure was initialized. Observe for CFL=5, 10, 20 the ACAP was never activated. Figure 4.11 shows the effect the CFL number had on engine performance.

![Figure 4.11: Stream Thrust](image)

In Figure 4.11, engine Stream thrust for the CFL=5, 10, 20 were identical, meaning CFL number had no impact on the solution. Engine performance was affected when using the
larger CFL numbers. Anywhere between an 8% and 10.5% decrease in steam thrust was observed by specifying the higher CFL numbers where ACAP was initiated. Notice the high speed non-reacting solution in the inlet and isolator was un-affected by the CFL number. This means only the kinetics model was being overstepped by the CFL number given the specified range of CFL numbers. The following set of figures shows some of the solution flow parameters. Mach number, pressure and temperature were affected by the higher CFL numbers, Figures 4.12-4.14. Most of this effect occurred at the second stage where greater dissipation resulted in less heat release.

Figure 4.12: Mach number
Figure 4.13: Static pressure
Due to the uncertainty in solutions where the ACAP becomes activated leads to the conclusion that NO results in this investigation were shown where the ACAP became activated. This makes the recommended value of CFL=20 an appropriate CFL number to perform analysis so long as the solution never activates the ACAP. Remember this particular value of CFL number was very sensitive to the kinetics model; other kinetics models may operate better at higher or lower CFL values.

Figure 4.14: Static Temperature
CHAPTER 5
PRELIMINARY DESIGN ANALYSIS

Introduction

Again to re-iterate the objectives of these results in a more concise fashion is as follows. First, to analyze the performance of each study, gain a better understanding of the flow dynamics and kinetics, geometrical considerations, observe changes in flight conditions and develop new design concepts. In this section titled “Preliminary design analysis” the original grid supplied by Corbin will be studied verses a geometrically modified grid, which later becomes the baseline grid for all future studies. This baseline grid/model will have a series of cases performed and those results will be presented in this section.

Second Cavity Study

The purpose of this study was to observe the effect a second cavity including its effect on overall performance and flame stability. These models were performed in 3D, since the 3D geometry would be more representative of the flow dynamics and the experimental work going on in Test Cell 22 at the Air Force Research Laboratories. The second cavity only contributed to a marginal performance gain. A 0.95% increase in thrust was observed with the second cavity in place with a corresponding increase in efficiency of 0.5%. A very small disruption in the flow was induced by the second cavity. The small disruption led to slightly better mixing. Mixing led to the marginal
gains in performance and was subsequently quantized. The second cavity’s temperature was elevated; however, the cavity did not provide flame holding since the flame remained lit at the second stage without the need of the second cavity. As shown in Figure 5.1, elevated temperatures are sustained inside the thermal boundary layer after the second injection without the cavity.

Figure 5.1: Static Temperature (2D slice along injector centerline)
The thermal boundary layer that formed from the reactions of the first fuel injection, traveled downstream to the second injector. Additional fuel was added from the second injection into this boundary layer. Figure 5.2, depicts the second injector (downstream injector location), it shows enough oxygen from the surrounding free stream had mixed with the combustion products within this boundary layer. This mixing further supported the addition and burning of more fuel. The temperatures within this boundary layer remained high enough to auto ignite the additional fuel without the need of the cavity. Remember, a cavity captures and circulates a small amount of fuel and air at very low Mach numbers to sustain a flame, this flame elevates the temperatures of the fuel/air mixture that exists in the free stream.
Figure 5.2: Mass Fraction of Oxygen

Figure 5.3 depicts air fuel equivalence ratio. These results show little difference in the flow dynamics (streamlines) between the two models. This means the fuel was mixing within the boundary layer for both models.
The efficiency, Figure 5.4, was affected very little by the removal of the second cavity. Only a marginal gain was observed at the outflow with no change in peak efficiency before the second injection. This means with or without the second cavity the first stage of the combustion process was unaffected by the second stage. The very small gain at the outflow can be attributed to mildly better mixing since the second cavity does disrupt the overall flow; however, this small gain was determined not to be worth the cost and overall complexity of implementing this second cavity. This conclusion about the second
cavity leads to the baseline/nominal configuration being with only one upstream cavity. All results from this point on will utilize this new baseline geometry.

![Graph showing combustion efficiency](image)

Figure 5.4: Combustion Efficiency

**Axisymmetric vs. Sector Models**

The purpose of this study was to point out the similarities and differences between models performed in 2D axisymmetric and 3D sector models. Axisymmetric models provided early ballpark estimations of overall solutions to a variety of models. From these estimations the most attractive models would be performed using the sector
geometry. This aided in model selection, since axisymmetric models can be run to completion in a number of hours where sector models take a number of days. Axisymmetric solutions provide rough approximations in applying the physics of the solution. Geometrically speaking for axisymmetric, the injector had to be represented as a thin slice that wraps all the way around the combustion section, where in a real application, such as the sector, there would be 8 equally spaced injectors around a single stage of the combustion section. Physically, the fuel was being injected at sonic M=1, for each geometry however, the mass for the axisymmetric was thinly spread out all the way around the combustor. For the sector the mass was concentrated at an injector. This corresponds to greater injection momentum at the injection centerline for the sector models, which yield greater free stream penetration. Surprisingly, parameters like pressure and Mach number match up very well between axisymmetric and sector analysis. The most noticeable difference in Figure 5.5 is a smaller pressure rise in the axisymmetric model at the second injector as compared to the second injector for the sector model. The pressure rise in the sector model corresponds nicely to a lower Mach number, Figure 5.6, where two thermal throats exist for the axisymmetric model and only one for the sector model. The difference at the second stage has a lot to do with mixing within the thermal boundary layer. Since the flow was being accelerated after the first stage of combustion it becomes important for fuel at the second injector to penetrate deep into the thermal boundary layer. This is important because the thermal boundary layer near the wall before injection, at the second stage has depleted air content. This was unlike the upstream location of the first stage, which had clean air near the wall.
Figure 5.5: Static Pressure
Figure 5.6: Mach number

Notice from Figure 5.7, the elevated temperatures near the wall for the sector model. The additional fuel injection at the second stage properly mixed (near stoichiometric) with most of the air inside the thermal boundary layer. This was unlike the axisymmetric model where average temperatures were significantly lower.
Figure 5.8 shows air fuel equivalence ratio contour plots. For ethylene an equivalence ratio greater than 6 will make the air fuel mixture too rich to burn; at the opposite end an equivalence ratio less than 0.3 will make the air fuel mixture too lean to burn. The most efficient burning (highest temperatures) occurs at an equivalence ratio of 1. Make note of the stark differences between the two models and the distribution of the fuel. Notice a fuel rich content $\Phi > 3$ exists near the wall for the axisymmetric, which propagates all the way to the outflow to the combustor. In the sector model, a fuel rich mixture exists farther into the boundary layer, however, by the time this mixture reaches the outflow to
the combustor it has mixed and reached levels of $\Phi < 3$. On the injection centerline of the sector model, the injection momentum was greater due to a higher concentration of mass in the free stream direction, which led to deeper penetration into this free stream. This is why the cavity is much leaner $\Phi = 0.5 - 0.6$ in the cavity for the sector model. In the axisymmetric, a thin width slit spans the entire combustor; therefore, less mass is injected at its centerline, which yields greater coupling between the injector and cavity. This coupling leads to the richer fuel content in the cavity for the axisymmetric model. The sector contour was a 2D slice taken along its injection centerline. However, if a slice is taken off the centerline of the sector model no momentum exists, only a wall.

Figure 5.8: Fuel Distribution ($\Phi$ contours along injector centerline)

The axisymmetric model has a constant mass concentration and mass flow no matter how far one moves away from its centerline. Therefore, the total injection momentum was the same for both the sector and axisymmetric. This was why after the first injection little
difference in performance was observed as seen in Figure 5.9. This is why the close agreement between the two models was surprising.

![Combustion Efficiency Graph](image)

**Figure 5.9: Combustion Efficiency**

Initially, the axisymmetric performs better because the majority of the fuel is being captured by the cavity increasing its duration time at the upstream location. The better mixing properties at the second stage of the combustor for the sector model yielded 8.3% greater efficiency at the outflow. The sector model generated 4.1% greater thrust than the
axisymmetric model. Despite some of these differences axisymmetric solutions would typically model a sector solution within 10% or less in performance. This makes axisymmetric solutions satisfactory solutions for approximating performance for sector models.

