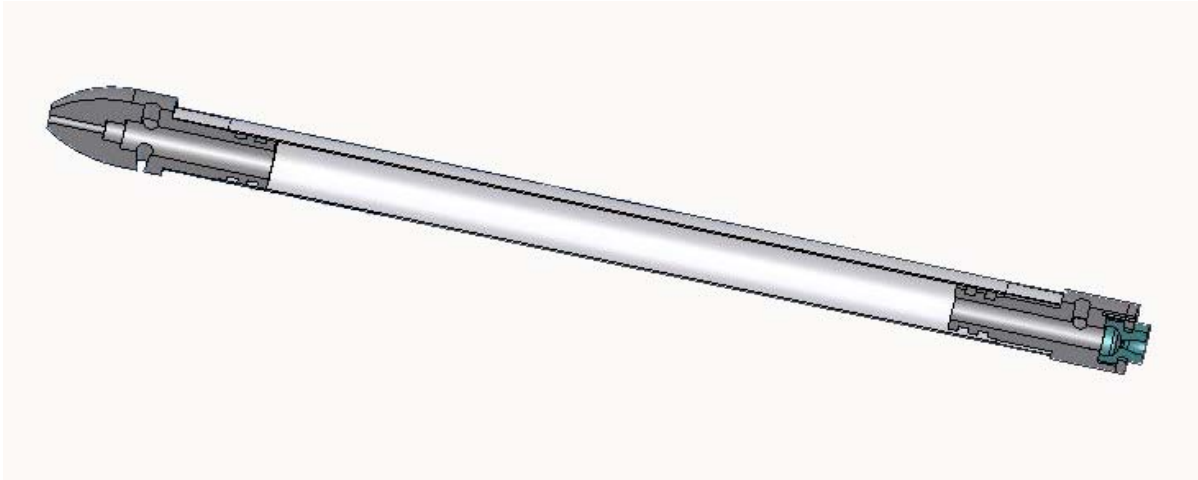# NUMERICAL MODELING OF A HYBRID ROCKET

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SPRING 2005

Contents

Section 1 - Thermochemical Calculations

This section models the combustion process occurring in a hybrid rocket utilizing nitrous oxide (N_2O) as an oxidizer, and paraffin wax ($C_{28}H_{58}$) as a propellant. General states of all reactants and products from the reaction are defined and used to calculate an adiabatic flame temperature. After an adiabatic flame temperature is found assuming a stoichiometric reaction, the process is refined to account for dissociation of minor species.

Comments: The results from Section 1 may be used to further understand the internal workings of a hybrid rocket; however this would require the application of a boundary layer energy balance. Currently, there is not enough information known to complete this study. Radiation, convection, and conduction models are needed to use the information from the thermochemical calculations and apply the results to the fuel grain and reacting gases. The completion of this model would enable the whole rocket to be numerically predicted.

Section 2 - Product Equilibrium Calculations

To account for the dissociation of minor species in a chemical reaction, element balances must be performed. Section 2 outlines the element balance performed for the overall reaction. These calculations enable mole numbers to be found for each exhaust gas constituent. With these equations defined, the combustion reaction may be modeled for varying oxidizer to propellant ratios.

Section 3 - Combustion Chamber Length Calculations

With the hope of manufacturing and testing a real hybrid rocket, certain design specifications needed to be made. This section derives a proper fuel grain size based on a desired burn time. The fuel grain manufacturing method (Roto-Molding) is also taken into account.

Section 4 - Igniter Calculations

This section attempts to find characteristics of the ignition process (sorbitol/potassium nitrate fuel). The combustion of an igniter is first modeled and the rate of heat generation is defined. Because the ignition process is transient, further modeling is required to obtain the state of a rocket after the ignition process.

Section 5 - Nitrous Oxide Injector Calculations

With information from the nozzle manufacturer, BETE, an injector nozzle is sized according to design specifications. Information is adapted to account for the flow of nitrous oxide instead of water. These calculations are valid for the current arrangement consisting of one injector nozzle directed straight into the fuel grain's annulus.

Section 6 - Nozzle Design Calculations

These calculations apply thermodynamic concepts to derive dimensions for a converging/diverging exhaust nozzle. The calculations also predict operating conditions of the nozzle assuming inlet conditions. Three different nozzles were designed based on varied operating pressures. The summary of results is given on the last page of this section.

Section 7 - Computational Evaluation of a Bell-Shaped Thrust Nozzle

The purpose of performing a computational evaluation on the thrust nozzle was to validate results from Section 6. This type of numerical method has the potential of better approximating operating conditions compared to hand calculations. The results are given in a visual format and do in fact validate calculations in Section 6. It is recommended that this numerical method be used to optimize the design of a thrust nozzle due to its flexibility. Experimental results may be applied to boundary and initial conditions to simulate actual rocket operation.

Section 8 - Thrust Calculations

This section initially defines thrust and approximates a value for the designed rocket. A graph is produced for the ideal exhaust gas mass flow rate of 0.166 kg/s comparing thrust to exit velocity. The next section outlines a method in which the exhaust gas velocity may be derived experimentally. Using data from the second firing of "Big Boy", an example is performed.

Section 9 - Calculation References

Acknowledgments

Thermochemical Calculations

Performed by: Ryan Erickson
Date: Spring 2005

Color Key for Values: Assumed   Referenced   Calculated

MathCAD Unit Defintions: $kJ := 10^3 J$ $kmol := 10^3 mol$ $MPa := 10^6 Pa$ $R_u := 8.314 \dfrac{kJ}{kmol \cdot K}$

Properties of Combustion Reactants:

Nitrous Oxide: Stored inside a high pressure holding tank in liquidous form at room temperature. The vaporization pressure of nitrous oxide at room temperature (295 K) is found to be 754.196 psi (5.20MPa) using data from [1]. Once expelled from the tank, the nitrous oxide expands and becomes a vapor. The vapor properties are assumed to be saturated and taken at 550 psi (3.8 MPa). This is the assumed combustion pressure.The new properties of the vapor are approximated using [1,2] to be:

$T_{n2o} := 280K$ $P_{n2o} := 550psi$ $R_{n2o} := 0.1889 \dfrac{kJ}{kg \cdot K}$

Assuming an ideal gas: $\dfrac{P}{\rho} := R \cdot T$

$\rho_{n2o\_ideal} := \dfrac{P_{n2o}}{R_{n2o} \cdot T_{n2o}}$ $\rho_{n2o\_ideal} = 71.695 \dfrac{kg}{m^3}$

Since the nitrous oxide is at a very high pressure, the ideal gas equation introduces a good amount of error. Therefore, the compressibility factor (Z) must be taken into account:

$P_{cr} := 7.245 MPa$ $T_{cr} := 309.57K$

These critical properties, from [2], are needed to find the reduced properties of nitrous oxide.

$P_r := \dfrac{P_{n2o}}{P_{cr}}$ $T_r := \dfrac{T_{n2o}}{T_{cr}}$ $P_r = 0.523$ $T_r = 0.904$

From [2] pg.867, the compressibility factor is found to be approximately: $Z := 0.7$

$Z := \dfrac{\rho_{ideal}}{\rho_{actual}}$ $\rho_{n2o} := \dfrac{\rho_{n2o\_ideal}}{Z}$ $\rho_{n2o} = 102.422 \dfrac{kg}{m^3}$

The mass flow rate of oxidizer will vary throughout, but is currently approximated as:

$m_{dot\_n2o} := 0.150 \dfrac{kg}{sec}$

Paraffin Wax: Initially assumed to be at room temperature (295 K) in solid form. The latent heat of fusion is assumed to be approximately 95 BTU/lb (220.97 kJ/kg) and the heat of combustion is 20,000 BTU/lb (46.52MJ/kg), both from [3].

Combustion:

The stoichiometric reaction for combustion in the rocket using nitrous oxide as an oxidizer and paraffin wax as a propellant is first defined to be:

$$85N_2O + C_{28}H_{58} \longrightarrow 85N_2 + 29H_2O + 28CO_2$$
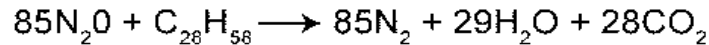
This balance is created assuming complete combustion comprising of:

Reactants: Nitrous Oxide(N_2O) and Paraffin Wax (approximated as $C_{28}H_{58}$)
Products: Diatomic Nitrogen(N_2), Water(H_2O), and Carbon Dioxide(CO_2)

Using the stoichiometric balance, the molal oxidizer to propellant ratio is found to be 85:1
On a mass basis, the ratio can now be computed as follows:

$$M_{n2o} := 44.013 \frac{kg}{kmol} \quad N_{n2o} := 85 \quad M_{c28h58} := 394.786 \frac{kg}{kmol} \quad N_{c28h58} := 1$$

$$OP_{ratio} := \frac{M_{n2o} \cdot N_{n2o}}{M_{c28h58} \cdot N_{c28h58}} \qquad OP_{ratio} = 9.476$$

The mass flow rate of paraffin wax can be approximated assuming stoichiometric combusiton as:

$$m_{dot\_wax} := \frac{m_{dot\_n2o}}{OP_{ratio}} \qquad m_{dot\_wax} = 0.016 \frac{kg}{s}$$

The Steady-Flow Energy Equation is now defined for use in later calculations.
(From [2], pg.716, eq.14-13)

$$Q - W := h_c^o + \sum_{Products} \left[N_i \cdot \left(h - h^o \right) \right] - \sum_{Reactants} \left[N_i \cdot \left(h - h^o \right) \right]^{\blacksquare} \qquad \left(\frac{kJ}{kmol} \right)$$

*In our process there is no external work (W=0), and adiabatic combustion will be assumed (Q_{out}=0) for simplicity. The Steady-Flow Energy equation can then be rewritten as:

$$h_c^o + \sum_{Products} \left[N_i \cdot \left(h - h^o \right) \right] := \sum_{Reactants} \left[N_i \cdot \left(h - h^o \right) \right]^{\blacksquare}$$

Before combustion calculations are performed, the coefficients of thermodynamic properties are defined. Knowing that combustion will occur at very high temperatures, properties are gathered from [4,1].

N_2: $a_{1\_n2} := 2.95257626$ $a_{2\_n2} := 1.39690057 \cdot 10^{-3} \frac{1}{K}$ $a_{3\_n2} := -4.92631691 \cdot 10^{-7} \frac{1}{K^2}$

$a_{4\_n2} := 7.86010367 \cdot 10^{-11} \frac{1}{K^3}$ $a_{5\_n2} := -4.60755321 \cdot 10^{-15} \frac{1}{K^4}$ $b_{1\_n2} := -9.23948645 \cdot 10^2 \cdot K$

$$h_{n2}(T) := R_u \cdot T \cdot \left(a_{1\_n2} + a_{2\_n2} \cdot \frac{T}{2} + a_{3\_n2} \cdot \frac{T^2}{3} + a_{4\_n2} \cdot \frac{T^3}{4} + a_{5\_n2} \cdot \frac{T^4}{5} + \frac{b_{1\_n2}}{T} \right)$$

H_2O: $a_{1\_h2o} := 2.67703787$ $a_{2\_h2o} := 2.97318329 \cdot 10^{-3} \frac{1}{K}$ $a_{3\_h2o} := -7.73769690 \cdot 10^{-7} \frac{1}{K^2}$

$a_{4\_h2o} := 9.44336689 \cdot 10^{-11} \frac{1}{K^3}$ $a_{5\_h2o} := -4.26900959 \cdot 10^{-15} \frac{1}{K^4}$ $b_{1\_h2o} := -2.98858938 \cdot 10^4 \cdot K$

$$h_{h2o}(T) := R_u \cdot T \cdot \left(a_{1\_h2o} + a_{2\_h2o} \cdot \frac{T}{2} + a_{3\_h2o} \cdot \frac{T^2}{3} + a_{4\_h2o} \cdot \frac{T^3}{4} + a_{5\_h2o} \cdot \frac{T^4}{5} + \frac{b_{1\_h2o}}{T} \right)$$

CO_2: $a_{1\_co2} := 4.63659493$ $a_{2\_co2} := 2.74131991 \cdot 10^{-3} \frac{1}{K}$ $a_{3\_co2} := -9.95828531 \cdot 10^{-7} \frac{1}{K^2}$

$a_{4\_co2} := 1.60373011 \cdot 10^{-10} \frac{1}{K^3}$ $a_{5\_co2} := -9.16103468 \cdot 10^{-15} \frac{1}{K^4}$ $b_{1\_co2} := -4.90249341 \cdot 10^4 \cdot K$

$$h_{co2}(T) := R_u \cdot T \cdot \left(a_{1\_co2} + a_{2\_co2} \cdot \frac{T}{2} + a_{3\_co2} \cdot \frac{T^2}{3} + a_{4\_co2} \cdot \frac{T^3}{4} + a_{5\_co2} \cdot \frac{T^4}{5} + \frac{b_{1\_co2}}{T} \right)$$

N_2O: $a_{n2o} := 24.11 \frac{kJ}{kmol \cdot K}$ $b_{n2o} := 5.8632 \cdot 10^{-2} \frac{kJ}{kmol \cdot K^2}$

$c_{n2o} := -3.562 \cdot 10^{-5} \frac{kJ}{kmol \cdot K^3}$ $d_{n2o} := 10.58 \cdot 10^{-9} \frac{kJ}{kmol \cdot K^4}$

$$C_{p\_n2o}(T) := a_{n2o} + b_{n2o} \cdot T + c_{n2o} \cdot T^2 + d_{n2o} \cdot T^3$$

$$\Delta h_{n2o}(T_{one}, T_{two}) := \int_{T_{one}}^{T_{two}} C_{p\_n2o}(T) \, dT \qquad\qquad T_{one} := 298K$$

The heat of combustion used for paraffin wax in this analysis comes from [3] and is:

$$h_{c\_given} := 20000 \, \frac{BTU}{lb} \qquad h_{c\_given} = 4.652 \times 10^4 \, \frac{kJ}{kg}$$

***This value must be converted to the molar heat of combustion:

$$h_c := -h_{c\_given} \cdot M_{c28h58} \qquad h_c = -1.837 \times 10^7 \, \frac{kJ}{kmol}$$

From the heat of combustion value, the enthalpy of formation must be calculated for paraffin wax. This is done using the definition of "heat of combustion" from [2] pg.713. Assuming the defined combustion happens with air, the stoichiometric balance and calculations are as follows:

$$42.5(3.76 \, N_2 + O_2) + C_{28}H_{58} \longrightarrow 159.8 N_2 + 29 H_2O + 28 CO_2$$
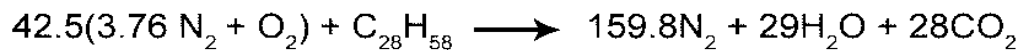
$$h_c := H_{products} - H_{reactants} \qquad \text{guess value:} \quad h_f := 350000 \, \frac{kJ}{kmol}$$

Given

$$h_c = 159.8 \cdot 0 \, \frac{kJ}{kmol} + 29 \cdot -241820 \, \frac{kJ}{kmol} + 28 \cdot -393520 \, \frac{kJ}{kmol} - -h_f$$

$$h_f := Find(h_f)$$

$$h_f = -3.341 \times 10^5 \, \frac{kJ}{kmol}$$

Adiabatic Flame Temperature (maximum temperature of products at constant pressure)

Recall the Steady-Flow Energy equation from [2]:
$$\sum_{Products} \left[N_i \cdot \left(h_f + \Delta h \right) \right] := \sum_{Reactants} \left[N_i \cdot \left(h_f + \Delta h \right) \right]$$

This equation can be conveniently reduced on the product side by using thermodynamic data from [4]. Here, the least-squares coefficients of species are given in a form that combines sensible enthalpies and energies of chemical and physical changes in one numerical value. This is represented in equations 5&6 of [4] as:

$$h^o(298.15) := \Delta_f \cdot h^o(298.15)$$

and

$$h^o(T) := h^o(298.15) + \left[h^o(T) - h^o(298.15) \right]$$

This is applied to the Steady-Flow Energy equation, which becomes:

$$\sum_{Products} \left[N_i \cdot h^o(T) \right] := \sum_{Reactants} \left[N_r \cdot \left(h_f + \Delta h \right) \right]$$

Guess $\quad T_{flame} := 2000K$

Given

$$85 \cdot h_{n2}(T_{flame}) + 29 \cdot h_{h2o}(T_{flame}) \ldots = 85 \cdot \Delta h_{n2o}(T_{one}, T_{n2o}) + 85 \cdot 82050 \cdot \frac{kJ}{kmol} + h_f$$
$$+ 28 \cdot h_{co2}(T_{flame})$$

$T_{flame} := Find(T_{flame})$

$$T_{flame} = 4.319 \times 10^3 \, K$$

***This is the calculated adiabatic flame temperature for ideal products of combustion.

The adiabatic flame temperature with nitrous oxide seems very high, so to verify its value I decided to calculate the combustion with air. For various hydrocarbons, the adiabatic flame temperatures have been published in such references as [5]. These values can be used to verify that my methodology is correct.

