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Numerical Simulation of UVA Ramjet/Scramjet Hypersonic Engine with Hydrogen-Air Combustion Using Wind-US

Vishal Anand Bhagwandin
Embry-Riddle Aeronautical University - Daytona Beach

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Numerical Simulation of UVA Ramjet/Scramjet Hypersonic Engine with Hydrogen-Air Combustion using Wind-US

by

VISHAL ANAND BHAGWANDIN

Thesis Submitted in Partial Fulfillment of the Requirements for the Degree of Master of Science in Aerospace Engineering

Embry-Riddle Aeronautical University Daytona Beach, Florida Fall 2008
Numerical Simulation of UVA Ramjet/Scramjet Hypersonic Engine
with Hydrogen-Air Combustion using Wind-US

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Vishal Anand Bhagwandin

This Thesis was prepared under the direction of the Candidate’s Thesis Committee
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approved by the members of his Thesis Committee. This Thesis was submitted to the
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ABSTRACT

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Year: 2008

The internal flowpath of University of Virginia’s Mach 5, direct-connect, dual-mode scramjet engine was simulated using Wind-US, a density-based Reynolds-Averaged Navier-Stokes flow solver. Detailed flowfield simulation results are directly compared to experimental data to evaluate the accuracy of the numerical model and to provide insight into the flowfield behavior. Four hydrogen-air reaction mechanisms were initially assessed using the Burrows-Kurkov case. An Evans-Schexnayder, 7-specie, 8-reaction set with third body efficiencies was then selected for the scramjet simulations. The scramjet simulations included one fuel-off case and two reacting cases with different equivalence ratios, all with clean, non-vitiated air supply. The strong sensitivity of the simulation results to the choice of turbulent Schmidt number is demonstrated. For low equivalence ratio, excellent agreement with experimental data is achieved. For high equivalence ratio, the results agree with that of experiment, however, this case shows large numerical and combustion instabilities.
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LIST OF SYMBOLS

\( K_B \) = Boltzmann Constant
\( \rho \) = Density
\( \Phi_{\text{CFD}} \) = Equivalence Ratio of CFD Simulation
\( \Phi_{\text{EXP}} \) = Equivalence Ratio of Experiment
\( D_f, D_b \) = Forward and Backward Reaction Activation Energies
\( C_f, C_b \) = Forward and Backward Reaction Rate Coefficients
\( S_f, S_b \) = Forward and Backward Reaction Rate Exponents
\( m, m_n \) = Fuel and Air Mass Flow Rates
\( \nu \) = Kinematic Viscosity
\( M \) = Mach Number
\( D \) = Mass Diffusivity
\( \omega \) = Specific Dissipation Rate
\( P_0, P \) = Total and Static Pressure
\( T_0, T \) = Total and Static Temperature
\( Pr_t, Pr_l \) = Turbulent and Laminar Prandtl Numbers
\( Sc_t, Sc_l \) = Turbulent and Laminar Schmidt Numbers
\( \varepsilon \) = Turbulent Dissipation
\( k \) = Turbulent Kinetic Energy
\( V \) = Velocity
\( \mu \) = Viscosity
\( \tau_c \) = Chemical Time Scales
\( Z \) = Compressibility Factor
\( Da \) = Damkohler Number
\( C_0 \) = Initial Concentration
\( n \) = Reaction Order
\( k \) = Reaction Rate Constant
\( R \) = Specific Gas Constant
\( t \) = Time
\( \tau_t \) = Turbulent Time Scales
\( u, v, w \) = \( x, y, z \) Velocity Components
\( \sim/\approx \) = approximately
1.0 INTRODUCTION

1.1 Thesis Objective

The aerospace community has long recognized the need for hypersonic flight, leading to a renaissance of development in scramjet technology. Various hypersonic programs include University of Queensland’s HyShot [38] in Australia where the first ever successful flight of a scramjet at speeds of Mach 7.6 in July 2002 was conducted. NASA’s Hyper-X [29] produced the successful flights of its X43-A, hydrogen-fueled, scramjet-powered aircraft in 2004, reaching speeds of Mach 7+ at about 95,000 feet. The Air Force Research Laboratory (AFRL) and the Defense Advanced Research Projects Agency (DARPA) have jointly developed the FALCON and X-51A programs [39, 21] which are now the mainstream of hypersonic activity today.

Scramjet development faces many challenges and current research demands efficient ways of evaluating scramjet performance. Consequently, numerical modeling via Computational Fluid Dynamics (CFD) is largely being developed and utilized for this purpose. CFD, as a complement to experimental tests, has the potential to provide valuable insight into the engine behavior and significantly improve the flowpath design process. One such CFD tool is Wind-US, a software capable of predicting and evaluating the performance of high-speed, air-breathing engines such as scramjets. The NPARC Alliance, a partnership between NASA Glenn Research Center (GRC), United States Air Force Arnold Engineering & Development Center (USAF AEDC), Boeing Phantom Works,
and funded by the United States Department of Defense (DoD), is assigned the task of augmenting and validating Wind-US [9, 13, 18, 25, 32, 33] to meet the challenges of hypersonic vehicle propulsion systems.

Wind-US is a density-based, Reynolds-Averaged Navier-Stokes (RANS) flow solver that uses finite-differencing numerical schemes. The code also supports equation sets governing turbulent and chemically reacting flows. The flow solution is computed iteratively on a computational grid, which is generated by an external software such as GridGen.

Previous studies such as that of Goyne et al [19, 20] and Baurle & Eklund [6], among many others, have utilized various numerical flow solvers to simulate scramjet flows by separately and sequentially simulating individual nozzle, isolator and combustor components. Validation studies of Wind-US in particular have previously been conducted by Georgiadis, Nelson, Lankford, Nichols, DalBello [11, 18, 25, 33], among others, where individual high-speed air-breathing engine components were simulated. Engblom et al [13] attempted to validate Wind-US for simulation of an entire scramjet flowpath, where all engine components were numerically coupled, but for only one run condition.

This thesis focused on simulating the entire 3-D internal flowpath of a dual-mode scramjet engine operating at about Mach 5 flight condition using WIND-US V3.0 Alpha. The scramjet model was based on the experimental configuration of University of
Virginia (UVA)’s Supersonic Combustion Facility [19, 20]. Experimental results obtained from UVA were used to validate the numerical results.

A numerical simulation entailed a sequence of modeling tools. Figure 1 outlines the steps taken in this process and provides a road map for this manuscript. Each step will be addressed in detail in later Chapters.

The scramjet model is based on University of Virginia’s experimental configuration. With the aid of NASA Glenn Research Center, 3-D CAD models were obtained and imported into GridGen.

GridGen is a mesh generation software that was used to apply a 3-D, structured, hexahedral grid to the entire scramjet geometry, as well as wall boundary conditions.

MADCAP is a CFD tool, specifically used in this case to couple mismatched zonal interfaces. These mismatched zones were created in GridGen and could not be defined or coupled by GridGen.

CFSPLIT is a WIND-US utility used to split the 18-zone grid into a 34-zone grid optimized to run on about 20 processors in parallel.

WIND-US is a compressible, Reynolds-Averaged Navier-Stokes numerical solver used to simulate the scramjet flowfield. User species geometry, numerics, chemical kinetics, turbulence & other physical models.

Fieldview & Tecplot are post-processing tools used for visualizing the spatial variation of physical variables.

MATLAB & CFPOST were used to process the time history files generated by UNIX bash scripts to monitor convergence.

