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Analysis of Auto-Ignition via Cavitation in Rocket Engines

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Analysis of Auto-Ignition via Cavitation in Rocket Engines

by

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Abstract

Cavitation in rocket propellants is a source of safety concerns, though also a source of potential utility. The phenomenon, wherein a pressure difference causes vapor to form in discrete bubbles throughout a liquid, can occur in liquid rocket propellants in various ways. Cavitation can occur in flow through valves as they open and close, around sharp corners, or in areas of changing flow such as venturis or during cryogenic tank depressurization. At the moment of implosion, cavitation bubbles can produce energies and temperatures that far exceed the ignition energies and temperatures of rocket propellants, with implosion pressures in particular reaching values on the order of hundreds to thousands of atmospheres. In volatile monopropellants or instantaneous bipropellant mixtures these high pressures, energies, and temperatures can induce autoignition, leading to explosion or detonation of the propellants and even the destruction of the launch vehicle. Conversely, cavitation may be used to produce controlled ignition of propellants, presenting an alternative means of ignition in rocket engines. Such an alternative would not involve additional subsystems (hypergolics, torch, arc, etc.) and would increase reliability and reduce cost. The purpose of this project is to model the implosion of a single cavitation bubble by calculating several physical and thermal properties of the bubble during the bubble's collapse. Analysis of the energetic behavior of a single cavitation bubble collapse will be presented, and future advancements on the modeling software will be discussed.

1. Nomenclature

W_P = work of compression
V_0 = initial bubble volume
V = bubble volume
P = bubble pressure
Q = initial bubble pressure
γ = specific heat ratio
$W_{adiabatic}$ = adiabatic work
W_{net} = net work
P_E = external pressure
KE = kinetic energy
ρ = liquid density
r = radius from center of bubble
u = velocity of liquid at radius r
R = bubble surface boundary
U = velocity of bubble surface
T = temperature in bubble
T_0 = initial bubble temperature
R_0 = initial bubble radius
P_{sat} = saturation pressure of liquid

2. Introduction

2.1. Previous Work

The software developed in this project is based primarily on prior work conducted by Dr. James Blackmon to develop a parametric model for cavitation bubble collapse. In his paper, Dr. Blackmon derives a means to characterize bubble collapse based on Lord Rayleigh's derivation of the inertia of implosion for compressed bubbles [1]. The derivation is summarized by equating the kinetic energy of the liquid boundary with the potential energy of the external pressure on the liquid. This equation is solved for the surface velocity of the bubble. The work done by an adiabatic gas is solved and subtracted from the work done by the external pressure to yield a net work. This energy is then equated with the kinetic energy of the liquid medium, and the velocity is solved for. This velocity is used on the parametric approach as a function of the radius ratio of the bubble to its original radius. From the velocity and radius other properties can be solved, such as temperature and pressure for the bubble. The derivation is given in brief below, beginning with the work of compression:

$$W_P = \int_V^{V_0} PdV \tag{1}$$

A substitution for the adiabatic assumption is made such that

$$P = Q\left(\frac{V_0}{V}\right)^{\gamma} \tag{2}$$

Which yields the integral

$$W_{adiabatic} = QV_0^{\gamma} \int V^{-\gamma} dv = \left(\frac{QV_0}{\gamma - 1}\right)\left(\left(\frac{V_0}{V}\right)^{\gamma - 1} - 1\right). \tag{3}$$

The net work of the liquid is the difference between the work done by the external pressure and the work done on the bubble,

$$W_{net} = P_E V\left(\frac{V_0}{V} - 1\right) - \left(\frac{QV_0}{\gamma - 1}\right)\left(\left(\frac{V_0}{V}\right)^{\gamma - 1} - 1\right). \tag{4}$$

The kinetic energy of the liquid is

$$KE = \frac{1}{2}\rho\int 4u^2\pi r^2 dr = 2\pi\rho U^2 R^4 \int_R^\infty r^{-2} dr = 2\pi\rho U^2 R^3 = \frac{3}{2}\rho U^2 V. \tag{5}$$

This kinetic energy can be equated with the net work of the liquid yielding the following relation, with volume in place of radius:

$$\frac{3}{2}\rho U^2 V = P_E V\left(\frac{V_0}{V} - 1\right)\left(\frac{QV_0}{\gamma-1}\right)\left(\left(\frac{V_0}{V}\right)^{\gamma-1} - 1\right). \tag{6}$$

Equation 6 is solved for U^2, yielding

$$U^2 = \left(\frac{2P_E}{3\rho}\right)\left(\frac{V_0}{V} - 1\right) - \left(\frac{2}{3\rho}\right)\left(\frac{Q\frac{V_0}{V}}{\gamma-1}\right)\left(\left(\frac{V_0}{V}\right)^{\gamma-1} - 1\right). \tag{7}$$