**Reduced Flight Enthalpy (M=3.0 vs. M=2.5 flight conditions)**

The purpose of this study was to make preliminary observations between Mach 2.5 and Mach 3.0 flight using an axisymmetric analysis. The nozzle being used for the Mach 2.5 investigation is still the Mach 1.8 nozzle, which makes this study a reduced flight enthalpy study. The total fuel air equivalence ratio remained constant at 0.8 for both flight conditions. Observing Figure 5.10 shows the shock train was approximately 5cm farther up into the isolator at the Mach 2.5 flight condition than the Mach 3.0. Also the Mach number for Mach 2.5 after the first injection did not accelerate as rapidly as the Mach 3.0. Two thermal throats exist at Mach 3.0 where only one exists at Mach 2.5. Static temperatures were down as well as depicted in Figure 5.11. With the movement of the shock train farther up in the isolator coupled with the decrease in temperatures corresponded to a combustor that is not performing as well at Mach 2.5 compared to Mach 3.0.
Figure 5.10: Mach Number
Figure 5.11: Static Temperatures
Figure 5.12 depicts overall combustion efficiency loss at the lower flight Mach number. Combustion efficiency was down 3% overall at Mach 2.5 conditions.

Figure 5.12: Combustion Efficiency

The decrease in combustion efficiency was not significant, which shows that the Dual Mode Scramjet is still capable of efficient operation at the lower flight Mach number.
Fuel Mixture

The use of a different fuel type was studied to observe the effect of introducing a less reactive fuel into the overall fuel mixture like a JP fuel. Clearly, the introduction of a 50/50 molecular split of ethylene and methane played a role in the performance and shock location, Figure 5.13 shows the shock location. The use of methane yielded less heat release, which resulted in lower temperatures (Figure 5.14). The decrease in temperature resulted in a decrease in performance, this decrease was anticipated since it is known that methane is less reactive and provides less energy when it does react. Stream thrust decreased by 5% for the 50/50 mixture model as compared to the ethylene model.
Figure 5.13: Mach Number
The contours, in Figure 5.15, show the mass fraction of methane to ethylene for the mixture model. In the mixture model, methane was being injected on a molar basis $X_{\text{CH}_4}=0.5$, $X_{\text{C}_2\text{H}_4}=0.5$, this corresponds to mass fractions of $Y_{\text{CH}_4}=0.364$, $Y_{\text{C}_2\text{H}_4}=0.636$. For equal consumption of the two fuels the ratio of the mass fractions should be maintained, approximately, at $Y_{\text{CH}_4}/Y_{\text{C}_2\text{H}_4} \approx 0.57$, everywhere throughout the model. This clearly was not the case. The reaction rate of methane was less than ethylene. This correlates nicely to the less reactive methane concentration being higher in the free stream as compared to ethylene.
Other studies examined involving fuel type mixing and splitting were a 100% and 80% by mol of methane, but both of these cases blew out the flame in the cavity. Another case with a fueling equivalence ratio of 0.6 and 0.2 between the first and second injector, respectively, using pure ethylene was attempted. This too yielded engine blowout because the flame could not sustain itself in the cavity. For axisymmetric analysis the cavity became too rich to sustain a flame at a fueling of $\Phi_1 = 0.6$ and $\Phi_2 = 0.2$. For the sector analysis the cavity became too lean to sustain the flame. This distinction between axisymmetric and sector models will have to be taken into serious consideration when performing future analysis.
CHAPTER 6
Detailed Geometrical Design Analysis

Introduction

Based on the preliminary design analysis, it should be possible to make the new baseline geometry/configuration more optimal in terms of overall performance. This analysis strictly takes into account new considerations such as injector placement, cavity feeding and fueling. Therefore, fuel type and flight condition are held constant in order to accurately analyze the geometrical changes. Like the second cavity preliminary study, a 3D sector analysis will be performed since they are geometrical studies that better reflect the experimental configurations from RC22 at the Air Force Research Laboratories.

Feeding the Cavity

As shown previously in the section titled “Axisymmetric vs. Sector,” the baseline sector cavity was lean having an equivalence ratio ranging from $\Phi = 0.5-0.6$. Attempts to further increase the amount of fuel at the upstream injector beyond $\Phi_1=0.4$ yielded over-penetration of the fuel, leading to leaner mixtures in the cavity that ultimately led to cavity blowout, therefore, the concept of placing a smaller feed injector upstream of the cavity will be investigated. The injector was placed at the same axial location as the first injector just upstream of the cavity. The feed injector is $\frac{1}{4}$ the diameter of the main injector. In a full 3D model two feed injectors would be placed in between each of the 8
primary injectors leading to a total of 16 feed injectors. Note, these are sector simulations and only a 3D pie slice of the geometry is being modeled. Feeding only took place at the first fuel injection stage. The downstream injector maintained the same baseline geometric configuration. Two different fuelings were used for the feed injector. First, was a feed injector fueling equivalence ratio of $\Phi=0.03$. Second, was a feed injector fueling equivalence ratio of $\Phi=0.07$. The fueling for the primary injectors remained the same as the baseline configuration of $\Phi_{1,2} = 0.4$. By only adjusting fueling of the feed injector accurate comparisons to the baseline were possible. The fuel type used for the comparison was ethylene and the flight condition was Mach 3.0 at the higher altitude of 52,000ft. The feeding geometry can be seen in Figure 6.1.

![Figure 6.1: Fuel Distribution (translucent $\Phi$ contours, displays feed injector)](image)
Figure 6.2 shows the mass conservation utility as a sanity check for obtaining a steady state solution. Also, fuel distribution is shown by equivalence ratio contours. This 2D slice of the sector geometry was taken along the primary injector centerline. On the centerline it appears the feed injector was having an effect by fueling the backside (downstream) of the cavity.

Figure 6.2: Mass Conservation “top” and Fuel Distribution (Φ contours) “bottom”
Figure 6.3 gives a 3D view of the cavity. At the lower feeding case of $\Phi=0.03$ the upstream portion of the cavity was better fueled at $\Phi=0.75$. The higher feeding case of $\Phi=0.07$ yielded higher cavity fuel penetration near the downstream portion of the cavity ($\Phi=0.75, 0.85, 0.95$) but not upstream. Off the main injector centerline the lower feeding case better fueled the cavity at $\Phi=0.45$. Both feeding cases proved beneficial in feeding the downstream portion of the cavity over the baseline, however, the upstream portion of the cavity was largely unaffected by the feeding.

Figure 6.3: Fuel Distribution ($\Phi$ contours) Feeding Effects
A good explanation as to why the feeding at $\Phi=0.03$ did a better job fueling the upstream portion has once again to do with fuel penetration. Since the equivalence ratio was lower the fuel jet from the wall did not penetrate as deep as the feeding at $\Phi=0.07$. More is not always better, however, near the very backside of the cavity the feeding at $\Phi=0.07$ did do a better job fueling the downstream portion of the cavity. It leads to the understanding that injecting more fuel $\Phi>0.07$ through the feed injector could lead to complete over penetration of the cavity, which would defeat the purpose of cavity feeding. Once again for these results to be valid the injectors do need to be choked at their exit at Mach=1 which they were for both the main and feed injectors for these three cases. Figure 6.4 illustrate the feed injection penetration for the two different types of fueling.
Now that the dynamics of the feeding have been looked at in detail it becomes necessary to observe the feeding effects on overall engine performance, Figure 6.5.
A 7% increase in stream thrust was observed by implementing the feeding of $\Phi=0.07$ over the baseline, which corresponded to a total $\Phi_t=0.87$. A 3.8% increase in stream thrust was observed by implementing the feeding of $\Phi=0.03$ over the baseline, which corresponded to a total $\Phi_t=0.83$. Overall combustion efficiency was largely unaffected by increases in fueling of the feed injector as compared to the baseline. Figure 6.6 shows static pressure. As expected the static pressure rise increased by increasing the amount of fuel. Shock position changed by increasing $\Phi$ as well, which was also expected. It appears shock displacement in the isolator is nonlinear with fueling/heat release.
Increasing the equivalence ratio by 0.03 via feeding, the shock train moved further upstream by 13cm as compared to the baseline. Next, the equivalence ratio was more than doubled via feeding to 0.07. This led to a shock displacement of 23cm as compared to the baseline. However, there was only a 10cm difference in shock location between the two feeding models. Once again this shows the non-linearity between heat release and the volumetric capacity of the isolator. The small increase in the amount of fuel (by feeding) shows how sensitive shock position is in the isolator.

![Static Pressure Graph](image)

Figure 6.6: Static Pressure
Figure 6.7 shows a corresponding temperature rise which led to greater engine performance.

![Figure 6.7: Static Temperature](image-url)
Injector Placement

The final geometry change explored was moving the second injector to reduce the length of the combustor. This involves moving the second injector closer to the first. Intuitively, reducing the gap between the first and second stage has two advantages. First, reducing the size of the combustor would lead to lower structural weight and engine bulk. Second, it would provide less surface area for heat to escape through the combustor wall between stages (note: heat losses are not being taken into account in these simulations but it is understood that heat losses will occur through the combustor walls during actual scramjet experiments). Despite these intuitive reasons for reducing combustor length, it is unknown what kind of an effect it will have on overall engine performance.