Figure 1: Simulation process overview.
1.2 Relevant Theory & Specific Issues

A scramjet engine generally consists of an inlet, isolator, combustor and exhaust nozzle, as shown in Figure 2. The inlet and isolator will decelerate oncoming supersonic air flow via a series of shock waves, converting kinetic energy into internal energy. The resulting air is higher in pressure, temperature and density. This air then enters the combustor where it is combined with fuel and burned. The hot, high pressure flow then accelerates via a divergent exhaust nozzle to the atmosphere. Thrust is generated since the exhaust flow has more momentum leaving than it did entering [3, 22].

![Figure 2: Major components of a typical scramjet engine mounted to the underside of a wave-rider type hypersonic vehicle [39].](image)

Scramjet implies that the core flow entering the combustor is supersonic. However, scramjets are usually designed to operate in ramjet mode as well, where the combustor entry core flow is subsonic. Such a hypersonic engine is referred to as a dual-mode scramjet. The simulations presented herein involve the UVA engine operating in both ramjet and scramjet mode, each with slightly different flowfield characteristics.
1.2.1 Isolator Shock Train & Turbulent Schmidt Number Sensitivity

The function of the isolator is to contain the shock train propagated upstream due to increased back pressures on the isolator exit. The shock train is a result of the flow attempting to equilibrate the low inlet pressure with the high isolator back pressures. The high back pressures are due to heat release from combustion. If the shock train reaches the scramjet inlet, the engine may unstart and can lead to loss of performance and/or failure. Also, associated with the shock train is boundary-layer flow separation (demonstrated in Figure 2) due to boundary-layer-shock interactions [1, 6, 26, 37].

Capturing the strength and hence leading edge of the isolator shock train has been an issue, not only for WIND-US, but for other flow solvers as well. Sensitivity studies presented herein show that the choice of turbulent Schmidt number is crucial to capturing the shock train. The turbulent Schmidt number (Sc\textsubscript{t}) is defined as the ratio of momentum diffusivity (or kinematic viscosity) to mass diffusivity [22]. Thus, varying the turbulent Schmidt number varies the mixing rate of fuel and air species relative to the flow momentum, thus varying the development of diffusion flames, and consequently the peak combustor pressure and shock train propagation. The dependence of turbulence/chemistry interactions on the turbulent Schmidt number has previously been demonstrated by studies such as that of Xiao et al [43] and Baurle et al [6].

1.2.2 Chemical Kinetics Model

Previous attempts at modeling the hydrogen-air combustion in the UVA engine had resorted to 1-step global kinetics mechanisms to ensure sustained flame-holding [20]. In
this study, an 8-reaction, 7-specie, hydrogen-air kinetics model from Evans & Schexnayder [15], modified to include third-body efficiencies, was employed for all reacting simulations. Although this model is theorized to more accurately capture the behavior of the actual kinetics than a model with fewer reaction steps, the dependence of the scramjet simulations on chemical kinetic models was not investigated. However, the choice of this kinetics model was not arbitrary. Using the Burrows-Kurkov supersonic combustion case [8], several kinetic models were assessed prior to the scramjet simulations, the results of which are also presented herein.

1.2.3 Combustion Instability

Combustion instabilities may be attributed to the acoustic-convective wave interactions between the fuel injection and subsonic flame zones as suggested by Li, Ma, Yang et al [27, 28]. Acoustic disturbances generated in the flame zone may propagate upstream altering the fuel distribution in the injection and mixing zones. This fluctuating fuel-air composition is then convected downstream and causes a heat-release fluctuation in the flame zone, which in turn produces acoustic waves propagating upstream, forming a feedback loop for driving flow oscillations. The simulations show numerically induced resonances which are an indication of experimental combustion instabilities. Since the simulations were time-accurate, then pseudo-steady-state convergences may be achieved when the oscillations display a constant amplitude and frequency.
2.0 UVA SCRAMJET CONFIGURATION

The scramjet model was based on the experimental configuration of the University of Virginia's (UVA) Supersonic Combustion Facility, shown in Figure 3 [19, 20, 26]. The schematic in Figure 4 shows the overall geometry and major components of this configuration. The convergent-divergent (C-D) nozzle was designed to deliver electrically heated, clean air at Mach 2 to the isolator. The constant-area isolator feeds this air to the rectangular combustor where it mixes with fuel and ignites. Combustion ignition was achieved via an 'oxygen-hydrogen wave igniter' that feeds hot combustion products into the fuel ramp recirculation region. Combustion was self-sustaining after ignition. The flow then exhausted to ambient conditions through a 2.9° divergent nozzle.

Hydrogen was delivered by a fuel injector (Figure 5) atop the scramjet. The fuel was introduced to the main airflow by a 1°, Mach 1.7, conical injection nozzle. The injector was accommodated by an unswept, 10° compression ramp having a width of 1.27 cm (0.5 in) and normal height of 0.635 cm (0.25 in). The normal ramp height (h) was used to normalize linear dimensions.

Pressure and temperature measurements were taken at various axial positions along the centerline of the top wall of the scramjet. Apart from the fuel injector and three optical windows, all components were water-cooled. Figure 6 also shows basic dimensions of the model. The width of the model (not shown) was constant and equal to 3.81 cm (1.5 in).
Figure 3: UVA Supersonic Combustion Facility (vertically mounted).

Figure 4: UVA scramjet configuration.
Figure 5: Fuel injector zoom.

Figure 6: Scramjet model dimensions.
3.0 GRID GENERATION FOR SCRAMJET MODEL

With the aid of UVA and NASA GRC, the geometrical model was constructed in GridGen V15.10 [36]. GridGen is a meshing software used to apply a three-dimensional, structured, hexahedral grid to the scramjet geometry. Since the model was symmetrical about a vertical plane through the x-axis (the z=0 plane), only half the model was used for meshing and CFD computation. An overview of the grid is shown in Figure 7.

The grid consisted of 3,481,928 hexahedral cells, divided among 31 zones. To capture wall boundary layer effects, the grid was clustered near all viscous walls in a direction perpendicular to the walls at 7.62E-4 cm (3.0E-4 in), and increased according to a hyperbolic tangent distribution. This was sufficient to ensure a y+ value of less than ~5 along all viscous walls for compatibility with a grid-to-wall strategy. The minimum and maximum grid spacing anywhere in the grid was 1.75E-4 and 3.83E-1 cm (6.898E-5 and 1.507E-1 in) respectively. Grid quality was partially ensured by Jacobian and aspect ratio analyses.

Several zones, mostly in the combustor region, were ‘mismatched’ at their boundary faces in order to conserve the number of grid cells and enhance computational efficiency. ‘Mismatched’ implies that the grid points at zonal interfaces were not point-to-point matched. Since GridGen does not couple mismatched zonal boundaries, MADCAP was used for this purpose. MADCAP (Modular Aerodynamic Design Computational Analysis Process) is a pre/post-processing tool supplied with WIND-US.
Figure 7: Zoom of grid in major components of the model. Grid shown only on symmetry plane and bottom wall. Zone boundaries are rendered in blue.
Figure 34 [APPENDIX B] shows details of the combustor and fuel ramp zones. These regions had the most complex grid, and proved to be the most numerically unstable. Since the injector consisted of two intersecting pipes, its complex geometry limited ways in which a structured grid can be applied. The result was very skewed grid cells, where the angle between the faces of some cells was almost 180°. The injector grid topology propagated through the injector exit plane and into the combustor (shown in Figure 34).

The largest source of numerical instability was the fuel-ramp region (just before the combustor, where the 10° ramp accommodates the fuel injector). The wedge shape geometry in this region forced construction of a line of singularity (see Figure 34), where a directly adjacent cell had five faces, with its sixth face considered to be a line. In addition to complex flow physics in this region, it is suspected that Wind-US does not adequately compensate for singular axes in the grid.