Put in terms of radius rather than volume, the equation solves to

$$U^2 = \left(\frac{2P_E}{3\rho}\right)\left(\left(\frac{R_0}{R}\right)^3 - 1\right) - \left(\frac{2}{3\rho}\right)\left[\frac{Q\left(\frac{R_0}{R}\right)^3}{\gamma-1}\right]\left(\left(\frac{R_0}{R}\right)^{3(\gamma-1)} - 1\right). \tag{8}$$

Equation 8 is used to determine the velocity of the bubble surface as a function of the ratio of the radius to the original bubble radius. Using the relation $U = \frac{dR}{dt}$, time steps for changes in speed and radius are calculated. These steps are not linear, as the variation of radius and velocity with time are not linear. Properties such as temperature, pressure, and energy density are calculated using the perfect gas law, shown below for temperature:

$$\frac{T}{T_0} = \left(\frac{R_0}{R}\right)^{3(\gamma-1)}. \tag{9}$$

Equations for the remainder of the calculated properties are provided in Section 2.3.

2.2. Objectives

Several objectives exist in this project, chief among them the development of a versatile, vetted, and expandable model for cavitation bubble collapse in both pure substances and mixtures. The existing method of calculation was spreadsheet-based, which does not lend itself to easy changes in radius step size. This limits the solution to steady state external pressure whereas this improved version can be used with varying pressures. The code is therefore applicable to acoustic variations as needed for

sonochemistry and rocket engine ignition. Versatility in the initial configuration of a simulation is also desired. To this end, the model was built in MATLAB, to take advantage of the ease of performing iterative calculations. The primary purpose of the development of a MATLAB script is to allow for varied and quick calculations of the potential temperatures and energies present in a single bubble collapse across many bipropellant combinations. Another primary objective is the production of consistent graphs displaying the thermal and physical characteristics of the implosion. The graphs must scale properly and automatically, as well as clearly label the parameters which are plotted. Such graphs are useful for two reasons; if unreasonable input parameters are entered, the model breaks down in a clearly visible way in the graphs of different properties, and the graphs are also useful for reading a quick maximum of a given property.

The script produced in this effort will be used to get order of magnitude estimates for pressure, temperature, energy density, and the speed of the bubble collapse to inform future test work in cavitation ignition. The user interface of the script must be intuitive and explicit when asking for initial inputs. As a goal, the number of user-configurable parameters should be as minimal as possible while still allowing the full range of temperature, pressure, and substance configurations. Parameters such as saturation pressure and partial pressure should be calculated from the inputs upon which they are dependent so as to minimize the ability for conflicting inputs to be entered. All user input parameters, as well as parameters directly calculated from inputs are provided in the graph outputs in order to keep a record of the inputs with their produced outputs.

2.3. Verification Methods

Verification of the model will be conducted by comparing the output to both Dr. Blackmon's original spreadsheet calculations, and to the sources of comparison used in his original paper. Of primary importance is an order of magnitude verification, as small differences in the curves used for vapor pressure or different specific heat ratios yield small changes well within an order of magnitude. The cases tested in this paper are therefore identical to the cases tested in Blackmon's paper. Additional cases of

interest are mentioned, and inputs which may prove important to bipropellant liquid rocket systems are discussed. The effect of condensation of gas in the bubble can be observed, as the code allows for condensation to be excluded at the user's discretion. A case can be tested with and without condensation to demonstrate the difference in behavior.

3. Model Development

3.1. Framework and Assumptions

The framework for this model is an iterative MATLAB script with user configurable inputs on the liquid medium, bubble medium, temperature of the bubble, external pressure, initial bubble radius, and a specific heat ratio. Each of these parameters is semi-independent; for a liquid oxygen-liquid methane (LOX-LNG) mixture, the bubble temperature will be near the boiling temperature of the LOX. A significantly higher temperature would be unreasonable, and would break the model, though the results of such a break are immediately noticeable in the numerical and graphical output of the script. Several assumptions are made based on Dr. Blackmon's original model. This model assumes a single bubble collapse, in the absence of any other bubble formation or existence, and with a large liquid volume relative to the size of the bubble. A cluster of bubbles would amplify the effect; as bubbles in the cluster imploded, they would exert pressure on surrounding bubbles and cause even greater pressures at implosion for those bubbles [1] [2].

The MATLAB script performs thousands of iterations over the collapse and subsequent re-expansion of a vapor bubble. The result is a symmetric profile for contraction and expansion properties, shown in Figure 2-1. This particular figure shows the temperature of the bubble as it undergoes adiabatic compression and then expansion. The script terminates calculations after the bubble re-expands to its starting radius as configured at the beginning of the script. The derivations in Section 1.1 assume an adiabatic gas, so the model is valid for an adiabatic gas. The adiabatic assumption of the model does not allow energy loss in the form of heat from the bubble to the surrounding liquid, so the effects of the bubble collapse on the liquid medium are not modeled. These effects are, however, discussed at length later in the report.

