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COMPUTATIONAL MODELING OF A LIQUID NITROUS OXIDE AND ETHANOL FUELED ROCKET ENGINE

Stewart H. Youngblood[*], Dr. Michael J. Hargather[†], Mark C. Grubelich[‡], and Venner Saul[§]

ABSTRACT

A comparative study of the modeling of a liquid rocket engine is performed using NASA CEA and Cantera, an open-source MATLAB-based code. The goal of this modeling is to demonstrate the ability of Cantera to accurately model the basic chemical equilibrium, thermodynamics, and transport properties for varied fuel and oxidizer operating conditions. Once validated for basic equilibrium, an expanded MATLAB code, referencing Cantera, is advanced beyond CEA's capabilities to include atomization and vaporization of propellant droplets, chemical kinetics, and heat transfer between the flow and chamber walls and nozzle. The developed computational code is utilized to analyze rocket engine performance across a range of operating pressures, fuel-oxidizer mixture ratios, and outlet nozzle configurations. In particular the code is used to evaluate performance of a novel nitrous oxide and ethanol rocket design. The computational performance predictions will be compared against experimental results for a small-scale rocket engine operating on nitrous oxide and ethanol with an average thrust of 667N (150 lbf) at the design condition. Interfaced with MATLAB, Cantera's predictions for equilibrium properties are almost exactly equal to those of CEA. Future testing with an experimental rocket engine will include measurement of the operating characteristics at the simulated conditions.

INTRODUCTION

NASA Lewis CEA (Chemical Equilibrium with Applications) is a well-known and widely-used computational program for performing chemical equilibrium and rocket performance calculations[6]. To perform these calculations, CEA references input files that contain thermodynamic data and transport property data for the chemical species present. Specific data set files can be used or created for these calculations or a standard NASA species data set may be used if the test scenario and reacting species fall within the NASA data set applicability range[7]. Test scenarios may be inputted by the user into CEA using a GUI interface or by using a command console to run a test scenario file, providing simplicity in performing calculations of reacting systems. However, the interfacing of CEA with other programs to expand CEA's capabilities or to use CEA for performing equilibrium calculations within a computational model can prove challenging as CEA is designed to function as a standalone program.

Cantera is an open source chemical equilibrium calculation code developed at the California Institute of Technology. Cantera is an object based software tool for solving chemically reacting flow problems involving thermodynamics, transport processes, and chemical kinetics, and was designed to be accessed by various environments, including C++, Fortan 90, MATLAB, and Python[2]. Reaction mechanism files, containing thermodynamic, transport process, and chemical kinetics data, are reference by Cantera when it makes chemical equilibrium calculations and flow property calculations. These reaction mechanism data files allow the user to use a predefined data file or create their own for a specific reaction process. Unlike CEA, Cantera is purely a chemical equilibrium and flow property solving software, relying on the user to write

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modeling code in their preferred operating environment and reference Cantera to perform the chemical reaction and flow property calculations. This requires more work from the user to perform calculations using the software, but provides the user with the ability to create advance models of thermodynamic flow systems. For this reason, Cantera was chosen by the New Mexico Tech team to be used in modeling the performance of a liquid nitrous oxide and ethanol fueled rocket engine. Using MATLAB as the computational environment, a computational model is developed that will include a user developed reaction mechanism file, a propellant droplet vaporization model, chemical kinetics, and heat transfer between the combustion gas flow and rocket combustion chamber and nozzle.

The idea of using Cantera for performing equilibrium calculations in rocket performance modeling has been discussed before[8], but Cantera has not formally been presented as an acceptable alternative to CEA. A primary goal of this work is to demonstrate Cantera's ability to provide comparable results to CEA for equilibrium and flow property calculations. With Cantera shown to be acceptable for equilibrium and flow property calculations, the developed MATLAB rocket engine model, referencing Cantera, must then be shown to provide comparable results to CEA for rocket performance calculations. With Cantera and the MATLAB/Cantera rocket engine model established as comparable to CEA, the developed rocket engine model can be advanced beyond CEAs capabilities. Ultimately the code developed here was used to design a small-scale experimental rocket engine being developed at New Mexico Tech. The computational performance results from this advanced model will be compared against the small-scale rocket engine operating with an average thrust of 667N (150lbf) at the design condition for validation.

II. COMPUTATIONAL METHODS

The computational work performed was completed using a desktop computer operating with a Windows 7 operating system. The computational rocket engine model was written using, and Cantera interfaced with, the MATLAB R2013a environment. The graphic user interface (GUI) version of CEA was used for making calculations with CEA.

