Computational Model of a HAN-based Satellite Thruster

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Abstract

Hydroxylammonium Nitrate (HAN) is a novel propellant for rocket engines. Due to the complexity of gathering experimental data quantifying the reaction and combustion of the fuel, many have turned to computational modeling. Through the use of Python 3.7 and Cantera 2.4.0, a model of the rocket engine chamber and HAN decomposition reaction has been created. From the model temperature, pressure, and composition gradients across the catalyst bed were generated and applied to calculate the thrust and specific impulse of the specified engine. Sensitivity analysis highlighted key inputs that engineers must focus on optimizing when designing the rocket engine chamber and choosing reaction conditions.

Keywords: HAN, Rocket Engine Model, Python 3.7, Cantera 2.4.0

For supplemental documents refer to HAN Solo GitHub Repository

1 Introduction

With growing concerns involving environmental safety and sustainability, many industries are reevaluating current practices to reduce emissions. The aerospace industry is no exception. NASA in particular launched in June 2019 a project titled Green Propellant Infusion Mission [1]. This project focused on testing alternative fuels to replace the costly, dangerous, and non-environmentally friendly hydrazine used in rocket engines.

Hydrazine is a highly efficient fuel that has been used since World War II [2]. The main concerns that engineers are trying to overcome is the chemical's toxicity and corrosivity. Hydrazine preparation is costly and difficult due to the complicated safety protocols, which commonly include the use of self contained atmospheric protective equipment, SCAPE, or gas bags and the evacuation of all non-essential personnel [3].

One of the alternative to hydrazine under investigation is Hydroxylammonium Nitrate, or HAN. While preliminary studies of HAN show promising results in efficiency, safety, and environmental friendliness, there are still many tests that need to be performed to

evaluate its feasibility. One important factor is the catalyst used in the HAN reaction. HAN typically requires iridium or platinum impregnated on alumina pellets as a catalyst. A major concern with this design is the operating temperature of the catalyst: if the reaction produces too much heat, the catalyst will deactivate or even fail catastrophically. Therefore, it is necessary to gain a greater overall understanding of the thermodynamic, kinetic, and transport processes involved in the reaction of HAN. The objective of this study is to use computer simulations to model a satellite-maneuvering thruster using HAN as the propellant, and investigate the impact of several input parameters on the performance and operating limit of the thruster.

2 Background

HAN has been looked at as a potential propellant for several decades, however there is still little known and agreed upon concerning the reaction kinetics. Various mechanisms have been proposed with different intermediates and overall reaction equations. The universally cited decomposition reaction for the chemical is shown below [4].

$$4\,\mathrm{HAN} \longrightarrow 3\,\mathrm{N_2O} + 2\,\mathrm{HNO_3} + 7\,\mathrm{H_2O}$$

While many agree that this is the overall reaction, there are many proposed mechanisms that detail the side reactions and intermediate steps. The team believes the mechanisms and analysis on the kinetic parameters proposed by Zhang and Thynell are most accurate and representative of HAN combustion. This study also looked into various reaction mechanisms, but most importantly, it also characterized relationships between the activation energy, temperature, and pre-exponential factor, A, in the Arrhenius Equation. Zhang and Thynell compared their study results and various others and were able to construct a linear plot showing a relationship between activation energy and pre-exponential factor. Figure 1 displays the plot they constructed and Equation 1 contains the fitted linear expression [4].