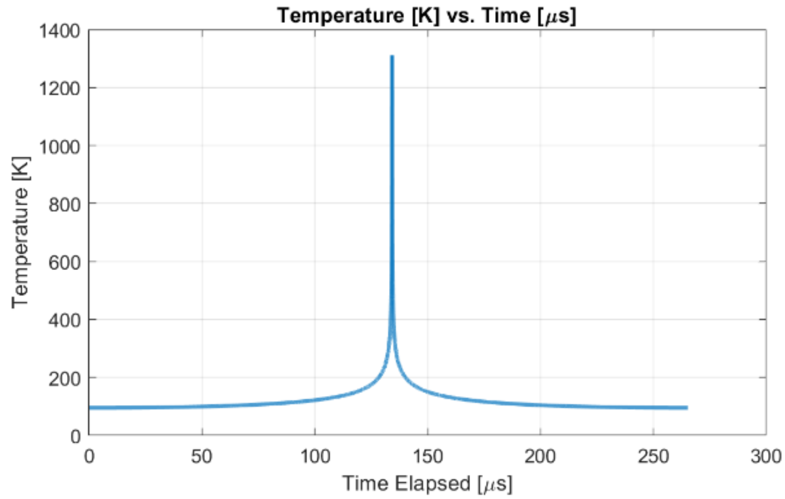

Figure 2-1: Temperature Profile During Collapse

Notably, the model excludes calculations for bubble surface tension and liquid viscosity. Blackmon's original paper excludes surface tension as well, noting that the parametric model held up to models of greater complexity even without the addition of surface tension. The parametric nature of the script would allow the addition of more physical phenomena to the model as needed. When the velocity term stops decreasing in magnitude, the bubble has reached the end of its collapse and has begun to re-expand. This is visualized by the peak in temperature in Figure 2-1. At this point the

3.2. Input Parameters

The inclusion of each input parameter is necessary for the model to run in its present state. The initial two inputs are the liquid and bubble media; these are selected from lists of options provided to the user. The included substances are shown in Figure 2-2, and are focused on potential bipropellant combinations. Additional substances such as water and air are added to facilitate calculations for tests with more inert substances, which may be conducted on small scales and without significant detonation risk.

```
Select a liquid medium:
    (1) LH2
    (2) LOX
    (3) LNG
    (4) RP-1
    (5) H20
    (6) Lead
Selection: 5

Select a bubble medium:
    (1) GH2
    (2) GOX
    (3) Methane
    (4) Air
    (5) Water vapor
Selection: 2
```

Figure 2-2: Liquid and Bubble Media

The external pressure (the pressure of the liquid medium) is configurable for the simulation of a pressurized propellant tank as might be found in a launch vehicle. The user can choose whether to simulate condensation of the gas in the bubble, which affects the pressure during collapse. The initial temperature of the bubble is also a user input. Initial bubble radius is configurable, as well as the value of the specific heat ratio, γ. The specific heat ratio is dependent on the substance and temperature of the gas bubble, but it is complicated by the potential for condensation and the low temperatures of cryogenic propellants, and is currently left to the user as an input. To compensate for this uncertainty in γ, the user can choose to perform a sensitivity analysis on the simulation by allowing the program to automatically alter γ slightly above and slightly below the user-provided value. A standard interaction with the script in setting these parameters is shown in Figure 2-3

```
External pressure [atm]: 68
Assume condensation (Y or N): n
Intial temperature [K]: 300
Initial radius of bubble [mm]: 2
Gamma: 1.4
Sensitivity analysis on gamma (Y or N): n
```

Figure 2-3: User Input Parameters

The sensitivity to γ is demonstrated by the output below. A case was run for a hydrogen and oxygen bubble in LOX, with a starting temperature of 79 K and an external pressure of 1 atm. Condensation is assumed and the initial bubble radius is set to 2 mm. The chosen value for the specific

heat ratio is γ = 1.358. This is based on a value chosen by Blackmon, and was derived from the assumed mixture of hydrogen and oxygen vapor in the bubble. If this value were slightly higher or lower, the effect on many properties would be noticeable, as shown in Figure 2-4. The temperature alone varies significantly for a small range of specific heat ratios. Results for the differences are summarized in Table 2-1.