Additional specific heat correlations needed:

N_2: $a_{n2} := 28.90 \dfrac{kJ}{kmol \cdot K}$ $\qquad$ $b_{n2} := -0.1571 \cdot 10^{-2} \dfrac{kJ}{kmol \cdot K^2}$

$c_{n2} := 0.8081 \cdot 10^{-5} \dfrac{kJ}{kmol \cdot K^3}$ $\qquad$ $d_{n2} := -2.873 \cdot 10^{-9} \dfrac{kJ}{kmol \cdot K^4}$

$C_{p\_n2}(T) := a_{n2} + b_{n2} \cdot T + c_{n2} \cdot T^2 + d_{n2} \cdot T^3$

$\Delta h_{n2}(T_{one}, T_{two}) := \displaystyle\int_{T_{one}}^{T_{two}} C_{p\_n2}(T) \, dT$

O_2: $a_{o2} := 25.48 \dfrac{kJ}{kmol \cdot K}$ $\qquad$ $b_{o2} := 1.520 \cdot 10^{-2} \dfrac{kJ}{kmol \cdot K^2}$

$c_{o2} := -0.7155 \cdot 10^{-5} \dfrac{kJ}{kmol \cdot K^3}$ $\qquad$ $d_{o2} := 1.312 \cdot 10^{-9} \dfrac{kJ}{kmol \cdot K^4}$

$C_{p\_o2}(T) := a_{o2} + b_{o2} \cdot T + c_{o2} \cdot T^2 + d_{o2} \cdot T^3$

$\Delta h_{o2}(T_{one}, T_{two}) := \displaystyle\int_{T_{one}}^{T_{two}} C_{p\_o2}(T) \, dT$

Guess $\quad T_{flame} := 2000K$

Given

$159.8 \cdot h_{n2}(T_{flame}) + 29 \cdot h_{h2o}(T_{flame}) \dots = 159.8 \cdot \Delta h_{n2}(T_{one}, 293.15K) + 42.5 \cdot \Delta h_{o2}(T_{one}, 293.15K) + h_f$
$+ 28 \cdot h_{co2}(T_{flame})$

$T_{flame} := Find(T_{flame})$

$\boxed{T_{flame} = 2.445 \times 10^3 \, K}$

**This adiabatic flame temperature is very similar to those hydrocarbons listed in Appendix D of [5]. This verifies that the methodology in previous calculations should also be accurate.

Equilibrium of Minor Species

The adiabatic flame temperatures previously found resulted from an exothermic reaction of ideal products. In real processes, the ideal products dissociate into minor species. The dissociation of species may have a significant effect on this reaction, so they are considered in the following calculations:

The "water-gas shift" reaction is commonly used to account for the presence of incomplete products in combustion [5]. This reaction defines an equilibrium balance between its components as shown below:

$$CO + H_2O \longrightarrow CO_2 + H_2$$
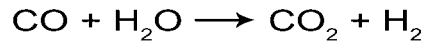
For rich combustion (no oxygen present in products), a coefficient (equilibrium constant) is developed that relates the mole numbers of CO_2, CO, H_2, and H_2O from the water-gas shift reaction. This relationship is given in [5] as:

$$K_p := \frac{n_{co2} \cdot n_{h2}}{n_{co} \cdot n_{h2o}} \qquad \text{where: } K_p \text{ is a function of temperature.}$$

The new combustion reaction needs to be written out with minor species included in order to find an equilibrium balance of products:

$$n_{N_2O}N_2O + C_{28}H_{58} \longrightarrow n_{co}CO + n_{CO_2}CO_2 + n_{H_2}H_2 + n_{H_2O}H_2O + n_{N_2}N_2$$
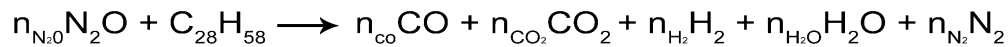
In order to the find the correct mole numbers for each component of the above reaction, an element balance is performed. Results of this element balance are given in terms of "K_p". This is because the final mole number and adiabatic flame temperature will be found using an iterative process. The symbolic calculations for the element balances are performed in "Product Equilibrium Calculations". Results of these calculations are summarized below:

$$n_{co2} := \frac{-57 + n_{n2o} - K_p \cdot n_{n2o}}{2 \cdot (1 - K_p)} + \frac{\sqrt{\left[57 + (K_p - 1) \cdot n_{n2o}\right]^2 - 4(1 - K_p) \cdot K_p \cdot 28(28 - n_{n2o})}}{\left[2 \cdot (1 - K_p)\right]}$$

$$n_{co} := 28 - n_{co2}$$

$$n_{h2o} := n_{n2o} - 28 - n_{co2}$$

$$n_{h2} := 57 - n_{n2o} + n_{co2}$$

Before the mole numbers are solved for, a relationship between temperature and the equilibrium constant "K_p" must be defined. Given on pg.40 of [5] as equation (2.66b):

$$K_p := e^{\dfrac{-\Delta G_T}{R_u \cdot T_{combustion}}}$$

where: ΔG_T is the standard-state Gibbs function change, and
R_u is the universal gas constant

The standard state Gibbs function change is then defined as:

$$\Delta G_T := \sum_{products} \left(N_i \cdot g_{f\_i}{}^o \right) - \sum_{reactants} \left(N_i \cdot g_{f\_i}{}^o \right)$$

where: g_f^o is the Gibbs function of formation, and
N is the mole number

The Gibbs functions of formation for each molecule may be calculated or referenced from tables. I have chosen to use values from tables for simplicity and time considerations. The mole numbers are found directly from the water-gas shift equation (above).

Assuming: $T_{combustion} := 4000K$

From Appendix A of [5]:

$\underline{CO}$	$\underline{H_2O}$	$\underline{CO_2}$	$\underline{H_2}$
$N_{co} := 1$	$N_{h2o} := 1$	$N_{co2} := 1$	$N_{h2} := 1$
$g_{f\_co} := -446291 \dfrac{kJ}{kmol}$	$g_{f\_h2o} := -18549 \dfrac{kJ}{kmol}$	$g_{f\_co2} := -393311 \dfrac{kJ}{kmol}$	$g_{f\_h2} := 0 \dfrac{kJ}{kmol}$

The standard-state Gibbs function change is now found:

$$\Delta G_T := N_{co2} \cdot g_{f\_co2} + N_{h2} \cdot g_{f\_h2} - N_{co} \cdot g_{f\_co} - N_{h2o} \cdot g_{f\_h2o}$$

$$\Delta G_T = 7.153 \times 10^4 \ \dfrac{kJ}{kmol}$$

The corresponding equilibrium constant "K_p" can now be defined as:

$$K_p := \exp\left(\dfrac{-\Delta G_T}{R_u \cdot T_{combustion}} \right) \qquad K_p = 0.116$$

This equilibrium constant is now substituted into the previously defined mole number relationships from the "Product Equilibrium Calculations". The results give mole numbers for each component of the combustion reaction as shown below:

Assume: $n_{n2o} := 70$

$$n_{co2} := \frac{-57 + n_{n2o} - K_p \cdot n_{n2o}}{2 \cdot (1 - K_p)} + \frac{\sqrt{\left[57 + (K_p - 1) \cdot n_{n2o}\right]^2 - 4(1 - K_p) \cdot K_p \cdot 28(28 - n_{n2o})}}{\left[2 \cdot (1 - K_p)\right]}$$

$n_{co} := 28 - n_{co2}$ $\qquad\qquad$ $n_{h2o} := n_{n2o} - 28 - n_{co2}$

$n_{h2} := 57 - n_{n2o} + n_{co2}$ $\qquad$ $n_{n2} := n_{n2o}$

Results

$n_{co} = 12.509$ $\qquad$ $n_{h2} = 2.491$ $\qquad$ $n_{n2o} = 70$

$n_{co2} = 15.491$ $\qquad$ $n_{h2o} = 26.509$ $\qquad$ $n_{n2} = 70$

These mole numbers are now used to calculate an adiabatic flame temperature. The calculation process is the same as before, however, it will require iteration. A combustion temperature of 4000 Kelvin was first assumed to find the mole numbers of reactants and products. Once the adiabatic flame temperature is known, the mole numbers will be recalculated and a new adiabatic flame temperature will be found. This process should yield converging results. Before the calculations begin, the coefficients for calculating thermodynamic properties of H_2 and CO must be defined from [4]. This is because H_2 and CO were not considered in the first set of calculations.

CO: $\quad a_{1\_co} := 3.04848583 \qquad a_{2\_co} := 1.35172818 \cdot 10^{-3} \frac{1}{K} \qquad a_{3\_co} := -4.85794075 \cdot 10^{-7} \frac{1}{K^2}$

$a_{4\_co} := 7.88536486 \cdot 10^{-11} \frac{1}{K^3} \quad a_{5\_co} := -4.69807489 \cdot 10^{-15} \frac{1}{K^4} \quad b_{1\_co} := -1.42661171 \cdot 10^4 \cdot K$

$$h_{co}(T) := R_u \cdot T \cdot \left(a_{1\_co} + a_{2\_co} \cdot \frac{T}{2} + a_{3\_co} \cdot \frac{T^2}{3} + a_{4\_co} \cdot \frac{T^3}{4} + a_{5\_co} \cdot \frac{T^4}{5} + \frac{b_{1\_co}}{T} \right)$$

H_2: $\quad a_{1\_h2} := 2.93286579 \qquad a_{2\_h2} := 8.26607967 \cdot 10^{-4} \frac{1}{K} \qquad a_{3\_h2} := -1.46402335 \cdot 10^{-7} \frac{1}{K^2}$

$a_{4\_h2} := 1.54100359 \cdot 10^{-11} \frac{1}{K^3} \quad a_{5\_h2} := -6.88804432 \cdot 10^{-16} \frac{1}{K^4} \quad b_{1\_h2} := -8.13065597 \cdot 10^2 \cdot K$

$$h_{h2}(T) := R_u \cdot T \cdot \left(a_{1\_h2} + a_{2\_h2} \cdot \frac{T}{2} + a_{3\_h2} \cdot \frac{T^2}{3} + a_{4\_h2} \cdot \frac{T^3}{4} + a_{5\_h2} \cdot \frac{T^4}{5} + \frac{b_{1\_h2}}{T} \right)$$

Recall the Steady-Flow Energy equation:

$$\sum_{Products} \left[N_i \cdot h^o(T) \right] := \sum_{Reactants} \left[N_i \cdot \left(h_f + \Delta h \right) \right]$$

Guess $\quad T_{flame} := 4000K$

Given

$$42.5 \cdot h_{n2}\left(T_{flame}\right) + 38.716 \cdot h_{h2o}\left(T_{flame}\right) \ldots = 42.5 \cdot \Delta h_{n2o}\left(T_{one}, T_{n2o}\right) + 42.5 \cdot 82050 \cdot \frac{kJ}{kmol} + h_f$$
$$+ 2.208 \cdot h_{co2}\left(T_{flame}\right) + 52.216 \cdot h_{co}\left(T_{flame}\right) \ldots$$
$$+ 16.708 \cdot h_{h2}\left(T_{flame}\right)$$

$$T_{flame} := Find\left(T_{flame}\right)$$

$$\boxed{T_{flame} = 3.542 \times 10^3 \, K}$$

This adiabatic flame temperature is then substituted back into the first step of the iterative process in order to find a new equilibrium constant and mole numbers. The iterative process is repeated until the results converge. The last iteration is shown below:

Assumed: $\quad T_{combustion} := 3550K$

From Appendix A of [5]:

$\underline{CO}$	$\underline{H_2O}$	$\underline{CO_2}$	$\underline{H_2}$
$N_{co} := 1$	$N_{h2o} := 1$	$N_{co2} := 1$	$N_{h2} := 1$
$g_{f\_co} := -411270 \frac{kJ}{kmol}$	$g_{f\_h2o} := -45050 \frac{kJ}{kmol}$	$g_{f\_co2} := -394504 \frac{kJ}{kmol}$	$g_{f\_h2} := 0 \frac{kJ}{kmol}$

$$\Delta G_T := N_{co2} \cdot g_{f\_co2} + N_{h2} \cdot g_{f\_h2} - N_{co} \cdot g_{f\_co} - N_{h2o} \cdot g_{f\_h2o}$$

$$\boxed{\Delta G_T = 6.182 \times 10^4 \, \frac{kJ}{kmol}}$$

$$K_p := \exp\left(\frac{-\Delta G_T}{R_u \cdot T_{combustion}} \right) \qquad \boxed{K_p = 0.123}$$

$$n_{h2} := 29 - \frac{1}{(4 \cdot K_p - 4)} \cdot \left(-27 K_p - 87 + \sqrt{729 K_p^2 + 11426 K_p + 841}\right)$$

$$n_{h2o} := \frac{1}{(4 \cdot K_p - 4)} \cdot \left(-27 \cdot K_p - 87 - \sqrt{729 \cdot K_p^2 + 11426 \cdot K_p + 841}\right)$$

$$n_{co} := \frac{27}{2} + \frac{1}{(4 \cdot K_p - 4)} \cdot \left(-27 \cdot K_p - 87 - \sqrt{729 \cdot K_p^2 + 11426 \cdot K_p + 841}\right) \qquad n_{n2o} := \frac{85}{2}$$

$$n_{co2} := \frac{29}{2} - \frac{1}{(4 \cdot K_p - 4)} \cdot \left(-27 \cdot K_p - 87 + \sqrt{729 \cdot K_p^2 + 11426 \cdot K_p + 841}\right) \qquad n_{n2} := \frac{85}{2}$$

Results

$n_{co} = 52.804$ $n_{h2} = 16.799$ $n_{n2o} = 42.5$

$n_{co2} = 2.299$ $n_{h2o} = 39.304$ $n_{n2} = 42.5$

Guess $T_{flame} := 4000K$

Given

$42.5 \cdot h_{n2}(T_{flame}) + 39.304 \cdot h_{h2o}(T_{flame}) \dots = 42.5 \cdot \Delta h_{n2o}(T_{one}, T_{n2o}) + 42.5 \cdot 82050 \cdot \frac{kJ}{kmol} + h_f$
$+ 2.299 \cdot h_{co2}(T_{flame}) + 52.804 \cdot h_{co}(T_{flame}) \dots$
$+ 16.799 \cdot h_{h2}(T_{flame})$

$T_{flame} := Find(T_{flame})$

$T_{flame} = 3.55 \times 10^3 \, K$

***This is the adiabatic flame temperature using the water-gas shift equilibrium
to account for minor species involved in combustion. All further calculations
will use this result as the temperature at which combustion occurs.***

Product Equilibrium Calculations   **Ryan Erickson**

$n_{N2O}N_2O + 1C_{28}H_{58} => n_{CO}CO + n_{CO2}CO_2 + n_{H2}H_2 + n_{H2O}H_2O + n_{N2}N_2$

<u>Mass Element Balances</u>

$C => 28 = n_{CO} + n_{CO2}$

$H => 58 = 2n_{H2} + 2n_{H2O}$

$O => n_{N2O} = n_{CO} + 2n_{CO2} + n_{H2O}$

$N => 2n_{N2O} = 2n_{N2}$ Therefore $n_{N2O} = n_{N2}$

also $n_{N2O} = 28 + 58/4$ from [5] (eq. 2.31)

<u>Water-gas Shift</u>

$CO + H_2O \Leftrightarrow CO_2 + H_2$ $\therefore K_p = \dfrac{n_{H2} \times n_{CO2}}{n_{H2O} \times n_{CO}}$

There are now 6 equations with 7 unknowns. K_p, however, can be found as a function of temperature with rather lengthy thermodynamic calculations. Solving for n_{H2} in terms of K_p will allow for the number of moles to be found for each constituent using an iterative process.

The calculations on the following page were performed with MathCAD software and give relationships for each constituent in terms of K_p. Only solutions that yield positive results are considered in further calculations.

Solve Block for Product Equilibrium Calculations

***equations from page 1 of "Product Equilibrium Calculations"

Given

$28 = n_{co} + n_{co2}$ $\qquad$ $58 = 2n_{h2} + 2n_{h2o}$ $\qquad$ $n_{n2o} = n_{co} + 2n_{co2} + n_{h2o}$

$2 \cdot n_{n2o} = 2n_{n2}$ $\qquad$ $K_p = \dfrac{n_{h2} \cdot n_{co2}}{n_{h2o} \cdot n_{co}}$

$$\text{Find}(n_{n2o}, n_{co}, n_{h2}, n_{n2}, n_{h2o}) \rightarrow \begin{bmatrix} \dfrac{\left(-784 \cdot K_p - 57 \cdot n_{co2} + K_p \cdot n_{co2}^2 - n_{co2}^2\right)}{\left(-28 \cdot K_p + K_p \cdot n_{co2} - n_{co2}\right)} \\ 28 - n_{co2} \\ 29 \cdot K_p \cdot \dfrac{\left(-28 + n_{co2}\right)}{\left(-28 \cdot K_p + K_p \cdot n_{co2} - n_{co2}\right)} \\ \dfrac{\left(-784 \cdot K_p - 57 \cdot n_{co2} + K_p \cdot n_{co2}^2 - n_{co2}^2\right)}{\left(-28 \cdot K_p + K_p \cdot n_{co2} - n_{co2}\right)} \\ -29 \cdot \dfrac{n_{co2}}{\left(-28 \cdot K_p + K_p \cdot n_{co2} - n_{co2}\right)} \end{bmatrix}$$

$$n_{n2o} = \frac{\left(-784 \cdot K_p - 57 \cdot n_{co2} + K_p \cdot n_{co2}^2 - n_{co2}^2\right)}{\left(-28 \cdot K_p + K_p \cdot n_{co2} - n_{co2}\right)}$$

$K_p := 0.125$ $\qquad$ $n_{n2o} := 85$

Solving this equation for n_{co2} yields:

$$n_{co2} := \frac{-57 + n_{n2o} - K_p \cdot n_{n2o}}{2 \cdot \left(1 - K_p\right)} + \frac{\sqrt{\left[57 + \left(K_p - 1\right) \cdot n_{n2o}\right]^2 - 4\left(1 - K_p\right) \cdot K_p \cdot 28\left(28 - n_{n2o}\right)}}{\left[2 \cdot \left(1 - K_p\right)\right]}$$

This can be checked by substituting in a K_p and n_{n2o} value: $\quad$ $n_{co2} = 28$

This satisfies the stoichiometric formula (for $n_{n2o} = 85$)!!!