Initially, there were 3 types of reductions, a 75% reduction, a 50% reduction and a 25% reduction in combustor length for the same baseline fueling of $\Phi_{1,2}=0.4$. The 75% reduction and 50% reduction model yielded unsteady results. Since these were unsteady results, they will only be mentioned in this document. The nature of unsteady results makes it difficult to analyze. The results showed that the cavity completely blew out and that the flame was trying to settle near the back of the combustor downstream of the second injector. For the 25% reduction model, the solution was still clearly unsteady and oscillating between two solutions, however, some flame was sustained in the cavity. The cavity became very lean and on the verge of blowout, then the fuel mixture would recover itself, which corresponded to a temperature recovery in the cavity. The solution kept oscillating between these two results. As a result of this oscillation, for the 25% reduction model, the amount of heat released at the first stage could be lowered by
reducing the equivalence ratio from $\Phi_1=0.4$ to $\Phi_1=0.325$. This reduction in the equivalence ratio would also reduce jet penetration and hopefully lead to enriching the fuel mixture in the cavity and achieving a steady solution. To make a proper baseline comparison, a baseline case with the original injector location was also performed at the reduced equivalence ratio $\Phi_1=0.325$. Figure 6.8 shows the steady state results for mass flow. Figures 6.8 thru 6.10 show strikingly different fuel distributions in the cavity.

Figure 6.8: Mass Flow Conservation and Fuel Distribution ($\Phi$ contours)
Figure 6.9: Fuel Distribution (Φ contours, 2D slice along injector centerline)
Observe a significant difference in cavity fuel distribution between the baseline geometric configuration and the injector placement configuration for the same equivalence ratio, $\Phi_1=0.325$ and $\Phi_2=0.4$. The cavity for the baseline configuration is closer to stoichiometric ($\Phi=1$) near the centerline as compared to the placement. Away from the injector centerline the equivalence ratios are approximately the same. Reducing overall $\Phi$ out of the upstream injector clearly had a beneficial effect in reducing jet penetration and fueling the cavity. This confirms that by moving the injector farther forward can lead to jet over penetration, which would lead to lean cavity mixtures and
possible cavity blowout. It appears moving the injector forward caused more of an interaction between the first and second injections.

Moving the injector forward 25% pushed the shock train approximately 15cm farther upstream into the isolator for the same equivalence ratio. This corresponded to a greater static pressure rise over the cavity as shown in Figure 6.11. Less fuel being injected at the first stage for the baseline configuration resulted in less heat release, which also corresponded to a lower static pressure rise as compared to the baseline fueling of $\Phi_{1,2}=0.4$.

Figure 6.11: Static Pressure
Slightly higher Mach number at the point of injection (Figure 6.12) would result in an increase in dynamic pressure. This is why much of the fuel went into the cavity and did not penetrate into the free stream for the baseline model at $\Phi_1 = 0.325$. Placing the injector farther forward had a beneficial effect on increasing static pressure between stages, which corresponded to a drop in Mach number.

![Figure 6.12: Mach Number](image)

The placement model led to greater heat release and an increase in static temperature at the second stage of the combustor. By lowering the equivalence ratio for the baseline
configuration at the first stage, this resulted in better cavity fueling closer to stoichiometric which led to higher cavity temperatures, Figures 6.13 and 6.14. Notice the flame began near the wall just upstream of the cavity for the baseline configuration at $\Phi_1=0.325$. The placement model had a beneficial impact on overall engine performance, Figure 6.15.

Figure 6.13: Static Temperature
Figure 6.14: Static Temperature (3D off centerline)
Stream thrust and combustion efficiency for the placement model were up 6.4% and 11%, respectively over the baseline configuration and it used LESS fuel. The combination of the temperature and pressure rise which led to greater thrust and efficiency proved that by using less fuel led to better burning which corresponded to greater heat release.
Baseline, Feeding and Placement

In this section, the baseline will be matched up against the feeding model at $\Phi_t = 0.03$ and the placement model from the previous section. This will be done to directly examine the best overall performer.

The placement model at a total equivalence ratio of $\Phi_t = 0.725$ outperformed not only the baseline as discussed previously but also outperformed the feeding model at a total $\Phi_t = 0.83$ by a small but noticeable 1.8% (Figure 6.16). Not shown is the feeding model of $\Phi_t = 0.87$, which would outperform the placement model in terms of stream thrust, however, it uses much more fuel. The explanation for this is greater heat release for the placement model, which resulted in greater combustion efficiency, Figure 6.17.

Figure 6.16: Stream Thrust

89
Combustion efficiency was approximately 10.5% greater for the placement model over the feeding model. Finally, the shock train did not move up as far in the isolator for the placement compared to the feeding, Figure 6.18. The placement, however, resulted in better overall performance.
Figure 6.18: Mach number
CHAPTER 7

CONCLUSIONS

“Preliminary Design Analysis”

Second Cavity Study

The marginal gain in performance by having the second cavity was not worth the cavity’s complexity of implementation. This small gain was due to the small disruption in flow induced by the second cavity, which led to slightly better mixing. The purpose of the second cavity was to provide flame holding capability, but the flame remained steady and lit at the second stage without the need of the additional cavity. The flame remained lit at the second stage due to elevated temperatures, inside the oxygenated thermal boundary, that was produced by the first stage of injection.

Axisymmetric vs. Sector Models

The difference in performance between an axisymmetric and sector model was minor for the configurations studied. This result was surprising considering the significant difference in the way the fuel was injected; therefore, the majority of the preliminary results presented are for axisymmetric configurations. Axisymmetric worked very well for the geometric configurations being analyzed, however, axisymmetric would not work well for more complex geometries such as introducing a strut or offsetting the injectors. The small differences between the two models in this study proved beneficiary, since axisymmetric models run much faster than sector models.
Reduced Flight Enthalpy ($M=3.0$ vs. $M=2.5$ flight conditions)

This study showed minimal decreases in performance. The flame was capable of sustaining itself at a low flight Mach number. This is beneficial to further extend the operating range of the DMSJ to lower flight Mach numbers. Physically, the shock train at Mach 2.5 moved farther up into the isolator with the same fuel air equivalence ratio as the Mach 3.0. This was an important observation because further reduction in flight Mach number could ultimately lead to unstart.

Fuel Mixture

The introduction of methane with ethylene into the free stream had differing effects on performance. The small decrease in thrust for the 50/50 mixture model, compared to the pure ethylene model, could be attributed to the lower heat of combustion of methane. The small decrease in performance by using a 50/50 mixture by mole, for the two fuels, proves helpful by possibly increasing the methane content for the use of methane as a possible fuel type in the future.

“Detailed Geometrical Design Analysis”

Feeding the Cavity

Feeding the cavity had a beneficial effect on fueling the downstream (backside) portion of the cavity by elevating the equivalence ratio closer to stoichiometric. This led to higher temperatures near the downstream portion of the cavity. The small amount of additional fuel injected by the feed injector had a significant impact on shock position in the isolator. Not only aiding in cavity flame development and stabilizing combustion, the
small increase in fuel via feed injection had a beneficial effect on performance by increasing stream thrust, however, combustion efficiency was largely left unchanged. This makes cavity feeding an attractive upgrade to the baseline configuration.

Injector Placement

Placing the injector 25% further upstream had several positive effects on performance. For a lower total equivalence ratio, $\Phi_t = 0.725$ for the placement geometry, stream thrust and combustion efficiency were increase 6.4% and 11%, respectively, over the baseline configuration which was at the higher total equivalence ratio of $\Phi_t = 0.8$. There was more interaction between the first and second stage for the placement configuration. The second stage injection influenced heat release, which corresponded to a static pressure rise at the first stage. The effect of placing the second stage injector closer to the first stage, for the lower equivalence ratio at the first stage, actually pushed the shock train further into the isolator as compared to the baseline shock location. This influenced fuel jet penetration at the first stage by causing a drop in dynamic pressure which leaned out the cavity.
Future Research

Further improvements to the baseline geometry can be made. It has been shown that cavity feeding has a beneficial effect on fueling the cavity and increasing stream thrust. Placing the second stage injectors further forward had exemplary gains in performance; not only in terms of stream thrust but also in terms of efficiency, which allowed for less fuel to be used. It may be possible to change the feeding strategy by fueling the cavity directly to better fuel the entire cavity not just the downstream portion. Continuing to move the second stage injectors closer to the first stage should prove to increase performance further. Moving the second stage injectors further upstream along with cavity feeding could help reduce the effect of leaning the cavity and starving it of fuel. Reducing the number of injectors at the second stage but increasing injector diameter to maintain injection area conservation could help improve burning radially near the centerline of the combustor.

After optimizing the baseline geometry the engine may then be more suitable for reducing flight Mach numbers and extending the range of the Dual Mode Scramjet. Finally, additional research into the effects of using different fuels and different fuel mixtures should be accomplished to provide a better understanding of the practical application of the DMSJ systems.
APPENDIX

INPUT FILE

An example of a CFD++ input file for a 3D sector model. The name of the file is “mcfd.inp” modifications to this input file can be made using Metacomp’s graphical interface or reading this input file directly from a linux machine.

