

Oxidizer-Fuel Optimization For Rotating Detonation Rocket Engines

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ABSTRACT

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Rotating detonation rocket engines have been a major topic of study in recent years due to potential boosts in efficiency. This paper will focus on researching RDREs, the respective theories supporting detonation engines, and simulating detonations with a variety of different reactant mixtures and ratios. Firstly, research is performed on both RDREs in terms of design as well as supporting theories and models such as Chapman-Jouguet detonation and the ZND model. This is followed by research into different oxidizer and fuel choices in terms of efficiency and drawbacks. Finally, CEARUN simulations are run on different oxidizer-fuel combinations as differing equivalence ratios until a select few are chosen as more specifically analysed to determine a potentially optimal choice for RDRE use. The CEARUN simulations in combination with research into prominent oxidizer and fuel options shows that a simple mixture with well-researched components like methane and dinitrogen tetroxide would be an optimal choice for potential RDRE designs.

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Nomenclature

Symbol	Definition	Units (SI)
p	Pressure	kPa
T	Temperature	K
u	Velocity	m/s
v	Specific Volume	m^3/kg
h/H	Enthalpy	J
s/S	Entropy	J/K
C	Chapman-Jouguet Velocity	m/s
Q	Heat Released per Unit Mass	J/(kg K)
R	Universal Gas Constant	$(gm^2)/(s^2molK)$
W	Average Molecular Weight	g/mol
d	Droplet Diameter	m
a	Speed of Sound	m/s
f	Friction Factor	-----
C_h	Heat Transfer Coefficient	-----
A_R	Surface Area of Reaction Zone	m^2
A_s	Frontal Area of Shockwave	m^2
ΔG	Change in Gibbs Free Energy	J/mol
K_p	Equilibrium Constant	$\sqrt{p}$
ϕ	Equivalence Ratio	-----
Subscripts		
X_H	Derivative on the Hugoniot	-----

X_{∞}	State of Fully Burnt Gas	-----
X_l	Liquid	-----
X_2	Value After Shockwave	-----
X_W	Value Relative to State 1	-----
X_1	Initial State	-----
X_3	Combustion Products	-----
X_D	Detonation Value	-----
X_i	I-th element of a set	-----
X_j	J-th element of a set	-----
Greek Symbols		
η	Efficiency	%
γ	Heat Capacity Ratio	Unitless
ρ	Density	kg/m^3
τ_b	Droplet Breakup Time	s
v	Stoichiometric Value	-----
Acronym		
RDRE	Rotating Detonation Rocket Engine	-----
OF	Oxidizer and Fuel	-----
CJ	Chapman-Jouguet	-----
DTD	Deflagration-To-Detonation	-----
FJ	Fickett-Jacobs	-----
CFD	Computation Fluid Dynamics	-----

ZND	Zeldovich, Neumann, and Doering	-----
LOX	Liquid Oxygen	-----
LH2	Liquid Hydrogen	-----
CTAP	Capillary Tube Average Pressure	-----
CEA	Chemical Equilibrium with Applications	-----
LPG	Liquified Petroleum Gas	-----
STP	Standard Temperature and Pressure	-----

Chapter 1: Introduction

1.1 Introduction and Motivation

The popularity of rotating detonation rocket engines, or RDREs, has been on the rise in recent years as the next major step in propulsion. What makes RDREs so revolutionary is the departure from using deflagration as a method of propulsion and rather utilizing detonation to garner thrust. By switching to detonation waves, RDREs gives the following advantages:

- simplifying both design and manufacturing,
- utilizing no moving components,
- higher rates of energy conversion,
- higher thermodynamic efficiency [1].

These advantages help promote RDREs as the next step of propulsion by offering an increase in efficiency versus traditional rocket propulsion with some theorizing that they will be 25-30% more efficient. To fully utilize detonation waves, RDREs are designed to rotate detonation waves around a chamber whilst injecting fuel to both sustain the detonation and produce thrust as seen in the schematic diagram below.