II.A. CEA and MATLAB/Cantera Equilibrium Calculations

Reaction scenarios were chosen for a gas phase mixture of nitrous oxide and ethanol that both CEA and Cantera would solve for comparison of the respective programs' results. These scenarios were chosen to be reasonably representative of conditions seen in rocket combustion processes. A direct comparison was performed using a short MATLAB script to reference Cantera's equilibrium and flow property functions and direct user input into the GUI version of CEA for these predetermined conditions. The reaction scenarios include three different stoichiometric mixtures reacting to equilibrium at five different pressures starting at an initial temperature of 298K (76.73°F). An oxidizer and fuel ratio (O/F) of 5.7 was chosen for a stoichiometric mixture of nitrous oxide and ethanol, and a fifty percent deviation from stoichiometric to fuel rich and oxidizer rich were chosen to be solved for equilibrium. The equilibrium calculations were made across a pressure range of one atmosphere to one hundred atmospheres in twenty five atmosphere steps. The reaction scenarios are outlined below:

Initial Temperature	Gas Mixture Stoichiometry	Initial Pressure
298K (76.73 °F)	2.85	0.101MPa (14.7psi)
	5.7	2.53MPa (367psi)
	8.55	5.06MPa (735psi)
		7.60MPa (1102psi)
		10.13MPa (1470psi)

Table 1. Reaction simulations for equilibrium calculations. 15 total simulations performed

Equilibrium was calculated for constant enthalpy and pressure of the gas mixture because this is what both CEA and the developed MATLAB/Cantera rocket engine model use

when solving for chemical equilibrium rocket performance calculations. The calculated results were tabulated and compared. The properties chosen to compare were final temperature, enthalpy, entropy, internal energy, Gibbs function, density, and specific heat (Cp). The standard NASA thermodynamic and transport process data file was used with CEA. For Cantera, a Lawrence Livermore National Labs (LLNL) developed reaction mechanism file for ethanol combustion was used[5]. This LLNL mechanism file was sourced directly from the LLNL website. The mechanism file was modified to be able to account for ethanol combustion with nitrous oxide, this included the addition of chemical species and the corresponding thermodynamic and transport process data to the LLNL mechanism file. Chemical species added and their respective property data included nitrous oxide (NO2), nitric oxide (NO), and nitrogen dioxide (NO2). The reaction equations for the added species break down to their respective radicals were also included. The choice for initial comparison to be made with the modified mechanism file was done to check that the mechanism file was functioning properly and calculations made using it compared well with CEA's calculations. Currently the modified LLNL file does not include chemical kinetic data such as rate constants for reactions, activation energy, or the effects of Arrhenius kinetics.

II.B. CEA and MATLAB/Cantera Rocket Performance Calculations

The first version of the developed MATLAB/Cantera rocket engine model code shares the same assumptions that govern CEA's rocket performance calculations: one-dimensional forms of the continuity, energy, and momentum equations, steady-state operation, homogeneous mixing, adiabatic combustion, complete combustion, isentropic flow through the nozzle, zero velocity at the combustion chamber inlet, infinite area combustor, and ideal gas behavior. In addition the same governing equations for rocket performance apply to both codes, sourced from Mcbride and Gorden[6] and Huzel and Huang[4]. The performance parameters include characteristic exhaust velocity (C^*), thrust coefficient (C_F), area ratio of the nozzle (A_{exit}/A^*), exit velocity of the gas from the nozzle (U_{exit}), and specific impulse (I_{sp}):

$$\boldsymbol{C^*} = \frac{(\boldsymbol{P_{inf}} \cdot \boldsymbol{A^*} \cdot \boldsymbol{g_c})}{\dot{\boldsymbol{m}}} \tag{1}$$

$$\boldsymbol{C_F} = \frac{\boldsymbol{U}}{\boldsymbol{C^*}} \tag{2}$$

$$\frac{\boldsymbol{A_{exit}}}{\boldsymbol{A^*}} = \frac{\boldsymbol{\rho^* \cdot U^*}}{\boldsymbol{\rho_{exit} \cdot U_{exit}}} \tag{3}$$

$$\boldsymbol{U_{exit}} = \sqrt{\boldsymbol{2 \cdot (H_\circ - H_{exit})}} \tag{4}$$

$$\boldsymbol{I_{sp}} = \frac{\boldsymbol{U_{exit}}}{\boldsymbol{g_c}} \tag{5}$$

Initial inputs for both codes are pre-combustion propellant temperature, propellants, mixture ratio, chamber pressure, and the ambient pressure of the environment the rocket will be operating in.