“mcfd.inp”

```plaintext
#--------------------------------------
# Input file created by CFD++ 7.1.1 GUI
#--------------------------------------
system begin
mc_filecopy cdepsout.bin cdepsin.bin
mc_filecopy cdaveout.bin cdavein.bin
mc_filecopy mcfd6dof.out mcfd6dof.inp
system end
#--------------------------------------
iofiles begin
lm_type STANDARD
lm_cells_limit 0
lm_cpus_limit 0
lm_ser2par 0
ifinbc 0
invoke_script 0
mcpusin_fn mcpusin.bin
nodesin_fn nodesin.bin
cellsin_fn cellsin.bin
exbcsin_fn exbcsin.bin
inbcsin_fn inbcsin.bin
ovsetin_fn ovsetin.bin
cdepsin_fn cdepsin.bin
pltosin_fn pltosin.bin
eqsetin_fn eqsetin.bin
zobcsin_fn zobcsin.bin
ovsetin_fn ovsetin.bin
blankin_fn blankin.bin
cgrpsin_fn cgrpsin.bin
#--------------------------------------
mcpusout_fn mcpusout.bin
nodesout_fn nodesout.bin
cellssout_fn cellsout.bin
exbcsout_fn exbcsout.bin
inbcsout_fn inbcsout.bin
ovsetout_fn ovsetout.bin
```
cdepsout_fn  cdepsout.bin
pltosout_fn  pltosout.bin
eqsetout_fn  eqsetout.bin
zobcsout_fn  zobcsout.bin
ovsetout_fn  ovsetout.bin
blankout_fn  blankout.bin
cgrpsout_fn  cgrpsout.bin
#---------------------------
iofiles end
#---------------------------
celltypes 1

celltype 0 fluxmasks 0 0 0 0 0 0

celltype 0 vtfpmasks 0 0 0 0 0 0

celltype 0 vtxpmasks 0 0 0 0 0 0 0 0 0 0
#

tsteps begin
istart 1
ntstep 6000
ntstop 0
ntsmin 0
ntrmin 0
dtsmoo 0
dtsmoo_iters 4
dtsmoo_param 0.6666667
runmod 1
dtauin -1.000000e+00
dtlomx 1.000000

cflbot 1.000000e-04
cfiller 0.950000
 rstcfl 1
 ntbcrlr 1
 nteclr 200
 cfllbg 1.000000e+00
cfllen 2.000000e+01
cflglo 1.000000e+15
 ilcfla 0
 igcfla 0
 itsync 0
ntbmdr 100
ntemdr 200
mdisbg 0.000000e+00
mdisen 0.000000e+00
ntbbfr 201
ntebrf 300
blfnbg 0.000000e+00
blfnen 1.000000e+00
cdepsave_compute 0
cdepsave_restart 1
cdepsave_ntsave 0
tsteps end
#

