

# Using CEQUEL for Thermochemistry Calculations in a Graduate Rocket Propulsion Course at UAH

Robert A. Frederick, Jr.<sup>1</sup>, Paige Berg<sup>2</sup>, and William Loeblich<sup>3</sup>  
*UAH Propulsion Research Center, Huntsville, Alabama, 35899, USA*

Advanced projects in rocket propulsion classes often require the calculation of thermochemical properties of the combustion gases and nozzle performance. While there are several codes available to do thermochemical calculations, difficulties often arise in interfacing the code results into the detailed trade study calculations of notional propulsion systems. The objective of this paper is to illustrate the use of a spreadsheet and Python-based code for a solid-fuel ramjet design project. The scope includes propellant characterization, time-dependent calculation of thermochemical properties, internal ballistics, and flight performance analysis. The code *Chemical Equilibrium in Excel* (CEQUEL<sup>TM</sup>) provided these on-demand calculations. The students evaluated different candidate solid fuels for an air-breathing ramjet concept and used the code to calculate the recovery properties of the inlet air, chamber properties, and nozzle performance into a flight simulation that compared range and time to target for each configuration. The paper illustrates the use of CEQUEL in both a spreadsheet approach as well as a Python-based implementation. Students could learn and successfully implement this program into their class project. The CEQUEL program allowed students to incorporate detailed thermochemical calculations into their time-dependent simulations without having to resort to table lookups or parametric curve fits of the thermochemical results. The code is an excellent fit for instructional courses in propulsion as well as research projects.

## I. Introduction

The University of Alabama in Huntsville (UAH) has a rich rocket propulsion heritage [1–7]. Dr. Wernher Von Braun and other community leaders facilitated state funding for the expansion of The University of Alabama in Huntsville to attract and further develop the workforce for the U.S. Space program. On June 20, 1961, Dr. Von Braun remarked, "It's not water, or real estate, or labor, or cheap taxes that bring industry to a state or city. It's brainpower." Over the past 30 years since the founding of the UAH Propulsion Research Center, MAE 440/540 (Rocket Propulsion I) [8] and MAE 640 (Rocket Propulsion II) in various forms have supported undergraduate and graduate degree programs in what is now The Department of Mechanical and Aerospace Engineering at the University of Alabama in Huntsville. In fact, as shown below, "Applied Aerodynamics and Propulsion," was in the 1968 UAH Course Catalogue.

The MAE 640 propulsion course covers propellant thermochemistry. The thermochemistry module covers the basic concepts, and it illustrates those concepts with homework. Here, the students calculate the adiabatic flame temperature

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<sup>1</sup> Professor of Mechanical & Aerospace Engineering/Director of the Propulsion Research Center, Department of Mechanical & Aerospace Engineering, 301 Sparkman Drive, Olin B. King Technology Hall, Room S226, Huntsville, AL 35899, and AIAA Associate Fellow.

<sup>2</sup> Graduate Research Assistant, Department of Mechanical & Aerospace Engineering, 301 Sparkman Drive, Olin B. King Technology Hall, Room S226, Huntsville, AL 35899, and AIAA Student Member.

<sup>3</sup> Graduate Research Assistant, Department of Mechanical & Aerospace Engineering, 301 Sparkman Drive, Olin B. King Technology Hall, Room S226, Huntsville, AL 35899, and AIAA Student Member.

and gas properties of a hydrogen and oxygen reaction. The first calculation is for no dissociation and the second is for limited dissociation. While this is very useful for students to understand the chemistry and thermodynamics of combustion, it is not practical for making hundreds of calculations that might be required to do a time-dependent simulation of a propulsion system. Over the years, the class has made use of many different codes to do these thermochemical calculations in a more automated fashion. We have used a FORTRAN and PC version of NASA-SP273 [9]. The Thermochemical Equilibrium Code (TEP), Stanjan, The Propellant Evaluation Program (PEP), and, in the past few years NASA's Chemical Equilibrium Analysis (CEA) and Chemical Equilibrium in Excel (CEQUEL™). These codes all generally use the minimization of Gibb's free energy to calculate combustion products and can subsequently calculate nozzle performance for frozen or equilibrium flow. They also include, to varying degrees, thermodynamic databases for propellants and combustion products of interest for rocket propulsion.

This paper illustrates the use of CEQUEL™ in our MAE 640 class in the spring of 2021. Students used the code to do the following calculations: 1) calculation of characteristic velocity and specific impulse for 50 common rocket propellant combinations, 2) calculation of characteristic velocity, specific heat ratio, and specific impulse as a function of air-to-fuel ratio for air-breathing solid fuel ramjet applications; and 3) calculation of time-dependent characteristic velocity, specific heat ratio, and thrust coefficient for internal ballistic/trajectory simulation of a solid propellant ramjet. The EXCEL version of CEQUEL™ provides the calculations for all of these tasks and some students tried out a Python version for the second task.

## **II. Approach to Using CEQUEL™**

### **A. CEQUEL™ Spreadsheet Environment**

CEQUEL™ is an add-in program for Microsoft Excel that performs thermochemistry calculations. In the Excel version of the program, there are two wizards; Equilibrium Wizard and Isobaric Mixing Wizard; that the user can use to perform calculations and insert the answer into a spreadsheet. The Isobaric Mixing Wizard calculates the final temperature, enthalpy, entropy, and specific heat capacity of a mixture of two or more nonreacting flow streams at different initial temperatures. This wizard can have up to five different streams with twenty-five different species in each stream. For the Equilibrium Wizard (shown in Figure 2) there are eleven different calculation types: Pressure-Temperature, Pressure-Enthalpy, Pressure-Entropy, Volume-Temperature, Volume-Internal Energy, Volume-Entropy, Rocket: Area Ratio, Rocket: Pressure/Pressure Chamber, Shock: Velocity, Shock: Mach #, and Detonation. For each of the calculations types the user has the option of seven mixture types: No Ratios, O/F Ratio, FA, Fuel Percent, Equivalence Ratio, Phi, and Tri-Propellant. CEQUEL™ has a built-in library of over 100 reactants. Figure 3 is an example of the Reactants Library window that is used when selecting reactants. The user inputs the percentage of the mixture for that reactant. If a reactant the user wants to use is not in the library, the reactant can be added by either using the "User Defined Reactant Wizard" button in the CEQUEL tab or by editing a reactant file in the library folder.

Ceque(R) Equilibrium Wizard: Reactant Input

Calculation Type  
 Rocket: Area Ratio

Reactant List Functions  
 Add Reactant  
 Edit Selected Reactant  
 Delete Selected Reactant  
 Delete All Reactants

Reactant List

Reactant	%	FOG
H2 (L)	100	F
O2 (L)	100	O

Total: FO: 100 / 100

Normalize

Mixture Fractions  
 Oxidizer  
 O / F: 4.13

Units  
☒ English ☐ SI

Mixture Type  
☐ No Ratios  
☒ O/F Ratio  
☐ FA  
☐ Fuel Percent  
☐ Equivalence Ratio  
☐ PHI  
☐ Tri-Propellant

Advanced Options

Cancel Next ->

Fig. 2. Equilibrium Wizard: Reactant Input Example.

Ceque(R): Reactants Library

Reactant List

- H2 #
- H2 (G)
- H2 (L)
- H2 (L) AT 298.15K
- H2+ #
- H2- #
- H2O6C274F342
- H2O6C12
- H2O6C12O45N
- H2O6C15FE
- H2O6C8PB
- H2O6C9
- H21C7O7PB
- H22C100F178
- H22C12
- H22C12O11
- H22C14O8
- H22C16O4
- H24C16O4
- H24C21O4

Search  
 h2

Composition

Element	Weight
H	2

☐ Modify Reactant Data

Reactant Libraries

Include User Reactants

Remove User Reactants

Mixture %  
 Cell Ref

Reactant Data

Phase  
☐ Solid  
☒ Liquid  
☐ Gas

Type  
☒ Fuel  
☐ Oxidizer  
☐ 2nd Fuel

Energy  
☐ Joules/Mole  
☒ Cal / Mole

Phase Data  
 Temperature (K) 20.27 Cell Ref  
 Heat of Formation (cal/Mole) -2153.92 Cell Ref  
 Density (gm/cm^3) (for density Isp only) 0 Cell Ref

Reactant Comment  
 HYDROGEN (L), MW= 2.0159

Cancel Add Selected

Fig. 3. CEQUEL™ Reactants Library.

Two calculation types that were of interest for the class were Rocket: Area Ratio and Rocket: Pressure/Pressure Chamber. The difference between these two calculation types is that for Area Ratio the user specifies the area ratio for the nozzle and for Pressure/Pressure Chamber the user specifies the pressure ratio. The chamber pressure is specified for both calculation types and can reference a cell in Excel or be entered in the wizard. In addition, the user can select the type of chemistry to be used i.e., Equilibrium, Frozen or Frozen Throat. Once these values are specified the user selects the outputs of the wizard. For these types of calculations Mixture Ratios, Rocket Properties or Combustion Products can be an output into Excel cells. A function similar to that shown in Figure 4. If the user knows the name of the reactant in the library, the reactant can be a cell reference as well. In addition, if the user knows how CEQUEL labels the different rocket properties such as characteristic velocity or “CSTAR”, or “ISPV” (vacuum specific impulse) can be a cell reference as well by modifying the command statement.

```
=CEQUEL("ROCKET","AR",Chart!$N$9,1,Chart!$O$9,"Mass",2,"H2 (L)",100,"O2 (L)",100,"OF",Chart!$M$11,1,0,"CSTAR",FALSE,FALSE)
```

**Fig. 4. Example CEQUEL**

### **L Function in a Cell.**

In each cell of a spreadsheet, one can specify or reference all the input parameters for the rocket calculations, the assumptions for the outpost, and then specify any one of the output results to be displayed in the cell. This has been a great utility for graphing, as well as making detailed calculation in preliminary design studies.