CEA uses the standard NASA data file, and solves for flow properties at three main points: the combustion chamber, the nozzle throat, and the nozzle exit. With the governing assumptions, constant enthalpy and pressure equilibrium of the propellant gas mixture is calculated for the combustion chamber. The resultant calculated thermodynamic and transport properties are used as the stagnation properties of the rocket for nozzle calculations. Throat conditions are calculated by an iterative method to determine the pressure for which the area ratio is a minimum, or alternatively, the flow conditions for which the gas velocity is equal to the local speed of sound of the flow. Equilibrium is calculated for the gas flow through the nozzle. Exit conditions are calculated and the area ratio determined by an iteration method to find the flow

pressure that corresponds to the user assigned pressure ratio (perfectly expanded for these cases) and the stagnation (combustion) entropy.

The MATLAB/Cantera rocket engine model iteration method differs in regards to what is used for determining convergence. First, combustion chamber properties are calculated for constant enthalpy and pressure equilibrium of the propellant gas mixture, and the resultant properties are used as the stagnation properties for later calculations. Secondly, the throat properties are solved using a "guess and check" iterative method. A gas flow temperature is guessed, and the pressure iterated, using a bisection method, until the entropy at the throat is within a predefined tolerance of the stagnation entropy. Equilibrium is calculated for each iterative step, and the enthalpy and the local speed of sound at the throat are compared against the stagnation enthalpy. Convergence at the throat is determined once two conditions are met:

$$\boldsymbol{abs}(\boldsymbol{S}_{\circ} - \boldsymbol{S}^{*}) < \boldsymbol{10^{-6}} \quad (6)$$

$$\boldsymbol{abs}(\boldsymbol{H}_{\circ} - (\boldsymbol{H}^{*} + \tfrac{\boldsymbol{1}}{\boldsymbol{2}}\boldsymbol{a^{2}})) < \boldsymbol{10^{-6}} \quad (7)$$

Finally, the exit properties are calculated by assuming the gas flow exiting the nozzle is perfectly expanded, such that the pressure of the gas flow is equal to the ambient pressure. The iterative method used is a bisection method that iterates the gas temperature from the nozzle throat top the nozzle exit. Equilibrium of the gas flow is calculated for that temperature and the exit pressure. The entropy of the exiting gas is then compared against the stagnation entropy of the flow. Convergence at the nozzle exit is determined when:

$$\boldsymbol{abs}(\boldsymbol{S}_{\circ} - \boldsymbol{S}_{\boldsymbol{exit}}) < \boldsymbol{10^{-6}} \quad (8)$$

Test scenarios were chosen for the rocket performance calculations that would be solved by both CEA and Cantera. These scenarios were chosen to check the applicability of the MATLAB/Cantera code across a range of rocket operating points. The conditions for each simulation can be found in table 2:

Initial Propellant Temperature	Mixture Ratio (O/F)	Chamber Pressure
298K (76.73 °F)	2.85	1.72MPa (250psi)
	5.7	3.45MPa (500psi)
	8.55	5.17MPa (750psi)
		6.89MPa (1000psi)

Table 2. Rocket simulations. 12 total simulations performed

The performance properties chosen for comparison were chamber temperature, throat temperature, exit temperature, exit Mach number, area ratio, characteristic exhaust velocity, coefficient of thrust, and specific impulse. Each mixture ratio is run at each of the four chamber pressures.

II.C. Advanced MATLAB/Cantera Rocket Engine Model

The MATLAB/Cantera rocket engine model was advanced in two steps. The first step was to modify the model to solve for chamber pressure using propellant rate and nozzle dimensions, specifically throat diameter. This would allow the effects of varying chamber flow rate to be observed and aid in the selection of operational flow rates for the experimental rocket engine under development. User inputs for initial conditions are: total propellant mass flow rate, initial propellant temperature, nozzle throat diameter, and mixture ratio. To solve for chamber pressure, the equation for isentropic choked flow was employed:

$$\dot{m}^* = \frac{A^* \cdot P_o}{\sqrt{T_o}} \cdot \sqrt{\frac{\gamma}{R}} * \left(1 + \frac{\gamma - 1}{2}\right)^{-\frac{\gamma+1}{2(\gamma-1)}} \quad (9)$$