To refine grid orthogonality and smoothness in the injector and combustor, GridGen’s elliptic partial differential equation methods was applied to the spacing of interior grid points. A suggested improvement would be to apply an unstructured tetrahedral grid in the fuel injector. This would not only improve grid quality where needed, but also would be much easier to construct. This in fact was attempted, however, WIND-US proved incapable of maintaining the total conditions (i.e. total pressure and temperature) at the fuel inflow plane.
4.0 SIMULATION METHODOLOGY

4.1 Flow Conditions

The UVA scramjet experiments involved several cases, three of which this study focused on. These three cases were defined by three equivalence ratios of 0, 0.260 and 0.397, referred to as Scans 4, 14 and 21 respectively according to UVA’s naming convention. Table 1 shows these cases with inflow, outflow and freestream conditions specified by UVA. Also supplied by UVA were axial pressure and temperature distributions which were used for comparison with simulation results.

<table>
<thead>
<tr>
<th>DATA</th>
<th>FUEL-OFF, PERFECT GAS FLOW -SCAN 4-</th>
<th>REACTING FLOW, LOW Φ -SCAN 14-</th>
<th>REACTING FLOW, HIGH Φ -SCAN 21-</th>
</tr>
</thead>
<tbody>
<tr>
<td>Equivalence Ratio, Φ</td>
<td>0</td>
<td>Φ_{exp} = 0.260</td>
<td>Φ_{exp} = 0.397</td>
</tr>
</tbody>
</table>
| Clean Air Inlet Total Conditions (Held Constant) | P_0=331 kPa  
T_0=1033 K  
\dot{m}=0.23 kg/s | P_0=330 kPa  
T_0=1203 K  
\dot{m}=0.203 kg/s | P_0=329 kPa  
T_0=1203 K  
\dot{m}=0.203 kg/s |
| H_2 Fuel Inlet Total Conditions (Held Constant) | No Fuel-Injector  
\dot{m}=0 | P_0=829 kPa  
T_0=297 K  
\dot{m}=1.54e-3 kg/s | P_0=1255 kPa  
T_0=298 K  
\dot{m}=2.34e-3 kg/s |
| Ambient Conditions | P_∞=101.35 kPa  
T_∞=294.4 K |

*Pressure & Temperature Error: ±3%; Equivalence Ratio Error: ±5%*
4.2 Chemistry Model

The fuel-off, $\Phi=0$ case modeled the air flow as a single-specie, thermally perfect gas. The fuel injector exit plane was modeled as a viscous wall, and the injector was removed from the computations.

For the reacting, $\Phi>0$ cases, the incoming clean air consisted of 21% oxygen ($O_2$) and 79% nitrogen ($N_2$), which combined with liquid hydrogen ($H_2$) in the combustor. The Burrows-Kurkov supersonic combustion case [8] was used to evaluate various hydrogen-air reaction mechanisms for use in the scramjet simulations. This pre-evaluation study is presented in Chapter 5. Based on those results, a 7-specie, 8-reaction kinetics model from Evans & Schexnayder [15, 16] modified to include the third-body efficiencies (other than unity) from the Jachimowski model [24] was chosen for the scramjet simulations.

Table 2 shows the details of this reaction mechanism and corresponding coefficients for the Arrhenius equation [42]. The thermodynamic properties of each species were derived from McBride et al, NASA TP-3287 [7]. Laminar viscosity and thermal conductivity coefficients were computed using Wilke’s Law [11].

To ignite and develop the flame in the combustor the activation energies ($D_i/K_b$) of the dissociation reactions (reactions 1-4 in Table 2) were reduced by about 50% for the first few hundred cycles, after which the simulations were run with standard activation energies until convergence. This numerical ‘spark plug’ proved to be necessary in some cases for ignition and flame holding, and is justified by the fact that the experiment utilized an ‘oxygen-hydrogen wave’ igniter as aforementioned.
Table 2: Modified Evans & Schexnayder H₂-Air Reaction Mechanism
Species: O, O₂, H, H₂, OH, H₂O, N₂

<table>
<thead>
<tr>
<th>#</th>
<th>REACTION</th>
<th>$S_I$</th>
<th>$S_B$</th>
<th>$D_I/K_B$</th>
<th>$D_B/K_B$</th>
<th>$C_I$</th>
<th>$C_B$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$O_2 + M \rightarrow O + O + M$</td>
<td>-1.0</td>
<td>-1.0</td>
<td>5.9340E+4</td>
<td>0.0</td>
<td>7.20E+18</td>
<td>4.00E+17</td>
</tr>
<tr>
<td></td>
<td>Third Body Efficiency</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$H_2, H_2O$ 16.25</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>1.0 for all others</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>$H_2 + M \rightarrow H + H + M$</td>
<td>-1.0</td>
<td>-1.0</td>
<td>5.1987E+4</td>
<td>0.0</td>
<td>5.50E+18</td>
<td>1.80E+18</td>
</tr>
<tr>
<td></td>
<td>Third Body Efficiency</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$H_2, H_2O$ 16.25</td>
<td></td>
<td></td>
<td></td>
<td></td>
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<td></td>
</tr>
<tr>
<td></td>
<td>1.0 for all others</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>$H_2O + M \rightarrow OH + H + M$</td>
<td>-1.5</td>
<td>-1.5</td>
<td>5.9386E+4</td>
<td>0.0</td>
<td>5.20E+21</td>
<td>4.40E+20</td>
</tr>
<tr>
<td></td>
<td>Third Body Efficiency</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$H_2, H_2O$ 16.25</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>1.0 for all others</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>$OH + M \rightarrow O + H + M$</td>
<td>-1.0</td>
<td>-1.0</td>
<td>5.0830E+4</td>
<td>0.0</td>
<td>8.50E+18</td>
<td>7.10E+18</td>
</tr>
<tr>
<td></td>
<td>Third Body Efficiency</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$H_2, H_2O$ 16.25</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>1.0 for all others</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>$O_2 + H \rightarrow OH + O$</td>
<td>0.0</td>
<td>0.0</td>
<td>8.4550E+3</td>
<td>0.0</td>
<td>2.20E+14</td>
<td>1.50E+13</td>
</tr>
<tr>
<td>6</td>
<td>$H_2 + O \rightarrow OH + H$</td>
<td>0.0</td>
<td>0.0</td>
<td>5.5860E+3</td>
<td>4.4290E+3</td>
<td>7.50E+13</td>
<td>3.00E+13</td>
</tr>
<tr>
<td>7</td>
<td>$H_2O + O \rightarrow OH + OH$</td>
<td>0.0</td>
<td>0.0</td>
<td>9.0590E+3</td>
<td>5.0300E+2</td>
<td>5.80E+13</td>
<td>5.30E+12</td>
</tr>
<tr>
<td>8</td>
<td>$H_2O + H \rightarrow OH + H_2$</td>
<td>0.0</td>
<td>0.0</td>
<td>1.0116E+4</td>
<td>2.6000E+3</td>
<td>8.40E+13</td>
<td>2.00E+13</td>
</tr>
</tbody>
</table>

4.3 Turbulence Model

The Shear Stress Transport (SST) turbulence model of Menter [30] was employed, with the compressibility corrections of Forsythe, Hoffmann and Suzen [17]. Menter’s SST model is a two-equation, eddy-viscosity model that uses a $k-\omega$ formulation in the inner boundary layer and a $k-\varepsilon$ formulation in the freestream.
The laminar Prandtl and Schmidt numbers were set at 0.72 for all cases. Base values for the turbulent Prandtl and Schmidt numbers were set at 0.9 for all cases. In addition, the turbulent Schmidt number was varied, typically from 0.5 to 1.7, for the reacting cases.