Combustion Chamber Length Calculations

Performed by: Ryan Erickson
Date: Spring 2005

A reasonable fuel grain length needs to be determined for the current rocket design specifications. This is because the length and surface area of a fuel grain controls the length of burn and also directly affects thrust characteristics. The fuel grain manufacturing process will consist of melting wax and spinning it inside a tube as it cools (roto-molding). As the wax solidifies, volumetric shrinkage occurs. These calculations simulate dimensions of the solid wax fuel grain assuming it has been formed into a cylindrical shape with a hollow core (due to shrinkage).

Given: $OD_{tube} := 2\,in$ $ID_{tube} := 1.866\,in$ $\%_{shrink} := 0.17$ $\rho_{paraffin} := 6.75\,\dfrac{lb}{gal}$

$m_{dot\_wax} := 0.016\,\dfrac{kg}{s}$ ***Derived from assumed oxidizer flow rate.
(See "Thermochemical Calculations")

First, the cross-sectional area inside the tube is found:

$$A_{initial} := \frac{\pi \cdot ID_{tube}^2}{4}$$ $A_{initial} = 1.764 \times 10^{-3}\,m^2$

The wax, while liquid, will fill this area. As it is spun, the wax will want to move away from the center of the cylinder. At the same time, it cools and shrinks about 17% by volume. A hollow core will be formed in the center of the tube with approximately the following diameter:

$$A_{final} := A_{initial} \cdot \left(1 - \%_{shrink}\right)$$ $A_{final} = 1.464 \times 10^{-3}\,m^2$

Guess diameter: $D_{core} := \dfrac{1}{8}\,in$

Given

$$A_{final} = \frac{\pi \cdot \left(ID_{tube}^2 - D_{core}^2\right)}{4}$$

$D_{core} := Find\left(D_{core}\right)$ $D_{core} = 1.954\,cm$ $D_{core} = 0.769\,in$

The required mass and volume of fuel is now determined for a specified burn time. If we choose to design this rocket motor to burn no more than 30 seconds, the following calculations are valid:

$t := 30s$ $m_{paraffin} := m_{dot\_wax} \cdot t$ $m_{paraffin} = 0.48\,kg$ $m_{paraffin} = 1.058\,lb$

$$V_{paraffin} := \frac{m_{paraffin}}{\rho_{paraffin}}$$ $V_{paraffin} = 593.451\,cm^3$

The required length of the fuel grain can now be estimated under some assumptions. Because of high temperatures and material properties, it is not advantageous to burn all of the paraffin wax. If we assume that a layer of wax is left so that the hollow inside core is 4.4 cm (1.75 in) in diameter, the length can be determined:

$$A_{fuel} := \frac{\pi \cdot \left[(1.75 \cdot in)^2 - D_{core}^2 \right]}{4} \qquad A_{fuel} = 12.519 \, cm^2$$

$$Length := \frac{V_{paraffin}}{A_{fuel}} \qquad \boxed{Length = 0.474 \, m} \qquad Length = 18.664 \, in$$

In hybrid rockets, it has been experimentally found that longer combustion chambers result in more stable combustion. For this reason, the fuel grain used will be lengthened from this calculation to try and help control combustion instabilities that are inherant in hybrids.
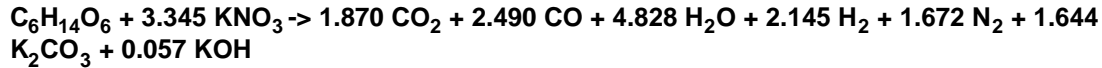
Igniter Calculations

Unit Definitions:

Performed by: Ryan Erickson
Date: Spring 2005

$$kJ := 10^3 J \quad kmol := 10^3 mol \quad R_u := 8.314 \frac{kJ}{kmol \cdot K}$$

For the KN-Sorbitol propellant, with an oxidizer-fuel (O/F) ratio of 65/35, the theoretical combustion equation is as follows:

$C_6H_{14}O_6$ + 3.345 KNO_3 -> 1.870 CO_2 + 2.490 CO + 4.828 H_2O + 2.145 H_2 + 1.672 N_2 + 1.644 K_2CO_3 + 0.057 KOH

First the mole fractions of each component are found:

$$N_{total} := 14.706 \qquad y_{co2} := \frac{1.870}{N_{total}} \qquad y_{co} := \frac{2.490}{N_{total}} \qquad y_{h2o} := \frac{4.828}{N_{total}}$$

$$y_{k2co3} := \frac{1.644}{N_{total}} \qquad y_{koh} := \frac{0.057}{N_{total}} \qquad y_{n2} := \frac{1.672}{N_{total}} \qquad y_{h2} := \frac{2.145}{N_{total}}$$

Thermodynamic Property Correlations of reacting components:

N_2: $\quad a_{1\_n2} := 2.95257626 \qquad a_{2\_n2} := 1.39690057 \cdot 10^{-3} \frac{1}{K} \quad a_{3\_n2} := -4.92631691 \cdot 10^{-7} \frac{1}{K^2}$

$$a_{4\_n2} := 7.86010367 \cdot 10^{-11} \frac{1}{K^3} \quad a_{5\_n2} := -4.60755321 \cdot 10^{-15} \frac{1}{K^4} \quad b_{1\_n2} := -9.23948645 \cdot 10^2 \cdot K$$

$$h_{n2}(T) := R_u \cdot T \cdot \left(a_{1\_n2} + a_{2\_n2} \cdot \frac{T}{2} + a_{3\_n2} \cdot \frac{T^2}{3} + a_{4\_n2} \cdot \frac{T^3}{4} + a_{5\_n2} \cdot \frac{T^4}{5} + \frac{b_{1\_n2}}{T} \right)$$

H_2O: $\quad a_{1\_h2o} := 2.67703787 \qquad a_{2\_h2o} := 2.97318329 \cdot 10^{-3} \frac{1}{K} \qquad a_{3\_h2o} := -7.73769690 \cdot 10^{-7} \frac{1}{K^2}$

$$a_{4\_h2o} := 9.44336689 \cdot 10^{-11} \frac{1}{K^3} \quad a_{5\_h2o} := -4.26900959 \cdot 10^{-15} \frac{1}{K^4} \quad b_{1\_h2o} := -2.98858938 \cdot 10^4 \cdot K$$

$$h_{h2o}(T) := R_u \cdot T \cdot \left(a_{1\_h2o} + a_{2\_h2o} \cdot \frac{T}{2} + a_{3\_h2o} \cdot \frac{T^2}{3} + a_{4\_h2o} \cdot \frac{T^3}{4} + a_{5\_h2o} \cdot \frac{T^4}{5} + \frac{b_{1\_h2o}}{T} \right)$$

CO_2: $\quad a_{1\_co2} := 4.63659493 \qquad a_{2\_co2} := 2.74131991 \cdot 10^{-3} \frac{1}{K} \qquad a_{3\_co2} := -9.95828531 \cdot 10^{-7} \frac{1}{K^2}$

$$a_{4\_co2} := 1.60373011 \cdot 10^{-10} \frac{1}{K^3} \quad a_{5\_co2} := -9.16103468 \cdot 10^{-15} \frac{1}{K^4} \quad b_{1\_co2} := -4.90249341 \cdot 10^4 \cdot K$$

$$h_{co2}(T) := R_u \cdot T \cdot \left(a_{1\_co2} + a_{2\_co2} \cdot \frac{T}{2} + a_{3\_co2} \cdot \frac{T^2}{3} + a_{4\_co2} \cdot \frac{T^3}{4} + a_{5\_co2} \cdot \frac{T^4}{5} + \frac{b_{1\_co2}}{T} \right)$$

CO: $a_{1\_co} := 3.04848583$ $\qquad a_{2\_co} := 1.35172818 \cdot 10^{-3} \frac{1}{K}$ $\qquad a_{3\_co} := -4.85794075 \cdot 10^{-7} \frac{1}{K^2}$

$\quad a_{4\_co} := 7.88536486 \cdot 10^{-11} \frac{1}{K^3}$ $\quad a_{5\_co} := -4.69807489 \cdot 10^{-15} \frac{1}{K^4}$ $\quad b_{1\_co} := -1.42661171 \cdot 10^{4} \cdot K$

$$h_{co}(T) := R_u \cdot T \cdot \left(a_{1\_co} + a_{2\_co} \cdot \frac{T}{2} + a_{3\_co} \cdot \frac{T^2}{3} + a_{4\_co} \cdot \frac{T^3}{4} + a_{5\_co} \cdot \frac{T^4}{5} + \frac{b_{1\_co}}{T} \right)$$

H₂: $a_{1\_h2} := 2.93286579$ $\qquad a_{2\_h2} := 8.26607967 \cdot 10^{-4} \frac{1}{K}$ $\qquad a_{3\_h2} := -1.46402335 \cdot 10^{-7} \frac{1}{K^2}$

$\quad a_{4\_h2} := 1.54100359 \cdot 10^{-11} \frac{1}{K^3}$ $\quad a_{5\_h2} := -6.88804432 \cdot 10^{-16} \frac{1}{K^4}$ $\quad b_{1\_h2} := -8.13065597 \cdot 10^{2} \cdot K$

$$h_{h2}(T) := R_u \cdot T \cdot \left(a_{1\_h2} + a_{2\_h2} \cdot \frac{T}{2} + a_{3\_h2} \cdot \frac{T^2}{3} + a_{4\_h2} \cdot \frac{T^3}{4} + a_{5\_h2} \cdot \frac{T^4}{5} + \frac{b_{1\_h2}}{T} \right)$$

KOH: $a_{1\_koh} := 8.917271950 \cdot 10^{5} \cdot K^2$ $\quad a_{2\_koh} := -2.334179072 \cdot 10^{3} \cdot K$ $\quad a_{3\_koh} := 7.972578710$

$\quad a_{4\_koh} := 1.038863156 \cdot 10^{-4} \frac{1}{K}$ $\quad a_{5\_koh} := -6.315893470 \cdot 10^{-8} \frac{1}{K^2}$ $\quad b_{1\_koh} := -1.443696469 \cdot 10^{4} \cdot K$

$\quad a_{6\_koh} := 1.027938106 \cdot 10^{-11} \frac{1}{K^3}$ $\quad a_{7\_koh} := -5.736685820 \cdot 10^{-16} \frac{1}{K^4}$

$$h_{koh}(T) := R_u \cdot T \cdot \left[\begin{array}{l} -a_{1\_koh} \cdot T^{-2} + a_{2\_koh} \cdot \dfrac{\ln\left(\dfrac{T}{K}\right)}{T} + a_{3\_koh} + a_{4\_koh} \cdot \dfrac{T}{2} + a_{5\_koh} \cdot \dfrac{T^2}{3} \cdots \\[3ex] + a_{6\_koh} \cdot \dfrac{T^3}{4} + a_{7\_koh} \cdot \dfrac{T^4}{5} + \dfrac{b_{1\_koh}}{T} \end{array} \right]$$

***This equation for enthalpy is modified due to the use of an alternate source of data.

K₂CO₃: $a_{1\_k2co3} := -3.26426316 \cdot 10^{5} \cdot K^2$ $\quad a_{2\_k2co3} := -1.521168973 \cdot 10^{3} \cdot K$ $\quad a_{3\_k2co3} := 1.712283562 \cdot 10^{1}$

$\quad a_{4\_k2co3} := -4.464580710 \cdot 10^{-4} \frac{1}{K}$ $\quad a_{5\_k2co3} := 9.833379630 \cdot 10^{-8} \frac{1}{K^2}$ $\quad b_{1\_k2co3} := -9.4882751 \cdot 10^{4} \cdot K$

$\quad a_{6\_k2co3} := -1.125478371 \cdot 10^{-11} \frac{1}{K^3}$ $\quad a_{7\_k2co3} := 5.210069120 \cdot 10^{-16} \frac{1}{K^4}$

$$h_{k2co3}(T) := R_u \cdot T \cdot \left[\begin{array}{l} -a_{1\_k2co3} \cdot T^{-2} + a_{2\_k2co3} \cdot \dfrac{\ln\left(\dfrac{T}{K}\right)}{T} + a_{3\_k2co3} + a_{4\_k2co3} \cdot \dfrac{T}{2} + a_{5\_k2co3} \cdot \dfrac{T^2}{3} \cdots \\[3ex] + a_{6\_k2co3} \cdot \dfrac{T^3}{4} + a_{7\_k2co3} \cdot \dfrac{T^4}{5} + \dfrac{b_{1\_k2co3}}{T} \end{array} \right]$$

KNO$_3$: $a_{1\_kno3} := -3.183682870 \cdot 10^5 \cdot K^2$ $\quad a_{2\_kno3} := -1.375234449 \cdot 10^3 \cdot K$ $\quad a_{3\_kno3} := 1.401587531 \cdot 10^1$

$$a_{4\_kno3} := -4.040660080 \cdot 10^{-4} \frac{1}{K} \quad a_{5\_kno3} := 8.900847780 \cdot 10^{-8} \frac{1}{K^2} \quad b_{1\_kno3} := -3.513853220 \cdot 10^4 \cdot K$$

$$a_{6\_kno3} := -1.018771993 \cdot 10^{-11} \frac{1}{K^3} \quad a_{7\_kno3} := 4.715982020 \cdot 10^{-16} \frac{1}{K^4}$$
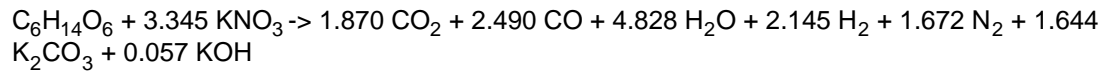
$$h_{kno3}(T) := R_u \cdot T \cdot \left(-a_{1\_kno3} \cdot T^{-2} + a_{2\_kno3} \cdot \frac{\ln\left(\frac{T}{K}\right)}{T} + a_{3\_kno3} + a_{4\_kno3} \cdot \frac{T}{2} + a_{5\_kno3} \cdot \frac{T^2}{3} \cdots \right. $$
$$\left. + a_{6\_kno3} \cdot \frac{T^3}{4} + a_{7\_kno3} \cdot \frac{T^4}{5} + \frac{b_{1\_kno3}}{T} \right)$$

$$h_{f\_sorbitol} := -1353.7 \cdot 10^3 \frac{kJ}{kmol}$$

Recall the Steady-Flow Energy equation from previous combustion calculations:

$$\sum_{Products} \left[N_i \cdot h^o(T) \right] + Q_{out} := \sum_{Reactants} \left[N_i \cdot \left(h_f + \Delta h \right) \right]$$

For the KN-Sorbitol propellant, with an oxidizer-fuel (O/F) ratio of 65/35, the theoretical combustion equation is as follows:

$C_6H_{14}O_6$ + 3.345 KNO_3 -> 1.870 CO_2 + 2.490 CO + 4.828 H_2O + 2.145 H_2 + 1.672 N_2 + 1.644 K_2CO_3 + 0.057 KOH

The combustion reaction can now be defined:

$$Q_{out}(T) := 1 \cdot h_{f\_sorbitol} + 3.345 \cdot h_{kno3}(T) - 1.870 \cdot h_{co2}(T) - 2.49 \cdot h_{co}(T) - 4.828 \cdot h_{h2o}(T) \cdots$$
$$+ -2.145 \cdot h_{h2}(T) - 1.672 \cdot h_{n2}(T) - 1.644 \cdot h_{k2co3}(T) - 0.057 \cdot h_{koh}(T)$$

According to the paper on sorbitol/potassium nitrate fuel, the chemical reaction occurs at 1600 Kelvin. This reaction would produce:

$$Q_{out}(1600K) = 6.291 \times 10^5 \frac{kJ}{kmol} \quad \text{(per kmol of sorbitol)}$$

The properties of the combustion reaction can be graphed as a function of reaction temperature:

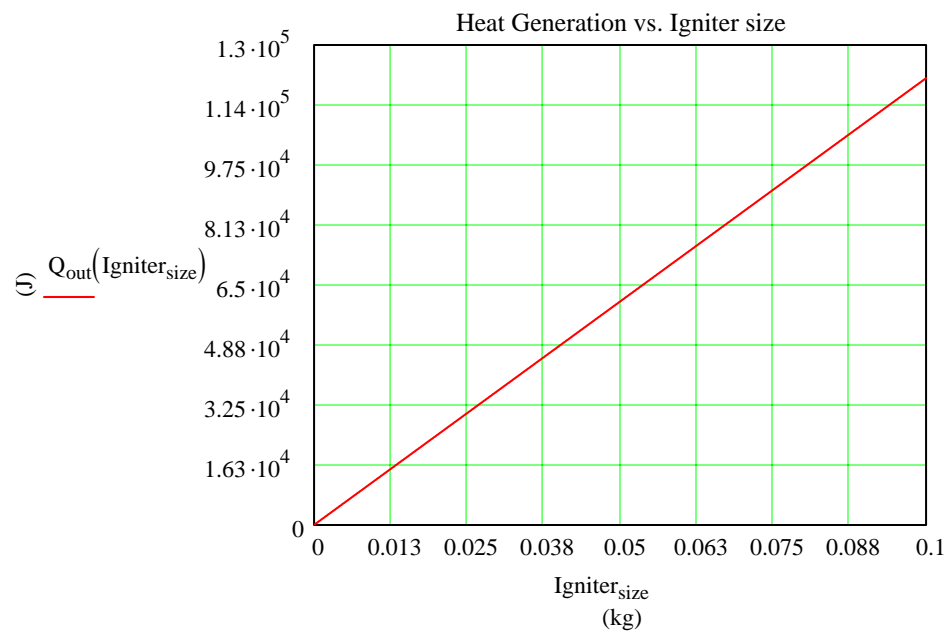$T := 1000K .. 3000K$

Heat Generation from Igniter
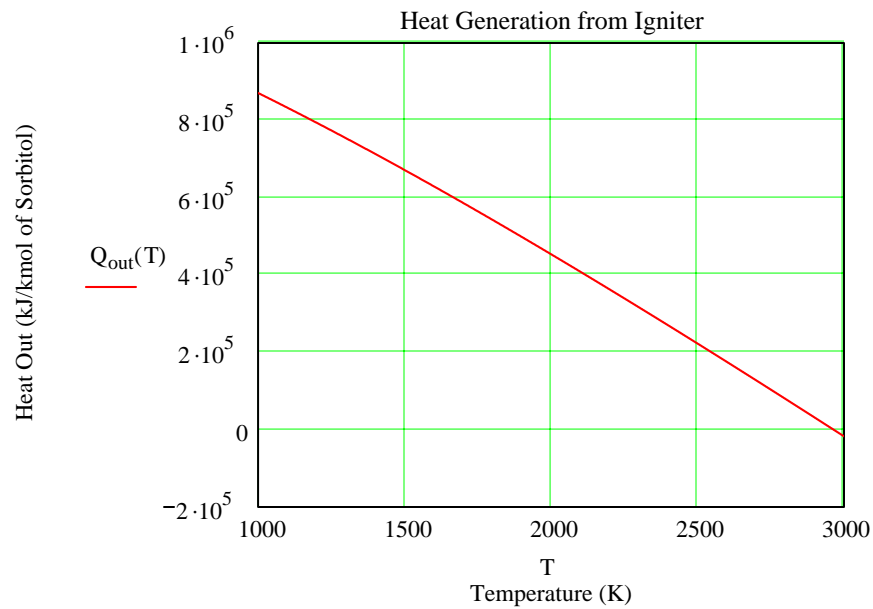
$MW_{sorbitol} := 182 \cdot \dfrac{gm}{mol}$ $Q_{out\_calculated} := 6.291 \cdot 10^5 \dfrac{kJ}{kmol}$ (per kmol of sorbitol)

$Sorbitol_{content}(Igniter_{size}) := \dfrac{0.35 \cdot Igniter_{size}}{MW_{sorbitol}}$ $Sorbitol_{content}(.03kg) = 0.058 \, mol$

$Q_{out}(Igniter_{size}) := Sorbitol_{content}(Igniter_{size}) \cdot Q_{out\_calculated}$

Heat Generation vs. Igniter size

Now using an experimentally found reaction rate for the solid fuel igniter, the rate of heat generation can be approximated:

$$\text{Burn}_{rate} := \frac{35.9\,\text{gm}}{6.72\,\text{s}} \qquad \text{Q}_{out\_mass} := \frac{\text{Q}_{out\_calculated}}{\text{MW}_{sorbitol}} \qquad \text{Q}_{out\_rate} := \text{Q}_{out\_mass} \cdot \text{Burn}_{rate}$$

$$\text{Q}_{out\_rate} = 18.466\,\text{kW} \qquad \text{This is the energy generation rate of the solid fuel.}$$

It is now desired to approximate the conditions inside the rocket after the igniter has been fired. This will initially be done by assuming the fluid in the rocket is air and that the rocket is completely enclosed (constant volume heat addition). Because this assumption is made, unrealistic results are likely. However, it is hoped that these results may aid in a future transient analysis of the system.

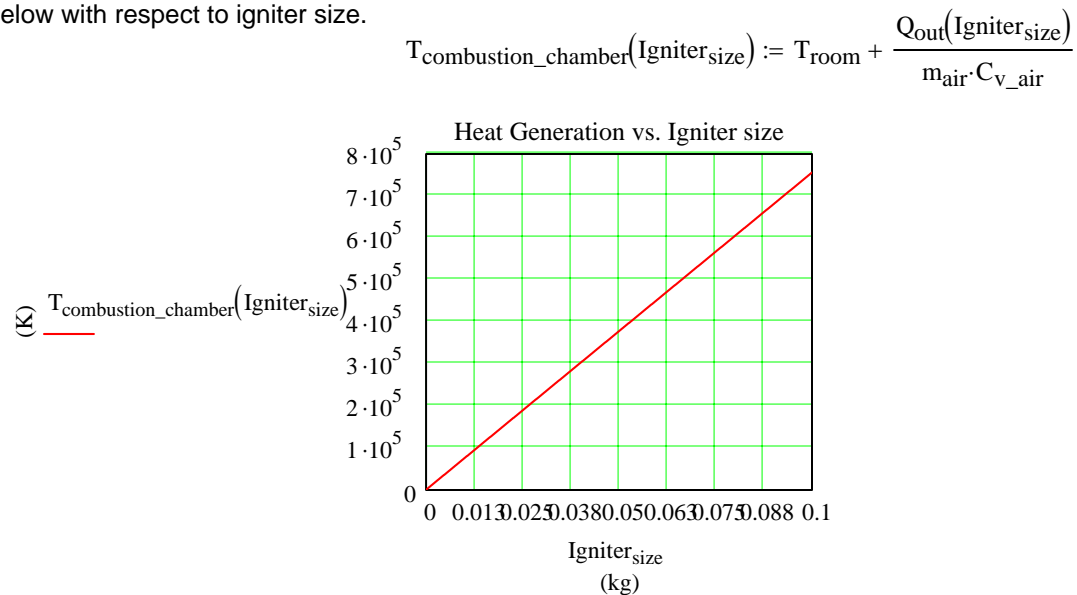The void (fluid) space inside the rocket is currently assumed to have a volume of: $11.5\,\text{in}^3$

$$11.4864\,\text{in}^3 = 1.882 \times 10^{-4}\,\text{m}^3 \qquad \text{V}_{air} := 1.882 \cdot 10^{-4}\,\text{m}^3$$

The definition of a closed thermodynamic system is now defined: $\quad \text{Q}_{out} := \text{m}_{air} \cdot \text{C}_v \cdot \Delta T$

$$\text{C}_{v\_air} := 0.718\,\frac{\text{kJ}}{\text{kg} \cdot \text{K}} \qquad \rho_{air} := 1.185\,\frac{\text{kg}}{\text{m}^3} \qquad \text{T}_{room} := (25 + 273)\,\text{K}$$

$$\text{m}_{air} := \rho_{air} \cdot \text{V}_{air} \qquad \text{m}_{air} = 2.23 \times 10^{-4}\,\text{kg}$$

The temperature change of the system, assuming the igniter is completely burned, is graphed below with respect to igniter size.

$$\text{T}_{combustion\_chamber}\left(\text{Igniter}_{size}\right) := \text{T}_{room} + \frac{\text{Q}_{out}\left(\text{Igniter}_{size}\right)}{\text{m}_{air} \cdot \text{C}_{v\_air}}$$

Heat Generation vs. Igniter size

The results of this analysis, as mentioned before, are not in any way physically realistic. It is possible that they will, however, be useful in a transient analysis completed in the future.

Nitrous Oxide Injector Calculations

Performed by: Ryan Erickson
Date: Spring 2005

The purpose of these calculations is to size the nitrous oxide injector nozzle to deliver the appropriate flow rate of N_2O into the rocket. The current bulkhead arrangement, where the N_2O enters the rocket, utilizes one injector. The injector directs N_2O straight down the fuel grain with minimal flow obstruction. The calculations are made using information from BETE, the nozzle manufacturer [7]. Because BETE's information is used, the calculations only hold for their nozzles (which are currently being used on the rocket).

The first step is to approximate the density of the N_2O flowing through the nozzle. This is done using information from Perry [8], assuming saturated liquid.

TABLE 2-291 Saturated Nitrous Oxide

Temp., °F	Pressure, psia	v_f, ft³/lb$_m$	v_g, ft³/lb$_m$	h_f, Btu/lb$_m$	h_g, Btu/lb$_m$	s_f, Btu/lb$_m$·°R	s_g, Btu/lb$_m$·°R
−127.2	14.70	0.01310	5.069	0.0	161.7	0.0000	0.4864
−100	33.68	0.01358	2.374	11.7	165.9	0.0304	0.4591
−80	56.79	0.01398	1.463	20.8	168.8	0.0634	0.4433
−60	90.29	0.01444	0.939	30.2	171.5	0.0782	0.4315
−40	136.68	0.01495	0.648	40.3	173.7	0.1044	0.4222
−20	198.62	0.01555	0.450	50.6	175.3	0.1296	0.4133
0	278.97	0.01625	0.316	60.5	176.2	0.1518	0.4036
20	380.88	0.01711	0.227	70.2	176.2	0.1718	0.3925
40	507.51	0.01819	0.164	80.3	175.0	0.1920	0.3815
60	662.69	0.01968	0.117	91.9	172.1	0.2145	0.3687
80	851.5	0.0222	0.0792	105.7	165.0	0.2382	0.3480
90	961.0	0.0247	0.0611	114.7	157.5	0.2523	0.3302
97.6^c	1052.2	0.0354	0.0354	136.4	136.4	0.2800	0.2800

Rounded and condensed from Couch, E. J. and K. A. Kobe, Univ. Texas Rep., Cont. DAI-23-072-ORD-685, June 1, 1956. c = critical point.

Specific Volume interpolation assuming saturated liquid:

$$v_1 := \frac{70-60}{80-60}\cdot(0.0222-0.01968)\cdot\frac{ft^3}{lb} + 0.01968\cdot\frac{ft^3}{lb} \qquad v_1 = 1.307\times10^{-3}\,\frac{m^3}{kg}$$

The density is now defined as:

$$\rho_{n2o} := \frac{1}{v_1} \qquad \rho_{n2o} = 764.97\,\frac{kg}{m^3}$$

With the density known, a mass flow rate is defined for future calculations. From the assumed mass flow rate, a volumetric flow rate is also found:

$$m_{dot\_required} := 0.15\,\frac{kg}{s} \qquad Q_{required} := \frac{m_{dot\_required}}{\rho_{n2o}} \qquad Q_{required} = 11.765\,\frac{L}{min}$$

Now that a desired volumetric flow rate of N_2O has been defined, a nozzle is ready to be sized. Since BETE nozzles are currently being used in the rocket, I found their spray characteristics from www.bete.com [7]. The published spray characteristics are for water flow, so some changes are required before they are used to find the fluid flow (Changes to "K" Factor). According to BETE, the volumetric flow rate of water through their nozzles varies according to:

$$Flow\ Rate\ (^{l}/_{min}) = K\ (bar)^{0.47}$$

The first consideration is whether or not nitrous oxide's viscous effects should be considered in calculations. To determine if they have a large impact on the flow, the Reynold's Number will be calculated. The Reynold's Number is a dimensionless value which can be though of as a ratio of intertial forces to viscous forces. Therefore, a large Reynold's Number represents a flow with overpowering inertial forces.

From pg. 441 of [9], the dynamic viscosity of N_2O at room temperature is: $\mu := 0.05 \cdot 10^{-3} poise$

The nitrous supply line dimensions are defined as: $D_{tube} := \frac{1}{8} in$ $\qquad A_{tube} := \frac{\pi \cdot D_{tube}^2}{4}$

The velocity of N_2O and Reynold's Number entering the nozzle are now defined as:

$$v := \frac{m_{dot\_required}}{\rho_{n2o} \cdot A_{tube}} \qquad v = 24.767\ \frac{m}{s}$$

$$Re := \frac{v \cdot D_{tube} \cdot \rho_{n2o}}{\mu} \qquad Re = 1.203 \times 10^7$$

At this high of a Reynold's Number, the K Factor can be assumed to vary as a function of density (neglecting viscous effects). The K Factor for N_2O can then be described as:

$$\rho_{water} := 1000\ \frac{kg}{m^3} \qquad K_{water} := 0.587 \qquad bar := \frac{1}{1.01325} atm$$

$$K_{n2o} := \frac{K_{water} \cdot \sqrt{\rho_{water}}}{\sqrt{\rho_{n2o}}} \qquad K_{n2o} = 0.671$$

With this K Factor defined for N_2O, BETE's flow characteristics may be used to predict flow through their nozzles. Note: In the formula provided by BETE for volumetric flow rate, the "bar" value is actually the differential pressure seen across the nozzle in bars (unit). At this time, the differential pressure seen across the nozzle during operation has been approximately 200 psi. This value will be assumed for all further calculations.

$$200psi = 13.79\ bar$$

The first nozzle evaluated will be type "WL 1/4" with an orifice diameter of 1.09 mm (0.043 in). The first step is to scale the K Factor for N_2O flow.

$$K_{water} := 0.587 \qquad K_{n2o} := \frac{K_{water} \cdot \sqrt{\rho_{water}}}{\sqrt{\rho_{n2o}}} \qquad K_{n2o} = 0.671$$

The differential pressure across the nozzle is defined as: $\quad P_{bar} := 13.79$

The volumetric flow rate through the nozzle is now solved: $\quad Q_{dot} := K_{n2o} \cdot P_{bar}^{0.47}$

$$Q_{dot} = 2.304$$

Working backwards, the mass flow rate that this nozzle will deliver is approximated to be:

$$Q_{dot} := 2.304 \frac{L}{min} \qquad m_{dot} := \rho_{n2o} \cdot Q_{dot} \qquad m_{dot} = 0.029 \frac{kg}{s}$$

This mass flow rate of N_2O is much smaller (around 5 times) than the designed flow rate. Therefore, a new nozzle should be considered.

The next nozzle evaluated will be type "WL 1/2" with an orifice diameter of 1.40 mm (0.055 in).
The first step is to scale the K Factor for N_2O flow.

$K_{water} := 1.17$ $\qquad K_{n2o} := \dfrac{K_{water} \cdot \sqrt{\rho_{water}}}{\sqrt{\rho_{n2o}}}$ $\qquad K_{n2o} = 1.338$

The differential pressure across the nozzle is defined as: $\qquad P_{bar} := 13.79$

The volumetric flow rate through the nozzle is now solved: $\qquad Q_{dot} := K_{n2o} \cdot P_{bar}^{0.47}$

$$Q_{dot} = 4.592$$

Working backwards, the mass flow rate that this nozzle will deliver is approximated to be:

$Q_{dot} := 4.592 \dfrac{L}{min}$ $\qquad m_{dot} := \rho_{n2o} \cdot Q_{dot}$ $\qquad m_{dot} = 0.059 \dfrac{kg}{s}$

This mass flow rate of N_2O is also smaller (around 4 times) than the designed flow rate.
Therefore, a new nozzle should be considered.

The third nozzle evaluated will be type "WL 3/4" with an orifice diameter of 1.83 mm (0.072 in). The first step is to scale the K Factor for N_2O flow.

$$K_{water} := 1.76 \qquad K_{n2o} := \frac{K_{water} \cdot \sqrt{\rho_{water}}}{\sqrt{\rho_{n2o}}} \qquad K_{n2o} = 2.012$$

The differential pressure across the nozzle is defined as: $\qquad P_{bar} := 13.79$

The volumetric flow rate through the nozzle is now solved: $\qquad Q_{dot} := K_{n2o} \cdot P_{bar}^{0.47}$

$$Q_{dot} = 6.907$$

Working backwards, the mass flow rate that this nozzle will deliver is approximated to be:

$$Q_{dot} := 6.907 \frac{L}{min} \qquad m_{dot} := \rho_{n2o} \cdot Q_{dot} \qquad m_{dot} = 0.088 \frac{kg}{s}$$

This mass flow rate of N_2O is slightly smaller than the designed flow rate of 0.15 kg/s. Therefore, a new nozzle should be considered.