Combined with the continuity equation, chamber pressure is iterated using a bisection method. After combustion of the propellants, the flow properties found are used in determining the specific heat ratio at the throat, and then the mass flow rate at the throat is calculated. Convergence is determined to be the point that the difference between the propellant mass flow and the mass flow at the throat are less than a predefined tolerance, as seen below:

$$abs\left(\dot{m}_{propellant} - \dot{m}^*\right) < 10^{-6} \quad (10)$$

The calculated chamber pressure for the inputted flow rate and initial conditions were then run through CEA to provide rocket performance values to compare with the results from the modified MATLAB/Cantera rocket engine model. Five propellant flow rates were chosen to be tested, starting at 0.181 kg/s (0.4 lbm/s) to 0.272 kg/s (0.6 lbm/s) in 0.022 kg/s (0.05 lbm/s) increments. These were calculated for a mixture ratio of 4.5 as this is the design condition for the experimental rocket currently under construction. This mixture ratio was chosen for fuel-film cooling and peak temperature concerns and followed the logic from previous work by Tokudome et al[8]. These run scenarios were performed to verify this method of calculating chamber pressure provided comparable results to CEA's predictions.

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III EXPERIMENTAL RESULTS

III.A. CEA and MATLAB/Cantera Equilibrium Calculation Results

Table 1, 2, and 3 present the percentage difference between the results produced by Cantera compared to CEA for constant enthalpy and pressure equilibrium. For the seven calculated properties, β, that were compared for the three different mixture stoichiometries, all differences remained under one percent, and the majority under 0.2 percent. For each mixture, the maximum calculated difference is highlighted. The difference percentage is calculated as:

$$Difference = \frac{\beta_{Cantera} - \beta_{CEA}}{\beta_{CEA}} * 100 \quad (11)$$

The two properties that exhibited large deviations between the results produced by Cantera and CEA were internal energy and specific heat (Cp). The maximum deviation observed being 0.919% less than CEA's result for the internal energy calculated by Cantera at 100 atmospheres and a mixture stoichiometry of 8.55. For temperature, enthalpy, entropy, Gibbs function, and density calculations, the calculated values exhibited less than a 0.2% difference.

The source of difference for the values calculated is believed to be a result of the differences in the thermodynamic and transport property data between the modified LLNL mechanism file used by Cantera and the NASA data file used by CEA. The modified LLNL file uses NASA thermodynamic and transport data for part of its chemical species data, however some of the chemical species included use data that is LLNL specific. This chemical species data is open source as is the overall LLNL mechanism file. However, the differences are small and the results presented below demonstrate Cantera's ability to provide comparable and often near exact results as the results produced by CEA. This shows Cantera as an alternative to CEA for making equilibrium calculations, and that it can be used in the development of the MATLAB based rocket engine modeling code.

Pressure (MPa, psi)	Temperature	Enthalpy	Internal Energy	Entropy	Gibbs	Density	Cp
0.101 (14.7)	0.115%	0.000%	0.369%	0.002%	0.117%	0.077%	0.346%
2.53 (367)	0.146%	0.000%	0.617%	0.006%	0.146%	0.138%	0.440%
5.06 (735)	0.152%	0.000%	0.692%	0.008%	0.152%	0.143%	0.458%
7.60 (1102)	0.157%	0.000%	0.735%	0.005%	0.158%	0.148%	0.471%
10.13 (1470)	0.156%	0.000%	0.767%	0.007%	0.159%	0.151%	0.471%

Table 3. Difference between Cantera's and CEA's results for equilibrium calculated for a gas mixture stoichiometry of 8.55

Pressure (MPa, psi)	Temperature	Enthalpy	Internal Energy	Entropy	Gibbs	Density	Cp
0.101(14.7)	-0.107%	0.000%	-0.919%	0.008%	-0.104%	0.074%	0.446%
2.53 (367)	-0.144%	0.000%	-0.798%	0.006%	-0.139%	0.151%	0.562%
5.06 (735)	-0.152%	0.000%	-0.794%	0.007%	-0.148%	0.000%	0.585%
7.60 (1102)	-0.157%	0.000%	-0.800%	0.007%	-0.152%	0.167%	0.597%
10.13 (1470)	-0.159%	0.000%	-0.802%	0.009%	-0.155%	0.171%	0.602%

Table 4. Difference between Cantera's and CEA's results for equilibrium calculated for a gas mixture stoichiometry of 5.7