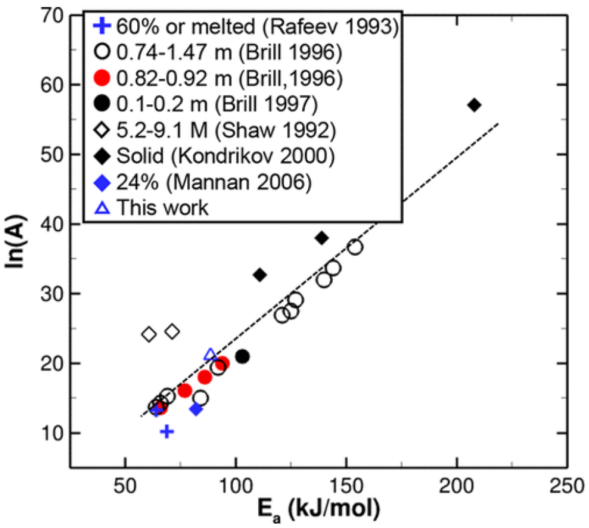

Figure 1: Summary of Arrhenius Parameters from literature

$$lnA = \alpha + \frac{E_a}{R\Theta} \tag{1}$$

From this expression, an approximate rate constant can be calculated using only activation energy and temperature. From the fitted expression, the study concluded that the constants in Equation 1 could be approximated to be α=-3.497 and Θ = 446.3K. Using the data generated, the rate constant and rate law can be calculated for HAN and the products. From the figure, it was estimated the overall value for ln(A) was 3.2 $\pm$ 0.05 and E_a was 8.86 $\pm$ 0.19 kJ/mol.

In order to model the reaction, thermodynamic data for all species involved was necessary too. In the same study by Zhang and Thynell, the heat of reaction for Equation 1 was determined to be -218.4 kJ/mol. In the reaction itself, there are four species for which data was needed for the program Cantera to work. Cantera was used by the team to calculate all thermodynamic values, such as heat capacity, molecular composition, density, etc. The four species needing to be characterized were HAN, HNO_3, H_2O, and N_2O. Cantera uses cti files to contain thermodynamic data on species and calculate values. Since all species, with the exception of water, were not found on the cti files in the Lawrence Livermore database [13], the team had to create a new cti file. This was done by using the data published in a report by NASA in 1993. The thermodynamic data for various species were reported in Chemkin format, including values for HNO_3, H_2O, and N_2O. An example of the format and species data can be seen below in Figure 2. [5]

TABLE I.– FORMAT FOR THERMODYNAMIC DATA COEFFICIENTS IN TABLE II

Record	Contents	Format	Columns
1	Species name	A15	1–15
	Reference/date code	A6	19–24
	Chemical formula: symbols and numbers	4 (A2, F3.0)	25–44
	"G" for gaseous species, "C" for condensed	A1	45
	Temperature range	2F10.3	46–65
	Molecular weight	F13.5	66–78
	Integer 1	I1	80
2	Coefficients $a_i (i = 1,5)$ in eq. (1) for $T \geq 1000$ K	5E15.8	1–75
	Integer 2	I1	80
3	Coefficients b_1 and b_2 in eqs. (2) and (3) for $T \geq 1000$ K	2E15.8	1–30
	Coefficients $a_i (i = 1,3)$ in eq. (1) for $T \leq 1000$ K	3E15.8	31–75
	Integer 3	I1	80
4	Coefficients $a_i (i = 4,5)$ in eq. (1) for $T \leq 1000$ K	2E15.8	1–30
	Coefficients b_1 and b_2 in eqs. (2) and (3) for $T \leq 1000$ K	2E15.8	31–60
	$H^o(298.15)/R$, K	E15.8	61–75
	Integer 4	I1	80

Example:

```
BeOH              J12/75BE 1.0  1.H  1.    0.O   300.000  5000.000      26.01952 1
 4.61167200E+00 2.39720130E-03-8.54891620E-07 1.43090620E-10-9.11123990E-15    2
-1.53618380E+04-1.98829219E+00 1.91391480E+00 1.35071590E-02-1.85316870E-05    3
 1.29424710E-08-3.54389610E-12-1.48196830E+04 1.09928304E+01-1.37885210E+04    4
```

Empirical equations for this example:

$$\text{Heat capacity}: \frac{C_p^o(T)}{R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \qquad (1)$$

$$\text{Enthalpy}: \frac{H^o(T)}{RT} = a_1 + a_2 \frac{T}{2} + a_3 \frac{T^2}{3} + a_4 \frac{T^3}{4} + a_5 \frac{T^4}{5} + \frac{b_1}{T} \qquad (2)$$

$$\text{Entropy}: \frac{S^o(T)}{R} = a_1 \ln T + a_2 T + a_3 \frac{T^2}{2} + a_4 \frac{T^3}{3} + a_5 \frac{T^4}{4} + b_2 \qquad (3)$$

Figure 2: Format for Thermodynamic Data Coefficients

The data from the Chemkin format can easily be converted into a cti file and used with Cantera. For the species HAN, it was approximated to similar to the thermodynamic data for nitric acid, which contains the same molecular weight. Therefore, the entry data for HNO_3 and HAN were the same. The printout for the HAN.cti file can be found in GitHub repository.