4.4 Wall Boundary Conditions

Wall boundary definitions were assigned by GridGen. There were five boundary types as depicted in Figure 8, viz, (i) the symmetry plane or reflection plane, (ii) two inflow planes, viz air and fuel inflows, (iii) the outflow or exit plane, (iv) two inviscid walls directly adjacent to the air inflow plane and perpendicular to the y-axis, and (v) viscous, no-slip walls, which constituted all other walls.

![Figure 8: Wall boundary assignment.](image)

The UVA scramjet experiments employed water-cooled mechanisms for all metal components, with the exception of the fuel injector insert. Certain observation windows
and instrumented walls in the vicinity of the combustor and fuel ramp region were also not water-cooled. Temperature readings were taken at specific points along the wall in the axial direction. Using the given information and suggestions from UVA, the wall temperature conditions were approximately modeled as follows. All walls from the end of the isolator to just downstream of the combustor were modeled as adiabatic. All other walls were modeled as isothermal to emulate the cooling mechanisms. Table 3 summarizes the wall temperatures specified for the various zones.

### Table 3: Wall Temperatures

<table>
<thead>
<tr>
<th>REGION</th>
<th>AXIAL SPAN, x/h</th>
<th>SCAN 4, Fuel-Off, Φ=0 Case 1</th>
<th>SCAN 14 Φ=0.260</th>
<th>SCAN 21 Φ=0.397</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inflow &amp; C-D Nozzle</td>
<td>-75.6:47.72</td>
<td>375</td>
<td>410</td>
<td>412</td>
</tr>
<tr>
<td>Isolator</td>
<td>-47.72:-5.84</td>
<td></td>
<td>428</td>
<td>468</td>
</tr>
<tr>
<td>Fuel Ramp Region &amp; Combustor</td>
<td>-5.84:9.96</td>
<td>Adiabatic</td>
<td>Adiabatic</td>
<td>Adiabatic</td>
</tr>
<tr>
<td>Exit Nozzle</td>
<td>9.96:57.76</td>
<td>400</td>
<td>500</td>
<td>495</td>
</tr>
<tr>
<td>Fuel Injector</td>
<td>-</td>
<td>Adiabatic</td>
<td>Adiabatic</td>
<td>Adiabatic</td>
</tr>
</tbody>
</table>

*All temperatures in K; h=0.635 cm/0.25 in; x/h=0 at fuel ramp base

### 4.5 Multi-Processor Decomposition

The 31-zone blocking topology of the numerical model was optimized for parallel computation on about 20 processors. The simulations were computed on Zeus Beowulf,
Embry-Riddle Aeronautical University’s supercomputer cluster consisting of 256 3.2-GHz Intel Xeon processors using MPICH for Myrinet parallel networking.

4.6 Numerics

The chosen inviscid flux function was Roe’s second-order, upwind-biased, flux-difference splitting algorithm, modified for stretched grids. A Total-Variation-Diminishing (TVD) limiter was used in conjunction with the Roe scheme to limit extrapolation of local maxima and minima flux quantities to acceptable values.

The default implicit time-advancement scheme was a spatially-split approximate factorization scheme. Local time-stepping was used to advance the solution towards steady-state, based on a chosen Courant-Friedrichs-Lewy (CFL) number which is a non-dimensional time step based on the local time-step, local grid spacing and local characteristic velocity [2]. CFL numbers as low as 0.5 were used at the inception of a simulation or when changing a significant modeling parameter. Once transients settle out, the CFL number was increased, typically up to 1.0.

4.7 Solution Advancement and Grid Sequencing

Wind-US’s grid sequencing capability allows use of every other grid point, or every two grid points, etc., to be used in the computations. Three grid levels were used, viz, coarse, medium and fine, consisting of approximately 54.4K, 435K and 3.48M grid cells respectively. Solution advancement involved obtaining a first-order accurate, followed
by a second-order accurate result for the course grid. From the latter, second-order
accurate medium and fine grid solutions were then successively generated.

4.8 Convergence Monitoring

The variables used to monitor convergence were (i) the mass flux of water through the
outflow plane since this is a main product of hydrogen-air combustion, (ii) the net mass
flux through the scramjet calculated by summing all inflow and outflow mass fluxes; the
conservation of mass dictates that the net mass flux must be zero, (iii) the maximum
residuals of the Navier-Stokes equations for each zone; these should decrease a few
orders of magnitude upon convergence, and (iv) successive axial pressure profiles along
the centerline of the top wall of the scramjet. For cases that showed a numerically
induced flow resonance, a pseudo-steady-state convergence was assumed when the
oscillating flowfield properties showed no significant change in amplitude and frequency
over a large number of computational cycles.

4.9 Post-processing and Visualization

Once convergence was reasonably achieved, the solution and grid files were processed
to create spatial rendering of flowfield variables. This was accomplished using Fieldview
V12, Tecplot 360, MATLAB R2007b and CFPOST (a Wind-US utility).
5.0 EVALUATION OF CHEMICAL KINETIC MODELS USING THE BURROWS-KURKOV BENCHMARK CASE

The performance of several hydrogen-air chemical kinetics models was assessed for supersonic combustion using Wind-US. Since the scramjet simulations were computationally expensive, the comparatively simpler Burrows-Kurkov case [8] was used for this purpose instead. The chemical kinetic models evaluated are depicted in Table 4.

Table 4: Hydrogen-Air Chemical Kinetic Models

<table>
<thead>
<tr>
<th>#</th>
<th>KINETICS MODEL</th>
<th>NUMBER OF SPECIES</th>
<th>NUMBER OF REACTIONS</th>
<th>SPECIES</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Evans-Schexnayder</td>
<td>7</td>
<td>8</td>
<td>O, O₂, H, H₂, OH, H₂O, N₂</td>
</tr>
<tr>
<td>2</td>
<td>Evans-Schexnayder w/ 3rd Body Efficiencies</td>
<td>7</td>
<td>8</td>
<td>O, O₂, H, H₂, OH, H₂O, N₂</td>
</tr>
<tr>
<td>3</td>
<td>Peters-Rogg w/ 3rd Body Efficiencies</td>
<td>13</td>
<td>27</td>
<td>H₂, O₂, OH, H, O, H₂O, HO₂, H₂O₂, CO, CO₂, HCO, HCHO, N₂</td>
</tr>
<tr>
<td>4</td>
<td>1-Step H₂-Air</td>
<td>4</td>
<td>1</td>
<td>**C₂H₄, O₂, CO, CO₂, H₂, H₂O, N₂</td>
</tr>
</tbody>
</table>

**All carbon species were neglected in the computations to facilitate a 1-step, 4-species mechanism.

The Burrows-Kurkov experiment is a benchmark case for supersonic combustion of vitiated air and hydrogen. Figure 9 shows a schematic of the experiment, while Figure 10 shows the computational domain which comprises the combustion chamber beginning from the point of hydrogen injection. Hot vitiated air enters the chamber at Mach 2.44 and mixes with cold pure hydrogen fuel injected at sonic velocity. The flow exhausts to ambient conditions at the exit. The boundary layer at the inflow was imposed using
digitized velocity and temperature profiles from the experiment, following the method of Engblom et al [13]. Ebrahimi [12] had demonstrated that the inflow boundary definition was crucial towards obtaining the correct combustor exit conditions. Table 5 summarizes all other simulation attributes.

Convergence was monitored via (i) comparing successive exit profiles and axial flame profiles of Mach number, total temperature, water and hydrogen mass fractions, (ii) net mass flux histories and, (iii) maximum residuals per cycle of the Navier-Stokes equations.

Figure 9: Schematic of the Burrows-Kurkov experiment [40].