options begin
ntdsko 250
ntdsks 0
ntplto 250
ntplts 0
ntpltt 0
dtpltt 0.000000e+00
ntdskc 0
ntdskr 0
ntacou 0
ntout1 20
ntout2 0
ntout3 0
ntout4 0
ntout5 0
ntout6 0
ntout7 0
ntout8 0
ntout9 0
ntout10 0
ntout11 0
ntout12 0
ntout13 0
ntout14 0
ntout15 0
ntout16 0
ntout17 0
ntout18 0
ntout19 0
ntout20 0
ntout21 0
ntout22 0
ntout23 0
ntout24 0
ntout25 0
ntout26 0
ntout27 0
ntout28 0
ntout29 0
nt6dof1 1
ntoutfv 0
ntsuffv 0
ntoutes 0
ntsufes 0
ntouttp 0
ntsuftp 0
ntoptrb 0
ntsptrb 0
bcsptrb 0
mpidri 0
mcpuse 0
mcgrps 9
#-----------------
nodebg 0
inbczr 0
autozb 0
osetyp 0
osetdb 0
osetbr 0
osetbc 0
osetbx 0
osetll 0
osetzo 0
osetsl 0
osetir 0
osnocn 1
osnosg 1
blnkdb 0
zobcdb 0
zobcty 2
iregrd 0
iregrq 1
irezon 0
reblnk 0
igrvs1 0
igrvs7 0
igrvs9 0
igrvs10 0
igrvs13 0
igrvs14 0
ifrbd1 0
#----------------
vicos 1
vibnew 1
ifmdis 1
mdislh 0.250000
disson 0.100000
ifmdps 1
mdisps 0.050000
mdtype 1
mdpscf 0.300000
mdpsmx 1.000000
ifmdcb 0
mdcbfr 0.250000
#----------------
xyzpol xyz
ispcac 2
ibblend 1
iblenz 0
blenzf 0.500000
bextac 1
bzonac 2
bzoncd 0
slidzb 0
arcozb 0
celpol 1
cenpol 2
nodnei 1
viscrs 0
vcropt 1
tvspol 1
celpoj 0
limfac 0
rhsopt 1
rhsink 0
tolpol 1.000000e-13
limtvd 3
tvdcmp 2.0
tvdphi 0.333330
cchkvol 1
tolvol 1.000000e-20
grqua1 0
grqua2 0
grqua3 0
grqua6 0
gq1dis 0.100000
gq2ang 2.000000
gq3dis 0.100000
gq6dis 0.100000
gq6ang 40.000000
#-----------------
rtcord 5.000000
convol 0
convol2 0
simstr 1
dultim 0
gltirc 0.100000
gloits 1
pc_method 0
mltlim 0
mlbfac 1.000000e-01
mlbglt 1
memopt1 0
method 2
itimac 2
impave 0
ifunlx 1
undrlx 0.750000
implic 1
impits 16
mg_mpio 1
fg_mpf 0
mg_mpf 0
mg_type 1
mg_lint 2
mg_itns 1
mg_levs 20
mg_mxcg 1048576
mg_cycl 6
mg_resc 5.000000e-01
mg_terc 1.000000e-01
mg_floc 1.000000e-10
fg_resc 5.000000e-01
fg_terc 1.000000e-01
fg_floc 1.000000e-10
mg_cvis 1.0
celord 1
subdomain_mode 0
options end
#---------------------------
insets 150
#----------------------------
seq.# 1 #vals 31 title eqnset_define
values 101 1 1 2 2
values 1 0 1 1 1
values 0 28 5 2 0
values 21 0 0 0 0
values 0 23 23 1 6
values 3 0 0 0 0
values 0
#----------------------------------------------------------
seq.# 2 #vals 4 title species_temperature_range_info
values 2 100.0 1000.0 5000.0
#----------------------------------------------------------
seq.# 3 #vals 1 title species_1_M wt1_H2
values 2.016
#----------------------------------------------------------
seq.# 4 #vals 6 title species_1_Sutherland6
values 8.45e-6 273.16 66.8 0.17290 273.16 175.3
#----------------------------------------------------------
seq.# 5 #vals 3 title species_1_Supercritical
values 33.2 0.0323 -0.22
#----------------------------------------------------------
seq.# 6 #vals 10 title species_1_Additional_Properties
values 3.5 0 0 0 2
values 0 0.0 0.0 0.0 0.0
#----------------------------------------------------------
seq.# 7 #vals 7 title species_1_Cp/R+HF+GF7_range_1
values 2.8460849 4.1932116e-03 -9.6119332e-06 9.5122662e-09 -3.3093421e-12
values -9.6725372e02 -1.4117850
#----------------------------------------------------------
seq.# 8 #vals 7 title species_1_Cp/R+HF+GF7_range_2
values 3.0436897e00 6.1187110e-04 -7.3993551e-09 -2.0331907e-11
values 2.4593791e-15
values -8.5491002e02 -1.6481339
#----------------------------------------------------------
seq.# 9 #vals 1 title species_2_M wt1_H
values 1.008
#----------------------------------------------------------
seq.# 10 #vals 6 title species_2_Sutherland6
values 7.63879e-6 273.16 154.8 0.23644 273.16 154.8
#----------------------------------------------------------
seq.# 11 #vals 3 title species_2_Supercritical
values 5. 0.0001 0.
#----------------------------------------------------------
seq.# 12 #vals 10 title species_2_Additional_Properties
values 2.5 0 0 0 1
values 0 0.0 0.0 0.0 0.0
#----------------------------------------------------------
seq.# 13 #vals 7 title species_2_Cp/R+HF+GF7_range_1
values 2.500000 0. 0. 0. 0.
values 2.5474390e4 -0.45989841
#----------------------------------------------------------
seq.# 14 #vals 7 title species_2_Cp/R+HF+GF7_range_2
values 2.500000 0. 0. 0. 0.
values 2.5474390e4 -0.45989841
<table>
<thead>
<tr>
<th>seq.#</th>
<th>#vals</th>
<th>title</th>
<th>values</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>1</td>
<td>species_3_Mwt1_O</td>
<td>16.0</td>
</tr>
<tr>
<td>16</td>
<td>6</td>
<td>species_3_Sutherland6</td>
<td>2.21761e-5</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>273.16</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>165.7</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.045558</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>273.16</td>
</tr>
<tr>
<td>17</td>
<td>3</td>
<td>species_3_Supercritical</td>
<td>5.0</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.0001</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.0</td>
</tr>
<tr>
<td>18</td>
<td>10</td>
<td>species_3_Additional_Properties</td>
<td>2.5</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.0</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>8.211e7</td>
</tr>
<tr>
<td>19</td>
<td>7</td>
<td>species_3_Cp/R+HF+GF7_range_1</td>
<td>3.0309401</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>-2.2525853e-3</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>3.982454e-6</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>-3.2604921e-9</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1.0152035e-12</td>
</tr>
<tr>
<td>20</td>
<td>7</td>
<td>species_3_Cp/R+HF+GF7_range_2</td>
<td>2.5342961</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>-1.2478170e-5</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>-1.2562724e-8</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>6.9029862e-12</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>-6.73797095e-16</td>
</tr>
<tr>
<td>21</td>
<td>1</td>
<td>species_4_Mwt1_O2</td>
<td>32.0</td>
</tr>
<tr>
<td>22</td>
<td>6</td>
<td>species_4_Sutherland6</td>
<td>1.919e-05</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>273.16</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>125.0</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.02449</td>
</tr>
<tr>
<td>23</td>
<td>3</td>
<td>species_4_Supercritical</td>
<td>154.6</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.00229</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.021</td>
</tr>
<tr>
<td>24</td>
<td>10</td>
<td>species_4_Additional_Properties</td>
<td>3.5</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>129</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1.543e7</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>3.771e7</td>
</tr>
<tr>
<td>25</td>
<td>7</td>
<td>species_4_Cp/R+HF+GF7_range_1</td>
<td>3.7189946</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>-2.5167288e-03</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>8.5837353e-06</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>-8.2998716e-09</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>2.7082180e-12</td>
</tr>
<tr>
<td>26</td>
<td>7</td>
<td>species_4_Cp/R+HF+GF7_range_2</td>
<td>3.5976129</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>7.8145603e-04</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>-2.2386670e-07</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>4.2490159e-11</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>3.3460204e-15</td>
</tr>
<tr>
<td>27</td>
<td>1</td>
<td>species_5_Mwt1_OH</td>
<td>17.008</td>
</tr>
<tr>
<td>28</td>
<td>6</td>
<td>species_5_Sutherland6</td>
<td>1.4005e-5</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>273.16</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>200.8</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.03581</td>
</tr>
<tr>
<td>29</td>
<td>3</td>
<td>species_5_Supercritical</td>
<td>5.0</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.0001</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.0</td>
</tr>
<tr>
<td>seq.#</td>
<td>vals</td>
<td>title</td>
<td>values</td>
</tr>
<tr>
<td>-------</td>
<td>------</td>
<td>-------</td>
<td>--------</td>
</tr>
<tr>
<td>30</td>
<td>10</td>
<td>species_5_Additional_Properties</td>
<td>0 0 0 0 2</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0 0.0 0.0 0.0 0.0</td>
</tr>
<tr>
<td>31</td>
<td>7</td>
<td>species_5_Cp/R+HF+GF7_range_1</td>
<td>3.873730  -1.3393772e-3  1.6348351e-6 -5.2133639e-10  4.1826974e-14</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>3.5802348e3  0.34202406</td>
</tr>
<tr>
<td>32</td>
<td>7</td>
<td>species_5_Cp/R+HF+GF7_range_2</td>
<td>3.8897814  1.005879e-3  1.6348351e-6 -5.2133639e-10  4.1826974e-14</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>3.8857042e3  5.5566420</td>
</tr>
<tr>
<td>33</td>
<td>1</td>
<td>species_6_Mwt1_H2O</td>
<td>18.02</td>
</tr>
<tr>
<td>34</td>
<td>6</td>
<td>species_6_Sutherland6</td>
<td>1.006e-5  1273.16  523.3  273.16  273.16  1276.0</td>
</tr>
<tr>
<td>35</td>
<td>3</td>
<td>species_6_Supercritical</td>
<td>647.3  0.00311  0.344</td>
</tr>
<tr>
<td>36</td>
<td>10</td>
<td>species_6_Additional_Properties</td>
<td>4.0  0  0  2</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0 0.0 0.0 0.0 0.0</td>
</tr>
<tr>
<td>37</td>
<td>7</td>
<td>species_6_Cp/R+HF+GF7_range_1</td>
<td>4.1565016  -1.7244334e-03  5.6982316e-6 -4.5930044e-9  1.4233654e-12</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>-3.0288770e04  6.8616246e-01</td>
</tr>
<tr>
<td>38</td>
<td>7</td>
<td>species_6_Cp/R+HF+GF7_range_2</td>
<td>2.6707532  3.0317115e-03  8.5351570e-7  1.1790853e-10  6.1973568e-15</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>-2.9888994e4  6.8838391</td>
</tr>
<tr>
<td>39</td>
<td>1</td>
<td>species_7_Mwt1_HO2</td>
<td>33.008</td>
</tr>
<tr>
<td>40</td>
<td>6</td>
<td>species_7_Sutherland6</td>
<td>1.4613e-5  656.0</td>
</tr>
<tr>
<td>41</td>
<td>3</td>
<td>species_7_Supercritical</td>
<td>5.  0.0001  0.</td>
</tr>
<tr>
<td>42</td>
<td>10</td>
<td>species_7_Additional_Properties</td>
<td>4.0  0  0  2</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0 0.0 0.0 0.0 0.0</td>
</tr>
<tr>
<td>43</td>
<td>7</td>
<td>species_7_Cp/R+HF+GF7_range_1</td>
<td>4.30178801  -4.74902008e-3  2.11579535e-5 -2.42759611e-8  9.29206702e-12</td>
</tr>
</tbody>
</table>
values 2.94808764e2 3.71670101
#---------------------------------------------------------
seq.# 44 #vals 7 title species_7_Cp/R+HF+GF7_range_2
values 1.7226593 1.88120976e-3 -3.46292968e-7 1.94685157e-11
1.76091525e-16
values -6.18188513e1 2.95779739
#---------------------------------------
seq.# 45 #vals 1 title species_8_Mwt1_H2O2
values 34.016
#---------------------------------------------------------
seq.# 46 #vals 6 title species_8_Sutherland6
values -1.334e-5 273.16 246.079 0.01598 273.16 1070.042
#---------------------------------------------------------
seq.# 47 #vals 3 title species_8_Supercritical
values 5. 0. 0.
#---------------------------------------
seq.# 48 #vals 10 title species_8_Additional_Properties
values 4.0 0 0 0 2
values 0 0.0 0.0 0.0 0.0
#---------------------------------------------------------
seq.# 49 #vals 7 title species_8_Cp/R+HF+GF7_range_1
values 3.4546633 5.5575930e-03 9.2103738e-07 -4.6279780e-09 2.145800e-12
values -1.7672328e4 6.8402452
#---------------------------------------------------------
seq.# 50 #vals 7 title species_8_Cp/R+HF+GF7_range_2
values 4.7928858 3.6300865e-3 -1.11136435e-6 1.4868513e-10 -6.8958511e-15
values -1.8132195e4 -0.51306415
#---------------------------------------------------------
seq.# 51 #vals 1 title species_9_Mwt1_CH3
values 15.024
#---------------------------------------------------------
seq.# 52 #vals 6 title species_9_Sutherland6
values -1.335e-05 273.16 169.6889 0.04777 273.16
values 743.6
#---------------------------------------------------------
seq.# 53 #vals 3 title species_9_Supercritical
values 5. 0.0001 0.
#---------------------------------------------------------
seq.# 54 #vals 10 title species_9_Additional_Properties
values 4.0 0 0 0 2
values 0 0.0 0.0 0.0 0.0
#---------------------------------------------------------
seq.# 55 #vals 7 title species_9_Cp/R+HF+GF7_range_1
values 0.34666350e+01 0.38301845e-02 0.10116802e-05 -0.18859236e-08
0.66803182e-12
values 0.16313104e+05 0.24172192e+01
#---------------------------------------------------------
seq.# 56 #vals 7 title species_9_Cp/R+HF+GF7_range_2
values 0.28400327e+01 0.60869086e-02 -0.21740338e-05 0.36042576e-09
-0.22725300e-13
values 0.16449813e+05 0.55056751e+01
#---------------------------------------------------------
seq.# 57 #vals 1 title species_10_Mwt1_CH4
values 16.04
#------------------------------------------------------
seq.# 58 #vals 6 title species_10_Sutherland6
values 1.024e-05 273.16 169.0 0.03069 273.16
values 2681.0
#------------------------------------------------------
seq.# 59 #vals 3 title species_10_Supercritical
values 190.4 0.00618 0.011
#------------------------------------------------------
seq.# 60 #vals 10 title species_10_Additional_Properties
values 4.0 0 0 0 2
values 0 0.0 0.0 0.0 0.0
#------------------------------------------------------
seq.# 61 #vals 7 title species_10_Cp/R+HF+GF7_range_1
values 4.2497678 -6.9126562e-03 3.1602134e-05 -2.9715432e-08
9.5103580e-12
values -1.0186632e04 -9.1754991e-01
#------------------------------------------------------
seq.# 62 #vals 7 title species_10_Cp/R+HF+GF7_range_2
values 1.1795744 1.0950594e-02 -4.0622131e-06 7.1370281e-10
4.7490353e-14
values -9.8556627e03 1.2505934e01
#------------------------------------------------------
seq.# 63 #vals 1 title species_11_Mwt1_CO
values 28.01
#------------------------------------------------------
seq.# 64 #vals 6 title species_11_Sutherland6
values 1.635e-05 273.16 253.0 0.0146 273.16
values 939.8
#------------------------------------------------------
seq.# 65 #vals 3 title species_11_Supercritical
values 132.9 0.00332 0.049
#------------------------------------------------------
seq.# 66 #vals 10 title species_11_Additional_Properties
values 3.5 0 0 0 2
values 0 0.0 0.0 0.0 0.0
#------------------------------------------------------
seq.# 67 #vals 7 title species_11_Cp/R+HF+GF7_range_1
values 3.7871332 -2.1709526e-03 5.0757337e-06 -3.4737726e-09
7.7216841e-13
values -1.4363508e4 2.6335459
#------------------------------------------------------
seq.# 68 #vals 7 title species_11_Cp/R+HF+GF7_range_2
values 2.9511519 1.5525567e-03 -6.1911411e-07 1.1350336e-10
7.7882732e-15
values -1.4231827e4 6.531445
#------------------------------------------------------
seq.# 69 #vals 1 title species_12_Mwt1_CO2
values 44.01
#------------------------------------------------------
seq.# 70 #vals 6 title species_12_Sutherland6
values 1.38e-05 273.16 253.0 0.0146 273.16
values 939.8
#------------------------------------------------------
seq.# 71 #vals 3 title species_12_Supercritical
values 304.2 0.00214 0.225
<table>
<thead>
<tr>
<th>Seq. #</th>
<th>#Vals</th>
<th>Title</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>72</td>
<td>10</td>
<td>species_12_Additional_Properties</td>
<td>3.5 0 0 0 2 0 0 0.0 0.0 0.0</td>
</tr>
<tr>
<td>73</td>
<td>7</td>
<td>species_12_Cp/R+HF+GF7_range_1</td>
<td>2.1701000 1.037815e-02 -1.0733938e-05 6.3459175e-09 -1.6280701e-12</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>-4.8352602e04 1.0664388e01</td>
</tr>
<tr>
<td>74</td>
<td>7</td>
<td>species_12_Cp/R+HF+GF7_range_2</td>
<td>4.129266 3.1922896e-03 -1.2978230e-6 2.4147446e-10 -1.6742986e-14</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>-4.8944043e04 -7.2875769e-01</td>
</tr>
<tr>
<td>75</td>
<td>1</td>
<td>species_13_Mwt1_CH2O</td>
<td>30.026</td>
</tr>
<tr>
<td>76</td>
<td>6</td>
<td>species_13_Sutherland6</td>
<td>1.248e-05 273.16 259.34 0.02047 273.16</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1133.9</td>
</tr>
<tr>
<td>77</td>
<td>3</td>
<td>species_13_Supercritical</td>
<td>408.00411 0.253</td>
</tr>
<tr>
<td>78</td>
<td>10</td>
<td>species_13_Additional_Properties</td>
<td>4.0 0 0 0 2 0 0.0 0.0 0.0 0.0</td>
</tr>
<tr>
<td>79</td>
<td>7</td>
<td>species_13_Cp/R+HF+GF7_range_1</td>
<td>3.7963783 -2.5701785e-03 1.8548815e-05 -1.7869177e-08 5.5504451e-12</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>-1.5088947e04 4.7548163</td>
</tr>
<tr>
<td>80</td>
<td>7</td>
<td>species_13_Cp/R+HF+GF7_range_2</td>
<td>2.8364249 6.8605298e-03 -2.6882647e-06 4.7971258e-10 -3.2118406e-14</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>-1.5236031e04 7.8531169</td>
</tr>
<tr>
<td>81</td>
<td>1</td>
<td>species_14_Mwt1_C2H2</td>
<td>26.04</td>
</tr>
<tr>
<td>82</td>
<td>6</td>
<td>species_14_Sutherland6</td>
<td>9.48e-06 273.16 320.0 0.01968 273.16</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>1465.0</td>
</tr>
<tr>
<td>83</td>
<td>3</td>
<td>species_14_Supercritical</td>
<td>308.3 0.0043 0.190</td>
</tr>
<tr>
<td>84</td>
<td>10</td>
<td>species_14_Additional_Properties</td>
<td>3.5 0 0 0 2 0 0.0 0.0 0.0 0.0</td>
</tr>
<tr>
<td>85</td>
<td>7</td>
<td>species_14_Cp/R+HF+GF7_range_1</td>
<td>7.9033340e-01 2.3466122e-02 -3.5541928e-05 2.7950550e-08 -8.4484125e-12</td>
</tr>
<tr>
<td>Seq.#</td>
<td>#Vals</td>
<td>Title</td>
<td>Values</td>
</tr>
<tr>
<td>-------</td>
<td>-------</td>
<td>------------------------------</td>
<td>-------------------------</td>
</tr>
<tr>
<td>86</td>
<td>7</td>
<td>species_14_Cp/R+HF+GF7_range_2</td>
<td>4.4965644 5.2698321e-03 -1.8402668e-06 3.1054295e-10 -2.0004309e-14</td>
</tr>
<tr>
<td>87</td>
<td>1</td>
<td>species_15_Mwt1_C2H4</td>
<td>28.032</td>
</tr>
<tr>
<td>88</td>
<td>6</td>
<td>species_15_Sutherland6</td>
<td></td>
</tr>
<tr>
<td>89</td>
<td>3</td>
<td>species_15_Supercritical</td>
<td></td>
</tr>
<tr>
<td>90</td>
<td>10</td>
<td>species_15_Additional_Properties</td>
<td>4.0 0 0 0 0 2</td>
</tr>
<tr>
<td>91</td>
<td>7</td>
<td>species_15_Cp/R+HF+GF7_range_1</td>
<td>1.2176600 1.3002675e-02 3.5037447e-06 -1.1155514e-08 4.7203222e-12</td>
</tr>
<tr>
<td>92</td>
<td>7</td>
<td>species_15_Cp/R+HF+GF7_range_2</td>
<td></td>
</tr>
<tr>
<td>93</td>
<td>1</td>
<td>species_15_Mwt1_C2H6</td>
<td>30.07</td>
</tr>
<tr>
<td>94</td>
<td>6</td>
<td>species_16_Sutherland6</td>
<td></td>
</tr>
<tr>
<td>95</td>
<td>3</td>
<td>species_16_Supercritical</td>
<td></td>
</tr>
<tr>
<td>96</td>
<td>10</td>
<td>species_16_Additional_Properties</td>
<td>4.0 0 0 0 2</td>
</tr>
<tr>
<td>97</td>
<td>7</td>
<td>species_16_Cp/R+HF+GF7_range_1</td>
<td></td>
</tr>
<tr>
<td>98</td>
<td>7</td>
<td>species_16_Cp/R+HF+GF7_range_2</td>
<td></td>
</tr>
<tr>
<td>99</td>
<td>1</td>
<td>species_17_Mwt1_HCCO</td>
<td></td>
</tr>
</tbody>
</table>
values 41.029
#
sequence 100 vals 6 title species_17_Sutherland
values 1.470e-05 273.16 216.31 0.02537 273.16
values 600.064
#
sequence 101 vals 3 title species_17_Supercritical
values 5.0 0.0001 0.0
#
sequence 102 vals 10 title species_17_Additional_Properties
values 4.0 0 0 0 2
values 0 0.0 0.0 0.0 0.0
#
sequence 103 vals 7 title species_17_Cp/R+HF+GF7_range_1
values 2.6901770 1.7680853e-02 -2.2749855e-05 1.4920568e-08 -3.7381925e-12
values 1.3683223e04 8.1338073
#
sequence 104 vals 7 title species_17_Cp/R+HF+GF7_range_2
values 6.0949501 3.9432428e-03 -1.4711438e-06 2.5294641e-10 -1.6446663e-14
values 1.2976907e04 -8.3285075
#
sequence 105 vals 1 title species_18_Mwt1_CH2CO
values 42.037
#
sequence 106 vals 6 title species_18_Sutherland
values 9.48e-06 273.16 247.83 0.01968 273.16
values 957.35
#
sequence 107 vals 3 title species_18_Supercritical
values 380.0 0.00344 0.21
#
sequence 108 vals 10 title species_18_Additional_Properties
values 0 0 0 0 2
values 0 0.0 0.0 0.0 0.0
#
sequence 109 vals 7 title species_18_Cp/R+HF+GF7_range_1
values 2.9749708 1.2118712e-02 -2.3450457e-06 6.466850e-09 3.9656492e-12
values -7.6326367e03 8.6735525
#
sequence 110 vals 7 title species_18_Cp/R+HF+GF7_range_2
values 6.0388174 5.8048405e-03 -1.9209538e-06 2.7944846e-10 -1.4588675e-14
values -8.5834023e03 -7.6575813
#
sequence 111 vals 1 title species_18_Mwt1_CH3CHO
values 44.05316
#
sequence 112 vals 6 title species_18_Sutherland
values 6.4075150E-05 2500.0 480.00 0.2729624 2500.0
values 1470.00
#
sequence 113 vals 3 title species_18_Supercritical
values 5.0 0.001 0.0
#-----------------------------------------------
seq.# 114 #vals 10 title species_19_Additional_Properties
values 4.0 0.0 0.0 0.0 2
values 0 0.0 0.0 0.0 0.0
#-----------------------------------------------
seq.# 115 #vals 7 title species_19_Cp/R+HF+GF7_range_1
values 0.47294595E+01 -0.31932858E-02 0.47534921E-04 -0.57458611E-07 0.21931112E+10
values -0.21572878E+05 0.41030159E+01
#-----------------------------------------------
seq.# 116 #vals 7 title species_19_Cp/R+HF+GF7_range_2
values 0.54041108E+01 0.11723059E-01 -0.42263137E-05 0.68372451E-09 -0.40984863E+13
values -0.22593122E+05 -0.34807917E+01
#-----------------------------------------------
seq.# 117 #vals 1 title species_20_Mwt1_C3H5
values 41.07270
#-----------------------------------------------
seq.# 118 #vals 6 title species_20_Sutherland6
values 4.54287292E-05 2500.0 390.00 0.2408058 2500.0
values 1330.00
#-----------------------------------------------
seq.# 119 #vals 3 title species_20_Supercritical
values 5.0 0.001 0.0
#-----------------------------------------------
seq.# 120 #vals 10 title species_20_Additional_Properties
values 4.0 0.0 0.0 0.0 2
values 0 0.0 0.0 0.0 0.0
#-----------------------------------------------
seq.# 121 #vals 7 title species_20_Cp/R+HF+GF7_range_1
values 0.13631835E+01 0.19813821E-01 0.12497060E-04 -0.33355555E-07 0.15846571E+10
values 0.19245629E+05 0.17173214E+02
#-----------------------------------------------
seq.# 122 #vals 7 title species_20_Cp/R+HF+GF7_range_2
values 0.65007877E+01 0.14324731E-01 -0.56781632E-05 -0.11080801E-08 -0.90363887E+13
values 0.17482449E+05 -0.11243050E+02
#-----------------------------------------------
seq.# 123 #vals 1 title species_21_Mwt1_C3H6
values 42.08064
#-----------------------------------------------
seq.# 124 #vals 6 title species_21_Sutherland6
values 0.331282E-04 1500.0 345.70 0.177752 1500.0
values 3233.47
#-----------------------------------------------
seq.# 125 #vals 3 title species_21_Supercritical
values 5.0 0.001 0.0
#-----------------------------------------------
seq.# 126 #vals 10 title species_21_Additional_Properties
values 4.0 0.0 0.0 0.0 2
values 0 0.0 0.0 0.0 0.0
#-----------------------------------------------
seq.# 127 #vals 7 title species_21_Cp/R+HF+GF7_range_1
values 0.28327856E+01 -0.52102746E-02 0.92958284E-04 -0.12275315E-06 0.49919115E-10
values 0.51952006E+04 0.10830670E+02
#--------------------------------------------
seq.# 128 #vals 7 title species_21_Cp/R+HF+GF7_range_2
values 0.62166329E+01 0.16539361E-01 -0.59007596E-05 0.94809547E-09 -0.56566174E-13
values 0.29593756E+04 -0.13604061E+02
#--------------------------------------------
seq.# 129 #vals 1 title species_22_Mwt1_N2
values 28.02
#--------------------------------------------
seq.# 130 #vals 6 title species_22_Sutherland6
values 1.656e-5 273.16 104.7 0.02407 273.16 values 178.1
#--------------------------------------------
seq.# 131 #vals 3 title species_22_Supercritical
values 126.2 0.00319 0.040
#--------------------------------------------
seq.# 132 #vals 10 title species_22_Additional_Properties
values 3.5 220 3.364e7 5.347e7 2
values 0 0.0 0.0 0.0 0.0
#--------------------------------------------
seq.# 133 #vals 7 title species_22_Cp/R+HF+GF7_range_1
values 3.6916148 -1.332552e-03 2.6503100e-06 -9.7688341e-10 -9.977234e-14
values -1.06283352e03 2.2874980
#--------------------------------------------
seq.# 134 #vals 7 title species_22_Cp/R+HF+GF7_range_2
values 2.8545761e00 1.5976316e-03 6.2566254e-07 1.1315849e-10 -7.6897070e-15
values -8.9017445e02 6.3902879
#--------------------------------------------
seq.# 135 #strs 11 title reaction_1_specification
strings 1.0 C2H4 + 1.0 O2 <-> 2.0 CO + 2.0 H2
#--------------------------------------------
seq.# 136 #vals 7 title reaction_1_parameters
values 2.10E20 0.0 1.497853294E8 0.5 0.5
values 1.0 0.0
#--------------------------------------------
seq.# 137 #strs 11 title modified_reaction_1_specification
strings 1.0 C2H4 + 1.0 O2 <-> 2.0 CO + 2.0 H2
#--------------------------------------------
seq.# 138 #vals 22 title reaction_1_3rdbody
values 1.0 1.0 1.0 1.0 1.0
values 1.0 1.0 1.0 1.0 1.0
values 1.0 1.0 1.0 1.0 1.0
values 1.0 1.0 1.0 1.0 1.0
values 1.0 1.0
#--------------------------------------------
seq.# 139 #strs 8 title reaction_2_specification
strings 2.0 CO + 1.0 O2 <-> 2.0 CO2
#--------------------------------------------
seq.# 140 #vals 7 title reaction_2_parameters
values 3.48E05 2.0 8.426467189E7 0.5 0.5
values 1.0 0.0
#--------------------------------------------
seq.# 141 #strs 8 title modified_reaction_2_specification