The fourth nozzle evaluated will be type "WL 1" with an orifice diameter of 2.08 mm (0.082 in).
The first step is to scale the K Factor for N_2O flow.

$$K_{water} := 2.35 \qquad K_{n2o} := \frac{K_{water} \cdot \sqrt{\rho_{water}}}{\sqrt{\rho_{n2o}}} \qquad K_{n2o} = 2.687$$

The differential pressure across the nozzle is defined as: $\qquad P_{bar} := 13.79$

The volumetric flow rate through the nozzle is now solved: $\qquad Q_{dot} := K_{n2o} \cdot P_{bar}^{0.47}$

$$Q_{dot} = 9.222$$

Working backwards, the mass flow rate that this nozzle will deliver is approximated to be:

$$Q_{dot} := 9.22 \frac{L}{min} \qquad m_{dot} := \rho_{n2o} \cdot Q_{dot} \qquad m_{dot} = 0.118 \frac{kg}{s}$$

This mass flow rate of N_2O is approaching the designed flow rate of 0.15 kg/s.

The fifth nozzle evaluated will be type "WL 1-1/2" with an orifice diameter of 2.77 mm (0.109 in).
The first step is to scale the K Factor for N_2O flow.

$$K_{water} := 3.52 \qquad K_{n2o} := \frac{K_{water} \cdot \sqrt{\rho_{water}}}{\sqrt{\rho_{n2o}}} \qquad K_{n2o} = 4.025$$

The differential pressure across the nozzle is defined as: $\qquad P_{bar} := 13.79$

The volumetric flow rate through the nozzle is now solved: $\qquad Q_{dot} := K_{n2o} \cdot P_{bar}^{0.47}$

$$Q_{dot} = 13.814$$

Working backwards, the mass flow rate that this nozzle will deliver is approximated to be:

$$Q_{dot} := 13.814 \frac{L}{min} \qquad m_{dot} := \rho_{n2o} \cdot Q_{dot} \qquad m_{dot} = 0.176 \frac{kg}{s}$$

This mass flow rate of N_2O is slighlty above the designed flow rate. Therefore, it can be concluded for the single nitrous injector nozzle arrangement, that the BETE "WL 1" and "WL 1 1/2" come closest to delivering the desired flow rate.

<div style="background-color: yellow;">

Nozzle Design

</div>

Performed by: Ryan Erickson
Date: Spring 2005

MathCAD Definitions: $kmol := 10^3 mol$ $kJ := 10^3 J$ $R_u := 8.314 \frac{kJ}{kmol \cdot K}$ $MPa := 10^6 Pa$

      In order to design a rocket nozzle with efficient thrust characteristics, supersonic flows must be achieved. This requires the design of a converging-diverging nozzle. The goal of a converging-diverging nozzle is to accelerate the exhaust gases to Mach 1 at the throat. This is the physical velocity limit in a converging nozzle which is known as "choked" flow. Once supersonic velocities are achieved at the throat, the fluid will actually accelerate through the diverging section of the nozzle. The following calculations are used to design the nozzle and approximate characteristic operating conditions for project "HERMES".

Initially, fluid properties of the exhaust gases must be defined. These gases are at extremely high temperatures, which require data from [4]. Combustion is assumed to occur <u>below</u> the adiabatic flame temperature previously calculated (See "Thermochemical Calculations"). This is because the adiabatic flame temperature occurs in the active combustion zone. The energy in that zone will diffuse into other system components besides the exhaust gases such as the fuel (shown in figure below). This results in a slightly lower exhaust gas temperature.
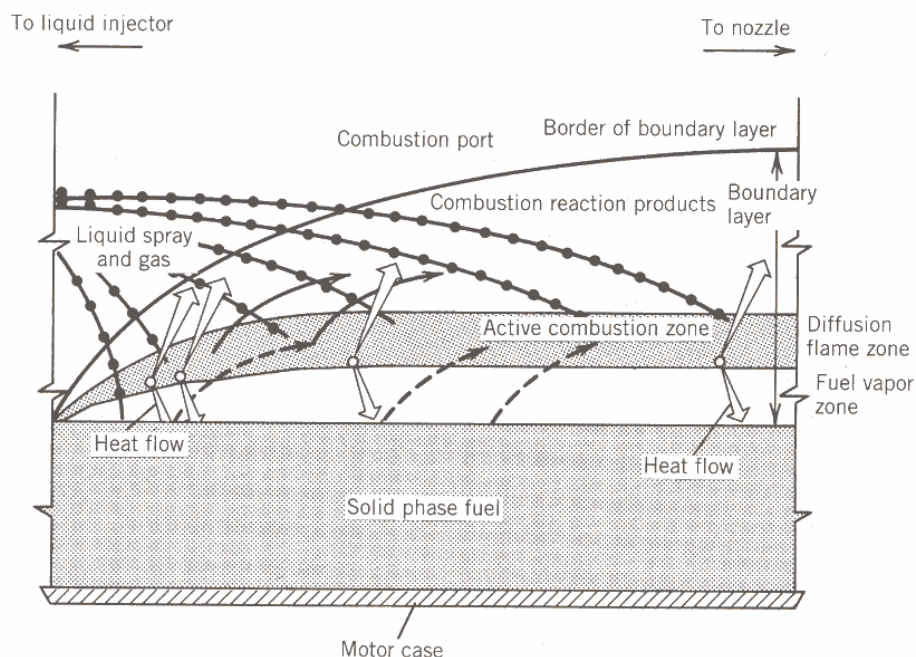
Assumed Nozzle Inlet Conditions: $T_{combustion} := 3000K$ $P_{combustion} := 500psi$

Thermodynamic properties of each exhaust gas component are first defined:

N_2: $a_{1\_n2} := 2.95257626$ $a_{2\_n2} := 1.39690057 \cdot 10^{-3} \dfrac{1}{K}$ $a_{3\_n2} := -4.92631691 \cdot 10^{-7} \dfrac{1}{K^2}$

$a_{4\_n2} := 7.86010367 \cdot 10^{-11} \dfrac{1}{K^3}$ $a_{5\_n2} := -4.60755321 \cdot 10^{-15} \dfrac{1}{K^4}$

$C_{p\_n2\_mol}(T) := R_u \cdot \left(a_{1\_n2} + a_{2\_n2} \cdot T + a_{3\_n2} \cdot T^2 + a_{4\_n2} \cdot T^3 + a_{5\_n2} \cdot T^4 \right)$

Assuming an ideal gas: $\dfrac{P}{\rho} := R \cdot T$ $P_{n2} := 500\text{psi}$ $T_{n2} := 3000K$ $R_{n2} := 0.2968 \dfrac{kJ}{kg \cdot K}$

$\rho_{n2\_ideal} := \dfrac{P_{n2}}{R_{n2} \cdot T_{n2}}$ $\rho_{n2\_ideal} = 3.872 \dfrac{kg}{m^3}$ $M_{n2} := 28.013 \dfrac{kg}{kmol}$

Since the nitrogen is at a very high pressure, the ideal gas equation introduces some error. Therefore, the compressibility factor (Z) must be taken into account. Nitrogen's critical properties are needed to find its reduced properties.

$P_{cr} := 3.39\text{MPa}$ $T_{cr} := 126.2K$

$P_r := \dfrac{P_{n2}}{P_{cr}}$ $T_r := \dfrac{T_{n2}}{T_{cr}}$ $P_r = 1.017$ $T_r = 23.772$

From [2] pg.867, the compressibility factor is found to be approximately: $Z := 1.02$

$Z := \dfrac{\rho_{ideal}}{\rho_{actual}}$ $\rho_{n2} := \dfrac{\rho_{n2\_ideal}}{Z}$ $\rho_{n2} = 3.796 \dfrac{kg}{m^3}$

$C_{p\_n2}(T) := \dfrac{C_{p\_n2\_mol}(T)}{M_{n2}}$ $C_{v\_n2}(T) := C_{p\_n2}(T) - R_{n2}$ $k_{n2}(T) := \dfrac{C_{p\_n2}(T)}{C_{v\_n2}(T)}$

H_2O: $a_{1\_h2o} := 2.67703787$ $a_{2\_h2o} := 2.97318329 \cdot 10^{-3} \dfrac{1}{K}$ $a_{3\_h2o} := -7.73769690 \cdot 10^{-7} \dfrac{1}{K^2}$

$a_{4\_h2o} := 9.44336689 \cdot 10^{-11} \dfrac{1}{K^3}$ $a_{5\_h2o} := -4.26900959 \cdot 10^{-15} \dfrac{1}{K^4}$

$C_{p\_h2o\_mol}(T) := R_u \cdot \left(a_{1\_h2o} + a_{2\_h2o} \cdot T + a_{3\_h2o} \cdot T^2 + a_{4\_h2o} \cdot T^3 + a_{5\_h2o} \cdot T^4 \right)$

Assuming an ideal gas: $\dfrac{P}{\rho} := R \cdot T$ $P_{h2o} := 500\text{psi}$ $T_{h2o} := 3000K$ $R_{h2o} := 0.4615 \dfrac{kJ}{kg \cdot K}$

$\rho_{h2o\_ideal} := \dfrac{P_{h2o}}{R_{h2o} \cdot T_{h2o}}$ $\rho_{h2o\_ideal} = 2.49 \dfrac{kg}{m^3}$ $M_{h2o} := 18.015 \dfrac{kg}{kmol}$

Since the water vapor is at a very high pressure, the ideal gas equation introduces some error. Therefore, the compressibility factor (Z) must be taken into account. Water's critical properties are needed to find its reduced properties.

$P_{cr} := 22.09 \, MPa$ $\quad$ $T_{cr} := 647.3 \, K$

$$P_r := \frac{P_{h2o}}{P_{cr}} \qquad T_r := \frac{T_{h2o}}{T_{cr}} \qquad P_r = 0.156 \qquad T_r = 4.635$$

From [2] pg.867, the compressibility factor is found to be approximately: $\quad Z := 1.0$

$$Z := \frac{\rho_{ideal}}{\rho_{actual}} \qquad \rho_{h2o} := \frac{\rho_{h2o\_ideal}}{Z} \qquad \rho_{h2o} = 2.49 \, \frac{kg}{m^3}$$

$$C_{p\_h2o}(T) := \frac{C_{p\_h2o\_mol}(T)}{M_{h2o}} \qquad C_{v\_h2o}(T) := C_{p\_h2o}(T) - R_{h2o} \qquad k_{h2o}(T) := \frac{C_{p\_h2o}(T)}{C_{v\_h2o}(T)}$$

CO_2: $\quad a_{1\_co2} := 4.63659493 \qquad a_{2\_co2} := 2.74131991 \cdot 10^{-3} \, \frac{1}{K} \qquad a_{3\_co2} := -9.95828531 \cdot 10^{-7} \, \frac{1}{K^2}$

$$a_{4\_co2} := 1.60373011 \cdot 10^{-10} \, \frac{1}{K^3} \qquad a_{5\_co2} := -9.16103468 \cdot 10^{-15} \, \frac{1}{K^4}$$

$$C_{p\_co2\_mol}(T) := R_u \cdot \left(a_{1\_co2} + a_{2\_co2} \cdot T + a_{3\_co2} \cdot T^2 + a_{4\_co2} \cdot T^3 + a_{5\_co2} \cdot T^4 \right)$$

Assuming an ideal gas: $\quad \dfrac{P}{\rho} := R \cdot T \qquad P_{co2} := 500 \, psi \qquad T_{co2} := 3000 \, K \qquad R_{co2} := 0.1889 \, \dfrac{kJ}{kg \cdot K}$

$$\rho_{co2\_ideal} := \frac{P_{co2}}{R_{co2} \cdot T_{co2}} \qquad \rho_{co2\_ideal} = 6.083 \, \frac{kg}{m^3} \qquad \qquad M_{co2} := 44.01 \, \frac{kg}{kmol}$$

Since the carbon dioxide is at a very high pressure, the ideal gas equation introduces some error. Therefore, the compressibility factor (Z) must be taken into account. Carbon dioxide's critical properties are needed to find its reduced properties:

$P_{cr} := 7.39 \, MPa$ $\quad$ $T_{cr} := 304.2 \, K$

$$P_r := \frac{P_{co2}}{P_{cr}} \qquad T_r := \frac{T_{co2}}{T_{cr}} \qquad P_r = 0.466 \qquad T_r = 9.862$$

From [2] pg.869, the compressibility factor is found to be approximately: $Z := 1.02$

$$Z := \frac{\rho_{ideal}}{\rho_{actual}} \qquad \rho_{co2} := \frac{\rho_{co2\_ideal}}{Z} \qquad \boxed{\rho_{co2} = 5.964 \; \frac{kg}{m^3}}$$

$$C_{p\_co2}(T) := \frac{C_{p\_co2\_mol}(T)}{M_{co2}} \qquad C_{v\_co2}(T) := C_{p\_co2}(T) - R_{co2} \qquad k_{co2}(T) := \frac{C_{p\_co2}(T)}{C_{v\_co2}(T)}$$

Now that properties of each exhaust gas constituent have been defined, the mixture must be analyzed as a whole. The property that is most important for nozzle design is the ratio of specific heats. In order to find the overall ratio, the total mole number and mole fractions must be determined:

$$N_{n2} := 85 \, mol \qquad N_{h2o} := 29 \, mol \qquad N_{co2} := 28 \, mol \qquad N_m := N_{n2} + N_{h2o} + N_{co2}$$

$$y_{n2} := \frac{N_{n2}}{N_m} \qquad y_{h2o} := \frac{N_{h2o}}{N_m} \qquad y_{co2} := \frac{N_{co2}}{N_m}$$

$$\boxed{y_{n2} = 0.599} \qquad \boxed{y_{h2o} = 0.204} \qquad \boxed{y_{co2} = 0.197}$$

$$C_{p\_mix}(T) := y_{n2} \cdot C_{p\_n2}(T) + y_{h2o} \cdot C_{p\_h2o}(T) + y_{co2} \cdot C_{p\_co2}(T)$$

$$\boxed{C_{p\_mix}\left(T_{combustion}\right) = 1.715 \; \frac{kJ}{kg \cdot K}}$$

$$k_{mix} := \Sigma y_i \cdot k_i^{\blacksquare}$$

$$k_{mix}(T) := y_{n2} \cdot k_{n2}(T) + y_{h2o} \cdot k_{h2o}(T) + y_{co2} \cdot k_{co2}(T)$$

$$\boxed{k_{mix}\left(T_{combustion}\right) = 1.238}$$

This is the ratio of specific heats for the exhaust gases at the combustion temperature. Its value will be used later on in nozzle design calculations. The overall density of the mixture can be found in the same manner:

$$\rho_{mix} := \Sigma y_i \cdot \rho_i^{\blacksquare}$$

$$\rho_{mix} := y_{n2} \cdot \rho_{n2} + y_{h2o} \cdot \rho_{h2o} + y_{co2} \cdot \rho_{co2}$$

$$\boxed{\rho_{mix} = 3.957 \; \frac{kg}{m^3}}$$

The gas constant for the exhaust mixture is also needed. It is approximated using mole fractions.

$$R_{mix} := y_{n2} \cdot R_{n2} + y_{h2o} \cdot R_{h2o} + y_{co2} \cdot R_{co2} \qquad \boxed{R_{mix} = 0.309 \; \frac{kJ}{kg \cdot K}}$$

Using this data, it is now possible to find the speed of sound in this medium (Mach 1):

$$C := \sqrt{k_{mix}(T_{combustion}) \cdot R_{mix} \cdot T_{combustion}} \qquad C = 1.072 \times 10^3 \frac{m}{s}$$

In order to design the internal dimensions of the nozzle, the exhaust gas velocity needs to be found. It will be denoted as v_{inlet} and is physically located at the nozzle inlet. The velocity distribution is assumed to be uniform. By applying the continuity equation for fluid flow through the combustion chamber, an exhaust gas velocity may be approximated.