3 Methodology

To model the decomposition of HAN in a rocket packed bed reactor, the team utilized several methods and assumptions. To simplify the reaction and math involved, assumptions concerning the reaction mechanism and transport equations were made along with characteristics about the reactor.

3.1 Assumptions

1. The catalyst bed is a cylinder with uniformly distributed catalyst pellets.
2. The catalyst pellets are made from Ir/Al_2O_3 (30% in mass metallic content) with a maximum operating temperature of 1600 K.
3. The HAN decomposition reaction is an elementary reaction with first order kinetics.
4. The system is at steady state.
5. The reaction is homogeneous and only occurs in the gas phase.

6. The heat transfer through the chamber wall is negligible.

7. The gas mixture is well mixed and thus temperature, pressure, and composition only changes in the axial direction with no radial variations.

Table 1 shows the constants used in the model.

Constants	Value
Bed diameter	5 cm
Nozzle diameter	6 cm
Volume void fraction	0.4
Area void fraction	0.3
Gas constant	8.314×10^{-2} $L \cdot bar/(K \cdot mol)$
Heat capacity of HAN	74.826 $J/(K \cdot mol)$

Table 1: Constants chosen based on similar rocket engine chambers and literature

3.2 Approach

In this study, we divided the satellite thruster into two regions: the catalyst bed region in which HAN is decomposed and the nozzle region in which the gas is accelerated to produce thrust. Figure 3 shows the design of a typical hydrazine thruster [6]:

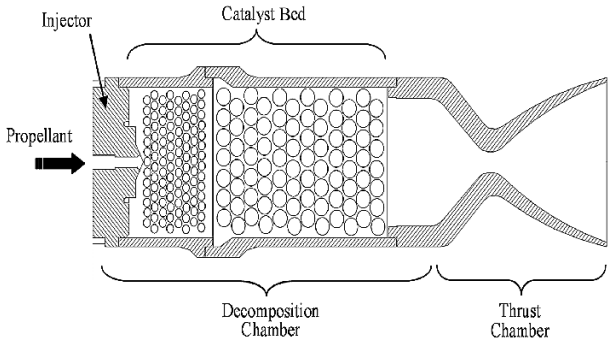

Figure 3: A typical hydrazine thruster design

Thrusters for satellite maneuvering typically employ this design due to its simplicity and re-ignitability. There is no pumping involved and the reaction starts spontaneously. The thruster model used in this study is similar to this design; but for simplicity it is assumed there is only one catalyst bed with pellets of the same size, unlike the two-stage design used in an actual thruster.

3.2.1 Catalyst Bed Region Simulation

Modeling a reaction such the decomposition of HAN is complicated and many simplifications were made. To design the code, the team selected several reactor geometry and feed parameters as the input, and chose temperature, pressure, and composition across bed

as the output. To bridge the gap between the inputs and outputs, a similar approach to a study performed by Makled and Belal was used [7]. The overall flow diagram of the code can be seen below (Figure 4).

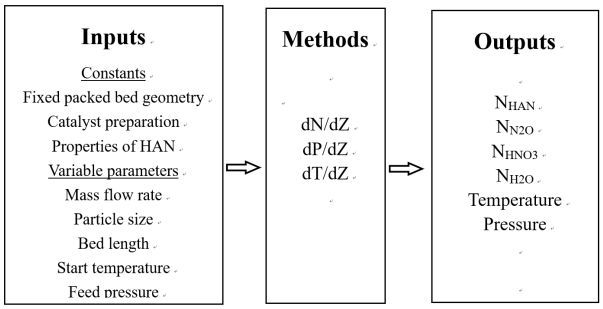

Figure 4: Flow diagram of catalyst bed region simulation

To apply the above methods, several expressions needed to be derived including the rate law, the change in molar flow rate, pressure, and temperature across the bed length.

First, the reaction rate law was determined using the global equation and parameters for the Arrhenius equation found by Zhang and Thynell. The rate law and rate constant k is shown below [7]:

$$r_{HAN} = -kC_{HAN} \tag{2}$$

in which

$$k = e^{\frac{-E_a}{RT}} \tag{3}$$

where k is the rate constant, C_{HAN} is concentration of HAN, E_a is the activation energy, R is the gas constant, and T is the absolute temperature.