110
strings 2.0 CO + 1.0 O2 <-> 2.0 CO2
#---------------------------------------------------------
seq.# 142 #vals 22 title reaction_2_3rdbody
values 1.0 1.0 1.0 1.0 1.0
values 1.0 1.0 1.0 1.0 1.0
values 1.0 1.0 1.0 1.0 1.0
values 1.0 1.0 1.0 1.0 1.0
values 1.0 1.0
#---------------------------------------------------------
seq.# 143 #strs 8 title reaction_3_specification
strings 2.0 H2 + 1.0 O2 <-> 2.0 H2O
#---------------------------------------------------------
seq.# 144 #vals 7 title reaction_3_parameters
values 3.0E14 -1.0 0.0 0.5 0.5
values 1.0 0.0
#---------------------------------------------------------
seq.# 145 #strs 8 title modified_reaction_3_specification
strings 2.0 H2 + 1.0 O2 <-> 2.0 H2O
#---------------------------------------------------------
seq.# 146 #vals 22 title reaction_3_3rdbody
values 1.0 1.0 1.0 1.0 1.0
values 1.0 1.0 1.0 1.0 1.0
values 1.0 1.0 1.0 1.0 1.0
values 1.0 1.0
#---------------------------------------------------------
seq.# 147 #vals 28 title primitive_variables_2
values 59000 414 100 0.0 0.0
values 6.000000e+00 1.469694e+04 0.0 0.0 0.0
values 0.232 0.0 0.0 0.0 0.0
values 0.0 0.0 0.0 0.0 0.0
values 0.0 0.0 0.0 0.0 0.0
values 0.0 0.0 0.0
#---------------------------------------------------------
seq.# 148 #vals 25 title ptot_ttot_etc.
values 337573 667.14 6.000000e+00 Æ.469694e+04 0.0
values 0.0 0.0 0.232 0.0 0.0
values 0.0 0.0 0.0 0.0 0.0
values 0.0 0.0 0.0 0.0 0.0
values 0.0 0.0 0.0 0.0 0.0
values 0.0 0.0 0.0 0.0 0.0
#---------------------------------------------------------
seq.# 149 #vals 25 title massrate_temp_etc.
values 0.00446 259 4.751556e+01 3.275320e+02 0.0
values 0.0 0.0 0.0 0.0 0.0
values 0.0 0.0 0.0 0.0 0.0
values 0.0 0.0 0.0 0.0 0.0
values 0.0 0.0 0.0 1.0 0.0
values 0.0 0.0 0.0 0.0 0.0
#---------------------------------------------------------
seq.# 150 #vals 25 title massrate_temp_etc.
values 0.00549 259 4.751556e+01 3.275320e+02 0.0
values 0.0 0.0 0.0 0.0 0.0
values 0.0 0.0 0.0 0.0 0.0
values 0.0 0.0 0.0 1.0 0.0
values 0.0 0.0 0.0 0.0 0.0
values 0.0 0.0 0.0 0.0 0.0
#---------------------------------------------------------
eqslct 101
icslct 147  
#  
mbcons 9  
seq# type modi info  
  1   43    0  148 Inflow  
  2  174    0    0 Outflow  
  3   58    0    0 Wall  
  4    6    0    0 Symmetry  
  5  98     0  149 Inj1_Inflow  
  6  98     0  150 Inj2_Inflow  
  7  38     0    0 Slip_Wall  
  8  58     0    0 hot_wall  
  9    6     0    0 symmetry_2  
#-----------------------------  
#seq_mtyp info  
#-----------------------------  
octree begin  
toldup 1.000000e-06  
tolins 1.000000e-06  
toldfn 1.000000e-06  
tolzco 1.000000e-06  
typzco 0  
trxdir 1  
trydir 1  
trzdir 1  
dfcmx 1.000000e+00  
octree end  
#-----------------------------  
physics begin  
meq_eqsets 0  
meq_eqsgrp 0  
meq_icslct 0  
meq_inityp 0  
cht_matprp 0  
absour 0  
absour_selftune 1  
cldriver 0  
rotor_model1 0  
anchor_pressure 0  
moddif 0  
moddif_type 2  
icsrot 0  
prerot 0  
preacc_opt 0  
preacc_dti 0.05  
pretyp 1  
ipreof 20  
prebet 5.000000e-02  
previs 5.000000e-02  
prevel 1.000000e-06  
prevl 1.000000e-03  
pfloor 0.000000e+00  
gasnam Air  
gasgam 1.400000  
gasmwt 28.950000  
advcon 1.000000e+00  