From previous calculations: $\qquad m_{dot\_n2o} := 0.150 \frac{kg}{s} \qquad m_{dot\_wax} := 0.016 \frac{kg}{s}$

$$m_{dot\_total} := m_{dot\_n2o} + m_{dot\_wax}$$

The diameter of the combustion chamber must now be assumed. According to the preliminary design, the actual internal diameter of the fuel grain will vary between 0.77 in and 1.75 in (see "Combustion Chamber Length" calculations). A larger flow area will result in a slower velocity for any given fluid. Because of this, I will take the conservative approach and use the largest internal diameter of the fuel grain for further calculations. This will ensure that exhaust gases accelerate through the nozzle to Mach 1 at even the slowest initial velocites.

$$D_{chamber} := 1.75in \qquad A_{chamber} := \frac{\pi \cdot D_{chamber}^2}{4} \qquad 1.75in = 4.445 \; cm$$

Knowing the initial mass flow rate of oxidizer and propellant, the continuity equation can be applied:

$$\text{Guess value:} \quad v_{inlet} := 100 \frac{m}{s}$$

Given

$$m_{dot\_total} = \rho_{mix} \cdot v_{inlet} \cdot A_{chamber}$$

$$v_{inlet} := Find(v_{inlet})$$

$$v_{inlet} = 27.036 \frac{m}{s}$$

This velocity corresponds to an inlet Mach number of (from pg.780 of [2]):

$$M_{inlet} := \frac{v_{inlet}}{C} \qquad M_{inlet} = 0.025$$

Using this information, a ratio of areas between the nozzle inlet and throat can be found assuming that the flow is accelerated to Mach 1 at the throat. Using equation 3.99 from [6] yields:

$$\frac{A_2}{A_1} := \frac{M_1}{M_2} \cdot \sqrt{\left(\frac{1 + \frac{k-1}{2} \cdot M_2{}^2}{1 + \frac{k-1}{2} \cdot M_1{}^2}\right)^{\left(\frac{k+1}{k-1}\right)}}$$

**An initial nozzle inlet dimension must be assumed. Due to design constraints, the largest inlet diameter possible is 1.125 inches. At this time, there is no reason to change this dimension so it will be used for further calculations.

$$D_{inlet} := 1.125\,in \qquad A_{inlet} := \frac{\pi \cdot D_{inlet}{}^2}{4} \qquad M_{throat} := 1$$

Rearranging and solving for the throat area (assuming Mach 1 at throat) gives:

Guess values: $\qquad A_{throat} := 1.2\,cm^2 \qquad k := k_{mix}(T_{combustion})$

Given

$$A_{throat} = \frac{A_{inlet} \cdot M_{inlet}}{M_{throat}} \cdot \sqrt{\left(\frac{1 + \frac{k-1}{2} \cdot M_{throat}{}^2}{1 + \frac{k-1}{2} \cdot M_{inlet}{}^2}\right)^{\left(\frac{k+1}{k-1}\right)}}$$

$$A_{throat} := Find(A_{throat})$$

$$A_{throat} = 0.274\ cm^2$$

This throat area can also be expressed in terms of throat diameter, given below:

Guess value: $\qquad D_{throat} := 0.5\,cm$

Given

$$A_{throat} = \frac{\pi \cdot D_{throat}{}^2}{4}$$

$$D_{throat} := Find(D_{throat})$$

$$D_{throat} = 0.6\ cm$$

Now that the throat dimensions have been determined, the diverging section of the nozzle needs to be designed. This requires a few assumptions, namely, that the ehaust gases will be released into ambient pressure and that the flow can be considered isentropic. Because the gases will expand to ambient pressure anyway, it is desired to accomplish this directly at the nozzle exit to optimize the thrust in the nozzle.

First, the stagnation properties are found at the inlet and throat of the nozzle (from pg.776 of [2]):

$$T_o := T_{combustion} + \frac{v_{inlet}^2}{2 \cdot C_{p\_mix}(T_{combustion})} \qquad T_o = 3 \times 10^3 \, K$$

**This shows that the inlet velocity is basically negligable. Therefore, P_o can be approximated as $P_{combustion}$.

$$P_o := P_{combustion} \qquad \rho_o := \rho_{mix}$$

The properties of the exhaust gases can now be approximated at the throat of the nozzle. Applying relationships from pg.787 of [2] yields:

$$T_{star} := \frac{2 \cdot T_o}{k_{mix}(T_{combustion}) + 1} \qquad T_{star} = 2.681 \times 10^3 \, K$$

$$P_{star} := P_o \cdot \left(\frac{2}{k_{mix}(T_{combustion}) + 1} \right)^{\frac{k_{mix}(T_{combustion})}{k_{mix}(T_{combustion}) - 1}} \qquad P_{star} = 1.921 \, MPa$$

$$\rho_{star} := \rho_o \cdot \left(\frac{2}{k_{mix}(T_{combustion}) + 1} \right)^{\frac{1}{k_{mix}(T_{combustion}) - 1}} \qquad \rho_{star} = 2.467 \, \frac{kg}{m^3}$$

$$v_{star} := \sqrt{k_{mix}(T_{star}) \cdot R_{mix} \cdot T_{star}} \qquad v_{star} = 1.014 \times 10^3 \, \frac{m}{s}$$

These properties at the throat can now be used to design the diffuser section of the nozzle. The only desired design condition at this time is that the exhaust gases exand to atmospheric pressure. This gives (from pg787 of [2]):

Known: $P_{exit} := 1 atm$ Guess: $M_{exit} := 10$

Given

$$P_o = P_{exit} \left[1 + \left(\frac{k_{mix}(T_{star}) - 1}{2} \right) \cdot M_{exit}^2 \right]^{\frac{k_{mix}(T_{star})}{k_{mix}(T_{star}) - 1}}$$

$$M_{exit} := Find(M_{exit})$$

$$M_{exit} = 2.857$$

Solving for the nozzle exit area with known Mach number yields:

Guess values: $A_{exit} := 3cm^2$ $k := k_{mix}(T_{star})$

Given

$$A_{exit} = \frac{A_{throat} \cdot M_{throat}}{M_{exit}} \cdot \sqrt{\left(\frac{1 + \frac{k-1}{2} \cdot M_{exit}^2}{1 + \frac{k-1}{2} \cdot M_{throat}^2} \right)^{\left(\frac{k+1}{k-1} \right)}}$$

$A_{exit} := Find(A_{exit})$

$A_{exit} = 1.367 \ cm^2$

This nozzle exit area can also be expressed in terms of diameter, given below:

Guess value: $D_{exit} := 0.5cm$

Given

$$A_{exit} = \frac{\pi \cdot D_{exit}^2}{4}$$

$D_{exit} := Find(D_{exit})$

$D_{exit} = 1.319 \ cm$

Now that the cross-sectional area dimensions for the whole nozzle have been determined, the lengths of each sections are needed to complete the design. According to [6], the nozzle length of the diffuser section is given by:

$L_n := \frac{D_{exit} - D_{throat}}{2 \cdot tan(\theta_{cn})}$ where: θ_{cn} is the half angle (Typically between 12 and 18 degrees)

Assuming an intermediate half angle yields: $\theta_{cn} := 15deg$

$L_n := \frac{D_{exit} - D_{throat}}{2 \cdot tan(\theta_{cn})}$ $L_n = 1.342 \ cm$

The nozzle dimensions should now be designed for different pressures than the assumed combustion chamber pressure of 500psi. The pressure range in which operating conditions occur must be assumed. I will choose a 200psi range which will allow for nozzle dimensions to be found at 400 and 600 psi, respectively.

$P_{combustion} := 400psi$ $T_{combustion} := 3000K$

First, the exhaust gas properties are found assuming the new combustion pressure. The ideal gas equation is used without a compressibility factor because it did not have a major impact in the first example.

N_2:

Assuming an ideal gas: $\dfrac{P}{\rho} := R \cdot T$ ■ $P_{n2} := 400psi$ $T_{n2} := 3000K$

$\rho_{n2} := \dfrac{P_{n2}}{R_{n2} \cdot T_{n2}}$ $\rho_{n2} = 3.097 \dfrac{kg}{m^3}$

H_2O:

Assuming an ideal gas: $\dfrac{P}{\rho} := R \cdot T$ ■ $P_{h2o} := 400psi$ $T_{h2o} := 3000K$

$\rho_{h2o} := \dfrac{P_{h2o}}{R_{h2o} \cdot T_{h2o}}$ $\rho_{h2o} = 1.992 \dfrac{kg}{m^3}$

CO_2:

Assuming an ideal gas: $\dfrac{P}{\rho} := R \cdot T$ ■ $P_{co2} := 400psi$ $T_{co2} := 3000K$

$\rho_{co2} := \dfrac{P_{co2}}{R_{co2} \cdot T_{co2}}$ $\rho_{co2} = 4.867 \dfrac{kg}{m^3}$

Now that the new properties of each exhaust gas constituent have been defined, the mixture must be analyzed as a whole. The only property that will change due to pressure is the density. The new exhaust gas density is given as:

$\rho_{mix} := \Sigma y_i \cdot \rho_i$ ■

$\rho_{mix} := y_{n2} \cdot \rho_{n2} + y_{h2o} \cdot \rho_{h2o} + y_{co2} \cdot \rho_{co2}$

$\rho_{mix} = 3.22 \dfrac{kg}{m^3}$

In order to design the internal dimensions of the nozzle, the exhaust gas velocity needs to be found. It will be denoted as v_{inlet} and is physically located at the nozzle inlet. The velocity distribution is assumed to be uniform. By applying the continuity equation for fluid flow through the combustion chamber, an exhaust gas velocity may be approximated.

From previous calculations: $m_{dot\_n2o} := 0.150 \frac{kg}{s}$ $m_{dot\_wax} := 0.016 \frac{kg}{s}$

$$m_{dot\_total} := m_{dot\_n2o} + m_{dot\_wax}$$

Just as before, the diameter of the combustion chamber is assumed:

$D_{chamber} := 1.75 in$ $A_{chamber} := \dfrac{\pi \cdot D_{chamber}^2}{4}$ $A_{chamber} = 15.518 \, cm^2$

Knowing the initial mass flow rate of oxidizer and propellant, the continuity equation can be applied:

Guess value: $v_{inlet} := 100 \dfrac{m}{s}$

Given

$$m_{dot\_total} = \rho_{mix} \cdot v_{inlet} \cdot A_{chamber}$$

$$v_{inlet} := Find(v_{inlet})$$

$$v_{inlet} = 33.216 \frac{m}{s}$$

This velocity corresponds to an inlet Mach number of (from pg.780 of [2]):

$M_{inlet} := \dfrac{v_{inlet}}{C}$ $M_{inlet} = 0.031$

Using this information, a ratio of areas between the nozzle inlet and throat can be found assuming that the flow is accelerated to Mach 1 at the throat. Using equation 3.99 from [6] yields:

$$\frac{A_2}{A_1} := \frac{M_1}{M_2} \cdot \sqrt{\left(\frac{1 + \frac{k-1}{2} \cdot M_2^2}{1 + \frac{k-1}{2} \cdot M_1^2}\right)^{\left(\frac{k+1}{k-1}\right)}}$$

**An initial nozzle inlet dimension must be assumed. Due to design constraints, the largest inlet diameter possible is 1.125 inches. At this time, there is no reason to change this dimension so it will be used for further calculations.

$$D_{inlet} := 1.125\,in \qquad A_{inlet} := \frac{\pi \cdot D_{inlet}^2}{4} \qquad M_{throat} := 1$$

Rearranging and solving for the throat area (assuming Mach 1 at throat) gives:

Guess values: $\qquad A_{throat} := 1.2\,cm^2 \qquad k := k_{mix}\left(T_{combustion}\right)$

Given

$$A_{throat} = \frac{A_{inlet} \cdot M_{inlet}}{M_{throat}} \cdot \sqrt{\left(\frac{1 + \frac{k-1}{2} \cdot M_{throat}^2}{1 + \frac{k-1}{2} \cdot M_{inlet}^2}\right)^{\left(\frac{k+1}{k-1}\right)}}$$

$1.125\,in = 2.857\ cm$

$$A_{throat} := Find\left(A_{throat}\right)$$

$$A_{throat} = 0.337\ cm^2$$

This throat area can also be expressed in terms of throat diameter, given below:

Guess value: $\qquad D_{throat} := 0.5\,cm$

Given

$$A_{throat} = \frac{\pi \cdot D_{throat}^2}{4}$$

$$D_{throat} := Find\left(D_{throat}\right)$$

$$D_{throat} = 0.655\ cm$$

Now that the throat dimensions have been determined, the diverging section of the nozzle needs to be designed. This requires a few assumptions, namely, that the ehaust gases will be released into ambient pressure and that the flow can be considered isentropic. Because the gases will expand to ambient pressure anyway, it is desired to accomplish this directly at the nozzle exit to optimize the thrust in the nozzle.

First, the stagnation properties are found at the inlet and throat of the nozzle (from pg.776 of [2]):

$$T_o := T_{combustion} + \frac{v_{inlet}^2}{2 \cdot C_{p\_mix}(T_{combustion})} \qquad T_o = 3 \times 10^3 \, K$$

**This shows that the inlet velocity is basically negligable. Therefore, P_o can be approximated as $P_{combustion}$.

$$P_o := P_{combustion} \qquad \rho_o := \rho_{mix}$$

The properties of the exhaust gases can now be approximated at the throat of the nozzle. Applying relationships from pg.787 of [2] yields:

$$T_{star} := \frac{2 \cdot T_o}{k_{mix}(T_{combustion}) + 1} \qquad T_{star} = 2.681 \times 10^3 \, K$$

$$P_{star} := P_o \cdot \left(\frac{2}{k_{mix}(T_{combustion}) + 1} \right)^{\frac{k_{mix}(T_{combustion})}{k_{mix}(T_{combustion}) - 1}} \qquad P_{star} = 1.536 \, MPa$$

$$\rho_{star} := \rho_o \cdot \left(\frac{2}{k_{mix}(T_{combustion}) + 1} \right)^{\frac{1}{k_{mix}(T_{combustion}) - 1}} \qquad \rho_{star} = 2.008 \, \frac{kg}{m^3}$$

$$v_{star} := \sqrt{k_{mix}(T_{star}) \cdot R_{mix} \cdot T_{star}} \qquad v_{star} = 1.014 \times 10^3 \, \frac{m}{s}$$

These properties at the throat can now be used to design the diffuser section of the nozzle. The only desired design condition at this time is that the exhaust gases exand to atmospheric pressure. This gives (from pg787 of [2]):

Known: $P_{exit} := 1 \, atm$ Guess: $M_{exit} := 10$

Given

$$P_o = P_{exit} \left[1 + \left(\frac{k_{mix}(T_{star}) - 1}{2} \right) \cdot M_{exit}^2 \right]^{\frac{k_{mix}(T_{star})}{k_{mix}(T_{star}) - 1}}$$

$$M_{exit} := Find(M_{exit})$$

$$M_{exit} = 2.732$$

Solving for the nozzle exit area with known Mach number yields:

Guess values: $A_{exit} := 3cm^2$ $k := k_{mix}(T_{star})$

Given

$$A_{exit} = \frac{A_{throat} \cdot M_{throat}}{M_{exit}} \cdot \sqrt{\left(\frac{1 + \frac{k-1}{2} \cdot M_{exit}^2}{1 + \frac{k-1}{2} \cdot M_{throat}^2} \right)^{\left(\frac{k+1}{k-1}\right)}}$$

$A_{exit} := Find(A_{exit})$

$A_{exit} = 1.436\ cm^2$

This nozzle exit area can also be expressed in terms of diameter, given below:

Guess value: $D_{exit} := 0.5cm$

Given

$$A_{exit} = \frac{\pi \cdot D_{exit}^2}{4}$$

$D_{exit} := Find(D_{exit})$

$D_{exit} = 1.352\ cm$

Now that the cross-sectional area dimensions for the whole nozzle have been determined, the lengths of each sections are needed to complete the design. According to [6], the nozzle length of the diffuser section is given by:

$$L_n := \frac{D_{exit} - D_{throat}}{2 \cdot \tan(\theta_{cn})}$$ where: θ_{cn} is the half angle (Typically between 12 and 18 degrees)

Assuming an intermediate half angle yields: $\theta_{cn} := 15deg$

$$L_n := \frac{D_{exit} - D_{throat}}{2 \cdot \tan(\theta_{cn})}$$ $L_n = 1.301\ cm$

Nozzle #3 Design

$P_{combustion} := 600psi$ $T_{combustion} := 3000K$

First, the exhaust gas properties are found assuming the new combustion pressure. The ideal gas equation is used without a compressibility factor because it did not have a major impact in the first example.

N_2:

Assuming an ideal gas: $\dfrac{P}{\rho} := R \cdot T$ $P_{n2} := 600psi$ $T_{n2} := 3000K$

$\rho_{n2} := \dfrac{P_{n2}}{R_{n2} \cdot T_{n2}}$ $\rho_{n2} = 4.646 \dfrac{kg}{m^3}$

H_2O:

Assuming an ideal gas: $\dfrac{P}{\rho} := R \cdot T$ $P_{h2o} := 600psi$ $T_{h2o} := 3000K$

$\rho_{h2o} := \dfrac{P_{h2o}}{R_{h2o} \cdot T_{h2o}}$ $\rho_{h2o} = 2.988 \dfrac{kg}{m^3}$

CO_2:

Assuming an ideal gas: $\dfrac{P}{\rho} := R \cdot T$ $P_{co2} := 600psi$ $T_{co2} := 3000K$

$\rho_{co2} := \dfrac{P_{co2}}{R_{co2} \cdot T_{co2}}$ $\rho_{co2} = 7.3 \dfrac{kg}{m^3}$

Now that the new properties of each exhaust gas constituent have been defined, the mixture must be analyzed as a whole. The only property that will change due to pressure is the density. The new exhaust gas density is given as:

$\rho_{mix} := \Sigma y_i \cdot \rho_i$

$\rho_{mix} := y_{n2} \cdot \rho_{n2} + y_{h2o} \cdot \rho_{h2o} + y_{co2} \cdot \rho_{co2}$

$\rho_{mix} = 4.831 \dfrac{kg}{m^3}$

In order to design the internal dimensions of the nozzle, the exhaust gas velocity needs to be found. It will be denoted as v_{inlet} and is physically located at the nozzle inlet. The velocity distribution is assumed to be uniform. By applying the continuity equation for fluid flow through the combustion chamber, an exhaust gas velocity may be approximated.