Pressure (MPa, psi)	Temperature	Enthalpy	Internal Energy	Entropy	Gibbs	Density	Cp
0.101 (14.7)	0.138%	0.029%	0.141%	0.002%	0.140%	0.117%	0.369%
2.53 (367)	0.148%	0.029%	0.154%	0.000%	0.150%	0.148%	0.412%
5.06 (735)	0.150%	0.029%	0.155%	0.001%	0.152%	0.150%	0.412%
7.60 (1102)	0.148%	0.029%	0.157%	0.002%	0.151%	0.151%	0.412%
10.13 (1470)	0.148%	0.029%	0.158%	0.000%	0.150%	0.152%	0.412%

Table 5. Difference between Cantera's and CEA's results for equilibrium calculated for a gas mixture stoichiometry of 2.85

III.B. CEA and Matlab/Cantera Rocket Engine Model Performance Results

Tables 4, 5, and 6 present the difference between the rocket performance results produced by the MATLAB/Cantera rocket engine model compared to the results from CEA. For all three mixture stoichiometries, the temperature calculations were a main source of difference and these differences carried through to later calculations. For each mixture, the maximum percentage difference is highlighted.

It is predicted that the method of initialization of the MATLAB/Cantera model and the methods of integration used are different enough from those used by CEA to produce noticeable difference in calculated temperatures. However, at a stoichiometric mixture of 5.7, the results from the MATLAB/Cantera model compare well to CEA. Despite a near four percent difference in the calculated exit temperature, the characteristic exhaust velocity, thrust coefficient, and specific impulse all compare well to the values produced by CEA. This demonstrates that the methods used for modeling rocket performance by the MATLAB/Cantera model as being acceptable and provides comparable results to CEA.

Chamber Pressure (Mpa, psi)	Temperature			Area Ratio	C^*	C_F	I_{sp}
	Chamber	Throat	Exit				
6.89 (1000)	0.912%	0.625%	2.191%	0.622%	1.446%	0.144%	0.860%
5.17 (750)	0.878%	0.571%	2.154%	0.548%	0.830%	0.077%	0.839%
3.45 (500)	0.831%	0.500%	2.073%	0.480%	0.859%	0.020%	0.813%
1.72 (250)	0.762%	0.401%	1.828%	0.343%	0.869%	-0.036%	0.763%

Table 6. Difference between Cantera's and CEA's results for rocket performance calculated for a gas mixture stoichiometry of 8.55

Chamber Pressure (Mpa, psi)	Temperature			Area Ratio	C^*	C_F	I_{sp}
	Chamber	Throat	Exit				
6.89 (1000)	0.289%	-0.167%	-3.103%	-2.739%	0.598%	-0.289%	0.234%
5.17 (750)	0.285%	-0.162%	-2.241%	-1.985%	0.492%	-0.107%	0.315%
3.45 (500)	0.276%	-0.187%	-1.040%	-1.171%	0.602%	-0.145%	0.393%
1.72 (250)	0.261%	-0.197%	-0.093%	-0.380%	0.535%	0.000%	0.460%

Table 7. Difference between Cantera's and CEA's results for rocket performance calculated for a gas mixture stoichiometry of 5.7

Chamber Pressure (Mpa, psi)	Temperature			Area Ratio	C^*	C_F	I_{sp}
	Chamber	Throat	Exit				
6.89 (1000)	-2.836%	-3.648%	-3.981%	-0.670%	-0.743%	-0.166%	-0.973%
5.17 (750)	-2.807%	-3.270%	-3.981%	-0.824%	-0.632%	-0.261%	-0.960%
3.45 (500)	-2.759%	-3.245%	-3.959%	-0.751%	-0.697%	-0.169%	-0.934%
1.72 (250)	-2.667%	-3.211%	-3.866%	-0.607%	-0.775%	-0.007%	-0.880%

Table 8. Difference between Cantera's and CEA's results for rocket performance calculated for a gas mixture stoichiometry of 2.85. Calculated values can be found in the appendix, table A6

III.C. Advanced MATLAB/Cantera Rocket Engine Model

The results from the modified MATLAB/Cantera model calculating rocket performance as a function of total propellant flow rate are compared to CEA's results and tabulated in Table 7. The calculated pressure from the MATLAB/Cantera model was used to make the CEA calculations for comparison. As with the previous version of the MATLAB/Cantera rocket engine model, the largest difference is seen with the calculated temperatures, notably the exit temperatures. The largest difference seen is a calculated exit temperature by the MATLAB/Cantera model as 4.20% less than CEA's predictions.