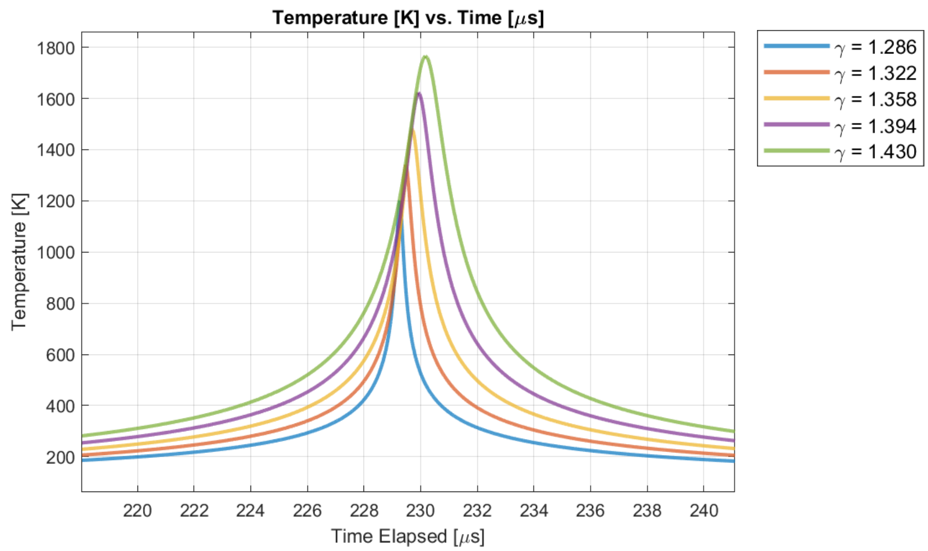

Figure 2-4: Temperature Variation with γ

Table 2-1: Variation of Properties with γ

γ	Max. Temp [K]	Max. Pressure [atm]	Min. Radius [mm]
1.2864	1201	3058	0.084
1.322	1341	1670	0.107
1.358	1482	1013	0.130
1.3938	1623	664	0.155
1.4296	1766	464	0.179

The trend is observed as follows: for higher values of γ, the maximum temperature will be higher, while the maximum pressure will be lower. This follows the expected relationship, and is observed throughout the test cases in this report. For higher values of γ, the minimum radius reached will be larger. Thus, for smaller γ values, the bubble will collapse to a much smaller size and will experience a much

higher pressure, but will maintain a lower temperature. It is notable that across the range of variation of the specific heat ratio, the bubble always reaches temperatures above the minimum ignition temperature for hydrogen of 833 K [3].

3.3. Modeled Characteristics

There are a number of useful parameters that are graphed, as well as a text output of the maximum and minimum points of interest for the run. The graphed properties plotted over time are as follows: bubble surface speed, bubble surface acceleration, bubble radius, bubble temperature, bubble pressure, compression energy, and compression energy density. The ratio of the compression energy to the minimum ignition energy (MIE) is also graphed with respect to time. Graphs are provided that zoom in on the peaks of the compression energy and energy density lines, for ease of interpretation of peaks that overlap in the case of a sensitivity analysis on γ. The bubble surface speed is graphed over the ratio of the radius of the bubble to its original radius, to characterize the speed of collapse at different points during the collapse. Parameter outputs provided in a text summary are the following: maximum temperature, maximum pressure, minimum radius, maximum energy, and maximum energy density. This output serves to provide a general summary of notable values upon a quick glance at results. The equations for bubble properties are shown below, beginning with the equation for pressure,

$$P = Q\left(\frac{V_0}{V}\right)^{\gamma} + P_{sat}. \tag{10}$$

The equation for the energy of the bubble is

$$W = \frac{4}{3}Q\pi\left(\frac{r_0}{\gamma-1}\right)\left(\left(\frac{V_0}{V}\right)^{\gamma-1} - 1\right) \tag{11}$$

And the equation for the energy density of the bubble is

$$\frac{W}{V} = \frac{3W}{4\pi r_i^3}. \tag{12}$$

These equations, as well as those in Section 1.1, are all the calculated properties of the bubble during collapse.

4. Results

Three test cases are run for common propellant combinations, with LOX as the oxidizer in all cases due to its ubiquity in large-scale bipropellant rockets. The results of each are compared to Blackmon's calculations and to the models used for verification in his paper. Applications of the script are discussed, and the implications of the temperatures and energies experienced during bubble collapse are analyzed. Future improvements to the model are suggested and plans to calculate the specific heat ratio are discussed.