### **B. CEQUEL™ Python Environment**

With a cursory knowledge of programming logic and the language of Python, one can easily become accustomed to the usage of Pyrho, especially with the help of a provided step-by-step manual detailing what commands to use in the Python code to execute Pyrho simulations. However, to accomplish tasks in Pyrho, a good understanding of the Excel version of the CEQUEL program is also warranted so that it is clear what potential options (like reactant names) may be chosen and in what format to create a desired model.

This section will go through part of an assigned problem for the MAE 640 class at UAH to demonstrate the use of Pyrho. The problem called for an analysis of how O/F ratio changes with respect to characteristic velocity ( $C^*$ ), vacuum specific impulse ( $I_{sp,vac}$ ), heat capacity ratio ( $\Gamma$ ), and vacuum thrust coefficient ( $C_f, vac$ ) by calculating each parameter through Pyrho and giving graphs as output. The problem used a fuel combination of 90% HTPB and 10% IPDI with heated air as an oxidizer, which can be seen as being selected as reactants by the code in Lines 17 through 20 in the screenshot of the code in the following example figure. The FOX value means the reactant is a fuel when set equal to “F” and an oxidizer when set equal to “O”. The reactant of aluminum was “commented out” with a # symbol on Line 19, showing the settings can be “saved” in this way in case one wanted to bring back what they were working on in the project.

A powerful way to harness the power of Pyrho are the loops inherent to programming, like the “for” loops in Figure 5. One was used to cycle through each iteration of O/F ratio and an extra outer loop was used to run the calculations for each of the  $\Gamma$ ,  $C^*$ , and  $I_{sp,vac}$  outputs.

```

1  import pyrho
2  import math
3  import numpy as np
4  from matplotlib import pyplot as plt
5  from scipy.interpolate import make_interp_spline as spl
6
7  OF_list = [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15]
8  Gamma = []
9  Cstar = []
10 IspV = []
11
12 for i in range(3):
13     for n in OF_list:
14         rocket = pyrho.problem(type="ROCKET_AR", AR=3, P=30, units="e dll")
15         mixture = pyrho.mixture(type="O/F", ratio=n)
16
17         HTPB = pyrho.reactant(name="HTPB", FOX="F", percent = 90)
18         IPDI = pyrho.reactant(name="IPDI (ARC)", FOX="F", percent = 10)
19         # Al = pyrho.reactant(name="AL (S)", FOX="F", percent = 30)
20         Air = pyrho.reactant(name="AIR (500 K)", FOX="O", percent = 100)
21         reactants = [HTPB, IPDI, Air]
22
23         mycalc = pyrho.calc(rocket, reactants, mixture)
24
25
26         if i == 0:
27             Gamma.append(mycalc.output["GAMMAG"][0])
28         elif i == 1:
29             Cstar.append(mycalc.output["CSTAR"][0])
30         elif i == 2:
31             IspV.append(mycalc.output["ISPV"][0])
32
33 CFV = np.divide(np.multiply(IspV, 32.2), Cstar)
34

```

**Figure 5. Screenshot of Pyrho Code for MAE 640 Thermochemistry Project Detailing Inputs**

One can set up initial conditions like the problem type (Line 14) as in temperature-pressure or rocket area ratio, and the  $C_{f,vac}$  (CFV) was also calculated with  $C_{fv} = \frac{I_{sp}g}{C^*}$ . A possible code segment for the plotting of these calculations is shown in the following figure:

```

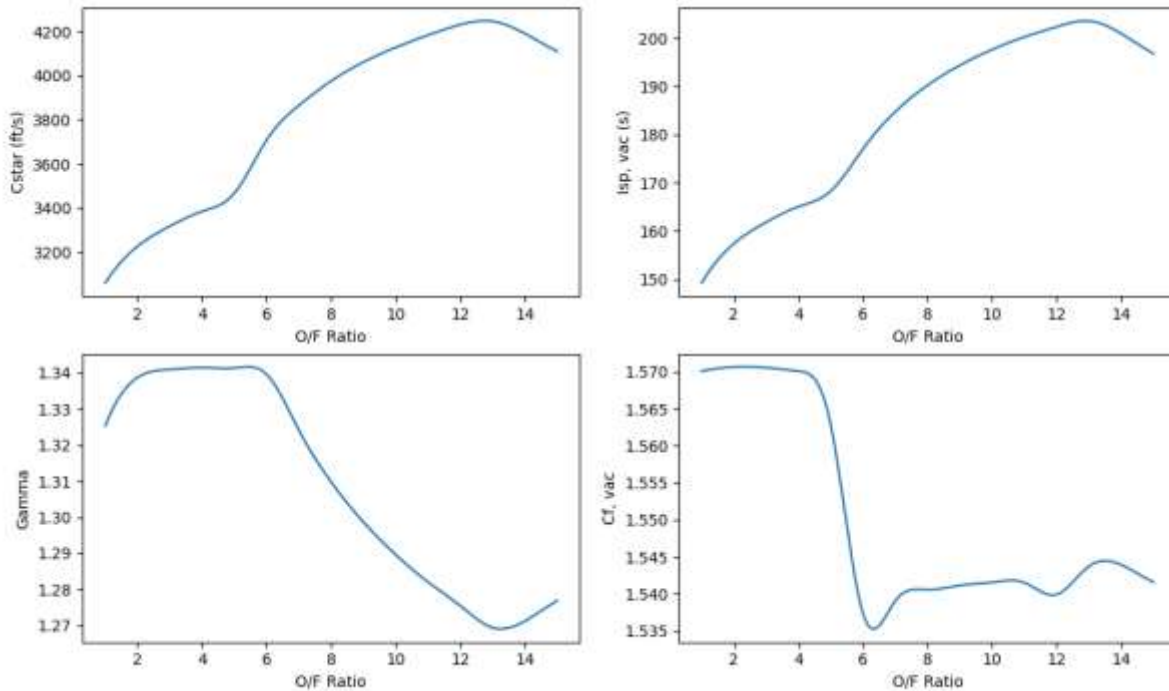
36 figure, axis = plt.subplots(2,2)
37
38 XY_Spline1 = spl(OF_list,Cstar)
39 OF_list1 = np.linspace(min(OF_list),max(OF_list),500)
40 Cstar_spl = XY_Spline1(OF_list1)
41 axis[0,0].plot(OF_list1,Cstar_spl)
42 axis[0,0].set_xlabel('O/F Ratio')
43 axis[0,0].set_ylabel('Cstar (ft/s)')

```

**Figure 6. Screenshot of the Another Part of Pyrho Code Showing Plotting Commands**

The plots were smoothed out plot with splining (“spl”) and “linspace” to make linearly equidistant intermediary points between two extremes of the O/F ratio plotted line.

The O/F ratio was made the x-axis and  $c^*$  the y-axis. One can make subplots (Line 36) to show more information on one window, like if it was desired to show  $c^*$ ,  $I_{sp,vac}$ , gamma, and  $C_f$ -vac as the y axis for each subplot as shown in the following figure. Most of the code in Figure 6 would be duplicated in order to output each of these parameters' graphs:



**Figure 7. Output of Pyrho Code Showing Subplots of O/F Ratio vs  $C^*$ ,  $I_{sp,vac}$ , Gamma, and  $C_f$ -vac**

In this example programming project, Figure 5 is where all of the Pyrho-specific code remains, and the plotting in Figure 6 required purely general Python knowledge. And so accordingly, one can use normal Python plotting features like overlapping graphs in case they wanted to compare data that way, such as comparing  $C^*$  and  $I_{sp,vac}$  for different propellant mixtures.

The Python objects being defined in Figure 5 like “problem”, “mixture”, and “reactant” are like selecting the options in the Excel version. Although it may be a slight drawback in time and effort spent in writing everything out instead of simply selecting radio buttons, Pyrho is like a superuser version of CEQUEL in that if one knows how CEQUEL works, they can do “heavy lifting” like calculating many things at once with loops and such. Having a written code also shows the settings and properties all at once in one script, so Pyrho can give a way to transfer a large amount of information about a simulation in a compact way with the easily transferable text file format.

### III. Example Applications of CEQUEL™

#### A. Reproducing Performance Predictions of Classic Rocket Propellant

To familiarize students with how to use CEQUEL, the first two oxidizers in the Pratt & Whitney theoretical performance of rocket propellant combinations chart (Figure 8) were replicated. Students were required to do the following:

- Run CEQUEL and calculate numbers at the mixture ratio and conditions shown in the chart on the next page. Use the propellant formulations shown
- Run all the cases for Liquid and Gaseous Oxygen (Sea Level and Vacuum)
- Comment on the % differences in your calculations with the ones Shown on the table.

For extra credit the students could replicate the entire chart including colors, footnotes, and headers but omitting the density as not every reactant has a density in the library. The bar graphs shown in the original chart could be embed in the chart or made separately.