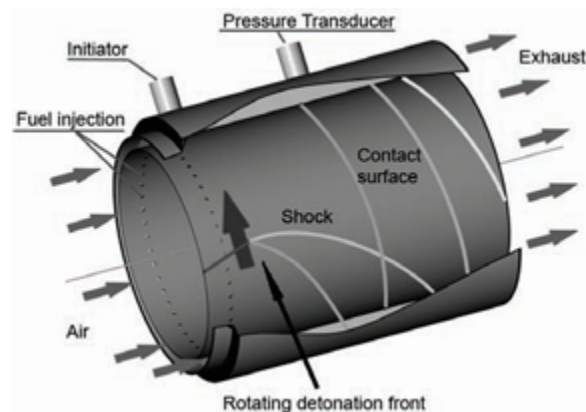


Figure 1.1 - Schematic of rotating detonation rocket engine [2]

Due to the inherent advantages, RDREs will play a major role in the upcoming years due to the ever increasing complexity of missions. With more focus than ever on extraplanar and deep space missions, more advanced technologies will be necessary to meet the standards of the respective mission statements. In addition, RDREs has applications in both the civil and military sectors. RDREs have the capacity to replace traditional turbojet engines in commercial aircraft as well as be implemented in both air-to-ground and air-to-air missiles as there are several key benefits versus traditional munitions such as increased range, compatibility, and ease of manufacturing [3]. Given how RDREs will allow for more complicated deep space missions to be undergone as well as RDRE powered weapons being capable of giving a paramount advantage to militaristic endeavours, RDREs are the next major technological advance for propulsion.

RDREs have been a concept for decades but serious endeavors have recently begun to further conceptualize and analyze the mechanics and properties of RDREs. While the core mechanics are well understood, research is still necessary to further advance and optimize RDREs in all regards. One of these topics concerns the fuel pumped into the detonation wave to both propagate the wave and create sufficient thrust through the exhaust. Given that RDREs utilize a detonation wave rather than deflagration, new combinations of oxidizers and fuels with new ratios may be considered optimal. There also exists the issue of mixing the oxidizer and fuel together before the detonation.

The main objective of this project is to perform a case study concerning the OF mixture for RDREs to determine the combinations and ratios for producing optimal thrust. This project will compare different oxidizers and fuels used in both traditional deflagration engines as well as currently tested RDREs to determine which scenario generates the most thrust whilst taking into account additional factors such as the toxicity and abundance of said materials. This process will utilize a combination of NASA's CEARUN and MATLAB's combustion toolbox to simulate different combinations of oxidizer and fuel with differing equivalence ratios in a detonation wave, recording key parameters such as thrust and specific impulse. With this data, a case study will be undertaken to determine a potential optimal combination that outputs high performance with minimal negative qualities such as toxicity, abundance, and ease-of-use.

1.2 Literature Review

This literature review is designed to research the two major topics of this paper: rotating detonation rocket engines and oxidizer-fuel mixtures. To be specific, the research will be focused on the following few topics:

- RDREs' design and function,
- the nature of detonation waves and how they affect airflow,
- OF choices, specifically how to choose mixture and ratio.

The literature review will also cover recent testing of RDREs for the purpose of comparison, investigating the decisions made by the respective engineering team, especially the choice of oxidizer and fuel. This acts as both a starting point for this project by utilizing already tested OF mixtures before simulating new combinations and ratios as well as a point of comparison to see whether any different combinations are more effective than previously testing mixtures.

1.2.1 Detonation Waves

As the name shows, detonation waves are the unique characteristic that separates RDRES from traditional rocket propulsion which utilize deflagration. It is in that difference and the nature of detonation waves that allows for RDREs to be far more efficient in producing thrust. The major difference between detonation and deflagration comes from the speed of the waves; deflagration is a subsonic combustion while detonation is a supersonic combustion. As a result, RDREs experience a shock reaction due to the detonation wave rather than a heat transfer reaction from the deflagration which results in an increase in thermodynamic efficiency. The increase in efficiency is a result of very fast material burning induced by the detonation wave which allows for a more compact system [4]. Due to the rapid burning of fuel, the system is unable to equalize the pressure which results in the reaction being closer to a constant volume process rather than a constant pressure process found in traditional propulsion systems. To illustrate the difference in efficiency between constant pressure versus constant volume, a comparison between idealized versions of the two thermodynamic cycles can be done. For this comparison, an equal amount of heat is provided to each of the two reactions with detonations being added as a point of comparison. When comparing the results, it is found that the thermodynamic efficiency of constant pressure is 27%, constant volume is 47% and detonation is 49%, showing a 20% increase purely from switching to constant volume from constant pressure.