From previous calculations:

$$m_{dot\_n2o} := 0.150\,\frac{kg}{s} \qquad m_{dot\_wax} := 0.016\,\frac{kg}{s}$$

$$m_{dot\_total} := m_{dot\_n2o} + m_{dot\_wax}$$

Just as before, the diameter of the combustion chamber is assumed:

$$D_{chamber} := 1.75\,in \qquad A_{chamber} := \frac{\pi \cdot D_{chamber}^2}{4} \qquad A_{chamber} = 15.518\,cm^2$$

Knowing the initial mass flow rate of oxidizer and propellant, the continuity equation can be applied:

Guess value: $v_{inlet} := 100\,\dfrac{m}{s}$

Given

$$m_{dot\_total} = \rho_{mix} \cdot v_{inlet} \cdot A_{chamber}$$

$$v_{inlet} := Find\left(v_{inlet}\right)$$

$$v_{inlet} = 22.144\,\frac{m}{s}$$

This velocity corresponds to an inlet Mach number of (from pg.780 of [2]):

$$M_{inlet} := \frac{v_{inlet}}{C} \qquad M_{inlet} = 0.021$$

Using this information, a ratio of areas between the nozzle inlet and throat can be found assuming that the flow is accelerated to Mach 1 at the throat. Using equation 3.99 from [6] yields:

$$\frac{A_2}{A_1} := \frac{M_1}{M_2} \cdot \sqrt{\left(\frac{1 + \frac{k-1}{2} \cdot M_2^2}{1 + \frac{k-1}{2} \cdot M_1^2}\right)^{\left(\frac{k+1}{k-1}\right)}}$$

**An initial nozzle inlet dimension must be assumed. Due to design constraints, the largest inlet diameter possible is 1.125 inches. At this time, there is no reason to change this dimension so it will be used for further calculations.

$$D_{inlet} := 1.125\,in \qquad A_{inlet} := \frac{\pi \cdot D_{inlet}^2}{4} \qquad M_{throat} := 1$$

Rearranging and solving for the throat area (assuming Mach 1 at throat) gives:

Guess values: $\quad A_{throat} := 1.2\,cm^2 \qquad k := k_{mix}(T_{combustion})$

Given

$$A_{throat} = \frac{A_{inlet} \cdot M_{inlet}}{M_{throat}} \cdot \sqrt{\left(\frac{1 + \frac{k-1}{2} \cdot M_{throat}^2}{1 + \frac{k-1}{2} \cdot M_{inlet}^2}\right)^{\left(\frac{k+1}{k-1}\right)}}$$

$$A_{throat} := Find(A_{throat})$$

$$A_{throat} = 0.225\ cm^2$$

This throat area can also be expressed in terms of throat diameter, given below:

Guess value: $\quad D_{throat} := 0.5\,cm$

Given

$$A_{throat} = \frac{\pi \cdot D_{throat}^2}{4}$$

$$D_{throat} := Find(D_{throat})$$

$$D_{throat} = 0.525\ cm$$

Now that the throat dimensions have been determined, the diverging section of the nozzle needs to be designed. This requires a few assumptions, namely, that the ehaust gases will be released into ambient pressure and that the flow can be considered isentropic. Because the gases will expand to ambient pressure anyway, it is desired to accomplish this directly at the nozzle exit to optimize the thrust in the nozzle.

First, the stagnation properties are found at the inlet and throat of the nozzle (from pg.776 of [2]):

$$T_o := T_{combustion} + \frac{v_{inlet}^2}{2 \cdot C_{p\_mix}(T_{combustion})} \qquad T_o = 3 \times 10^3 \, K$$

**This shows that the inlet velocity is basically negligible. Therefore, P_o can be approximated as $P_{combustion}$.

$$P_o := P_{combustion} \qquad \rho_o := \rho_{mix}$$

The properties of the exhaust gases can now be approximated at the throat of the nozzle. Applying relationships from pg.787 of [2] yields:

$$T_{star} := \frac{2 \cdot T_o}{k_{mix}(T_{combustion}) + 1} \qquad T_{star} = 2.681 \times 10^3 \, K$$

$$P_{star} := P_o \cdot \left(\frac{2}{k_{mix}(T_{combustion}) + 1} \right)^{\frac{k_{mix}(T_{combustion})}{k_{mix}(T_{combustion}) - 1}} \qquad P_{star} = 2.305 \, MPa$$

$$\rho_{star} := \rho_o \cdot \left(\frac{2}{k_{mix}(T_{combustion}) + 1} \right)^{\frac{1}{k_{mix}(T_{combustion}) - 1}} \qquad \rho_{star} = 3.012 \, \frac{kg}{m^3}$$

$$v_{star} := \sqrt{k_{mix}(T_{star}) \cdot R_{mix} \cdot T_{star}} \qquad v_{star} = 1.014 \times 10^3 \, \frac{m}{s}$$

These properties at the throat can now be used to design the diffuser section of the nozzle. The only desired design condition at this time is that the exhaust gases exand to atmospheric pressure. This gives (from pg787 of [2]):

Known: $P_{exit} := 1 \, atm$ Guess: $M_{exit} := 10$

Given

$$P_o = P_{exit} \left[1 + \left(\frac{k_{mix}(T_{star}) - 1}{2} \right) \cdot M_{exit}^2 \right]^{\frac{k_{mix}(T_{star})}{k_{mix}(T_{star}) - 1}}$$

$$M_{exit} := Find(M_{exit})$$

$$M_{exit} = 2.959$$

Solving for the nozzle exit area with known Mach number yields:

Guess values: $\quad A_{exit} := 3cm^2 \qquad k := k_{mix}(T_{star})$

Given

$$A_{exit} = \frac{A_{throat} \cdot M_{throat}}{M_{exit}} \cdot \sqrt{\left(\frac{1 + \frac{k-1}{2} \cdot M_{exit}^2}{1 + \frac{k-1}{2} \cdot M_{throat}^2}\right)^{\left(\frac{k+1}{k-1}\right)}}$$

$A_{exit} := Find(A_{exit})$

$A_{exit} = 1.275 \ cm^2$

This nozzle exit area can also be expressed in terms of diameter, given below:

Guess value: $\quad D_{exit} := 0.5cm$

Given

$$A_{exit} = \frac{\pi \cdot D_{exit}^2}{4}$$

$D_{exit} := Find(D_{exit})$

$D_{exit} = 1.274 \ cm$

Now that the cross-sectional area dimensions for the whole nozzle have been determined, the lengths of each sections are needed to complete the design. According to [6], the nozzle length of the diffuser section is given by:

$$L_n := \frac{D_{exit} - D_{throat}}{2 \cdot \tan(\theta_{cn})} \qquad \text{where: } \theta_{cn} \text{ is the half angle (Typically between 12 and 18 degrees)}$$

Assuming an intermediate half angle yields: $\quad \theta_{cn} := 15deg$

$$L_n := \frac{D_{exit} - D_{throat}}{2 \cdot \tan(\theta_{cn})} \qquad L_n = 1.398 \ cm$$

COMPUTATIONAL EVALUATION OF A BELL-SHAPED THRUST NOZZLE

A SUMMARY OF RESULTS

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INDEPENDENT STUDY
SPRING 2005

Introduction: This study was performed to evaluate a thrust nozzle designed for the project HERMES hybrid rocket. The nozzle was designed from calculations in the "Nozzle Design" section of this report. Once the nozzle had been designed, it was desired to compare hand calculations to a computational evaluation of the identical nozzle using Computational Fluid Dynamics software.

Approach and Procedure: The first step of this study was to define the bell-shaped thrust nozzle geometry to be evaluated. This was done through initial research from references [1, 2, 3, and 4] and further calculations. From the calculations, a drawing of the nozzle geometry required was created with vertices labeled (Figure 1).
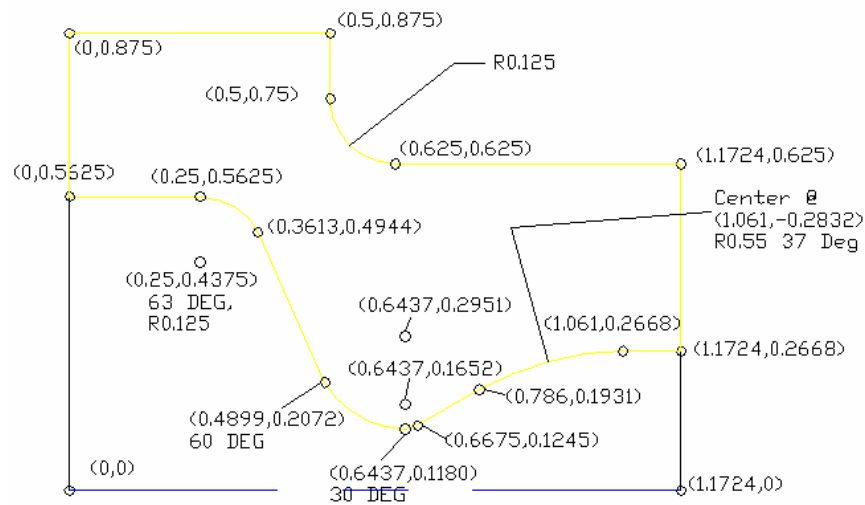
Figure 1. Nozzle Geometry with vertices

The coordinates of vertices were then used in the Gambit software to develop a meshed geometry (Figure 2). This geometry is used to define boundary conditions within the nozzle. Note that only half of the thrust nozzle needed to be evaluated because it is an axis-symmetric problem.
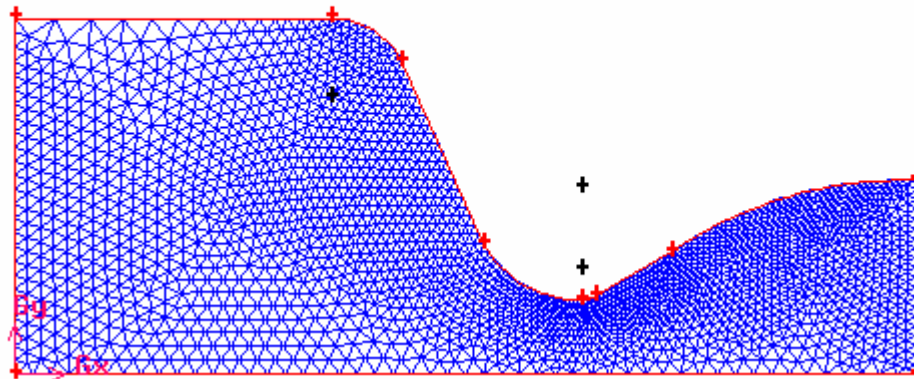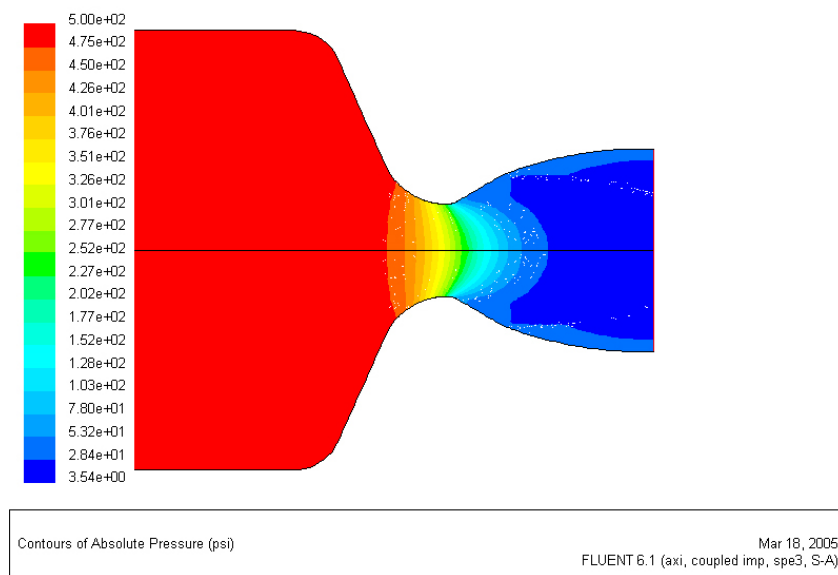

Figure 2. Meshed thrust nozzle (exported from Gambit 2.2.30)

Once the mesh was created, it was imported into the Fluent 6.1.22 software. Standard procedures within Fluent were followed to define the models, materials, boundary conditions, grid adaptation, and units for calculations. Solutions were found for both constant and variable fluid properties. The two fluids analyzed were air and an exhaust gas mixture of CO_2, N_2, and H_2O vapor. The end goal was to solve the nozzle using the exhaust gas mixture as the operating fluid with variable properties.

Results of this problem proved to be very interesting and provoked further study regarding fluid flow external to the nozzle. The same approach was used to generate a mesh within Gambit and define methods in Fluent. The new mesh consisted of both the thrust nozzle and a large space of air surrounding it. This solution was only solved using CO_2 as the fluid with variable properties due to time and computational constraints.

Results: The solutions for fluid flow internal to the nozzle will first be displayed. The boundary conditions for this problem were defined as follows:

- Pressure Inlet at 500 psia
- Inlet Temperature of 3000 Kelvin
- Pressure Outlet at 14.7 psia

Contours of Absolute Pressure (psi)   Mar 18, 2005
                                         FLUENT 6.1 (axi, coupled imp, spe3, S-A)

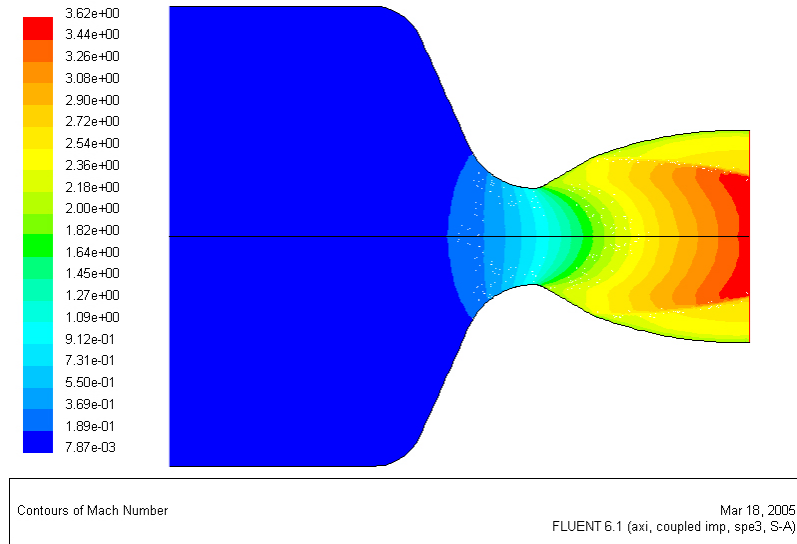**Figure 3.** Absolute Pressure Contours (psia)

Figure 4. Mach Number Contours

Both Figures 3 and 4 visually display the definition of a thrust nozzle. As explained by Sutton [2], "a nozzle increases a fluids velocity at the expense of pressure". In the case of a rocket, the nozzle transforms hot exhaust gases into thrust. Thrust, in this case, is predominately a function of exit velocity.
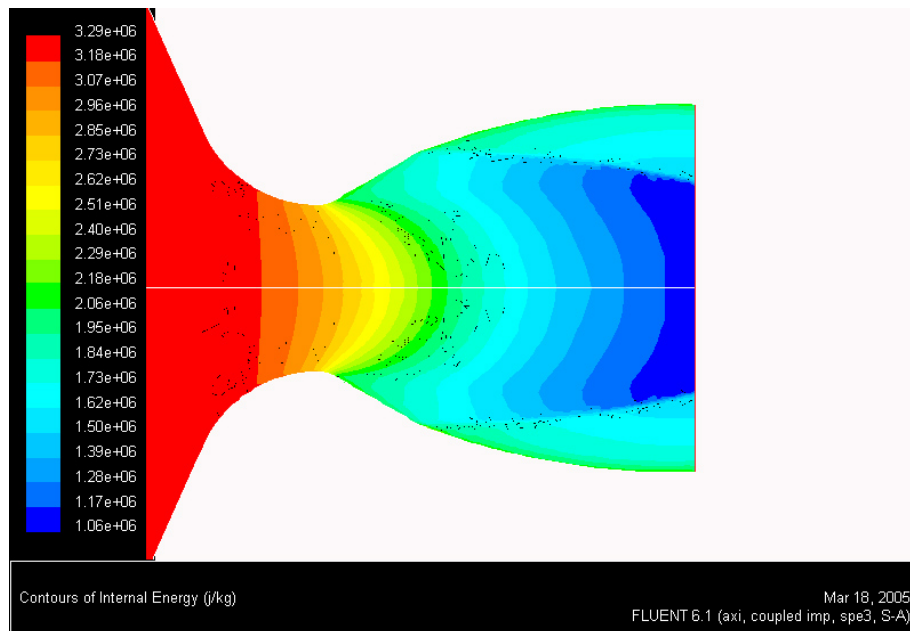


Figure 5. Internal Energy Contours (j/kg)

Figure 5 displays the conversion of the fluid's internal energy into flow work. Since internal energy is related to a fluid's temperature, the internal temperature contours behave similarly.