The characteristic exhaust velocity, coefficient of thrust, and specific impulse all compare well with CEA's predictions for performance at the corresponding chamber pressure, with the maximum difference being the coefficient of thrust as 0.54% less than CEA's predictions. Despite the area ratio exhibiting nearly a two percent difference compared to CEA, solving for the exit ratio diameter yields a difference of less than one percent. For this reason this version of the code was used for designing the test rockets nozzle. The only difference being performance calculations to be used for design were made for perfectly expanded nozzle flow at an altitude of 1371.6 meters (4500ft), which is approximately the altitude of the rocket test facility.

Propellant Flow (kg/s, lbm/s)	Chamber Pressure (MPa, psi)	Temperature		
		Chamber	Throat	Exit
0.272(0.6)	6.93(1005)	-0.64%	-1.52%	-4.20%
0.249(0.55)	6.35(921)	-0.62%	-1.51%	-4.17%
0.227(0.5)	5.76(836)	-0.60%	-1.50%	-4.15%
0.204(0.45)	5.18(752)	-0.59%	-1.26%	-4.11%
0.181(0.4)	4.60(667)	-0.39%	-1.42%	-4.09%

Table 9. Difference between Cantera's and CEA's temperature results for varied propellant flow rate. Calculated chamber pressure by MATLAB/Cantera model inputted into CEA as method of comparison

Propellant Flow (kg/s, lbm/s)	Chamber Pressure (MPa, psi)	Area Ratio	C^*	C_F	I_{sp}
0.272(0.6)	6.93(1005)	-1.76%	0.07%	-0.45%	-0.44%
0.249(0.55)	6.35(921)	-1.84%	0.11%	-0.47%	-0.44%
0.227(0.5)	5.76(836)	-1.88%	0.19%	-0.54%	-0.42%
0.204(0.45)	5.18(752)	-1.82%	0.09%	-0.43%	-0.40%
0.181(0.4)	4.60(667)	-1.72%	0.06%	-0.36%	-0.37%

Table 10. Difference between Cantera's and CEA's rocket performance results for varied propellant flow rate. Calculated chamber pressure by MATLAB/Cantera model inputted into CEA as method of comparison

The MATLAB/Cantera model predicts well at the design condition, and for this reason performance calculations were made across a range of mixture ratios to develop a sense of varied rocket performance and aid in design. Various throat diameters were tried and the chamber pressure calculation checked for determining the required throat diameter that would provide the desired chamber pressure for the design condition. This design condition was 6.89MPa (1000psi) chamber pressure at a mixture ratio of approximately 4.5 that could be supplied by the constructed fuel system. A throat diameter of 8.89mm (0.35") was found to meet the design condition and Figure 1 is the resultant chamber pressure plot.

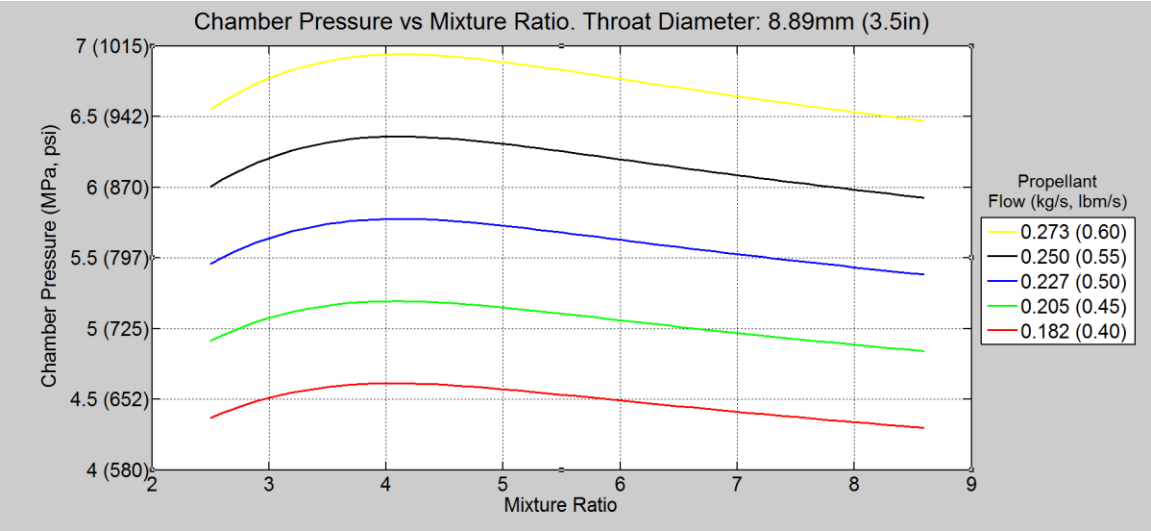

Figure 1. Chamber pressure versus mixture ratio for total propellant flow rates from 0.182kg/s (0.4lbm/s) to 0.273kg/s (0.6lbm/s). Stoichiometric is a mixture ratio of 5.7