Using Eqn.(2) and the stoichiometric ratios given in the global reaction, the rate law for the decomposition products can be obtained,

$$r_{N_2O} = \frac{3}{4}kC_{HAN} \tag{4}$$

$$r_{HNO_3} = \frac{1}{2}kC_{HAN} \tag{5}$$

$$r_{H_2O} = \frac{7}{4}kC_{HAN} \tag{6}$$

Then the governing differential equations of molar flow rate of species across the length of the packed bed can be obtained. The equations used can be seen below for all species of the reaction:

$$\frac{dN_{HAN}}{dZ} = r_{HAN}A_c \tag{7}$$

$$\frac{dN_{N_2O}}{dZ} = -\frac{3}{4}\frac{dN_{HAN}}{dZ} \tag{8}$$

$$\frac{dN_{HNO_3}}{dZ} = -\frac{1}{2}\frac{dN_{HAN}}{dZ} \tag{9}$$

$$\frac{dN_{H_2O}}{dZ} = -\frac{7}{4}\frac{dN_{HAN}}{dZ} \tag{10}$$

To relate pressure drop across the length of the reaction, the Ergun equation is used for calculating the pressure drop through the packed bed. Using the Reynolds number, flow patterns can be predicted:

$$Re = \frac{\rho v_s D}{\mu} \tag{11}$$

where ρ is density, v_s is effective velocity, D is particle diameter, and μ is dynamic viscosity. The flow tends to be laminar flow in this model. Therefore, the Ergun equation can be simplified as:

$$\frac{dP}{dZ} = \frac{-2G}{\rho r_p}\left(\frac{1-\varphi}{\varphi^3}\right)\left(\frac{300(1-\varphi)\mu}{r_p}\right) \tag{12}$$

where G is loading factor (mass flow rate divided by cross-section area), ρ is the average density, r_p the radius of particle, φ is void fraction, and μ is viscosity of mixture.

Then using the energy balance the temperature change across the packed bed reaction can be determined by:

$$\frac{dT}{dZ} = \left(\frac{\sum_{i=1}^{n}(-r_{ij})[-\Delta H_{Rxij}(T)]}{\sum_{i=1}^{m}(N_j)(C_{p,j})}\right) A_c \tag{13}$$

where $\Delta H_{Rxij}(T)$ is the heat of the reaction, N is the molar flow rate of species, C_p is the specific heat of species, and A_c is the cross-section area.

To solve the equations, Cantera was used to get properties of gaseous mixtures at different temperatures and pressures, including density and heat capacity. The heat of reaction assumed to be -218.4 kJ/mol at 298K from the findings of Zhang and Thynell, so the heat of reaction at other temperatures is given by the equation below.

$$\Delta H_{Rxn}(T) = \Delta H_{Rxn}(298K) + \int_{298K}^{T} C_p dT \tag{14}$$

One of the limitations of using Cantera for only thermodynamic calculations is the system cannot calculate viscosity for a mixture. While Cantera normally can get viscosity of a mixture, there needs to be enough transport data to calculate the viscosity of each component. Since some of the species in the reaction, such as HAN or HNO_3, are not as frequently used in the industry, there is no data online for transport properties. Therefore, the following expression was used to calculate the viscosity of gases [8].

$$\mu = \frac{2}{3\pi^{\frac{3}{2}}}\left(\frac{\sqrt{mkT}}{d_{mol}^2}\right) \tag{15}$$

where m is mass of molecules and d_{mol} is diameter of molecules, both of which are given in Table 2.

Molecules	N_2O	HNO_3	H_2O
m(g)	44.01	63.01	18.015
d_{mol} $\times 10^{-12}$(m)	330	550	140

Table 2: Mass and diameter of gases

Eqn. (15) utilizes the molecular weight and molecule diameter of a species to calculate the viscosity of the pure substance. This equation was used for H_2O, N_2O, and HNO_3. The viscosity of HAN was approximated to be that of liquid water at a higher pressure. This is a common assumption that many papers researching HAN tend to make due to the lack of experimental data. In particular, one paper cited that HAN could be compared to water at a pressure of 27.5 MPa for a range of temperatures[4]. Therefore, a new function was created for the viscosity of HAN based on research of water viscosity found on the DIPPR database [9]. Figure 5 show the expression, associated coefficients, and temperature ranges for water which were used to approximate HAN viscosity.