Figure 10: Computational grid for the Burrows-Kurkov combustion chamber.
Table 5: Burrows-Kurkov Simulation Attributes

<table>
<thead>
<tr>
<th>ATTRIBUTE</th>
<th>INPUT</th>
</tr>
</thead>
<tbody>
<tr>
<td>Numerical Scheme</td>
<td>Roe 2nd Order, Upwind, TVD Compression, CFL ~0.5</td>
</tr>
<tr>
<td>Turbulence Model</td>
<td>Menter’s Shear Stress Transport, Pr, 0.7, Sc, 0.7</td>
</tr>
<tr>
<td>Walls Boundary Conditions</td>
<td>Viscous, Isothermal Temperature of 298 K</td>
</tr>
<tr>
<td>Freestream</td>
<td>Mach 2.44, P$_s$=101.35 kPa, T$_s$=1270 K</td>
</tr>
<tr>
<td>Air Inflow</td>
<td>Vitiated, P$_s$=101.35 kPa</td>
</tr>
<tr>
<td></td>
<td>25.76% O$_2$, 48.62% N$_2$, 25.62% H$_2$O</td>
</tr>
<tr>
<td>Fuel Inflow</td>
<td>Pure H$_2$, Mach 1, P$_s$=101.35 kPa, T$_s$=254 K</td>
</tr>
<tr>
<td>Computational Domain</td>
<td>2-D, ~17,000 Cells, Single Zone, Single Processor</td>
</tr>
</tbody>
</table>

Figure 11 shows the exit profiles for total temperature, Mach number, water and hydrogen mole fractions. The Evans & Schexnayder with third-body efficiencies [15, 16] and the Peters & Rogg [35] kinetics models both capture the position and peak temperature of the flame fairly well. It is noted that the Peters & Rogg model produces slightly better exit profiles.

Figure 12 and Figure 13 show total temperature and water mass fraction contours respectively. It is evident that the flame ignition point varies significantly with kinetics model. The Evans & Schexnayder model with third-body efficiencies almost exactly captures the flame ignition point, which was at x=25 cm in the experiment.
In addition to producing early ignition, the Peters & Rogg model would be far more computationally expensive since it has 13 species and 27 reactions as compared to 7 and 8 respectively for the Evans & Schexnayder reaction set.

Based on the assessments made herein, it was determined that the Evans & Schexnayder model with third body efficiencies would be the best choice for use in the scramjet simulations.

Figure 11: Exit profile comparison for various chemical kinetic models.
Figure 12: Total temperature contours for various kinetic models.

Figure 13: Water mass fraction contours for various kinetic models.
6.0 RESULTS OF THE FUEL-OFF CASE: $\Phi_{\text{EXP}} = 0$

The following presents and discusses the results of the UVA scramjet simulations for the fuel-off, $\Phi=0$ case namely Scan 4 (refer to Table 1, Section 4.1). This run involves non-vitiated air and no fuel injection. Thermally and calorically perfect gas is assumed due to expected modest temperature variation. For this case, the fuel injector exit plane was modeled as a viscous wall and the injector zones were ignored in the computations. Grid independence was verified by comparing results obtained with the medium and fine grid levels. The results shown herein are for the fine grid level.

Two variants on this simulation were performed, viz 'Case 1' and 'Case 2' (refer to Table 3, Section 4.4). Case 1 employs adiabatic walls for the combustor and fuel ramp zones, and isothermal walls otherwise according to Table 3. Case 1 attempts to more accurately emulate the cooled and uncooled components of the experiment. Case 2 employs uniform isothermal walls everywhere at a spatially-averaged temperature of 389 K.

Figure 14 compares the experimental static pressure along the axial centerline of the top wall of the scramjet with that of the two $\Phi=0$ simulations. For both cases, the streamwise pressure fluctuates significantly downstream of the isolator. Since there is no combustion, this is strongly attributed to shock and expansion waves generated by the fuel-ramp protruding into the main airflow, as Figure 16 shows.
Excellent agreement is obtained with available pressure readings in the isolator and early combustor regions for both cases. However, the pressures for the first two peaks in the profiles are different between the two Cases; there is no experimental data in either of these regions to validate either simulation result. For the reacting cases ($\Phi > 0$), to alleviate uncertainties, the more accurate wall temperature modeling, as in Case 1, was chosen.

Another discrepancy for both cases occurs in the exit nozzle downstream of $x/h=24$. The higher static pressures in this region are due to flow separation evident in Figure 15. The reason for this numerically induced phenomenon is still unclear.

![STATIC PRESSURE PROFILE](image)

Figure 14: Wall static pressure along axial centerline for $\Phi=0$. 

No experimental data exist in the fuel ramp region to justify simulation discrepancy.

Discrepancy probably due to flow separation in exit nozzle.
Figure 15: Mach number contours for Case 1.

- Mach 1 at nozzle throat
- Mach 2 flow through isolator
- Subsonic recirculation region behind fuel ramp
- Core flow remains supersonic
- Flow separation evident, likely a numerical artifact resulting in increased static pressures
Figure 16: Static pressure contours (kPa) on symmetry plane (z=0) with zoom of shock and expansion waves in combustor and nozzle regions for Case 1.
Contour plots for both Cases 1 and 2 are qualitatively similar, and therefore only that of Case 1 are shown. Figure 15 shows Mach number contours on the symmetry plane and on cross-sectional planes in the exit nozzle. The supply air is accelerated via the convergent-divergent nozzle to approximately Mach 2 at the entrance of the isolator. The isolator inlet pressure provided by the supply nozzle matches the experiment (Figure 14). The inlet nozzle therefore sufficiently emulates the conditions in the UVA experiment.

Figure 15 shows that the core flow is predominately supersonic until it separates along the upper right corner of the exit nozzle. The onset of flow separation approximately coincides with the beginning of the static pressure discrepancy observed in Figure 14, downstream of x/h=24.

Figure 35 [APPENDIX C] show the net mass and net x-momentum fluxes through the engine for both Cases. The final net mass fluxes are within 1.7% and 0.2% of the air inflow mass fluxes for Cases 1 and 2, respectively, adequately satisfying the law of conservation of mass.

Figure 36 [APPENDIX C] shows the decadic logarithm of the absolute value of the maximum residual of the Navier-Stokes equations for each zone of Case 1 (Case 2 shows similar trends). The maximum residuals decreased by several orders of magnitude for all zones, except in zones 8 and 10. Zones 8 and 10 comprised the fuel ramp region directly upstream of the combustor and proved to be the more numerically unstable zones. This was probably attributed to one or more of several factors, viz, (i) numerical stiffness due
to fine grid spacing in the near-field mixing region downstream of the injector exit, (ii) a singular axis in the grid due to the wedge-shaped fuel ramp, and (iii) multiple shock and expansion waves generated by the fuel ramp. The spikes in the residuals observed in Figure 36 occur when increasing to a finer grid level.

Cycle times averaged 3.5 seconds with local minimum and maximum time-steps of 6.155E-11 and 9.734E-07 seconds respectively.
7.0 RESULTS OF THE REACTING CASES: $\Phi_{\text{exp}} = 0.260 & 0.397$

The following presents and discusses the results of the UVA scramjet simulations for equivalence ratios 0.260 and 0.397 - Scans 14 and 21 respectively (refer to Table 1, Section 4.1). The sensitivity of the results to the turbulent Schmidt number ($S_c$) is first demonstrated. Combustion instability, convergence and grid independence is then addressed. Finally, internal flowfield characteristics of the engine are presented.

7.1 Turbulent Schmidt Number Sensitivity Analysis

Figure 17 and Figure 18 compare the experimental static pressure, measured axially along the centerline of the top wall of the scramjet, with that of the simulations. These results were computed using the medium grid resolution of ~435K grid cells (grid independence to be discussed in Section 7.3). Since some simulations showed fluctuations in pressures (to be discussed in Section 7.2), pressures were usually averaged over the final 5000 iterations/cycles.