The approach used for replicating the chart was to use the O/F or r ratio in the chart and a chamber pressure of 1000 psi for both types of rocket calculations. In addition, the reactants entered in Excel were the names for the reactants in the CEQUEL library. For example, for the LOX section of the chart the oxidizer was listed as “O<sub>2</sub> (L)” and for the fuel it was listed “H<sub>2</sub> (L)”. The first property that was inserted into the spreadsheet was the specific impulse (Isp) value for liquid oxygen and liquid hydrogen. The function was then modified to all for the function to be dragged down to perform calculations for the remaining reactants in the chart. The function was also dragged over to other columns to calculate the chamber temperature and characteristic velocity (C\*) and the part of the function indicating the property to be output was changed to a cell reference. The temperature in the Pratt and Whitney chart was in Fahrenheit and CEQUEL only outputs Rankine for the English units, therefore the CEQUEL answer needed to be converted to Fahrenheit. This process was then repeated for both the pressure ratio chart and the area ratio chart. Bar graphs were created by using the impulse for each fuel and oxidizer mixture and placing it alongside the finished charts. The fully replicated Pratt and Whitney chart can be found in Figure 9. The percent difference between the values calculated using CEQUEL and the Pratt and Whitney chart was calculated using Equation 1. Based on this calculation it was determined that CEQUEL values and that of the Pratt and Whitney chart matched for most of the fuel and oxidizer variations. However, for oxygen difluoride and ethane, the chamber temperature and C\* value for the area ratio calculations had at least a 10% difference and for the pressure ratio for the same mixture the chamber temperature had a difference of 9%.

$$\text{Percent Difference} = \frac{\text{CEQUEL Value} - \text{Pratt \& Whitney Value}}{\text{Pratt \& Whitney Value}} \times 100 \quad (1)$$