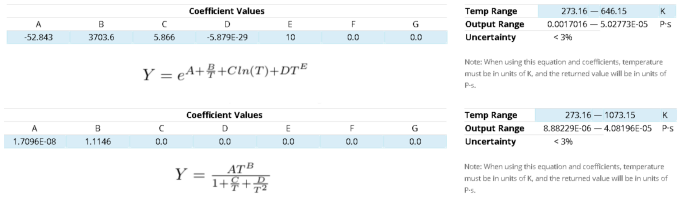

Figure 5: Temperature dependent properties for water

3.2.2 De Laval Nozzle Region Simulation

In a rocket engine, thrust is produced by the expansion of hot gas produced in the combustion chamber exiting a rocket nozzle, in which heat energy is converted to kinetic energy. The most common rocket engine nozzle design is the de Laval nozzle, developed by Gustaf de Laval in the 19th century. A de Laval nozzle consists of three sections:

1. The convergent region where hot, slow-moving gas is accelerated due to decreasing cross-section area, but the velocity stays below the speed of the sound (Mach < 1);

2. The throat region where the cross-section area is at its minimum and gas velocity is limited to the speed of the sound (Mach number $= 1$), a condition known as choked flow;

3. The divergent region where the gas expands and is further accelerated to supersonic velocities (Mach number > 1). The temperature and pressure of the gas decreases rapidly, converting most of the heat energy to kinetic energy.

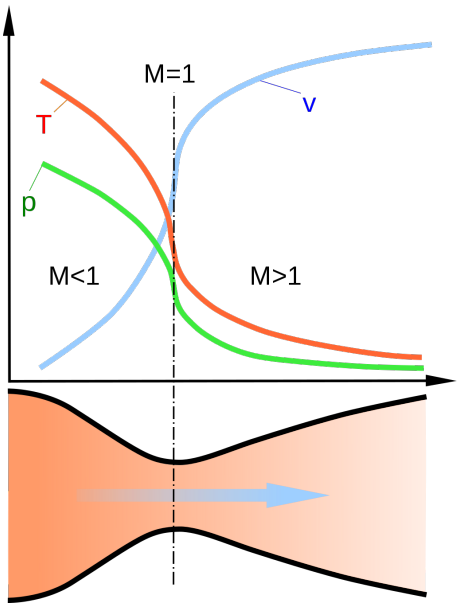

Figure 6: Diagram of a de Laval nozzle showing the evolution of temperature, pressure, and velocity in different nozzle regions.

From Newton's Third Law, the thrust of the rocket engine can be calculated as [10]

$$F = \dot{m}V_e + (P_e - P_0)A_e \tag{16}$$

where $\dot{m}$ is the mass flow rate, V_e is the velocity at the nozzle exit, p_e is the pressure at the nozzle exit, p_0 is the ambient pressure, and A_e is the area of the nozzle.

The exit velocity depends on the Mach number and the speed of the sound given in the equation below:

$$V_e = M_e\sqrt{\gamma R T_e} \tag{17}$$

where M_e is the Mach number, γ is the specific heat ratio of the exhaust, and T_e is the temperature at the nozzle exit.

The specific heat ratio is the ratio of the specific heat of the gas at constant pressure C_p and that at constant volume C_v. The difference between C_p and C_v is usually assumed to be equal to the ideal gas constant R. Therefore γ can be calculated by

$$\gamma = \frac{C_p}{C_p - R} \tag{18}$$

The exit temperature and exit pressure can be calculated given the Mach number:

$$T_e = T_c(1 + \frac{\gamma - 1}{2}M_e^2)^{-1} \tag{19}$$

$$P_e = P_c(1 + \frac{\gamma - 1}{2}M_e^2)^{\frac{-\gamma}{\gamma - 1}} \tag{20}$$

where T_c and P_c are the temperature and pressure at the entrance of the nozzle (also the exit of the catalyst bed), respectively.