4.1. LOX-LH2

The liquid oxygen-liquid hydrogen (LOX-LH2) case is run with the following input parameters shown in Figure 3-1, to match the inputs of Blackmon's simulation and align with the results from Osipov, 2018, whose paper sought to model the explosion of the Challenger Shuttle's hydrogen tank [4]. The output of the script is provided in Figure 3-2. Notable are the high temperatures of the bubble during implosion, and the high ratio of the energy of the bubble to the minimum ignition energy of hydrogen in the presence of oxygen.

```
Select a liquid medium:
    (1) LH2
    (2) LOX
    (3) LNG
    (4) RP-1
    (5) H20
    (6) Lead
Selection: 2

Select a bubble medium:
    (1) GH2
    (2) GOX
    (3) Methane
    (4) Air
    (5) Water vapor
Selection: 1

External pressure [atm]: 1
Assume condensation (Y or N): y
Intial temperature [K]: 78.62
Initial radius of bubble [mm]: 2
Gamma: 1.358
Sensitivity analysis on gamma (Y or N): n
```

Figure 3-1: LOX-LH2 Inputs

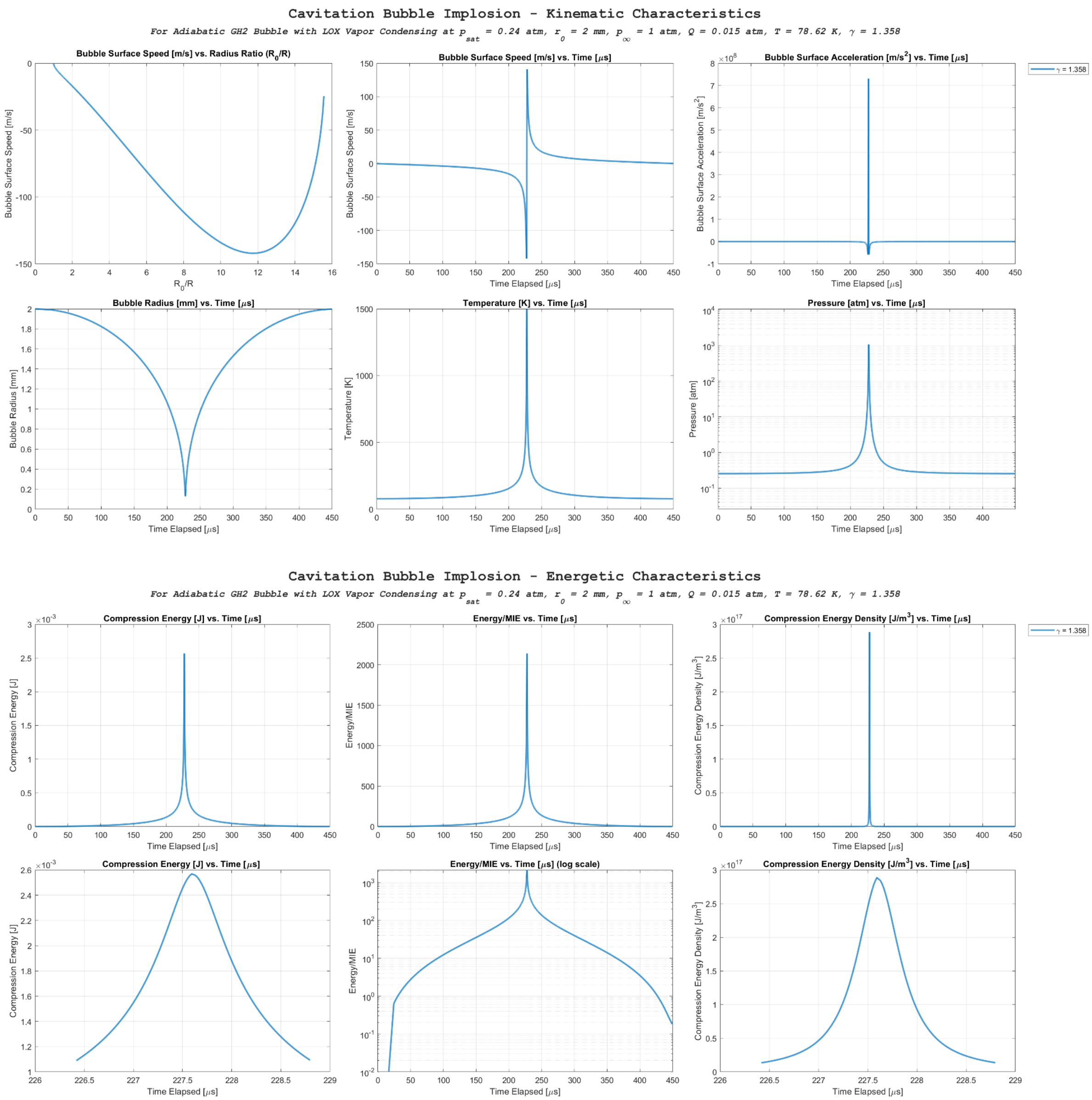

Figure 3-2: LOX-LH2 Graph Outputs

A summary of the important parameters is provided in Table 3-1, with a comparison to the values calculated by Blackmon [1] and Ospiov [4]. The minimum ignition energy of hydrogen in oxygen is 1.2 μJ, which is quite low compared to most substances in the presence of oxygen [5]. The relative agreement between the script results and Blackmon's results indicate faithful representation of Blackmon's model. The automatic calculation of vapor pressure for condensation modeling is sufficient to maintain the integrity of the model. Differences between Osipov's calculations and the Blackmon method are perhaps due to the inclusion of surface tension in Osipov's calculations. Particularly notable from Figure 3-2 is the