It is evident that the accuracy of the simulations is strongly dependent on the turbulent Schmidt number. The trends generally show that decreasing the turbulent Schmidt number increases static pressures in the isolator and combustor regions. This is explained by the fact that decreasing the turbulent Schmidt number increases mass diffusion between fuel and air species relative the flow momentum, leading to increased combustion. The latter implies greater heat release, which accelerates the flow through the combustor and increases the static pressures in these regions.
Figure 17: Wall static pressure along axial centerline for $\phi=0.260$.

Figure 18: Wall static pressure along axial centerline for $\phi=0.397$. 
Concerning the isolator, increased combustion due to lower turbulent Schmidt numbers incurs larger adverse pressure gradients on the isolator exit. This results in a stronger shock train in the isolator which propagates further upstream to capture the pressure gradient. The leading edge of this shock train approximately coincides with the abrupt static pressure rise in the isolator where boundary-layer-shock interactions on the isolator wall begin to cause flow separation [1, 22, 26, 37]. Figure 19 and Figure 20 show the flow separating further upstream in the isolator along the lower right corner as the turbulent Schmidt number is decreased.

Note that it is critical that Wind-US be able to predict the extent of the isolator shock train, since engine unstart can occur if the shock train reaches the inlet. Engine unstart can lead to loss of engine performance and possible engine failure [22]. The strong sensitivity of these results to the turbulent Schmidt number suggests that the representation of mass diffusivity effects is crucial for scramjet propulsion simulations using RANS.

For Φ=0.260, it is evident from Figure 17 that Scₜ=1.1 provides an excellent match with experiment, except for some small discrepancy in the exit nozzle downstream of x/h≈40.

For Φ=0.397, Figure 18 seems to indicate that Scₜ=1.7 provides an excellent match with experiment, except in the exit nozzle region downstream of x/h≈23. However, this is an averaged pressure profile as aforementioned, and in fact, the pressures fluctuate to a large enough extent to consider this result questionable. This will be explained more in Section 7.2.
Figure 19: Mach number comparison on z=1.524 cm/0.6 in (80%) plane for Φ=0.260.

Figure 20: Mach number comparison on z=1.524 cm/0.6 in (80%) plane for Φ=0.397.
7.2 Combustion Instability and Solution Convergence

Figure 21: Mass flux of water through the exit plane for $\Phi=0.260$.

Figure 22: Mass flux of water through the exit plane for $\Phi=0.397$. 
Water is a major product of hydrogen-air reactions, and is thus a measure of sustained combustion, as well as solution convergence. Figure 21 and Figure 22 show the mass flux of water at the exit plane of the engine for Φ=0.260 and Φ=0.397, respectively, for the various Schmidt numbers.

For Φ=0.260, Figure 21 shows that combustion instability decreases with increasing turbulent Schmidt number; steady-state convergence is reached for $Sc_t=1.1$, which Figure 17 shows to provide the best match with experimental data.

For Φ=0.397, Figure 22 shows that combustion instability increases with increasing turbulent Schmidt number (opposite to the trend for the Φ=0.260 case). This introduces a numerical challenge since increasing the turbulent Schmidt number appears to provide a better match with experimental data according to Figure 18, but at the expense of increased combustion instability. The latter has made difficult increasing the turbulent Schmidt number higher than about 1.1, as this leads to questionable numerical instabilities and pressure fluctuations. For this reason, for the Φ=0.397 case, the $Sc_t=1.1$ result will be used in subsequent Chapters for analyses.

Where strict steady-state convergence could not be achieved, convergence was assumed when there was no significant change in the amplitude and frequency of the oscillations over a large number of computational cycles, i.e., a pseudo-steady-state convergence was achieved. Although the experiment very likely has inherent combustion instabilities/resonances, the results in Figure 21 and Figure 22 reflect a numerically induced combustion resonance since the simulations were not time-
accurate (i.e., local time-stepping was used). Time-accurate simulations coupled with experimental investigation of combustion instabilities in the UVA engine would perhaps lend to more accurate studies.

This numerically induced resonant behavior can only be speculated at this point. Li, Ma, Yang et al [27, 28] have suggested that combustion resonance may be attributed to the acoustic-convective wave interactions between the ‘fuel injection zones’ and subsonic ‘flame zones’. Disturbances generated in the flame zone may propagate upstream altering the fuel distribution in the ‘injection’ and ‘mixing zones’. This fluctuating fuel-air composition is then convected downstream and causes a heat-release fluctuation in the flame zone, which in turn produces acoustic waves propagating upstream, forming a feedback loop for driving the flow oscillations. Further investigation is needed to determine whether this is the responsible mechanism.

Figure 37 [APPENDIX D] and Figure 39 [APPENDIX E] show the histories of the net mass fluxes and net $x$-momentum fluxes through the entire engine for both $\Phi$-cases. The trends are similar to that of the water mass flux histories. The average net mass flux for all Schmidt numbers were within 1% of the air inflow mass flux at convergence for both $\Phi$-cases. The latter therefore adequately satisfies the law of conservation of mass.

Figure 38 [APPENDIX D] and Figure 40 [APPENDIX E] show the decadic logarithm of the absolute value of the maximum residual for each zone for both $\Phi$-cases. The graphs are only a sample plot for the $Sc_t=1.1$, fine grid case, but the trends for all cases were similar. Most zones show a decrease in residuals of 5-10 orders of magnitude. The
largest fluctuations occur in the combustor (zones 12-21), likely because these regions are numerically ‘stiff’ due to finer grid resolution and larger flow gradients.

The fuel ramp zone (zone 11), just upstream of the combustor, shows the least reduction in residuals and proved to be the most numerically unstable. This was probably due to the same reasons indicated in Section 6.0, Page 29 for the fuel-off case. The success of a simulation was very sensitive to this zone.

7.3 Grid Sensitivity Analysis for $\text{Sc}_t=1.1$

As mentioned, all results presented so far were generated using a medium grid level of $\sim 435K$ grid cells. To demonstrate grid independence, solutions for a single turbulent Schmidt number were generated on three grid levels, viz, course ($\sim 54.4K$ cells), medium ($\sim 435K$ cells) and fine ($\sim 3.48M$ cells).

It should be noted that the fine grid results showed more combustion instabilities (larger numerical resonances) as compared to the medium grid level. This may be expected since a courser grid is usually more dissipative. For this reason, the pressure profiles are again an average of the final 5000 cycles/iterations.

For $\Phi=0.260$, Figure 23 shows that grid independence is not firmly established when the medium and fine grids are compared. The fine grid predicts that the isolator pressure rise begins at approximately $3h$ (1.905 cm) downstream of that predicted by the medium grid. It may be inferred that the fine grid predicts a slightly weaker isolator shock train, as well as a slightly larger heat release profile in the combustor and exit.
nozzle. Although not shown, grid independence was more firmly established for lower turbulent Schmidt numbers for the Φ=0.260 case.

For Φ=0.397, Figure 24 shows that grid independence is firmly established when the medium and fine grid solutions are compared.

It is noted that the fine grid yields a better resolution of the isolator shock train (evidenced by the peaks and valleys in the isolator pressure profile) for both Φ-cases. Therefore, the flowfield analyses to be presented in Section 7.4 will constitute that of the fine grid solutions.

Table 6 shows that the computational expense of the fine grid is significantly larger, with cycle times about 7-9 times that of the medium grid. CFL numbers ranged between 0.5 and 1.0 depending upon whether or not numerical instabilities arise.