The Mach number can be solved from the equation below:

$$\frac{A_e}{A^\star} = (\frac{\gamma+1}{2})^{-\frac{\gamma+1}{2(\gamma-1)}} \frac{(1+\frac{\gamma-1}{2}M_e^2)^{\frac{\gamma+1}{2(\gamma-1)}}}{M_e} \tag{21}$$

where A_e is the nozzle area, $A^\star$ is the throat area, and the ratio of of the two variables is known as the expansion ratio. The higher the expansion ratio the more efficient the engine, since the exhaust gas expands more and more heat energy is converted to kinetic energy. The equation above could not be solved analytically and thus the Mach number is solved numerically given the expansion ratio and the specific heat ratio.

Finally, the throat area is given in the equation below:

$$A^\star = \dot{m}\frac{\sqrt{T_c}}{p_c}\sqrt{\frac{\gamma}{R}}(\frac{\gamma+1}{2})^{\frac{\gamma+1}{2(\gamma-1)}} \tag{22}$$

The thrust and the engine can then be determined by solving Eqn. (16) to (22) in reverse order.

Besides thrust, another important criteria to evaluate rocket engine performance is the specific impulse (I_{sp}), which measures the ratio of thrust generated and the amount of propellant used. The specific impulse is given in the equation below:

$$I_{sp} = \frac{F}{\dot{m}g} \tag{23}$$

where g is the gravitational acceleration. A higher specific impulse means the engine generates more thrust for a given fuel flow, thus it is more efficient. Monopropellant thrusters for satellites usually have I_{sp} values between 120 s and 240 s [11], depending on the type of propellant used. Main engines used on rockets and spaceships have I_{sp} values between 250 s and 450 s, however these engines are very complicated and do not scale down well. Therefore, the low efficiency of satellite thrusters is usually considered a worthy trade-off for simplicity and ease of operation.

4 Results and Discussion

4.1 Single-pass Engine Parameter calculator

To validate the model, the team passed through a set of parameters based on the upper limits of the system. The parameters chosen were the minimum particle diameter, and the maximum bed length, feed temperature, feed pressure, and mass flow rate defined for the model. This was done to ensure that Cantera and the model the team designed could handle the most extreme values. Table 3 below details the specific inputs that were chosen for the single pass through the model.

Input	Value
Particle diameter	2 mm
Bed length	20 cm
Feed temperature	473 K
Feed pressure	50 bar
Mass flow rate	100 g/s

Table 3: Specific inputs for the single-pass model

From the single pass analysis, the following results were obtained. The overall molar flow rate of each species, temperature and pressure were all looked at across the catalyst bed. As seen in the respective figures below (Figure 7), the compositions of the species behave as expected, with HAN decreasing and the products increasing according to their stoichiometry. The simplicity of the plot and linear nature is most likely due to the simplified reaction rate law that is being used. If a more complex law and reaction mechanism were assumed, it is probable that the change of molar flow for each species would become more exponential in growth and decay before plateauing.

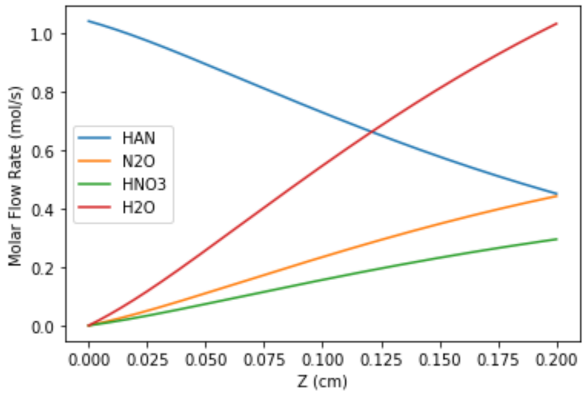

Figure 7: Molar flow rate of species changed with bed length

The temperature profile similarly acts as expected for the reaction (Figure 8). The upward trend matches the consumption of HAN in a manner that suggests the model is accurately translating the heat generated from the reaction to the temperature change of the catalyst. Additionally, the pressure behaves in a manner one would expect from a catalyst based reaction (Figure 9). The pressure drop associated with the reaction drives the combusted fuel out the nozzle, giving the rocket its thrust.