energy density of the bubble compression. At the peak of collapse, the energy density is $2.8 * 10^{17} J/m^3$. Based on a 2012 report by the city of Los Angeles, the yearly energy use of the city was 22,000 GWh [6]. The energy density of the bubble compression is therefore equivalent to the entire energy use of Los Angeles, for a year, packed within a single cubic foot. Cavitation implosion produces extremely high values which are difficult to compare to, due to the small scale of an implosion and relatively high energy given the scale.

Table 3-1: Comparison of Results for LOX-LH2

	Osipov	**Blackmon**	**MATLAB Script**
Max. Pressure [atm]	510	1047	1076
Max. Temperature [K]	1450	1484	1498
Minimum Radius [mm]	0.165	0.129	0.129
Collapse Time [ms]	0.23	0.23	0.23
Max. Energy/MIE	—	2118	2141

4.2. LOX-LNG

A LOX-LNG case was run for a 2-mm methane and oxygen bubble in liquid oxygen. LOX-LNG is a forthcoming choice of propellant in the new class of launch vehicles being built by several private entities. Liquid oxygen exists from 54.35 K to 90.15 K, while liquid methane exists from 90.7 K to 111.65 K, at an external pressure of 1 atm [7]. The two substances can be a liquid at nearly the same temperature, permitting the use of a common bulkhead in propellant tanks in order to save weight. This common bulkhead is an interface which could fail, and serve as a mixing point for LOX and methane. The input conditions and output graphs are shown below in Figure 3-3 and Figure 3-4.

```
Select a liquid medium:
    (1) LH2
    (2) LOX
    (3) LNG
    (4) RP-1
    (5) H20
    (6) Lead
Selection: 2

Select a bubble medium:
    (1) GH2
    (2) GOX
    (3) Methane
    (4) Air
    (5) Water vapor
Selection: 3

External pressure [atm]: 1
Assume condensation (Y or N): y
Intial temperature [K]: 78.618
Initial radius of bubble [mm]: 2
Gamma: 1.25
Sensitivity analysis on gamma (Y or N): n
```