<table>
<thead>
<tr>
<th>Table 6: Sample CFD Temporal Data for Various Grid Levels</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Number of Grid Cells</strong></td>
</tr>
<tr>
<td>Course</td>
</tr>
<tr>
<td>~54.4K</td>
</tr>
<tr>
<td>Cycle Time (s)</td>
</tr>
<tr>
<td>Minimum Time-Step (s)</td>
</tr>
<tr>
<td>Maximum Time-Step (s)</td>
</tr>
<tr>
<td>CFL #</td>
</tr>
</tbody>
</table>
Figure 23: Static pressure profile showing grid sensitivity for $\Phi=0.260$, $Sc_t=1.1$.

Figure 24: Static pressure profile showing grid sensitivity for $\Phi=0.397$, $Sc_t=1.1$. 
7.4 Equivalence Ratio Summary & Flowfield Analyses for $Sc_t=1.1$

![Equivalence Ratio Comparison for $Sc_t=1.1$](image)

Figure 25: Static pressure profile for all $\Phi$'s at $Sc_t=1.1$ on the fine grid.

Table 7: Experimental & CFD Equivalence Ratios Compared

<table>
<thead>
<tr>
<th>$\Phi_{\text{EXP}} \pm 5%$</th>
<th>$\Phi_{\text{CFD}}$</th>
<th>Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.260</td>
<td>0.266</td>
<td>+2.3%</td>
</tr>
<tr>
<td>0.397</td>
<td>0.403</td>
<td>+1.5%</td>
</tr>
</tbody>
</table>

Figure 25 compares results for $\Phi=0$, 0.260 and 0.397 at $Sc_t=1.1$ using the fine grid level.

For $\Phi=0$, there is no combustion and the comparatively small pressure fluctuations are primarily due to shock and expansion waves generated by the presence of the injector ramp. As $\Phi$ is increased (say from 0.260 to 0.397), higher fuel mass flow into the main
airstream increases the number of combustion reactions. Consequent increased heat release accelerates the flow resulting in a higher combustor peak pressure as Figure 25 indicates. To capture the gradient between the inlet pressure and the higher combustor pressure, the resulting isolator shock train is stronger and its leading edge moves upstream. Consequently, shock-induced flow separation and the accompanying static pressure rise also moves upstream.

Table 7 compares the equivalence ratios of the simulations with that of the experiments. Nominal simulation Φ-values are well within the ±5% error range of the experimental Φ-values. The simulations’ equivalence ratios were calculated based on a stoichiometric fuel-air ratio of 0.0291 for a hydrogen-air reaction [22].

Figure 26 to Figure 33 show Mach number, static pressure, static temperature and water mass fraction contours on symmetry and cross-sectional planes throughout the UVA engine for Φ=0.260 and Φ=0.397. These results are again for Scₙ=1.1 on the fine grid level.

For both Φ-cases, the inlet nozzle supplies approximately Mach 2 air to the entrance of the isolator. The isolator inlet pressure provided by the supply nozzle matches that of the experiment (Figure 25), while the inlet mass flow rate of 0.206 kgs⁻¹ is within +1.5% of the experimental value.

For Φ=0.260, Figure 26 shows that the combustor entry Mach number of the core flow is just supersonic, indicating operation in scramjet mode or possibly the transition mode between ramjet and scramjet. The isolator shock train, evident in Figure 26 and Figure
28, appears to be a sequence of oblique shocks followed by progressively weak normal shocks that propagates into the combustor. The shock train first incurs flow separation at $x/h = -21$, coinciding with the initial static pressure rise indicated in Figure 25. The core flow remains just supersonic in the combustor and exit nozzle until $x/h = 46$, where there appears to be a weak normal shock, with corresponding static pressure rise (Figure 25 and Figure 28) to capture the ambient pressure.

For $\Phi = 0.397$, Figure 27 shows that the combustor entry Mach number of the core flow is subsonic, indicating operation in ramjet mode. The isolator shock train, evident in Figure 27 and Figure 29, appears to have an oblique shock structure. In the simulations, the shock train appears to first incur flow separation at $x/h = -44$, coinciding with the static pressure rise observed in Figure 25. However, the experimental data indicates that the leading edge of the shock train is in the vicinity of $x/h = -35$. The core flow in the combustor/exit nozzle appears to accelerate from subsonic to supersonic due to heat release from combustion, indicating the presence of a thermal throat in this region (similar to the Rayleigh flow phenomenon [22]). Before exiting the engine, Figure 27 shows that the core flow decelerates back to subsonic speeds by the apparent weak normal shock at $x/h = 44$, where the pressure then rises (Figure 25 and Figure 29) to equilibrate with the ambient back pressure. However, this normal shock at $x/h = 44$ may be a numerical artifact, since Figure 25 shows that from $x/h = 30:50$, there is no drop and subsequent rise in the experimental pressures. It may be that the flow is separated in this region in the experiment. The reasons for the observed discrepancies between the experiment and the simulations for the $\Phi = 0.397$ case are still unclear. It is possible that
heat transfer to the walls of the combustor and exit nozzle are inadequately modeled in the simulations due to a lack of thermocouple readings in this region; and/or structural deformation due to thermal stresses is altering the flow behavior in the experiment; and/or the chemical kinetic model used is not capturing the correct heat release profile. It is apparent that further investigation is necessary.

Figure 26 to Figure 29 also show the under-expanded, supersonic, hydrogen fuel-stream penetrating into the main air-stream with a ‘diamond-pattern’ sequence of shocks. Just downstream of the fuel ramp base is a region of low-speed, recirculating flow which would assist in flame holding. The fuel reacts with the main airstream and its mass fraction reaches less than 5% by $x/h=20$ and $x/h=40$ for $\Phi=0.260$ and $\Phi=0.397$, respectively.

The temperature and water contours indicate that the flame ignites just downstream of the injector exit, first on the ‘top side’ of the fuel-air shear layer. This may be related to stronger velocity gradients (and turbulent mass diffusion) between the fuel jet and the subsonic flow in the recirculating region behind the fuel ramp. The flame then propagates with increasing annular to circular cross-section through the combustor and exit nozzle. Maximum combustion temperatures reach approximately 2363 K & 2347 K for $\Phi=0.260$ & $\Phi=0.397$, respectively. These are within -0.9% & -1.6%, respectively, of the adiabatic flame temperature of 2384 K for stoichiometric hydrogen-air combustion at initial conditions of 1 atm and 298 K [22]. The water vapor mass fraction reaches a maximum of about 0.23 through most of the flame zone for both $\Phi$-cases.
Figure 26: Mach # contours on cross-sectional & symmetry planes for Φ=0.260.
Figure 27: Mach # contours on cross-sectional & symmetry planes for $\Phi=0.397$. 
Figure 28: Pressure [kPa] contours on symmetry plane for Φ=0.260.
(Maximum static pressure = 828.92 kPa).
Figure 29: Pressure [kPa] contours on symmetry plane for $\Phi=0.397$.
(Maximum static pressure = 1254.95 kPa).
Figure 30: Static temperature [K] in the exit nozzle for $\Phi=0.260$.

Figure 31: Static temperature [K] in the exit nozzle for $\Phi=0.397$. 
Figure 32: Water mass fraction in exit nozzle for $\Phi=0.260$.

Figure 33: Water mass fraction in exit nozzle for $\Phi=0.397$. 
8.0 CONCLUSIONS & RECOMMENDATIONS

The internal flowpath through University of Virginia’s direct-connect, dual-mode scramjet engine was numerically simulated using Wind-US flow solver for three different run conditions, viz, one fuel-off and two reacting cases with different equivalence ratios.

For the fuel-off case, pressure distributions along the flowpath were predicted with excellent accuracy according to available experimental data, except in the exhaust nozzle region where there is a large region of numerically induced separated flow. The reason/s for the latter is/are yet to be resolved, but it is plausible that this discrepancy is related to the exhaust boundary condition treatment.