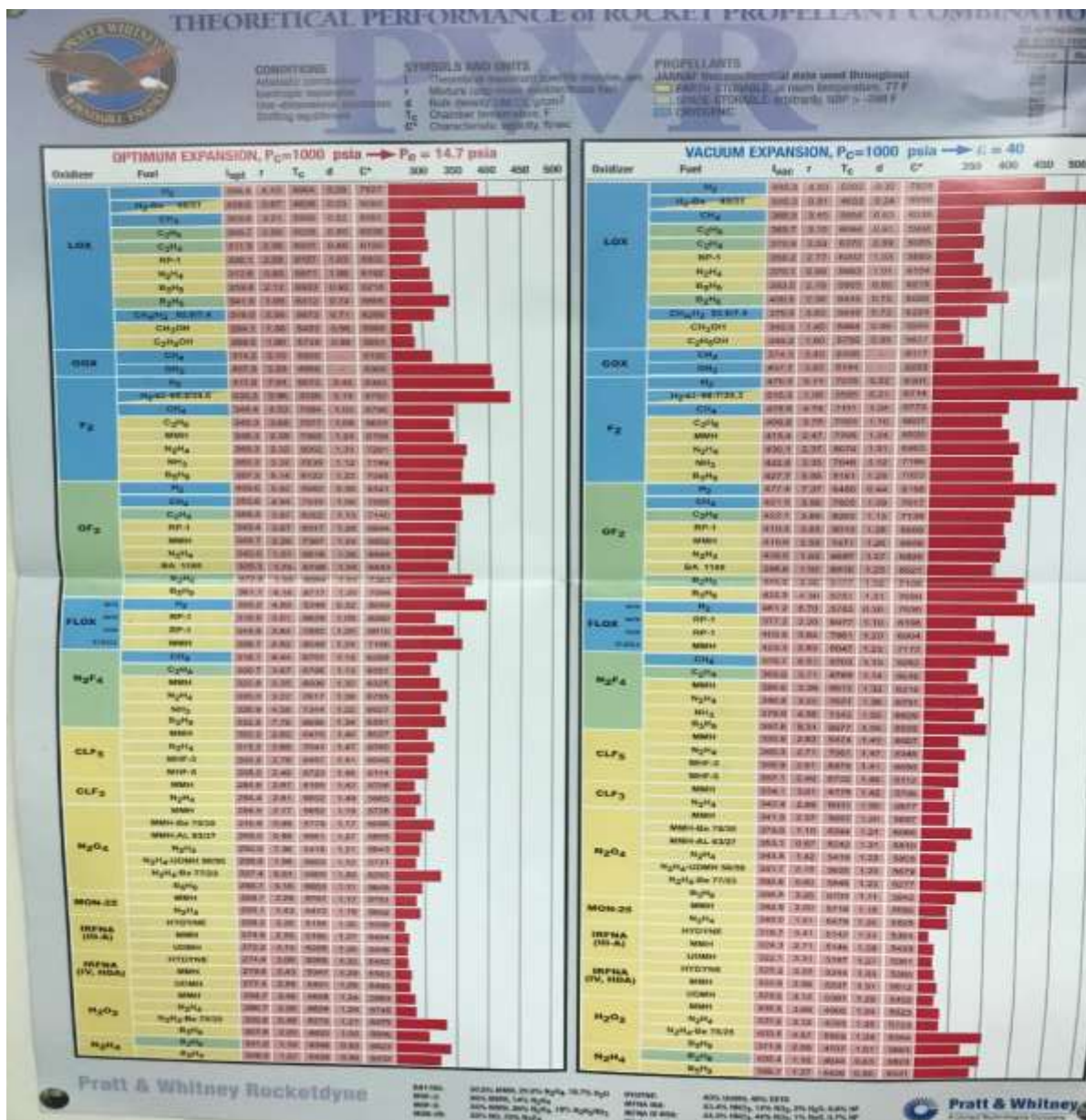


Fig. 8. Pratt & Whitney Poster of Thermochemical Calculations



CONDITIONS		SYMBOLS AND UNITS						DIFFERENCES		PROPELLANTS													
Adiabatic combustion		I Theoretical maximum specific impulse, sec						≥10% Difference		CEQUEL thermochemical data used throughout													
Isentropic expansion		r Mixture ratio-mass oxidizer/mass fuel						≥9% Difference		EARTH-STORABLE: at room temperature, 77 F													
One-dimensional expansion		d Bulk density [M/V], g/cm <sup>3</sup>						Difference in values that seem significant as well		SPACE-STORABLE: arbitrarily, NBP > -288 F													
Shifting equilibrium		T <sub>c</sub> Chamber temperature, F						but not under other categories		CRYOGENIC													
						C* Characteristic velocity, ft/sec																	
OPTIMUM EXPANSION, P <sub>c</sub> =1000 psia → P <sub>c</sub> =14.7 psia												VACUUM EXPANSION, P <sub>c</sub> =1000 psia → P <sub>c</sub> =14.7											
Oxidizer	Fuel	I <sub>sp</sub>	r	T <sub>c</sub>	d	C*				Oxidizer	Fuel	I <sub>sp</sub>	r	T <sub>c</sub>	d	C*							
LOX	H <sub>2</sub>	389.1	4.13	4938	0.29	7917				LOX	H <sub>2</sub>	455.1	4.83	5365	0.32	7813							
	H <sub>2</sub> -Be 49/51	454.9	0.87	4672	0.24	9207					H <sub>2</sub> -Be 49/51	540.1	0.91	4672	0.24	9427							
	CH <sub>4</sub>	309.2	3.21	5880	0.81	6083					CH <sub>4</sub>	368.5	3.45	5937	0.83	6022							
	C <sub>2</sub> H <sub>6</sub>	306.5	2.89	5996	0.89	6032					C <sub>2</sub> H <sub>6</sub>	365.6	3.10	6051	0.90	5978							
	C <sub>3</sub> H <sub>8</sub>	311.2	2.38	6295	0.88	6140					C <sub>3</sub> H <sub>8</sub>	370.6	2.59	6359	0.89	6076							
	RP-1	299.6	2.58	6140	1.02	5888					RP-1	357.7	2.77	6185	1.03	5838							
	N <sub>2</sub> H <sub>4</sub>	312.4	0.93	5661	1.07	6189					N <sub>2</sub> H <sub>4</sub>	369.9	0.98	5674	1.07	6151							
	B <sub>2</sub> H <sub>6</sub>	317.7	2.12	6935	0.90	6188					B <sub>2</sub> H <sub>6</sub>	382.3	2.16	6967	0.90	6182							
	B <sub>2</sub> H <sub>4</sub>	340.6	1.96	6347	0.75	6671					B <sub>2</sub> H <sub>4</sub>	408.1	2.06	6456	0.76	6654							
	CH <sub>4</sub> /H <sub>2</sub> 92.6/7.4	318.5	3.36	5852	0.71	6287					CH <sub>4</sub> /H <sub>2</sub> 92.6/7.4	379.1	3.63	5929	0.72	6220							
GOX	CH <sub>3</sub> OH	283.9	1.36	5443	0.96	5556				GOX	CH <sub>3</sub> OH	339.3	1.40	5454	0.97	5541							
	C <sub>2</sub> H <sub>5</sub> OH	289.3	1.80	5729	1.03	5658					C <sub>2</sub> H <sub>5</sub> OH	346.1	1.90	5749	1.04	5624							
	CH <sub>4</sub>	313.0	3.30	5922	-	6171					CH <sub>4</sub>	373.2	3.40	6007	-	6096							
	GH <sub>2</sub>	407.7	3.29	4853	-	8356					GH <sub>2</sub>	474.6	3.92	5135	-	8259							
F <sub>2</sub>	H <sub>2</sub>	412.1	7.94	6680	0.46	8385				F <sub>2</sub>	H <sub>2</sub>	479.7	9.74	7212	0.52	8303							
	H <sub>2</sub> -Li 65.2/34.8	437.4	0.96	9411	0.19	8865					H <sub>2</sub> -Li 65.2/34.8	513.2	1.08	3514	0.20	8803							
	CH <sub>4</sub>	345.8	4.53	6972	1.03	6671					CH <sub>4</sub>	413.6	4.74	7049	1.04	6631							
	C <sub>2</sub> H <sub>6</sub>	337.7	3.68	6876	1.10	6519					C <sub>2</sub> H <sub>6</sub>	404.8	3.78	6889	1.10	6508							
	MMH	347.3	2.39	7425	1.24	6778					MMH	414.8	2.47	7462	1.25	6775							
	N <sub>2</sub> H <sub>4</sub>	365.5	2.32	8084	1.31	7280					N <sub>2</sub> H <sub>4</sub>	430.4	2.37	8098	1.31	7270							
	NH <sub>3</sub>	360.4	3.32	7862	1.12	7196					NH <sub>3</sub>	422.9	3.35	7869	1.12	7193							
	B <sub>2</sub> H <sub>6</sub>	356.7	5.14	8995	1.22	7008					B <sub>2</sub> H <sub>6</sub>	427.9	5.58	9077	1.24	6995							
OF <sub>2</sub>	H <sub>2</sub>	409.9	5.92	5990	0.38	8343				OF <sub>2</sub>	H <sub>2</sub>	477.7	7.37	6487	0.44	8195							
	CH <sub>4</sub>	355.8	4.94	7413	1.06	7082					CH <sub>4</sub>	421.8	5.58	7625	1.09	7019							
	C <sub>2</sub> H <sub>6</sub>	352.6	3.87	7444	1.11	7015					C <sub>2</sub> H <sub>6</sub>	412.0	3.86	7538	1.11	6979							
	RP-1	349.6	3.87	8038	1.28	6993					RP-1	410.5	3.85	8052	1.28	6992							
	MMH	349.8	2.28	7382	1.24	6952					MMH	415.2	2.58	7487	1.26	6911							
	N <sub>2</sub> H <sub>4</sub>	345.1	1.51	6823	1.26	6848					N <sub>2</sub> H <sub>4</sub>	409.2	1.65	6906	1.27	6826							
	BA 1185	343.8	1.75	6803	1.24	6737.00					BA 1185	405.7097	1.92	6908.9531	1.250997	6723							
	B <sub>2</sub> H <sub>6</sub>	371.1	3.95	8071	1.02	7322					B <sub>2</sub> H <sub>6</sub>	443.7	3.90	8044	1.02	7322							
	B <sub>2</sub> H <sub>4</sub>	359.9	4.16	8695	1.19	7065					B <sub>2</sub> H <sub>4</sub>	431.3	4.30	8734	1.19	7060							
	30/70 FLOX 30/70	H <sub>2</sub>	394.8	4.80	5534	0.32	8039					30/70 FLOX 30/70	H <sub>2</sub>	461.0	5.70	5762	0.36	7918					
RP-1		316.3	3.01	6623	1.09	6245				RP-1	376.9		3.30	6671	1.10	6191							
RP-1		344.5	3.84	7897	1.20	6904				RP-1	403.6		3.84	7897	1.20	6904							
MMH		359.8	2.82	8068	1.24	7170				MMH	423.5		2.83	8071	1.24	7170							
70/30 87.8/12.2	CH <sub>4</sub>	319.1	6.44	6580	1.16	6240				70/30 87.8/12.2	CH <sub>4</sub>	377.8	6.51	6583	1.17	6235							
	C <sub>2</sub> H <sub>6</sub>	309.2	3.67	6635	1.15	6001					C <sub>2</sub> H <sub>6</sub>	369.0	3.71	6638	1.16	5998							
	MMH	323.4	3.35	7015	1.34	6326					MMH	382.1	3.39	7025	1.35	6324							
	N <sub>2</sub> H <sub>4</sub>	336.7	3.22	7672	1.40	6779					N <sub>2</sub> H <sub>4</sub>	392.6	3.25	7675	1.40	6774							
	NH <sub>3</sub>	328.8	4.58	7404	1.30	6656					NH <sub>3</sub>	382.4	4.58	7404	1.30	6656							
	B <sub>2</sub> H <sub>6</sub>	334.3	7.76	8651	1.35	6568					B <sub>2</sub> H <sub>6</sub>	400.7	8.31	8700	1.37	6557							
	MMH	301.5	2.82	6362	1.40	5985					MMH	355.6	2.83	6364	1.40	5984							
	N <sub>2</sub> H <sub>4</sub>	313.5	2.66	7055	1.47	6349					N <sub>2</sub> H <sub>4</sub>	365.7	2.71	7075	1.47	6346							
CLF <sub>1</sub>	MHF-3	302.7	2.78	6406	1.41	6011				CLF <sub>1</sub>	MHF-3	356.7	2.81	6416	1.41	6008							
	MHF-5	305.0	2.46	6741	1.45	6114					MHF-5	357.2	2.49	6751	1.46	6112							
	MMH	287.8	2.97	6172	1.43	5742					MMH	338.7	3.01	6181	1.44	5740							
	N <sub>2</sub> H <sub>4</sub>	298.6	2.81	6730	1.50	6040					N <sub>2</sub> H <sub>4</sub>	347.8	2.89	6759	1.51	6048							
CLF <sub>2</sub>	MMH	288.4	2.17	5642	1.20	5720				CLF <sub>2</sub>	MMH	341.5	2.37	5646	1.21	5653							
	MMH-Be 70/31	309.1	0.99	5658	1.15	5906					MMH-Be 70/31	318.9	1.10	6160	1.22	6029							
	MMH-Al 63/27	294.5	0.85	5850	1.27	5820					MMH-Al 63/27	351.6	0.87	5897	1.23	5821							
	N <sub>2</sub> H <sub>4</sub>	292.0	1.36	5406	1.22	5833					N <sub>2</sub> H <sub>4</sub>	343.8	1.42	5408	1.22	5801							
N <sub>2</sub> O <sub>4</sub>	N <sub>2</sub> H <sub>4</sub> -UDMH 50/50	288.8	1.98	5589	1.19	5737				N <sub>2</sub> O <sub>4</sub>	N <sub>2</sub> H <sub>4</sub> -UDMH 50/50	341.7	2.15	5594	1.20	5675							
	N <sub>2</sub> H <sub>4</sub> -Be 77/23	325.5	0.51	5291	1.21	6166					N <sub>2</sub> H <sub>4</sub> -Be 77/23	392.6	0.60	5792	1.22	6263							
	B <sub>2</sub> H <sub>6</sub>	298.0	3.18	6622	1.09	5822					B <sub>2</sub> H <sub>6</sub>	357.7	3.26	6657	1.10	5815							
	MMH	293.6	2.28	5739	1.17	5756					MMH	345.1	2.50	5730	1.18	5681							
MON-25	N <sub>2</sub> H <sub>4</sub>	294.7	1.43	5495	1.20	5863				MON-25	N <sub>2</sub> H <sub>4</sub>	345.5	1.51	5488	1.20	5817							
	HYDINE	269.1	3.26	5148	1.30	5331					HYDINE	318.8	3.43	5129	1.31	5295							
	MMH	274.4	2.59	5146	1.28	5456					MMH	324.3	2.71	5131	1.28	5419							
	UDMH	272.0	3.13	5193	1.25	5397					UDMH	322.1	3.31	5174	1.26	5353							
IRFNA (III-A)	HYDINE	274.8	3.06	5282	1.30	5469				IRFNA (III-A)	HYDINE	325.8	3.25	5286	1.31	5435							
	MMH	279.9	2.43	5269	1.28	5590					MMH	331.0	2.58	5278	1.29	5356							
	UDMH	277.7	2.95	5319	1.25	5531					UDMH	329.0	3.12	5328	1.27	5499							
	MMH	284.3	3.46	4905	1.26	5650					MMH	336.4	3.69	4881	1.27	5610							
H <sub>2</sub> O <sub>2</sub>	N <sub>2</sub> H <sub>4</sub>	286.4	2.05	4781	1.27	5733				H <sub>2</sub> O <sub>2</sub>	N <sub>2</sub> H <sub>4</sub>	337.4	2.12	4771	1.27	5712							
	N <sub>2</sub> H <sub>4</sub> -Be 75/25	333.3	0.48	5063	1.22	6301					N <sub>2</sub> H <sub>4</sub> -Be 75/25	399.1	0.57	5104	1.23	6244							
	B <sub>2</sub> H <sub>6</sub>	305.4	2.20	4806	1.02	5955					B <sub>2</sub> H <sub>6</sub>	368.9	2.09	4682	1.01	5920							
	B <sub>2</sub> H <sub>4</sub>	341.3	1.16	4142	0.64	6836					B <sub>2</sub> H <sub>4</sub>	403.6	1.16	4142	0.64	6836							
N <sub>2</sub> H <sub>4</sub>	B <sub>2</sub> H <sub>6</sub>	328.7	1.27	4534	0.79	6495				N <sub>2</sub> H <sub>4</sub>	B <sub>2</sub> H <sub>6</sub>	391.6	1.27	4534	0.79	6495							
BA1185:		50.5% MMH, 29.8% N <sub>2</sub> H <sub>4</sub> , 19.7% H <sub>2</sub> O										HYDINE:		60% UDMH, 40% DETA									
MHF-3:		86% MMH, 14% N <sub>2</sub> H <sub>4</sub>										IRFNA III-A:		83.4% HNO <sub>3</sub> , 14% NO <sub>2</sub> , 2% H <sub>2</sub> O, 0.6% HF									
MHF-5:		55% MMH, 26% N <sub>2</sub> H <sub>4</sub> , 19% N <sub>2</sub> H <sub>4</sub> /NO <sub>2</sub>										IRFNA IV-HDA:		54.3% HNO <sub>3</sub> , 44% NO <sub>2</sub> , 1% H <sub>2</sub> O, 0.7% HF									
MON-25:		25% NO <sub>2</sub> , 75% N <sub>2</sub> O <sub>4</sub>										RP-1:											

## B. Calculating the Properties of Solid fuel Candidates for a Ramjet

Students were asked to do the following using the EXCEL and Python version of CEQUEL and compare the results for the five solid fuels and air at 500K for O/F from 1 to 15,  $P_c=30$  psi, and  $\varepsilon = 3.0$

- B1: 90% HTPB, 10% IPDI
- B2: 63% HTPB, 7% IPDI, 30% Aluminum
- B3: 63% HTPB, 7% IPDI, 30% Boron
- B4: 63% HTPB, 7% IPDI, 30% Boron Carbide
- B5: 81% HTPB, 9% IPDI, 10% Magnesium

A sample of the Excel and Pyrho inputs are shown in Figure 4 in which the  $c^*$  and  $I_{sp-vac}$  were calculated for each of the mentioned propellant combinations. Only combinations B2 through B5 are shown in this example. The Pyrho code is the same as shown in Figure 5 but is put side-by-side with the Excel version GUI for comparison. The results of these two methods are shown in Figure 10. As previously hinted, going through the menus and buttons of the Excel-based GUI are equivalent to the lines of code in Pyrho derived from the manual that the creator of Pyrho provided.