When discussing how to utilize a continuous detonation wave in an RDRE, the geometry of the combustion chamber plays a paramount role. Many different geometries are considered viable for RDREs but most recent experimentations utilized an annular approach, complete with an inner and outer cylinder. Unfortunately, throwing two cylinders together is considered a suboptimal approach to this problem. However, in a study conducted by Kudo et al., a “critical” parameter exists which allows for a stable propagation of detonation waves [5]. Through experimentation, it was determined that for rectangular-cross-section tubes, if the inner wall had a curvature radius as between 14-40 times the detonation cell width, the oblique detonation waves would be stable. While this experiment operated on conditions not native to RDREs, it did lay the groundwork for later experimentation such as the work done by Kawasaki et. al. [6]. This experiment built upon the previous experiments and attempted to apply the concept of a critical condition for RDREs. For this experiment, testing was done on multiple configurations of RDREs, with inner radii ranging from 0 mm, or no inner cylinder, to 31 mm. In these trials, the mass flow rate and equivalence ratio were kept within a certain range with only the radius drastically changing between experiments as shown in Fig. 1.2. Through this experiment, it was determined that the critical condition, in this case an inner radius of 15 mm, was the most suitable more efficient thrust production as it avoided the complications associated with the

subcritical and supercritical trials. For the subcritical values, it was determined that the specific impulse generated was less than 80% the ideal value due to the existence of deflagration. While deflagration existed in the critical trial as well, it was far less pronounced as the lack of space forced most of the fuel to react with the detonation wave; Fig. 1.2 demonstrates this by showing the deflagration zone for the three trials, with the zone becoming smaller and smaller as the inner circle encroaches the space. As for the supercritical trials, while exceeding 80% ideal output alongside the critical trial, having a large inner radius is suboptimal due to the detonation wave attaching to the inner cylinder wall. When the detonation wave attaches to the inner radius, it produces additional acoustic, cooling, and stability complications in addition to the complications the detonation creates innately. In conclusion, keeping the inner radius of the annulus with the critical threshold is paramount for optimal performance.

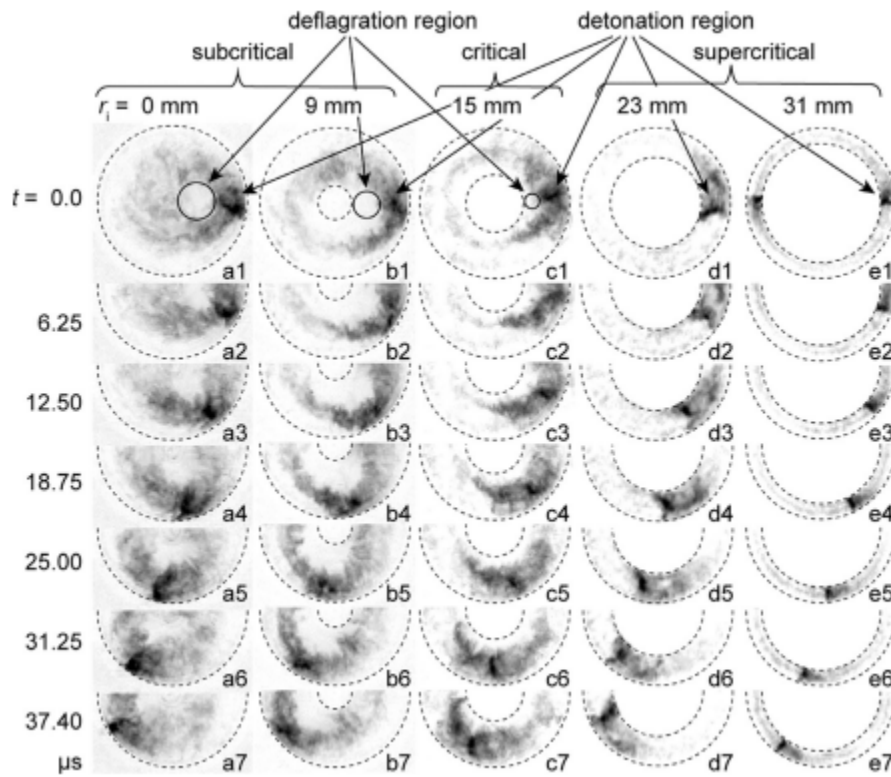


Figure 1.2 - Axial imaging of RDRE combustion chambers with varying inner radii [6]

1.2.2 Mechanics of Rotating Detonation Rocket Engines

Rotating detonation rocket engines are designed to utilize detonation waves as a method of producing thrust. To explain this proficiently, resources and information will be taken from a study done by the University of Texas concerning RDREs [1]. Put simply, RDREs create propulsion by feeding a detonation wave into an annular chamber as a method for converting energy. As mentioned above, detonation waves act as a near constant volume thermodynamic reaction, similar to a shockwave. It is this shockwave-like behavior, typically referred to as

detonation-shock waves or detonation wavelets, is where the efficiency of RDREs is derived; Fig. 1.3 below shows a cross-section of how the airflow and detonation wavelet appears in an RDRE.