Figure 3-3: LOX-LNG Inputs

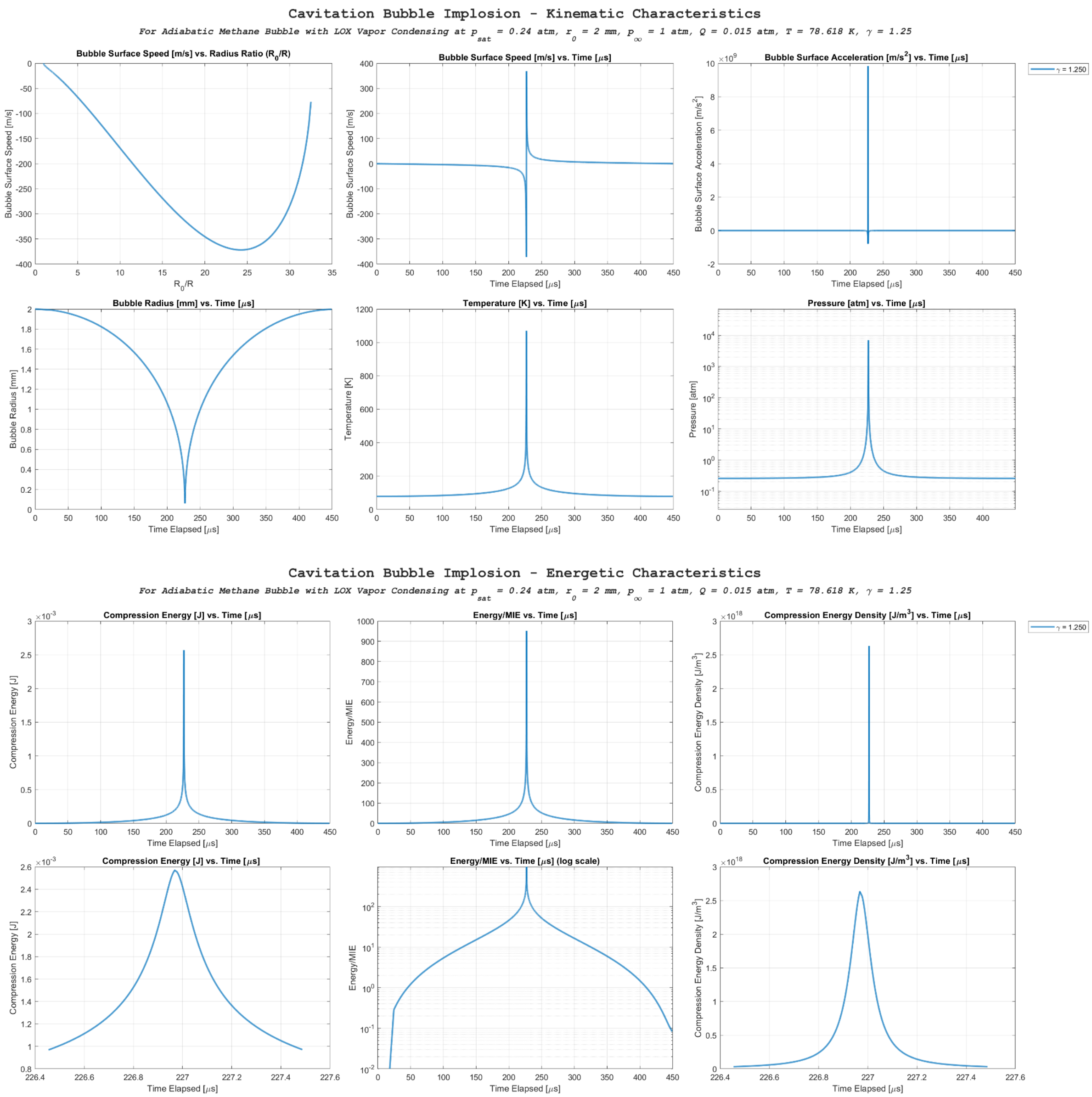

Figure 3-4: LOX-LNG Graph Outputs

Again, the maximum properties and general behavior of the collapse are similar to Blackmon's results. The addition of Antoine equations for calculating the saturation pressure of the liquid medium is likely responsible for the difference. This difference is negligible, and the use of different Antoine coefficients would result in different maximum values [8]. The discrepancy is noted but is not a source of serious concern. The high pressure experienced by the bubble during implosion is significantly higher than the hydrogen bubble pressure by a factor of 7. The minimum autoignition temperature of 853 K for methane in oxygen, and the temperature of the bubble at its smallest size is above this by a significant

margin [1]. The collapse time is short, nearly the same as the hydrogen bubble. As both bubbles began at the same initial radius, this follows.

Table 3-2: Comparison of Results for LOX-LNG

	Blackmon	**MATLAB Script**
Max. Pressure [atm]	6725	7009
Max. Temperature [K]	1061	1070
Collapse Time [ms]	0.221	0.227

4.3. LOX-RP1

A final case was run for a LOX-RP1 mixture, which is perhaps the most common propellant combination throughout history and at the present moment. This combination differs from the hydrogen and methane fuel combinations in that RP-1 (a refined kerosene) is not cryogenic. The case is also different in setup; a bubble of gaseous oxygen (GOX) is surrounded by RP-1, rather than LOX serving as the liquid medium. Input conditions are given in Figure 3-5 and the graph output is shown in Figure 3-6.

```
Select a liquid medium:
    (1) LH2
    (2) LOX
    (3) LNG
    (4) RP-1
    (5) H20
    (6) Lead
Selection: 4

Select a bubble medium:
    (1) GH2
    (2) GOX
    (3) Methane
    (4) Air
    (5) Water vapor
Selection: 2

External pressure [atm]: 1
Assume condensation (Y or N): n
Intial temperature [K]: 300
Initial radius of bubble [mm]: 2
Gamma: 1.35
Sensitivity analysis on gamma (Y or N): n
```