These plots also served as checks that the model provided proper performance trends. Of importance to check were thrust and specific impulse to identify whether the proper trends were exhibited. Figure 8 and 9 show that thrust and specific impulse both peak at a mixture ratio of approximately 5.2. This corresponds to a fuel-oxidizer equivalency of approximately 1.1, or slightly fuel rich. It is here that the combination of temperature and average molecular weight of the product species reaching a maximum, resulting in the peaks in the thrust and specific impulse we see.

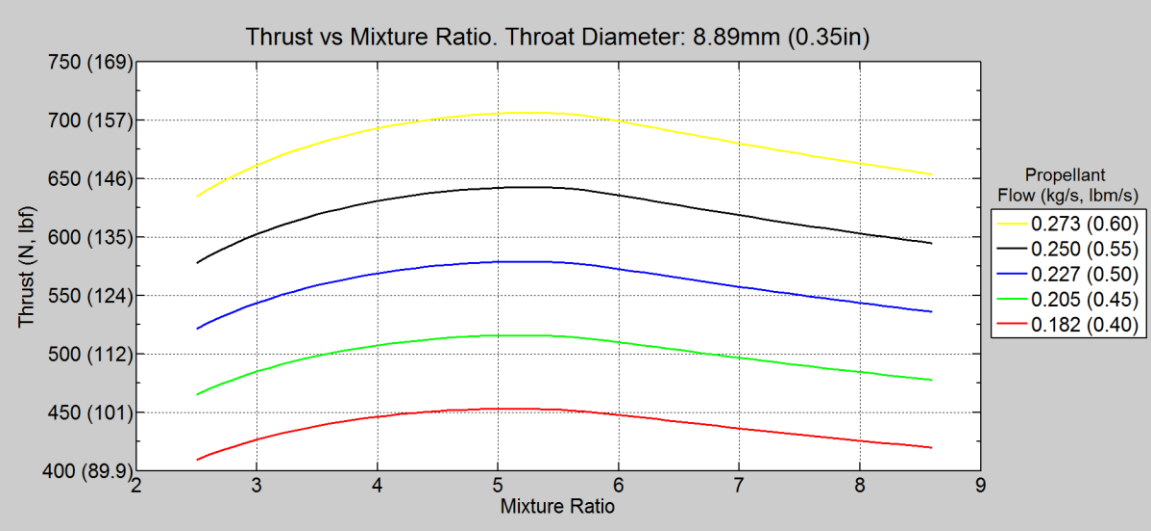

Figure 2. Thrust versus mixture ratio for total propellant flow rates from 0.182kg/s (0.4lbm/s) to 0.273kg/s (0.6lbm/s). Stoichiometric is a mixture ratio of 5.7