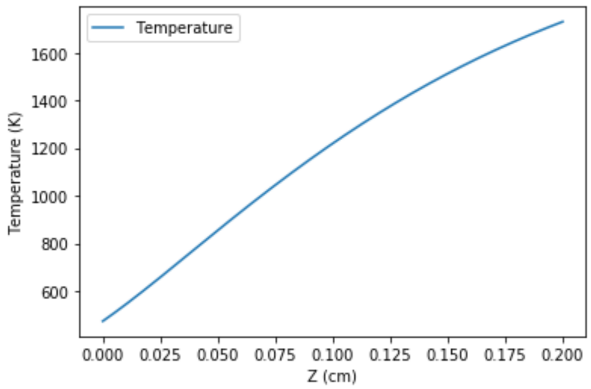

Figure 8: Temperature changed with bed length

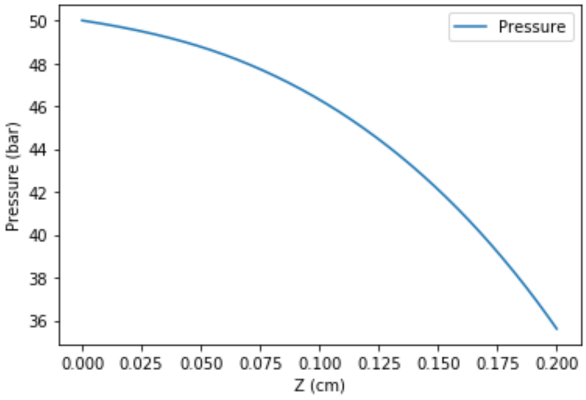

Figure 9: Pressure changed with bed length

Another important takeaway from the single pass analysis is that the performance of the thrust modelled is similar to that of a real world hydrazine thruster [12]. A comparison is shown in Table 4. Although the specifications of the modelled thruster and the real world thruster don't completely match, it's important to note that these numbers are of similar orders of magnitude and thus the model is a reasonably good approximation.

Thruster	Model	Real World
Bed diameter	5.0 cm	5.3 cm
bed length	20 cm	6.1 cm
Mass flow rate	100 g/s	155 g/s
Feed temperature	473 K	300 K
Feed pressure	50.0 bar	35.0 bar
Chamber pressure	35.6 bar	14.0 bar
Thrust	183 N	360 N
Specific impulse	186 s	225 s

Table 4: Performance comparison between the modelled thruster and a real world hydrazine thruster

4.2 Sensitivity Analysis

To characterize the reaction of HAN in a rocket, the team designed a program that returns the overall change in temperature, pressure, and composition for all components across the reactor bed based on the inputs of bed length, catalyst particle diameter, mass flow rate, and entering feed temperature and pressure. The design of the rocket's reaction chamber is an important aspect, and being able to see how different inputs affect efficiency and safety of operation is an appealing trait to engineers. Therefore, the program was also designed to accept the following range for the inputs (Table 5).

Parameters	min	max
Particle diameter	2 mm	5 mm
Bed length	5 cm	20 cm
Start temperature	323 K	473 K
Feed pressure	20 bar	50 bar
Mass flow rate	50 g/s	100 g/s

Table 5: Range of variable parameters

For ease of use, sliders were used to allow the user to change the inputs. In addition to visually being able to see how different inputs affect the overall efficiency and results of the reaction, a sensitivity analysis was performed on the program. The results of the analysis can be broken down into five sections. Each section was performed with the same generated 7000 sample sets. In respective order the sensitivity results detail how the inputs effect the exit temperature, exit pressure, conversion of HAN, thrust, and specific impulse. The results of the analysis can be seen in the two figures below (Figure 10,11).

Sobol Sensitivity Analysis for Temperature

Name	1st	Total	Mean of Input
bed length	0.41	0.46	(12.50)
particle diameter	0.24	0.28	(3.50)
mass flow rate	0.00	0.00	(74.99)
feed temperature	0.06	0.06	(125.01)
feed pressure	0.23	0.28	(35.02)

Sobol Sensitivity Analysis for Pressure

Name	1st	Total	Mean of Input
bed length	0.01	0.01	(12.50)
particle diameter	0.01	0.01	(3.50)
mass flow rate	0.01	0.01	(74.99)
feed temperature	0.00	0.00	(125.01)
feed pressure	0.97	0.97	(35.02)

Sobol Sensitivity Analysis for Conversion of HAN

Name	1st	Total	Mean of Input
bed length	0.05	0.07	(12.50)
particle diameter	0.03	0.04	(3.50)
mass flow rate	0.86	0.88	(74.99)
feed temperature	0.00	0.00	(125.01)
feed pressure	0.03	0.04	(35.02)