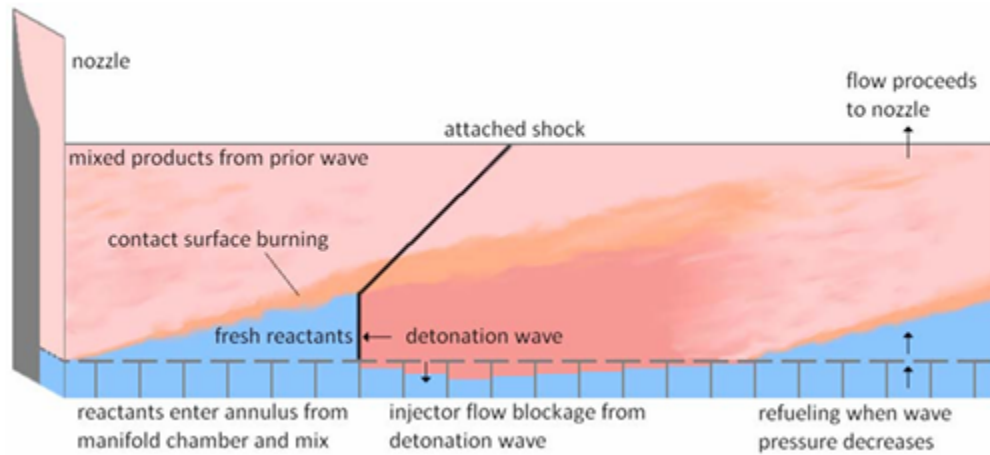


Figure 1.3 - Cross section of detonation wave in RDRE [1]

To explain further, a detonation wave is induced into the annular chamber, referred to as the annulus, placed near the exit of the injectors. From there, fuel is fed into the annulus, symbolized by the blue coloration, before reacting with the detonation wave to create a region of high-pressure, high-temperature airflow. After the collision is the detonation wave, the pressure begins to drop as it moves towards the nozzle, resulting in a new low-pressure region which allows for more reactant to flow into the annulus, restarting the cycle when the detonation wave completes its cycle around the annulus. However, providing OF to a RDRE has its complications, amplified by the detonation wave. While there exists multiple difficulties, this paper will focus on three: poor OF mixing, parasitic/commensal combustion, and wall curvature.

1.2.2.1 Oxidizer and Fuel Mixing

Due to the rapid nature in which RDREs cycle a detonation wavelet around the annulus, the distance in which oxidizer and fuel needs to be mixed is far smaller than in systems using deflagration. The mixing of the OF mixture is paramount for optimal thrust as insufficient mixing can lead to decrease stability and speed of the detonation wave, limiting the speed of the airflow exiting the annulus. As mentioned in a report concerning OF mixing in RDREs from Queen's University, incomplete mixing was a major contributor to suboptimal conditions in experimental testing [7]. In this report, different scenarios are tested using different dimensions and techniques to investigate potential design choices for future RDREs. In almost all cases, an incomplete mixing of oxidizer and fuel results in reduced strength and steadiness of detonation propagating which inhibits optimal performance. This unsteady detonation wavelet, which is sometimes referred to as "chugging," is a problem needing to be addressed; fortunately, premixing the OF mixture has been noted to help reduce chugging. By premixing, RDREs are

capable of producing faster detonation velocities while non-premixed RDREs struggle with chugging as non-premixed tests, “typically produce average combustion front velocities substantially below the CJ detonation velocity [...], up to 50% below in some cases.” Before moving on, for clarity’s sake, the CJ detonation velocity is a reference to the Chapman-Jouguet condition which states that a detonation propagates at a velocity where the reactants will just reach sonic speed as the reaction ceases [8].

Premixing the OF mixture helps to prevent unstable detonation waves by homogenizing fuel-rich and fuel-lean regions in the annulus. When fuel and oxygen is mixed locally in the annulus, it is often inhomogeneous which results in two different types of regions forming: fuel-rich zones and fuel-scarce or fuel-lean zones. These local inhomogeneous zones, or stratification, can lead to both chugging as well as altering the characteristics of the detonation wavelet [9]. On the low end, this results in a reduction in the ideal Chapman-Jouguet velocity and on the high end, with a large enough gradient, a multi-headed detonation wave can form in the annulus. However, by premixing the OF mixture in a prior chamber, stratification can be reduced, allowing for a more constant detonation velocity as shown below.