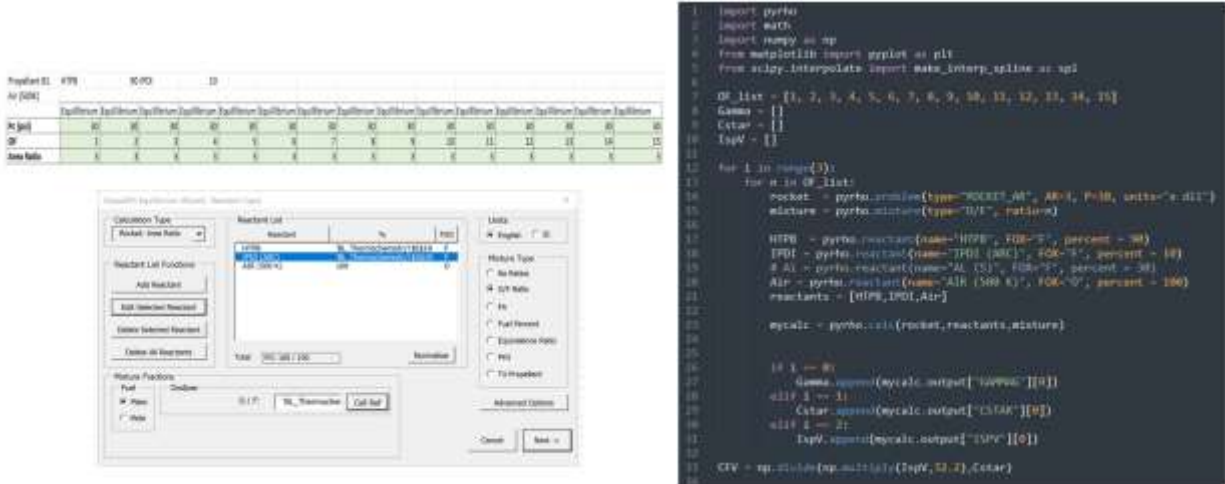


Fig. 10. Example Input Wizard and Python Code

The results are shown in Figure 10 below:

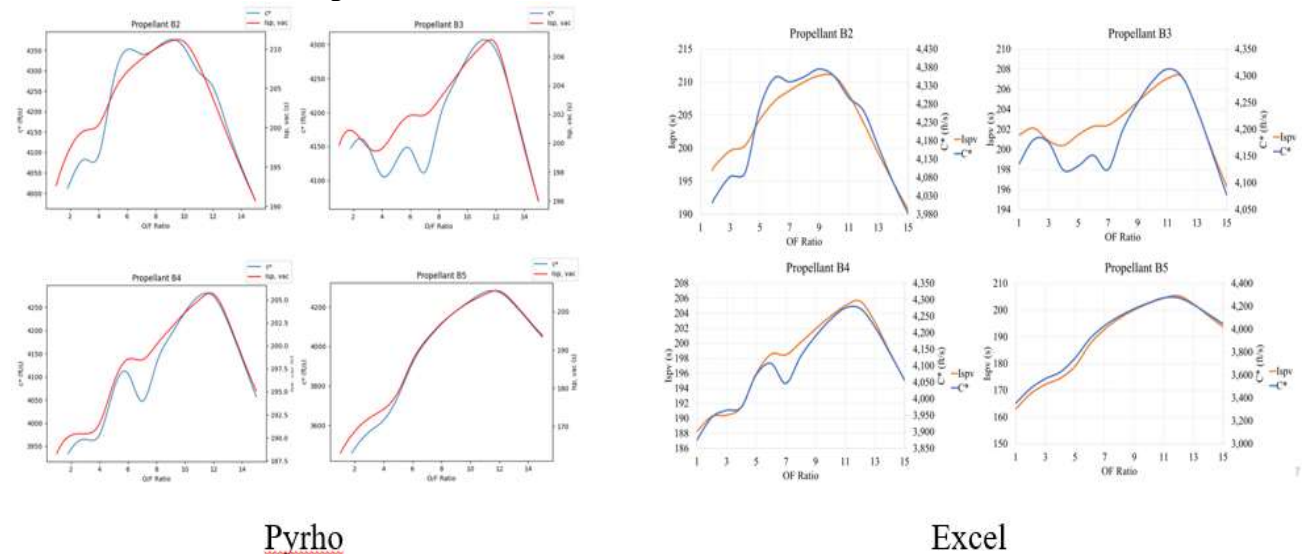


Fig. 11. Comparison of EXCEL and Python Results

It can be seen in Figure 11 that the charts between the two methods are essentially identical, save a slight difference in scaling which can be changed in the Pyrho script with simple Python graph scale code.

### C. Simulating the Flight Performance of a Solid Fuel Ramjet

Appendix A shows the concept of operations, guidelines and assumptions, and the candidate solid fuels for the ramjet engine. The overall objectives are to maximize the range of the entire system under the design constraints shown using an integral baseline solid boost system and considering four candidate solid fuels. Figure A1 shows solid propellant boosted ramjet that a center-perforated solid propellant grain (the gray portion) at burns on both ends is cast over a solid fuel grain (shown in green) for the ramjet.

The students evaluated three missions. Mission A was an all-solids mission using two center-perforated grains. This illustrated the range limitation of a pure rocket-based system for the mission selected. The instructor provided the internal ballistic calculations for the solid boost phase based on concepts the students had completed in MAE 540 (Prerequisite class). Mission B provided a Baseline Mission so that all students could work on the same design to establish and debug their calculations for the internal ballistics and trajectory calculations. Mission C was the Design Mission where each project Team did trade studies on the fuel candidates provided and changed input parameters within the guidelines and assumption of the project to find a maximum range.

For calculating the both the baseline and alternative formulation missions, it was assumed that the vehicle was launched horizontally at 33,000 feet. A one-dimensional analytic approach was used in this model meaning only movement in the horizontal direction was considered and gravity was ignored in the analysis. When the solid fuel in the ramjet is combusting, a web step is used for the modeling of the regression of the fuel. At each web step the burn area, air to fuel ratio, chamber pressure, and area ratio changes. The area ratio is changing since nozzle erosion is assumed to occur. Since these factors affect the thermochemical calculations CEQUEL was used at each step to calculate the vacuum specific impulse and the characteristic velocity. The characteristic velocity was then used to calculate chamber pressure at each step and the specific impulse was used to calculate the thrust coefficient. Since CEQUEL requires an initial chamber pressure the first guess for chamber pressure was 42.9 psi. After the initial pressure guess the chamber pressure from the previous web step was used. The summary of the equations used for this model can be found in the appendix.

To ensure that students had correctly created the model a baseline mission was made. The baseline mission used propellant B1-90% HTPB and 10% IPDI. The baseline model was completed in three assignments in the class and the solution for each was posted for the students to compare to. Once the students had the same results as the solution, the alternative mission could be created. Students were also required to perform a trade study to determine what would maximize the total impulse and range. The students could do this by changing the propellant formulation, grain design and or nozzle design from the baseline mission at the student's discretion. The trade study discussed here held the geometries from the baseline mission constant and varied the propellant formulation from the provided formulations. The alternative formulations provided were: B2-63% HTPB, 7% IPDI, and 30% Aluminum, B3-63% HTPB, 7% IPDI, and 30% Boron, 63% HTPB, 7% IPDI, and 30% Boron Carbide, and 81% HTPB, 9% IPDI, and 10% Magnesium. The results of the trade study for the range can be found in the top right image of Figure 1.2 in Figure 12. Based on the trade study, Propellant B2 was selected for Mission C in the project.

The baseline ramjet mission and the increased range mission were compared to a solid propellant mission that was provided by the instructor. The range, time to target, initial mass, and maximum Mach number (summarized in Figure 1.1 in Figure 12) were compared for each mission. In addition, a plot of the Mach number and range versus time was used as a visual representation of the difference in missions. Mission C with propellant B2 had the farthest range that was 5% farther than the baseline mission. Comparing the ramjet missions, the alternative propellant has a shorter time to target and a higher maximum Mach number than the baseline. However, the baseline mission has a lower initial fuel mass. The advantage of using all solids is its compact size, maximum Mach number and a lower time to target than the other missions. The advantage of using a ramjet is that the range increase to almost double the range even for the baseline mission. However, a disadvantage of the baseline mission is that the air at the inlet port is choked. A disadvantage of the alternative propellant for the ramjet is that a greater amount of fuel is required.