112
difcon 1.000000e+00
ed_con 1.000000e+00
ed_cap 0.000000e+00
iunits 0
lenuni m
masuni kg
temuni K
timuni s
grduni m
inityp 0
qcvrti 0
qcvrto 0
ifrpow 0
ifreac 1
ifrebx 0
frctin 2
frcuserf 1
frcnumjaco 1
temulx 2.000000e-01
frcint 1
frclim 0
frclif 0.050000
frccfl 1
ifscon 1
iftrds 0
ifrsrc 0
ifvols 0
ifvelp 0
ifrmai 0
frcxmn 0.000000e+00
frcxmx 0.000000e+00
frcymn 0.000000e+00
frcymx 0.000000e+00
frczmn 0.000000e+00
frczmx 0.000000e+00
frsrcu 0.000000
frsrcl 1.000000
frsrct 1.000000
frsrcm 1.000000
istiff 0
sureac 0
surspe 0
surmap 0
toltem 1.000000e-05
tolfrc 1.000000e-05
tnoneq_numeqns 0
edp_yesno 0
edp_model 0
edp_coefvm 0.500000
edp_coefcl 0.500000
edp_ifbuoy 0
edp_gravtx 0.000000
edp_gravty 0.000000
edp_gravtz 0.000000
sourc1 0
sourc2 0
ifaxix 0
ifaxy 0
ifwzro 0
ifaxst 0
ifaxsw 0
ifswrl 0
swrxmn 0.000000e+00
swrxml 0.000000e+00
swrymn 0.000000e+00
swrymx 0.000000e+00
swrzmn 0.000000e+00
swrzmx 0.000000e+00
swreta 0.500000
ifblck 0
blkxmn 0.000000e+00
blkxmx 0.000000e+00
blkymn 0.000000e+00
blkymx 0.000000e+00
blkszmn 0.000000e+00
blkszmx 0.000000e+00
ipbulk 0
bulkpr 0.000000
irbulk 0
bulkro 0.000000e+00
bulktm 2.880000e+02
presab 0.000000
presmn -1.000000e+20
presmx 1.000000e+20
templmn -1.000000e+00
tempmx 1.000000e+20
univgc 8314.000000
refmwt 1.000000
reflen 1.000000
reftem 1.000000
refden 1.000000
refvel -1.000000
refpre 1.000000
refpgf 101325.000000
ifbuoy 0
gravtx 0.000000
gravty 0.000000
gravtz 0.000000
grvcnx 0.000000e+00
grvcny 0.000000e+00
grvcnz 0.000000e+00
grvbet 0.003000
liqgas 0
vislaw 0
refmuu 1.000000e+00
refkap 1.000000e+00
prndtl 0.72
prlatu 0.800000
schmla 1.000000
schmtu 0.500000
rmuusl 1.716000e-05
tmuusl 273.110000
smuusl 111.000000
rkapsl 2.410000e-02
tkapsl 273.110000
skapsl 194.000000
liqtl0 0.0
liqtlp 5000.0
yppfac 1.000000
ifporo 0
ifpmut 0
isporo 0
ifcjhlt 0
iflnlas 0
ls_numeqns 0
ntrbst 11
ifftold 0
smagcf 0.050000
instyp 1
lnsdtnm 1
lnsbox 0
mnfltr 0.000000e+00
sync_alpha 1
nlas_allscals 0
rfg_sample_modes 100
mulnyq 1
inlns 0
rfg_rseed 1234567
ifmuon 0
ifdpds 0
ifwfe0 2
ifwf00 1
ifwbfc 1
ifcomp 0
ifmccw 1
ifskar 0
ifpope 0
ifbrad 0
iftran 0
ifrat 0
iftrfs 0
ifmbsl 0
iftcon 1
iftcrf 0
turbf0 1.000000
turbf1 1.000000
turbf2 1.000000
turbf3 1.000000
turbf4 1.000000
turbf5 1.000000
turbf6 1.000000
turbf7 1.000000
tunrlx 0.5
tururlx 1.000000
kmxval 1.0000000e+20
tmnval 1.0e-12
maxmut 1.0000000e+05
turlim 100.000000
turxyz 0
cgtsof 0
turxmn 0.000000e+00
turxmx 0.000000e+00
turymn 0.000000e+00
turymx 0.000000e+00
turzmn 0.000000e+00
turzmx 0.000000e+00
sa_cb1 0.135500
sa_sig 0.666667
sa_cb2 0.622000
sa_kap 0.410000
sa_cw2 0.300000
sa_cw3 2.000000
sa_cv1 7.100000
sa_ct3 1.100000
sa_ct4 2.000000
shaper 0