Upon further review of the internal-flow results, a supersonic phenomenon known as an oblique shockwave was discovered. The shockwave can be seen in Figure 6 as a dense line of velocity vectors. Shockwaves are very serious performance inhibitors in nozzles because they significantly reduce a fluid's velocity.
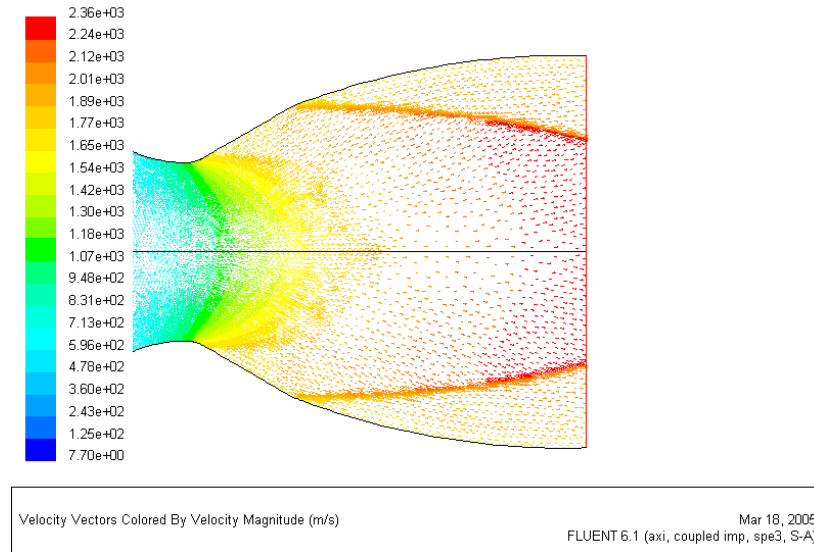
**Figure 6.** Velocity Vectors with Oblique Shockwave (m/s)

The occurrence of an oblique shockwave was actually unexpected. In the process of defining the thrust nozzle's geometry, calculations were made to ensure that normal shockwaves would not be present. To find the origin of this oblique shockwave, Figure 6 was zoomed in along the nozzle's wall. The result is displayed in Figure 7. From this view, it is apparent that the shockwave is created by a sudden change in the nozzle's wall angle. The point of concern occurs at the intersection of a parabolic function and straight line which do not meet tangent to each other. With the oblique shockwave's origin now determined, the geometry could be changed to eliminate its occurrence in further studies.
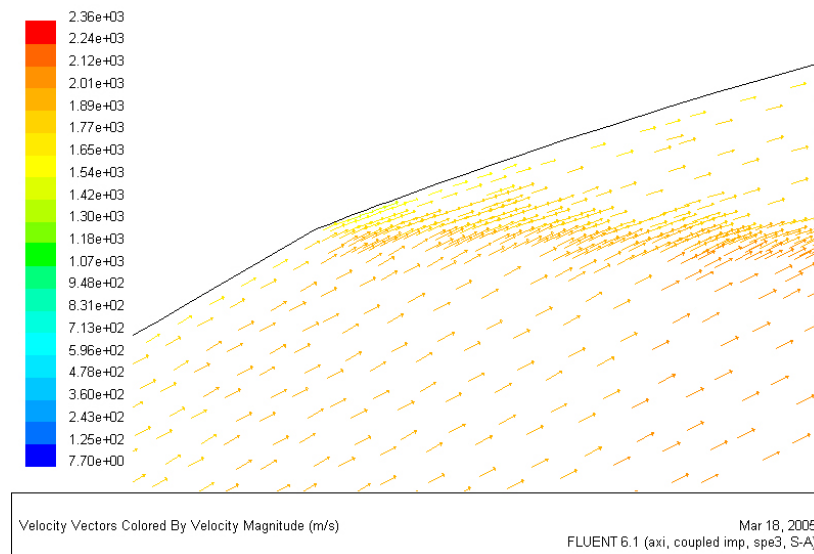
**Figure 7.** Velocity Vectors along Nozzle Wall (m/s)

The next section displays results of fluid flow external to the nozzle. Similar internal nozzle behavior should also be noted for these solutions.

Figure 8 shows the static temperature distribution of the fluid passing through the nozzle. Because the internal energy of the fluid is being converted into flow work, the static temperature decreases along the nozzle.
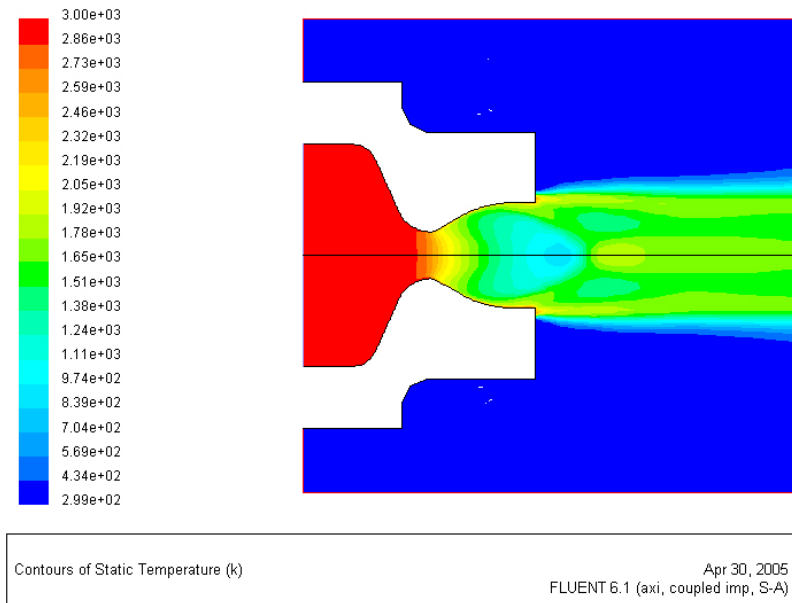
Figure 8. Static Temperature Contours (Kelvin)

When a fluid's kinetic energy is considered, the stagnation properties are found. Figure 9 shows the stagnation temperature distribution resulting from the flow.
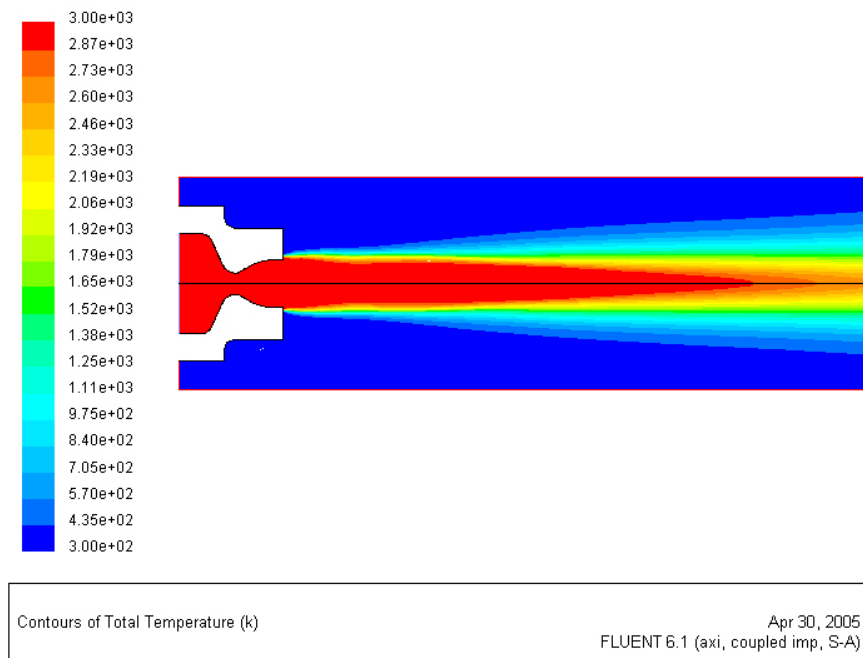
Figure 9. Stagnation Temperature Contours (Kelvin)

To view the fluid's velocity dissipation, a contour of the Mach number is displayed in Figure 10. This picture also shows the flow separation resulting from the fluid and atmospheric air.
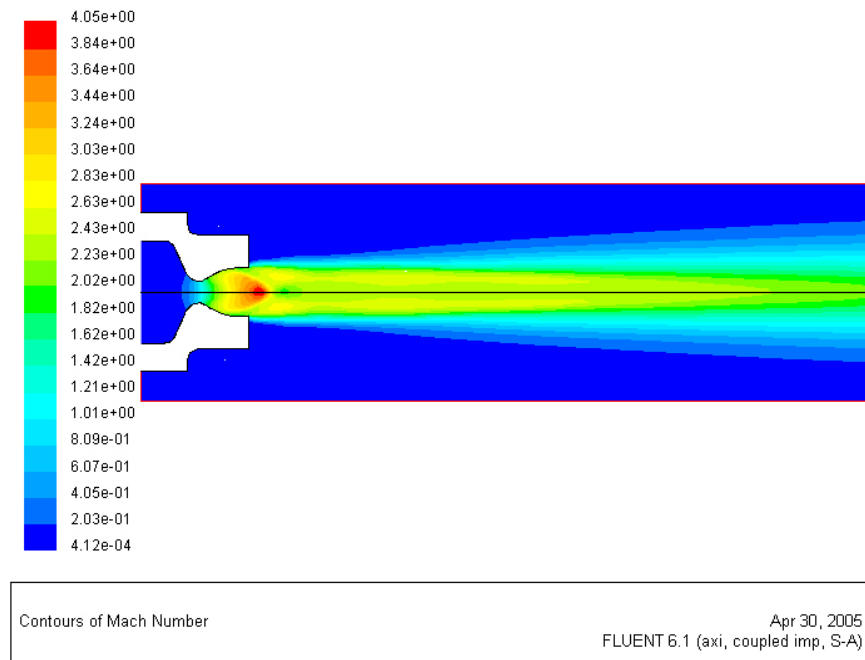

Figure 10. Mach Number Contours

Summary: This study successfully modeled the operating characteristics of a bell-shaped thrust nozzle assuming operating conditions. Not only were the solutions helpful in visualizing fluid behavior, but also in indicating design concerns such as wall contours. Utilizing the study's results, a nozzle was designed and manufactured. Coupled into the design process, the analysis using numerical methods proved to be a very rewarding tool.

Recommendations: Because a real nozzle has been manufactured, it would be advantageous to run operational experiments and compare results with the CFD model. Initial conditions for the CFD model may be changed to find solutions under various operating conditions. The model could then be used to optimize the nozzle's design based on performance and geometrical changes.

References:

[1]   Humble, Ronald; Henry, Gary; and Larson, Wiley; *Space Propulsion Analysis and Design*, McGraw Hill, 1995

[2]   Sutton, George; Biblarz, Oscar; *Rocket Propulsion Elements*, Wiley, 2000

[3]   Cengel, Yunus A.; Boles, Michael; *Thermodynamics-An Engineering Approach*, McGraw Hill, 2001

[4]   Cengel, Yunus A.; *Heat Transfer-A Practical Approach*, McGraw Hill, 2002

Thrust Calculations

Performed by: Ryan Erickson
Date: Spring 2005

These calculations serve as a guide to approximating the thrust produced by a rocket. Once the thrust equation is defined, two uses will be shown. The first is to approximate an ideal hybrid rockets thrust, and the second is to derive an exhaust gas velocity from a thrust measurement.

Thrust is defined on pg.484 of [2] as: $F := m_{dot\_total} \cdot (v_{exit} - v_{inlet})$

This equation assumes perfect expansion, which is valid in the case of the HERMES thrust nozzle. From previous calculations, all variables have been determined in the thrust equation. They are defined as:

From "Thermochemical Calculations": $m_{dot\_n2o} := 0.150 \frac{kg}{s}$ $m_{dot\_wax} := 0.016 \frac{kg}{s}$

$m_{dot\_total} := m_{dot\_n2o} + m_{dot\_wax}$ $m_{dot\_total} = 0.166 \frac{kg}{s}$

From "Nozzle Design Calculations": $v_{inlet} := 27.036 \frac{m}{s}$ $v_{exit} := 3062.7 \frac{m}{s}$ "Mach 2.857"

The thrust is now calculated: $F_{thrust} := m_{dot\_total} \cdot (v_{exit} - v_{inlet})$ $F_{thrust} = 113.286 \, lbf$

The thrust can now be graphed versus exit velocity: $F_{thrust}(v_{exit}) := m_{dot\_total} \cdot (v_{exit} - v_{inlet})$

Thrust vs. Exit Velocity

(Newtons) $F_{thrust}(v_{exit})$

v_{exit}
(m/s)
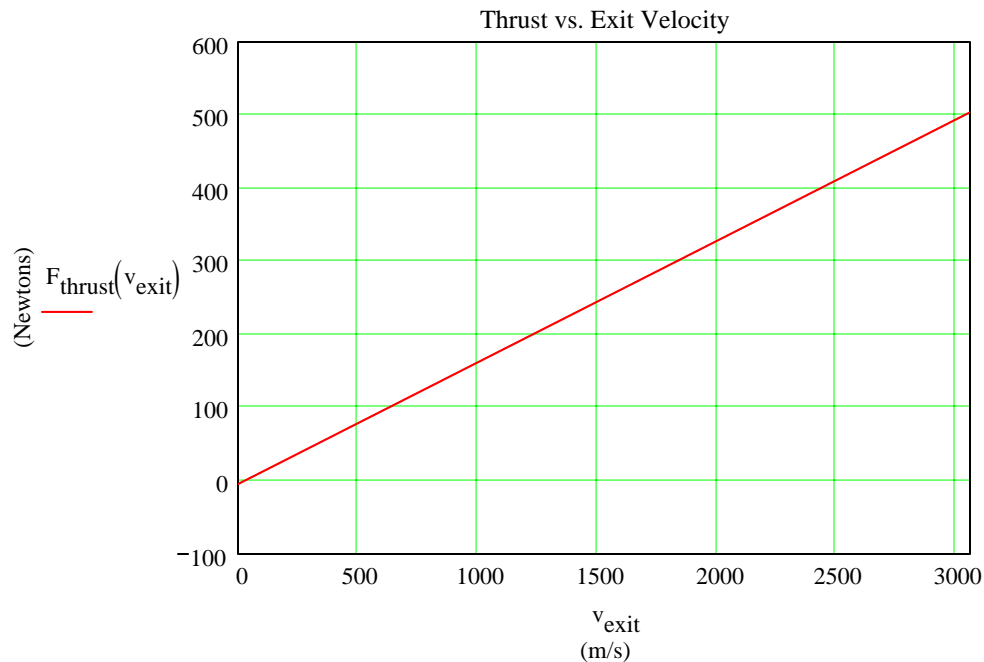
The second application of the thrust equation is to find an exhaust gas velocity from a thrust measurement and oxidizer/propellant flow rate. These values will be found experimentally.

There are two approaches to defining the total flow rate of exhaust: (1) Stoichiometric combustion can be assumed, or (2) the mass of fuel can be averaged over the burn time. In the case of the first assumption, the total mass flow rate is by the following method:

1.) Define oxidizer flow rate: $m_{dot\_n2o} := 0.15 \frac{kg}{s}$

2.) Define total mass flow rate: $m_{dot\_total} := m_{dot\_n2o} + \frac{m_{dot\_n2o}}{9.476}$

$$m_{dot\_total} = 0.166 \frac{kg}{s}$$

The second method is applied the following way:

1.) Define oxidizer flow rate: $m_{dot\_n2o} := \frac{1.5 lb}{12 sec}$ $m_{dot\_n2o} = 0.057 \frac{kg}{s}$

2.) Average fuel mass used over time: $m_{dot\_wax} := \frac{600 gm}{12 sec}$ $m_{dot\_wax} = 0.05 \frac{kg}{s}$

   ***Note: these are the approximate conditions observed in Big Boy's 2nd firing.

3.) Define the total mass flow rate: $m_{dot\_total} := m_{dot\_n2o} + m_{dot\_wax}$

$$m_{dot\_total} = 0.107 \frac{kg}{s}$$

4.) Define the average thrust measurement: $F_{thrust} := 37 lbf$

5.) Apply to rearranged for of thrust equation:

$$v_{exit} := \frac{F_{thrust}}{m_{dot\_total}} + v_{inlet}$$

$$v_{exit} = 1.57 \times 10^3 \frac{m}{s}$$

The result is the average velocity seen at the exit of the thrust nozzle. According to these calculations, Big Boy's exhaust velocity was somewhere around Mach 1. Note that the speed of sound varies with temperature. This method may be applied to each firing, as long as the oxidizer used per time, fuel used per time, and thrust are recorded. It would also be advantageous to evaluate the speed of sound in this medium at the exhaust temperatures. The proper equations to do that are already defined in the "Nozzle Design" calculations.

Calculation References

The following references were used in calculations. All reference numbers from calculation sections (excluding "Computational Evaluation of a Bell-Shaped Thrust Nozzle") correspond to these references.

[1]   Kobe, K.A.; Hirth, L.J.; Couch, E.J.; *Volumetric Behavior of Nitric Oxide*, *Journal of Chemical Engineering, 1961*, 6, 229

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