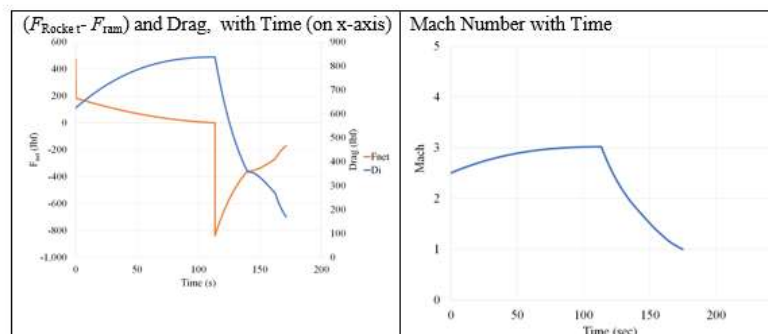
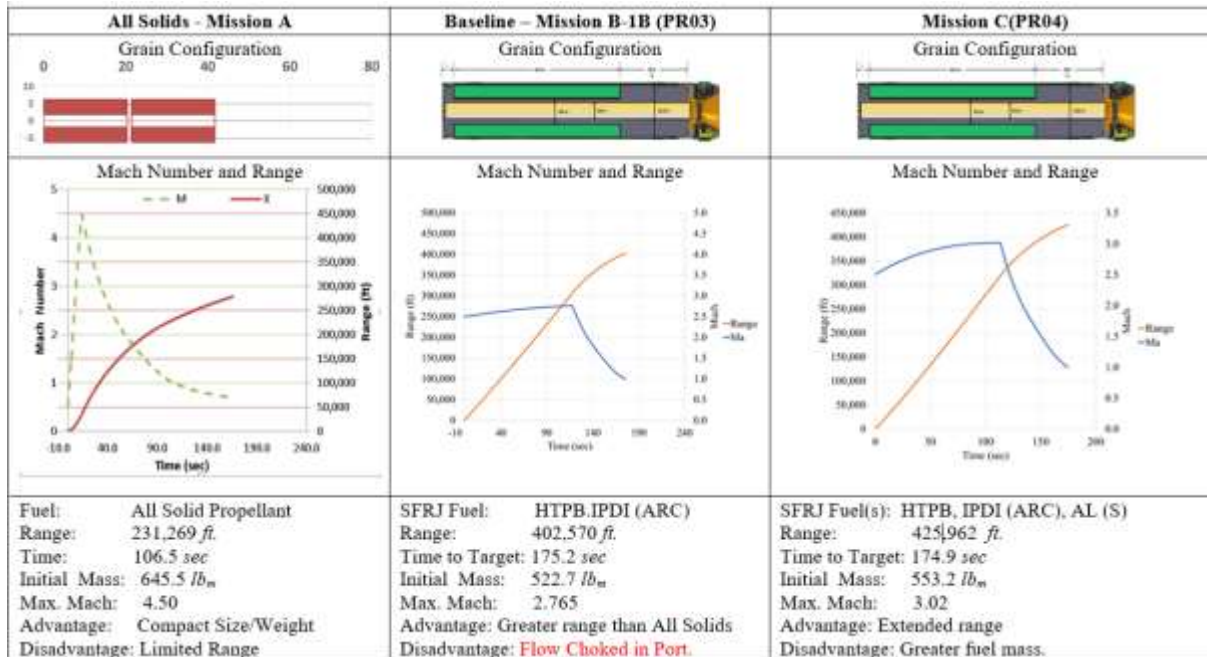


Figure 1.1] – Performance Plots Summary [Berg, Cox, Loeblich]

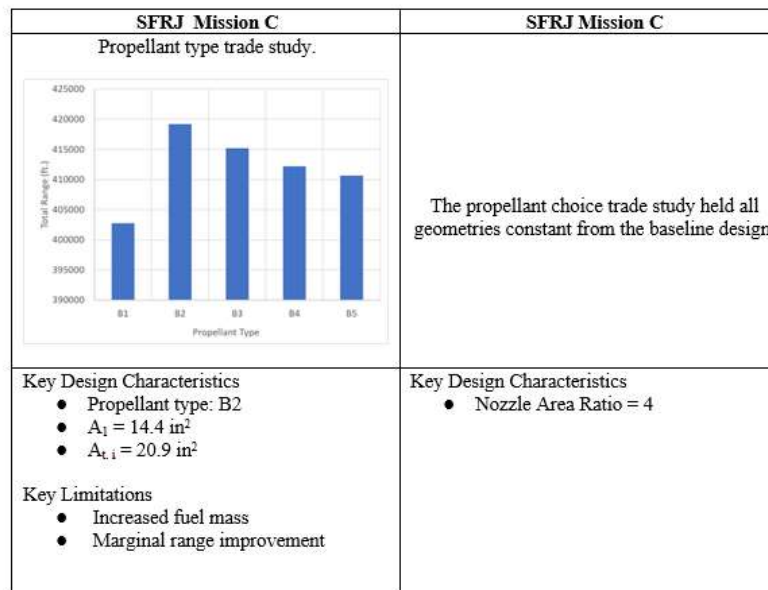


Fig. 12. Summary of Solid Fuel Ramjet Simulations supported by CEQUEL

### III. Final Remarks

The use of CEQUEL allowed students to quickly learn how to perform detailed thermochemical calculations. They applied this to calculated properties of over 50 different propellant combination, evaluate four candidate solid fuels for a ramjet propulsion system, and perform time-dependent calculation of internal ballistic/trajectory predictions for a class design project. The Excel version is easy to learn and integrate into graphics and detailed simulations. The Python version provides even more power for detailed simulations for the initial tests studied in this class, such as through looping to run more calculations at once. It also provides a new way to quickly share simulation information, showing all of the inputs at once in one script, and custom graphs can be created from the output.

### Acknowledgements

Thank you to Jonathan French at Praegysis for providing CEQUEL for student use during the class and for the technical support.

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## Appendix A

## UAH MAE 640 SFRJ 2021 Class Project Guidelines and Assumptions

### 1. Mission Requirements

- 1.1. Maximize the total impulse and range of the ramjet engine
- 1.2. Mission A is a Total Solid Propellant Mission (Data Provided by the Instructor)
- 1.3. Mission B's are Baseline Missions (Project Assignment's 01, 02, 03)
- 1.4. Mission C's is Team Design Mission to Maximize Total Impulse (range) by changing propellant (Project Assignment 04) formulation, grain design, and nozzle design.
- 1.5. Air Launch at 33,000 ft. (~10 Km)
- 1.6. The minimum takeover velocity for ramjet operation is Mach = 2.5
- 1.7. The mission is complete when Mach number descends to 1.0.
- 1.8. Propulsion system inner diameter and inner length is the same for all missions
- 1.9. Assume: horizontal flight with no induced drag from the angle of attack
- 1.10. Maximum Mach number for any flight is 4.5.
- 1.11. ~~Baseline Solid Propellant Mission (Mission A) is 90% HTPB/10% IPDI~~ (See section 6)
- 1.12. Review and Summarize Literature on at least 10 papers, reports, chapters, or articles on ramjet engines citing at least 5 in the references in Final Report.

### 2. Solid Propellant Booster (The Booster Information will be Provided))

#### 2.1. Propellant Properties

- 2.1.1. Propellant Temperature Coefficient,  $a_0 = 0.030 (in/s)[(lb/in^2)^{-n}]$
- 2.1.2. Propellant Pressure Exponent,  $n = 0.35$
- 2.1.3. Propellant Temperature Sensitivity,  $\sigma_p = 0.001 -/F$ ;
- 2.1.4. Propellant Characteristic Velocity,  $c^* = 5210 ft/s$
- 2.1.5. Propellant Gas Specific Heat Ratio,  $k = 1.3$
- 2.1.6. Propellant Reference Temperature,  $T_{b,0} = 70 ^\circ F$
- 2.1.7. Propellant Actual Initial Temperature,  $T_b = 70 ^\circ F$

#### 2.2. Chamber Requirements

- 2.2.1. Maximum Chamber Pressure,  $P_{1,max}$  is 1000 psi
- 2.2.2. Maximum Empty Chamber Inner Radius,  $R_f$  is 6.0 inches
- 2.2.3. Maximum Chamber Inner length for propellant,  $L_0$  is 68.0 inches
- 2.2.4. Minimum Boost Propellant Initial Bore Radius,  $R_{i,min}$  for structural integrity is 2.0 inches.
- 2.2.5. Maximum Mach Number in Boost Propellant Port is  $M_{port,max}$  is 0.5

### 3. Solid Fuel Ramjet Properties

- 3.1. The ramjet fuel is a center-perforated cylinder that only burns on the bore (see dimensions in Baseline Configuration Drawing)
- 3.2. Baseline Ramjet fuel, Propellant A, is 90% HTPB/(10% IPDI(ARC))
- 3.3. Propellant A Burning Rate Equation is  $r = 0.104 G_{air} 0.686 P_c 0.33 T_{air} 0.711 1000.335300.71$  where  $r$  {in/s};  $P_c$  {psia}; and  $T_c$  {R}
- 3.4. Propellant A solid density is  $0.0331 lb_m/in^3$
- 3.5. Thermochemical properties: Determined in CEQUEL using equilibrium calculations.
- 3.6. Ramjet  $c^*$  efficiency is 75% to 95%
- 3.7. Maximum Mach number in SFRJ Propellant Port is  $M_{port,max}$  is 0.5
- 3.8. HTPB  $c^*$  and specific heat ratio should be calculated from CEQUEL using "HTPB" and "IPDI(ARC)" fuel and "AIR(500K)" at a chamber pressure of 25 psi and use GAMMA for the specific heat ratio.