physics end
#-------------------------------------
probe begin
probe end
#-------------------------------------
default begin
debug end
#-------------------------------------
guiopts begin
turbi_lev 1
turbi_len 1
turbi_mutmu 50.000000
turbi_jet 0
turbi_int 1
turbi_tlev 2.000000e-02
turbi_tlen 1.000000e-03
turbi_tfrs 1.000000e-04
turbi_yp 1.000000e+00
turbi_replen 1.000000e+00
auto_pres 1.013250e+05
auto_temp 2.880000e+02
auto_u 3.000000e+01
auto_v 0.000000e+00
auto_w 0.000000e+00
auto_tvl 1.000000e-02
auto_tlnl 1.000000e-03
auto_tl 1
auto_lt 0
auto_eqinf 0
auto_ininf 0
auto_bpinf 0
aero_intyp 1
aero_unit 1
aero_pres 1.013250e+05
aero_temp 2.880000e+02
aero_deltat 0.000000e+00
aero_u 3.000000e+01
aero_v 0.000000e+00
aero_w 0.000000e+00
aero_tlv1 2.000000e-02
aero_tlnl 1.000000e-03
aero_t1 1
aero_lt 0
aero_eqinf 0
aero_ininf 0
aero_bcinf 0
aero_altid 1.000000e+01
aero_ma 8.000000e-01
aero_alpha 0.000000e+00
aero_beta 0.000000e+00
aero_plane 0
aero_re 1.000000e+06
aero_mutmu 30.000000
incomp_tlv1 5.000000e-02
incomp_tlnl 1.000000e-02
incomp_eqinf 0
incomp_ininf 0
incomp_bpinf 0
guiopts end
#-------------------------------------

system begin
system end
#-------------------------------------
REFERENCES