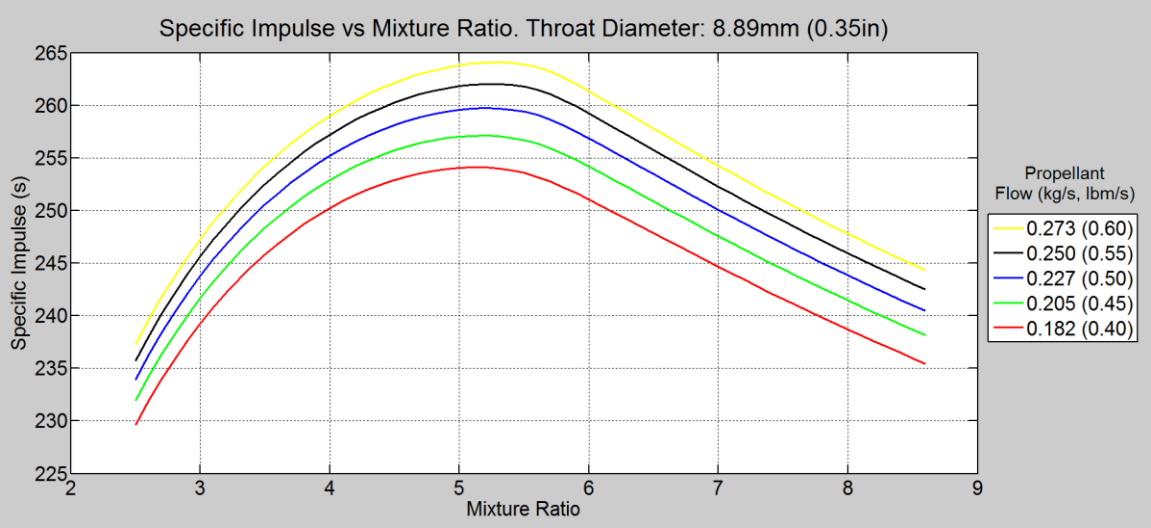

Figure 3. Specific impulse versus mixture ratio for total propellant flow rates from 0.182kg/s (0.4lbm/s) to 0.273kg/s (0.6lbm/s). Stoichiometric is a mixture ratio of 5.7

IV CONCLUSION

Cantera has been established as an acceptable alternative to CEA for making equilibrium calculations and solving for thermodynamic and transport properties of a fluid system. Interfacing Cantera with MATLAB, it is possible to develop a computational rocket engine model that produces results comparable to CEA with the added benefit of ease in incorporation of more advance modeling aspects then CEA is equipped with.

Results from the calculations made with Cantera interfaced with MATLAB were compared against CEA and found that for equilibrium, thermodynamic, and transport property calculations, Cantera compares exceptionally well with difference in results from CEA less than one percent, and the majority of differences less than 0.2 percent. The modified LLNL mechanism file involved the addition of three chemical species and their respective thermodynamic and transport data. The results obtained from the Cantera and CEA comparison demonstrate that the modified LLNL mechanism file performs well and provides adequate results.

The developed rocket engine model using MATLAB and Cantera produced results that compared well with CEA, and continued to do so when modified to solve rocket performance based on total propellant flow rate. The results showed promise in the development of the model and that with refinement the model could provide more accurate results. With the addition of the droplet evaporation model, heat transfer modeling, and chemical kinetics, validation of the model can commence by comparing actually rocket performance to the models results.

FUTURE WORK

Development of the MATLAB/Cantera model will continue, with primary focus on debugging and advancement of the droplet vaporization model. This will include accounting for vaporization of both the ethanol and liquid nitrous oxide droplets. The governing equations for this system will be derived with respect to the combustion chamber length using methods described by Turns[10] and solved using an Euler method. Thermodynamic and transport properties for the propellants in liquid phase will be acquired using Turns[10] and Dillon and Penoncello[1] for ethanol properties, and Walterm[11] for nitrous oxide properties, and the use of high speed schlieren imaging and possibly PIV of the actual injector operating will be used in determining more applicable initial conditions (average droplet diameter, droplet speed, etc) for the propellant droplets entering the combustion chamber. Following this, a heat transfer model for heat flow between chamber gases and the combustion chamber walls and nozzle will be derived and incorporated into the model. Finally, chemical kinetics will be added to the modified LLNL reaction mechanism file.

Work on the rocket test facility will continue, and with completion of this facility, characterization of the rocket engine performance can take place. Data will be collected, to include thrust, chamber pressure, rocket temperatures, and high speed schlieren imaging of the exhaust plume, and compared to the MATLAB/Cantera model predictions for validation of the rocket engine model.

NOMENCLATURE

C^*	Characteristic Exhaust Velocity
C_F	Thrust Coefficient
A_{exit}	area of nozzle exit
A^*	area of nozzle throat
A_{exit}/A^*	nozzle area ratio
U	flow velocity
U_{exit}	exhaust flow exit velocity
I_{sp}	specific impulse
P_{inf}	ambient pressure
$P_\circ$	stagnation pressure
g_c	earth gravitational acceleration
$\dot{m}$	mass flow
$\dot{m}^*$	mass flow at nozzle throat
$\dot{m}_{propellant}$	total mass flow of propellants entering combustion chamber

ρ^*	density of gas flow at nozzle throat
ρ_{exit}	density of gas flow at nozzle exit
U^*	flow velocity at nozzle throat
$H_\circ$	stagnation enthalpy
H_{exit}	enthalpy of gas flow at nozzle exit
H^*	enthalpy of gas flow at nozzle throat
$S_\circ$	stagnation entropy
S_{exit}	entropy of gas flow at nozzle exit
S^*	entropy of gas flow at nozzle throat
a	local speed of sound of gas flow
$T_\circ$	stagnation temperature
γ	specific heat ratio
R	gas constant
β	property for CEA/Cantera comparison

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