- 3.9. At SFRJ burnout assume that the ram drag is equal to the pressure and momentum thrust (no net thrust). So only aerodynamic drag is operating after SFRJ burnout.
- 3.10. The SFRJ chamber pressure must always be less than or equal to the chamber recovery pressure at any point in the SFRJ operation.
4. **Baseline Vehicle Aerodynamic Properties**
- 4.1. Atmospheric Properties at 33,000 ft. altitude (NASA 1976 Atmosphere)
- 4.1.1. Ambient Pressure,  $P_a = 3.800 \text{ lb}_f/\text{in}^2$
- 4.1.2. Ambient air density,  $\rho_a = 0.02560 \text{ lb}_m/\text{ft}^3$
- 4.1.3. Ambient Temperature,  $T_a = 400.987 \text{ R}$
- 4.1.4. Ambient Speed of Sound,  $a_a = 981.655 \text{ ft/s}$
- 4.1.5. The specific heat ratio of ambient air is 1.4

4.2. **Baseline External Axial Drag Coefficient for Configuration without an Inlet**

Mach Number	Cd
0	0.15
0.6	0.15
1.2	0.42
1.8	0.25
>4.0	0.175

Referenced to the German V-2 missile (Figure 4-3 Sutton 8<sup>th</sup> Edition)

Assume the drag coefficient is linearly interpolated between points (EXCEL Example)

- CD=IF(A2<0.6, 0.15, IF(A2<1.2, -0.12+0.45\*A2, IF(A2<1.8, 0.76 -0.283\*A2, IF(A2<4, 0.311-0.034\*A2, 0.175))))
- Where “A2” = Mach Number

4.3. **Baseline External Axial Drag with an Inlet Included**

- 4.3.1. Baseline Drag Coefficient with a single scoop external inlet during solid boost is assumed to be 125% of the Drag Coefficient without an Inlet data and use the changing the reference vehicle cross-sectional area as the drag calculation without the inlet.
- 4.3.2. Missile Cross Section;  $A_{\text{missile}} = 0.92175 \text{ ft}^2$  (Based on 13.0-in diameter)
- 4.3.3. At burnout of the SFRJ, the drag coefficient properties do not change (4.3.1 still applies)

4.4. **Baseline Inlet Aerodynamic and Recovery Properties**

- 4.4.1.  $P_{0a} = P_{\text{ambient}}[1 + 0.5 (\gamma - 1) * M^2]^{[\gamma / (\gamma - 1)]}$
- 4.4.2. Pressure recovery factor is  $[P_{01}/P_{0a}]_{\text{shock}} = 1.0 - 0.075 (M_a - 1)^{1.35}$
- 4.4.3. The maximum area of air inlet port is 50% of the initial ramjet port area to provide flame holding.
- 4.4.4.  $T_{01} = A_{\text{ambient}}[1 + 0.5 (\gamma - 1) * M^2]$
- 4.4.5.  $\dot{m}_{\text{air}} = P_{01} * A_{\text{inlet}} / c^*_{\text{act}}$
- 4.4.6. Assume  $c^*$  CEQUEL for Air is always (500K, 25 psia) for the purposes of calculating the inlet mass flow rate.

5. **Mass and External Dimensional Properties of Vehicle**

5.1. **Baseline SFRJ Dimensional Properties**

- 5.1.1.  $R_i = 3.0$  inches
- 5.1.2.  $R_f = 6.0$  Inches
- 5.1.3.  $L_o = 52$  inches

## 5.2. BASELINE SFRJ Mass Properties

5.2.1. Takeoff Mass in Baseline Ramjet Configuration: includes the following:

5.2.1.1. Inlet mass,  $m_{inlet}$ ;

5.2.1.2. Booster Propellant Initial mass,

5.2.1.3.  $m_{BP,o}$  and SFRJ Initial Propellant Mass,

5.2.1.4.  $m_{SFRJ,o}$ , the Mass of the structure,

5.2.1.5.  $m_{struc.}$  and the mass of the payload,  $m_{pl}$ .

5.2.2. Mass in Inlet Hardware,  $m_{inlet} = 20 \text{ lb}_m$

5.2.3. Boost Propellant Initial Mass,  $m_{P,o}$  is initial volume of Boost Propellant time density of Boost propellant (See Figure 1 for configuration)

5.2.4. SFRJ Propellant Initial Mass,  $m_{SFRJ,o}$  is the initial volume of SFRJ Propellant time density of SFRJ propellant (See Figure 1 for configuration)

5.2.5. The mass of the structure is 159.14  $\text{lb}_m$

5.2.6. The mass of the payload is 220.00  $\text{lb}_m$ .

## 5.3. Baseline All Solid Mass Properties

5.3.1. Takeoff mass,  $m_o$  is the mass of the structure,  $m_{struc.}$ , plus the solid propellant mass,  $m_{p,o}$ .

5.3.2. The instructor will provide final mass properties in the Project Report template.

## 6. Nozzle(s)

6.1.1. Maximum Exit Area of Nozzle:  $A_2 = 0.7845 \text{ ft}^2$

6.1.2. Assume: Nozzle Exit Area does not Erode

6.1.3. Nozzle throat diameter erosion is based on  $dt, t+1=dt, i+0.000087*tt+1-ti*Pc,i$ , where pressure is in  $\text{lb}_f/\text{in}^2$  and  $d$  is the nozzle diameter in inches.

6.1.4. Thrust Coefficient is based on CEQUEL

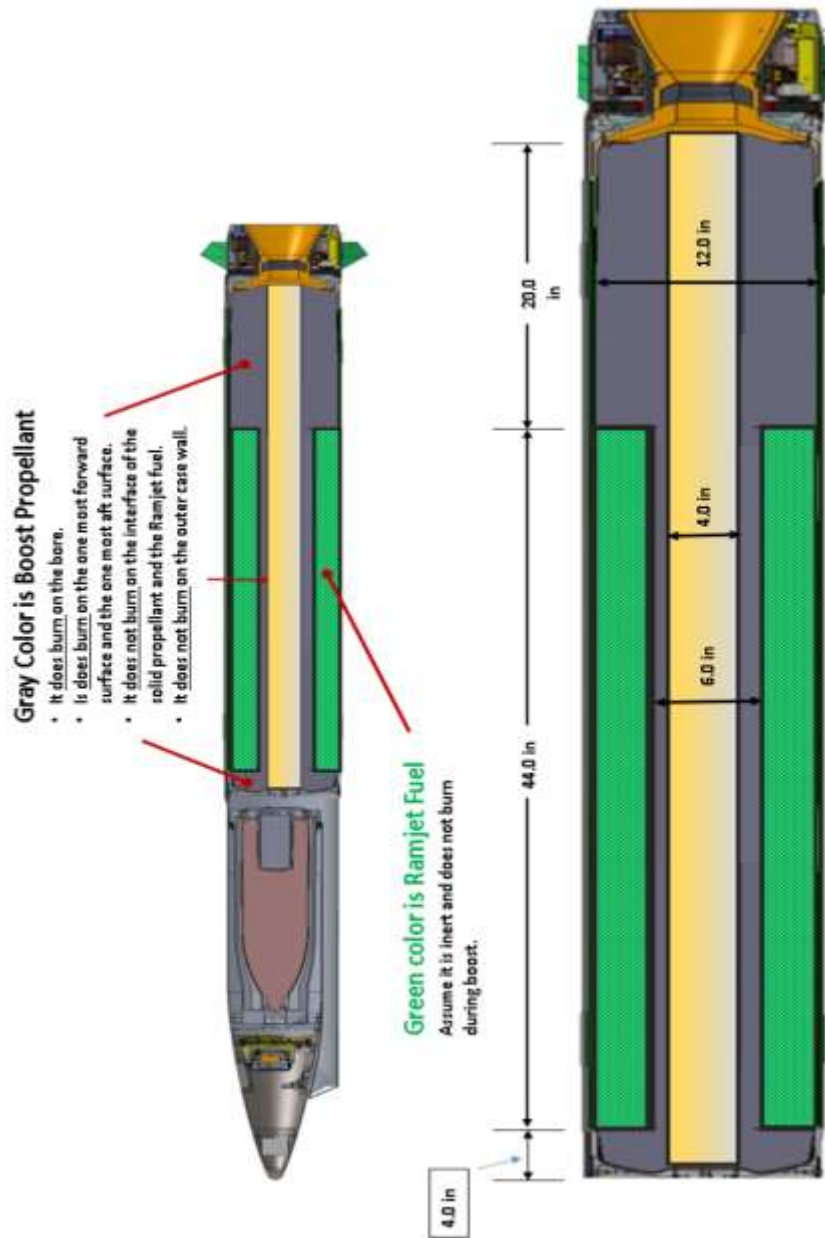
6.1.5. Minimum Thrust Coefficient for flow separation is based on 33%  $P_e/P_a$

6.1.6. The throat area can be instantly enlarged, and the area ratio changed at the beginning of the SFRJ operation to be best suited for the lower pressure combustion.

6.1.7. The area ratio of the nozzle must always be greater than or equal to 1.0 so if erosion causes the throat to grow past the size of the initial exit area, the exit area must be enlarged to keep the throat area ratio at 1.0

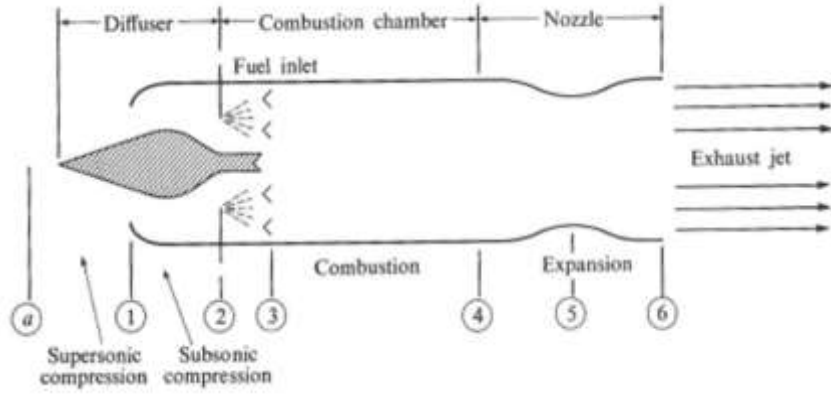
## 7. Candidate Solid Fuels

Ingredient	Baseline B	Prop. C	Prop. D	Prop. E	Prop. F
HTPB/IPDI	90%/10%	63%/7%	63%/7%	63%/7%	81%/9%
Aluminum	-	30%	-	-	-
Boron	-	-	30%	-	-
Boron Carbide	-	-	-	30%	-
Magnesium	-	-	-	-	10%



**Figure A1 – Baseline Solid Propellant Boosted Solid Fuel Ramjet**

shows the station convention used for this analysis.