Figure 10: Sobol Sensitivity Analysis for Temperature, Pressure, and HAN Conversion

Sobol Sensitivity Analysis for Thrust

Name	1st	Total	Mean of Input
bed length	0.26	0.29	(12.50)
particle diameter	0.15	0.17	(3.50)
mass flow rate	0.23	35.06	(74.99)
feed temperature	0.27	20.44	(125.01)
feed pressure	0.18	0.21	(35.02)

Sobol Sensitivity Analysis for Isp

Name	1st	Total	Mean of Input
bed length	0.39	0.44	(12.50)
particle diameter	0.22	0.26	(3.50)
mass flow rate	-0.31	29.96	(74.99)
feed temperature	0.33	18.32	(125.01)
feed pressure	0.26	0.31	(35.02)

Figure 11: Sobol Sensitivity Analysis for Thrust and Isp

From the analysis it can be seen that of the inputs, feed pressure, mass flow rate, and bed length have the most significant effect on the exit temperature, pressure, and conversion of HAN. With respect to thrust and specific impulse, feed temperature and mass flow rate are the most influential variables towards the result of the analysis. While many of these variables are influenced by each other, it makes sense that pressure and mass flow rate are some of the most influential of the inputs. Additionally, one could reason that particle diameter is the least influential overall due to its independence from the other variables. Temperature or pressure change isn't going to influence the diameter of the catalyst, so it stands to reason that the sensitivity for the variable would be one of the lower values.

5 Conclusion

HAN is a relatively new source of fuel in the aerospace industry. As a result, there is a need for a greater understanding of the decomposition reaction of HAN and effects of different engine geometry on overall rocket engineer efficiency. The proposed model by the team encompasses the above needs by showing the change in composition, temperature, and pressure across a specified rocket engine chamber. It additionally outputs the thrust and specific impulse of the rocket engine using the calculated temperature, pressure, and composition gradients. By conducting a sensitivity analysis, the team was able to identify key inputs for the reaction conditions and rocket engine geometry. It was found that overall, catalyst diameter was not as important as optimizing mass flow rate of the fuel or feed temperature. For efficiency in thrust and specific impulse, these two variables are extremely important to optimize.

5.1 Next Steps

Although the team was able to model the decomposition reaction of HAN in a rocket reaction chamber, there are still some areas in the research and code that could be improved. In future iterations, the following advice and methods would ideally be explored.

One of the main issues of complications in the code concerned the assumptions made in the reaction mechanism. The proposed mechanism of a first order reaction with the rate constants specified by Zhang and Thynell resulted in an oversimplified expression of HAN decomposition. In earlier attempts to code the reaction, the temperature and pressure would inflate exponentially after reaching around 800K. This was due to the assumptions made, which in turn caused Cantera to produce an error message. If the reaction were more complicated, there would be more limitations on the reaction, such as saturation of catalyst surface sites, which would prevent it from running away so suddenly and violently. In the future, the team advises that the eight step reaction mechanism proposed by Lee and Litzinger be used instead of the assumed first order global decomposition of HAN [14].

Additional ways to make the model more robust and versatile include incorporating the following changes. The team would like to see the incorporation of an expression to model heat transfer from the combustion reaction into the solid particles of the catalyst. This would make the estimate of the heat generation and transfer across the bed more accurate. Currently the model assumes that the temperature of the gas is equal to the temperature of catalyst surface. While this simplifies the expressions, it does not account for the heat lost to the solids in the reaction chamber. Additionally, the team would like to incorporate the presence of water in the feed to the reaction chamber. It has been stated in several studies that HAN is most stable when mixed with water, therefore, it would be worth investigating how such a change would affect the model and whether the HAN/H_2O ratio will influence results. It should also be investigated if having water present in the initial feed would result in a cheaper, but as efficient rocket fuel source.

The final piece of advice the team would recommend to future endeavors to model the reaction is to find expressions that account for non-steady state. Due to the complexity of

the expressions found and the lack of information needed, the team was not able to model the start up or shut down of the reactor. While steady state calculations still offer a lot to learn for the design of the catalyst bed, more information can be gained by looking at the reaction in a transient state.

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