For the reacting cases, the numerical model is very sensitive to the choice of turbulent Schmidt number. This mass diffusion control parameter significantly influences combustion levels altering combustor peak pressures and isolator shock strengths. Although a local time-step procedure was implemented, the results suggest that combustion instabilities (and sometimes numerical instabilities) also arise as the turbulent Schmidt number is varied. Such instabilities were a limiting factor for the higher equivalence ratio case.

Specifically, for the low equivalence ratio case, the pressure distribution along the flowpath was predicted with excellent accuracy provided a turbulent Schmidt number of 1.1 is chosen. However, a denser grid may be necessary to facilitate better grid
independence of the solutions. The engine was determined to be operating in scramjet mode (or possibly near transition mode) for this run condition.

For the higher equivalence ratio case, the pressure profile is mostly captured with a turbulent Schmidt number of 1.7, but was deemed suspect due to the extent of numerically-induced combustion resonances and accompanying pressure fluctuations. As stated, this case needs more investigation. The engine was determined to be operating in ramjet mode for this run condition.

Some recommendations include (i) multi-disciplinary CFD approaches using conjugate heat transfer with RANS to more accurately model thermal boundary conditions, (ii) investigation of thermal stresses on the combustor and exit nozzle components, (iii) using a non-uniform total temperature profile at the inflow plenum based on the fact that the incoming air may not be uniformly mixed by this point, (iv) more accurately modeling the outflow boundary condition, (v) determining the ability of the chemical kinetic model to capture the correct heat release profile, (vi) time-accurate simulations to capture combustion resonances/instabilities, supplemented by experimental investigations, and (vii) use of a Damkohler number whenever combustion instability limits numerical convergence. The Damkohler number is defined as the ratio of fluid-dynamic time scales to chemical-reaction time scales. Thus, reducing the Damkohler number proposes to limit chemical kinetic rates relative to the fluid advection rates, reducing numerical stiffness in reacting regions and maintaining practical time-steps [14].
It should be mentioned that grid quality plays a crucial role in simulation success. The relatively complex geometry of the fuel injector and the fuel ramp configuration can easily render increased numerical stiffness and instability. It is recommended for future simulations that an unstructured tetrahedral grid be used in the fuel injector. This would drastically improve grid orthogonality in the combustor, and hence numerical stability and convergence.

Future work involves using the Peters & Rogg, 13-species, 27-reaction set for the scramjet simulations. This kinetic mechanism proves to more accurately predict experimental results for the low equivalence ratio case, provided a turbulent Schmidt number of 2.0 is chosen. It also induces less combustion instabilities and more stable numerics. In addition, this mechanism will allow future simulations with vitiated air supply, i.e., with water vapor and carbon species. Figure 41 and Figure 42 [APPENDIX F] show a preview of the pressure distributions and Mach number contours, respectively, for \( \Phi=0.260 \) with clean air supply using the Peters & Rogg kinetics.

Simulations of dual-mode scramjet engines with combusting flow presents many challenges. The accuracy of the numerical model varies with chemical kinetic mechanisms, turbulence models, numerical schemes, grid topology, etc. While noting that there is room for further improvements, this study shows that CFD numerical prediction via Wind-US can adequately supplement theory and experiment for the development of hypersonic vehicle propulsion systems.
REFERENCES


34. NPARC Alliance, “WIND-US Documentation,” 2007


APPENDIX A : Sample Wind-US Input Data File

/ This is a comment line

UVA Scramjet Hydrogen-Air Supersonic Combustion
3D Struc Grid, 31 Zones, 20 Proc
Scan 14. Phi 0.260, Evan-Schex, Sc(t)=1.1

/Zone 1, 2, 3   Air Inflow
/Zone 26   Outflow
/Zone 27   Fuel Inflow

/ SPAWNED OUTPUT
spawn "./spawn.script1" frequency 1000 /save solution file every 1000 cycles
spawn "./spawn.script2" frequency 100 /compute axial press/temp profile every 100 cycles

/ NUMERICS
/rhs roe first
rhs roe second
converge level 1.0e-9
cfl 1.00
cycles 10000 print frequency 1
iterations per cycle 1
/sequence 1 1 1

/ LIMITERS
dq limiter on drmax 0.1 dtmax 0.1
test 71 5
/fixer print zone all
/tvd factor 2 zone all

PRANDTL 0.72 0.9
SCHMIDT 0.72 1.1

/ INLET CONDITIONS
freestream static 1.4 14.7 530.0 0.0 0.0
/initialize along minus j zone 27

/ OUTFLOW CONDITIONS
downstream pressure 14.7 extrapolate supersonic zone 26

/ WALL TEMP
wall temperature 738 zone 1:5
wall temperature 770 zone 6:8
wall temperature 900 zone 21:26

/ CHEMISTRY
chemistry
/frozen
finite rate
file h2air-7sp-std-15k-3rdbodyeff-NEW.chm local
/file ignite.chm local
species O2 0.21 H 0.0 H2 0.0 H2O 0.0 OH 0.0 O 0.0 N2 0.79
diffusion single
viscosity wilke
endchemistry

/ ARBITRARY INFLOW
arbitrary inflow
total
hold_totals
direction specified
zone 1
  uniform 1.00 47.80 2165.4 0.0 0.0
  0.21 0.0 0.0 0.0 0.0 0.0 0.79
zone 2
  uniform 1.00 47.80 2165.4 0.0 0.0
  0.21 0.0 0.0 0.0 0.0 0.0 0.79
zone 3
  uniform 1.00 47.80 2165.4 0.0 0.0
  0.21 0.0 0.0 0.0 0.0 0.0 0.79
zone 27
  uniform 0.50 120.21 535.34 -90.0 0.0
  0.0 0.0 1.0 0.0 0.0 0.0 0.0
endinflow

/ TURBULENCE MODEL
turbulence sst
/turbulence model chien

/ LOADS OUTPUT
loads
pressure offset 0.0
print planes totals frequency 1
reference area 1.0
reference length 1.0
reference moment center 0.0 0.0 0.0
zone 1
  surface i 1 mass force momentum
zone 2
surface i 1 mass force momentum
zone 3
  surface i 1 mass force momentum
zone 26
  surface i last mass force momentum
zone 27
  surface j last mass force momentum
zone 31
  surface i last mass force momentum
endloads

end
Figure 34: Grid details of the fuel ramp, fuel exit plane and combustor regions. Some connectors have been deleted to facilitate visual rendering.
APPENDIX C: Convergence of Φ=0 Case

Figure 35: Mass & x-momentum net fluxes for Φ=0, fine grid.

Figure 36: Maximum residuals of the Navier-Stokes equations for Case 1.
APPENDIX D: Convergence of Φ=0.260 Case

Figure 37: Mass & x-momentum net fluxes for Φ=0.260, medium grid.

Figure 38: Max residuals of the Navier-Stokes eqns for Φ=0.260, ScT=1.1, fine grid.
APPENDIX E: Convergence of $\Phi=0.397$ Case

Figure 39: Mass & $x$-momentum net fluxes for $\Phi=0.397$, medium grid.

Figure 40: Max residuals of the Navier-Stokes eqns for $\Phi=0.397$, $Sc_t=1.1$, fine grid.
APPENDIX F : Preview of Results using Peters & Rogg Kinetics

Figure 41: Wall static pressure along axial centerline for $\Phi=0.260$, medium grid.

Figure 42: Mach number contours for $\Phi=0.260$, $Sc_t=2.0$, fine grid level.
“The process of scientific discovery is, in effect, a continual flight from wonder.”

-Albert Einstein