**Figure A-2 Station Convention for the Analysis**

### Appendix B-Basic Equations

The propellant volume is multiplied by the propellant density to calculate the propellant mass. The equation for propellant mass as a function of web distance is

$$m_{p,i} = [V_i]\rho_b = A_i L_i \rho_b = \pi [R_o^2 - (R_i + w_i)^2] L_o \rho_b \quad (1)$$

Since the solid propellants are composed of various substances the bulk density of the propellant needs to be calculated. Equation 2 is used to calculate bulk density based on the mass fraction or percentages of each component.

$$\rho_b = \frac{1}{\frac{x_1}{\rho_1} + \frac{x_2}{\rho_2} + \frac{x_3}{\rho_3}} \quad (2)$$

The web distance is incremented as the propellant burns using

$$w_{i+1} = w_i + \Delta w \quad (3)$$

Maximum web thickness is limited by the initial amount of propellant and be determined using Equations 4 and 5.

$$w_{max} = R_o - R_i \quad \text{if } R_o - R_i \leq \frac{L_o}{2} \quad (4)$$

$$w_{max} = \frac{L_o}{2} \quad \text{if } \frac{L_o}{2} > R_o - R_i \quad (5)$$

For the prediction of the performance of the propellant, the propellant burn rate needs to be calculated using

$$r_i = \frac{0.104 G_{03,i}^{0.686} p_{03,i}^{0.33} T_{03,i}^{0.71}}{100^{0.33} 530^{0.71}} \quad (6)$$

The air mass flux is calculated using

$$G_{03,i} = \frac{\dot{m}_{03,i}}{\pi R_i^2} \quad (7)$$

Since burning surface area is a function of propellant web, radius, and length, it is calculated using Equation 8.

$$A_{b,i} = 2\pi R_i L_o \quad (8)$$

The radius at the step  $i$  can be calculated using

$$R_i = R_1 + w_i \quad (9)$$

The bore area can be ascertained from

$$A_{bore,i} = \pi R_i^2 \quad (10)$$

Fuel mass flow rate needs to be calculated to determine the oxidizer to fuel ratio and total mass flow rate. Equation 11 is used to calculate fuel mass flow rate.

$$\dot{m}_{f,i} = 2\pi\rho_f R_i L_i \frac{0.104 G_{03,i}^{0.686} P_{03,i}^{0.33} T_{03,i}^{0.71}}{100^{0.33} 530^{0.71}} \quad (11)$$

The oxidizer to fuel ratio is calculated using

$$OF = \frac{\dot{m}_{03,i}}{\dot{m}_{f,i}} \quad (12)$$

Total mass flow rate can be calculated from

$$\dot{m}_4 = \dot{m}_3 + \dot{m}_f \quad (13)$$

Chamber pressure is needed to calculate the rocket engine thrust. Equation 14 is used to calculate chamber pressure.

$$P_{c,i} = \frac{C_4^* (\dot{m}_{1,i} + \dot{m}_{f,i}) \eta_{c^*}}{A_{5,i}} \quad (14)$$

Net force on the missile for internal ballistic analysis can be calculated using the following equations

$$F_{net} = F_{rocket} - F_{ram} \quad (15)$$

$$F_{net} = \dot{m}_6 u_6 - \dot{m}_1 u_1 + (P_6 - P_a) A_6 \quad (16)$$

The thrust of the rocket can be calculated using

$$F_{rocket,i} = C_{f,i} P_{c,i} A_{5,i} \quad (17)$$

In Equation 17, thrust coefficient is determined from

$$C_{f,i} = C_{fv,i} - \frac{P_a}{P_{c,i}} \varepsilon_i \quad (18)$$

Vacuum thrust coefficient can be determined from

$$C_{fv,i} = \frac{I_{sp}}{C_{act}} \quad (19)$$

Initial throat area is calculated using the provided initial throat diameter for the baseline was calculated using the provided throat diameter and Equation 20.

$$A_{5_0} = \frac{\pi}{4} d_{5,o}^2 \quad (20)$$

Throat diameter is a function of time which during the internal ballistic analysis is a function of web as can be seen below.

$$t_{i+1} = t_i + \frac{w_{i+1} - w_i}{r_i} = t_i + \frac{\Delta w}{r_i} \quad (21)$$

The new throat diameter is calculated from

$$d_{5,i+1} = d_{5,i} + 0.000087(t_{i+1} - t_i)p_{c,i} = d_{5,i} + 0.000087 \frac{w_{i+1} - w_i}{r_i} p_{c,i} \quad (22)$$

Exit area of the nozzle is assumed to be constant for the analysis and can be found from

$$\varepsilon_o A_{5,o} = A_{6,o} \quad (23)$$

Using the calculated nozzle exit area and calculating the new throat area, the new area ratio can be calculated using

$$\varepsilon_i = \frac{A_{e,0}}{0.25\pi d_{t,i}^2} \quad (24)$$

The total impulse of each time step can be determined using Equation 25.

$$I_i = \frac{F_i + F_{i-1}}{2} (t_i - t_{i-1}) \quad (25)$$

The system total impulse can be calculated by summing the total impulse for each time step as seen below.

$$I = \sum_1^k I_i = \sum_1^k \frac{F_i + F_{i-1}}{2} (t_i - t_{i-1}) \quad (26)$$

The average specific impulse can be calculated from

$$I_{sp,ave} = \frac{I}{(m_{p0} + m_1)g_e} \quad (27)$$

The initial weight of the missile is determined by

$$m_i = m_{p,i} + m_{struc} + m_{inlet} + m_{payload} \quad (28)$$

The ramjet drag can be calculated as seen below.

$$F_{ram} = \dot{m}_{1,i} u_{1,i} \quad (29)$$

The velocity used to calculate ramjet drag can be found from Equation 30.

$$u_{o,a} = M_{a,o} a_a \quad (30)$$

Once the velocity is calculated for the initial conditions the inlet area can be determined using

$$A_1 = \frac{\dot{m}_{o,a}}{\rho_a u_{o,a}} \quad (31)$$

Mass flow rate of air can be calculated using

$$\dot{m}_{a,i} = \rho_a M_a a_a A_1 = \rho_a v_i A_1 \quad (32)$$

The drag experienced by the missile can be computed from

$$D_i = 0.5 * \rho_{a,i} * C_{d,i} * u_i^2 * A_{missile} \quad (33)$$

Drag coefficient is a piecewise function based on the Mach number. This function is characterized in Equations 34 to 38.

$$C_{d,i} = 0.15 * 1.25 \{0 \leq M_i < 0.6\} \quad (34)$$

$$C_{d,i} = (-0.12 + 0.45 * M_i) * 1.25 \{0.6 \leq M_i < 1.2\} \quad (35)$$

$$C_{d,i} = (0.76 - 0.283M_i) * 1.25 \{1.2 \leq M_i < 1.8\} \quad (36)$$

$$C_{D,i} = (0.311 - 0.034M_i) * 1.25 \{1.8 \leq M_i < 4\} \quad (37)$$

$$C_{d,i} = 0.175 * 1.25 \{M_i \geq 4\} \quad (38)$$

Acceleration of the missile in the x-direction can be ascertained from

$$a_{xi} = \frac{F_{rocket,i}}{m_i} - \frac{F_{ram,i}}{m_i} - \frac{D_i}{m_i} \quad (39)$$

Initial velocity of the missile is determined from Equation 40.

$$v_{0,i} = M_{a,0} a_a \quad (40)$$

The new velocity of the missile is calculated using the time step, acceleration, and the previous velocity.

$$v_{i+1} = v_i + a_i(t_{i+1} - t_i) \quad (41)$$

The stagnation pressure at station a in the above section was calculated from Equation 42.

$$P_{0a} = P_a \left(1 + 0.5(\gamma - 1)M_a^2\right)^{\frac{\gamma}{\gamma-1}} \quad (42)$$

Stagnation temperature can be calculated from Equation 43 and will remain constant through all of the stations. However, stagnation temperature will change as Mach number changes.

$$T_{0a} = T_a \left(0.5(\gamma - 1)M_a^2\right) \quad (43)$$

Stagnation pressure ratio between station 1 and station a is

$$\frac{P_{01}}{P_{0a}} = 1 - 0.075(M_a - 1)^{1.35} \quad (44)$$

Stagnation pressure at station 3 can be calculated using Equations 45.

$$P_{03,i} = P_a \left(1 + \frac{\gamma-1}{2}M_a^2\right)^{\frac{\gamma}{\gamma-1}} \left(1 - 0.075(M_{aq} - 1)^{1.35}\right) (0.8)(0.95) \quad (45)$$

Diffuser throat area can be computed using the equation below.

$$A_{2,a} = A_2 \left(\frac{1}{M_{2a}}\right) \left(\frac{2+(\gamma-1)M_{2a}^2}{\gamma+1}\right)^{\frac{\gamma+1}{2(\gamma-1)}} \quad (46)$$

Equation 47 is used to compute the range of the missile.

$$X_{x,i+1} = 0.5(v_i + v_{i+1})(t_{i+1} - t_i) + X_i \quad (47)$$