Figure 3-5: LOX-RP1 Inputs

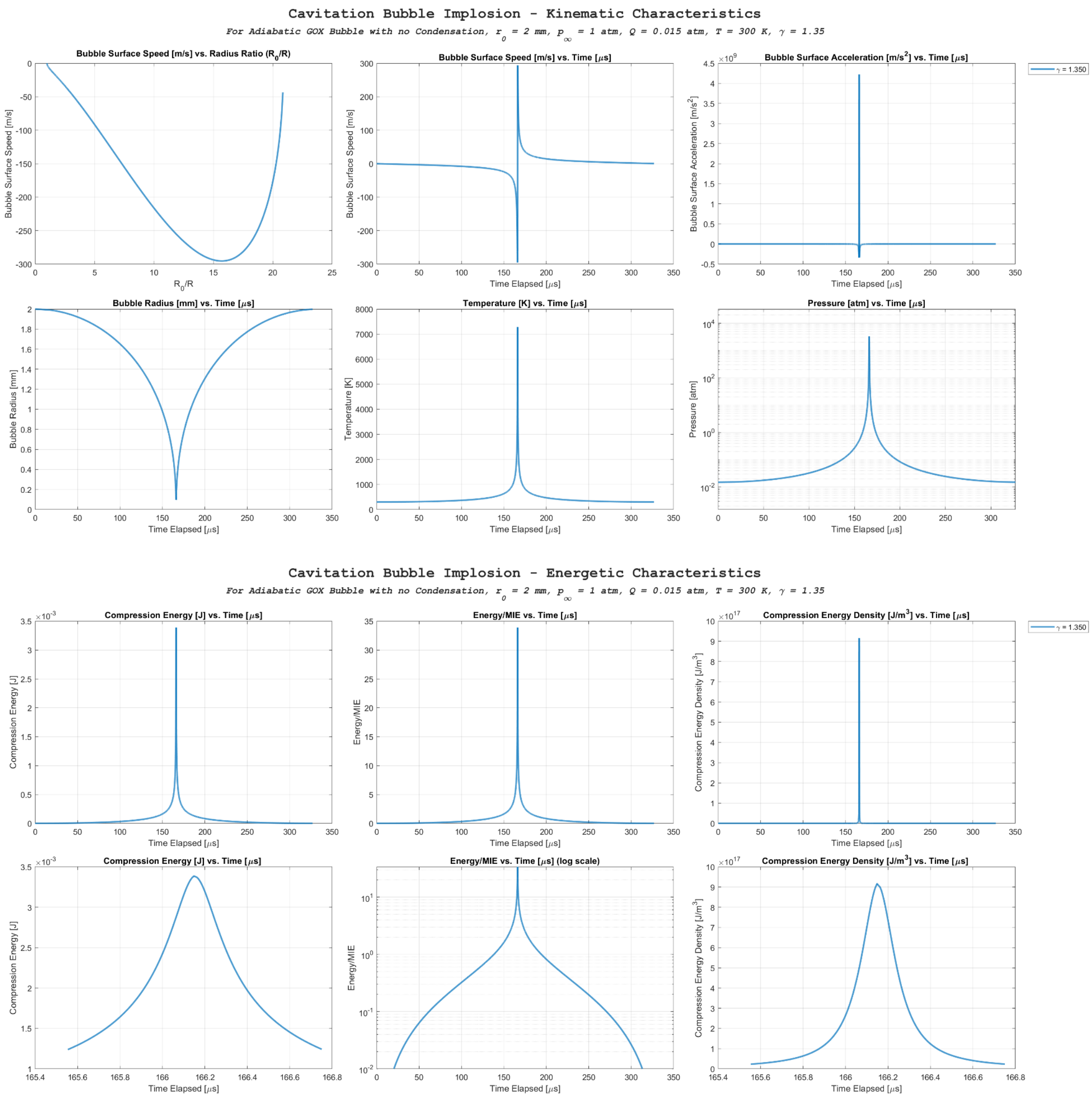

Figure 3-6: LOX-RP1 Graph Outputs

The maximum properties are provided at the smallest radius during implosion. Notable here is the extremely high temperature reached relative to the autoignition temperature RP-1 of 483 K [3]. The temperature is significantly higher than the temperatures reached by the cryogenic fuels, in part due to the higher starting temperature of the RP-1. Collapse times are on the same order of magnitude as the cryogenic fuels.

Table 3-3: Comparison of Results for LOX-RP1

	Blackmon	MATLAB Script
Max. Pressure [atm]	3332	3301
Max. Temperature [K]	7299	7282
Collapse Time [ms]	0.157	0.166

4.4. Applications and Future Work

The application of the script and its graphical output is the provision of a quick order of magnitude estimate for the conditions experienced during a cavitation bubble collapse. These estimates may be used to infer autoignition of a propellant combination, or for a combination such as an air bubble in water, could be used to estimate heating in the bubble. Insofar as the accuracy of the model is concerned, it matches Blackmon's results to within a percent. Blackmon's results are verified for a number of cases against results from other publications, including Osipov.

Several improvements to the program are planned for the near future, as the software will be used to inform test setups and potential physical demonstrators. The first addition will be the automatic calculation of the specific heat ratio based on the input substances, the initial temperature, and the consideration of condensation. Another improvement which is in development is a finer density calculator for liquids, and a more accurate determination of the minimum ignition energy and pressure for a given combination of liquid and gas bubble. The addition of surface tension terms into the calculation is also underway.

5. Acknowledgements

I would like to thank Dr. James Blackmon for his mentorship, his patience, and his incredibly gracious investment in my future. It was Dr. Blackmon who provided the idea for this project and fostered in me the excitement for the implications of cavitation ignition. I would also like to thank Dr. Blackmon for his recommendation which resulted in my hiring at Bangham Engineering Inc, where I am continuing full-time employment. I am equally grateful to Dr. David Lineberry for his mentorship and his recommendation to reach out to Dr. Blackmon initially.

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