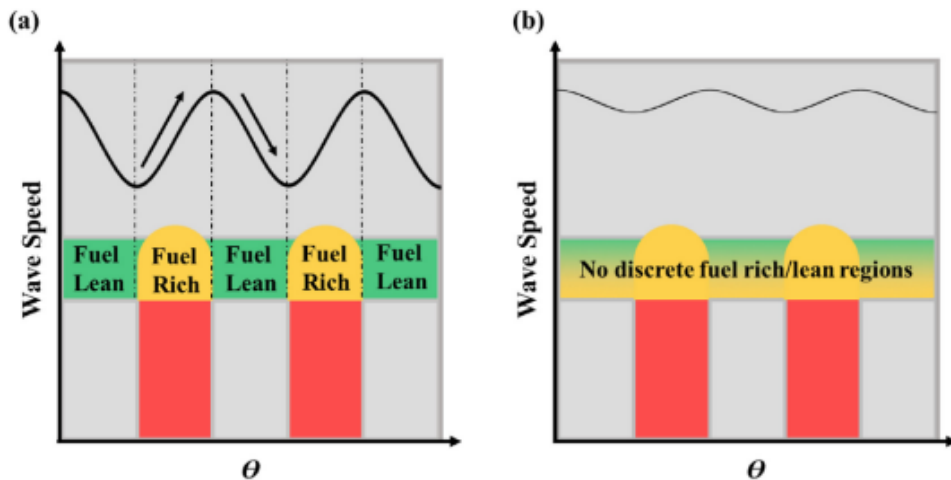


Figure 1.4 - Comparison of locally mixed to premixed oxidizer-fuel mixture for rotating detonation rocket engine [9]

When the oxidizer and fuel is properly mixed before injecting into the annulus, the stratification becomes far less discrete which results in a more stable detonation wave speed. It should be noted that wave speed is still oscillatory in nature as this scenario only performs a low level of premixing. While a higher level of mixing can be utilized to remove the oscillations entirely, this is unnecessary as it will only increase performance marginally. A low level of mixing is capable of marginalizing stratification which was the major complication which led to chugging and potential multi-headed detonations.

1.2.2.2 Parasitic and Commensal Combustion

Parasitic and commensal combustion refers to undesirable deflagration of reactants inside the annulus. This typically occurs due to the highly complex flow field of the RDRE which can result in a stabilized deflagration front burning the reactants before the detonative wave [10]. When discussing this secondary combustion, it is referred to as either parasitic combustion or commensal combustion depending on when it occurs. As shown in Fig. 1.5, parasitic combustion occurs before the detonation wave while commensal combustion occurs after the detonation wave.

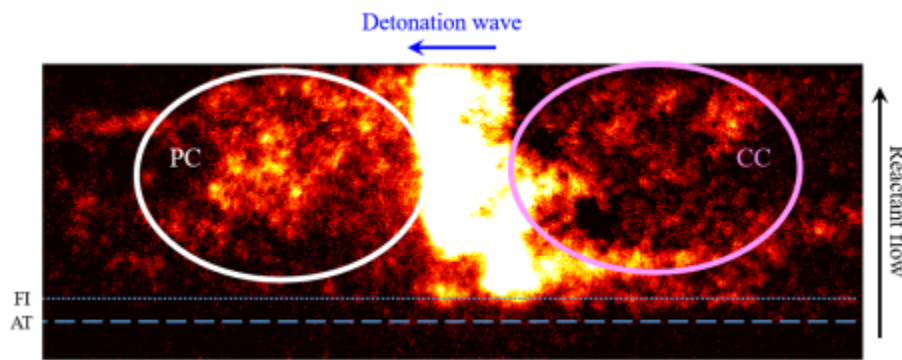


Figure 1.5 - Imaging of detonation wave with both parasitic (PC) and commensal (CC) combustion [10]

Concerning the effects imposed by each type of secondary combustion, as the names suggest, only the parasitic combustion actively hinders the detonation wave. Parasitic combustion occurs when injected reactants experience deflagration, potentially due the heat emitted by the detonation wave or residual heat from previous rotations. This, in turn, drastically inhibits the performance of the RDRE due to the reactants being consumed by the deflagration rather than helping to propagate the detonation wave which can lead to instability, decreased wave speed, and a lower CJ state pressure. On the other hand, commensal combustion occurs after the detonation wave and doesn't cause any direct loss to the detonation and merely represents deflagration occurring as a consequence of reactant or heat leaking from the detonation wavelet.

When parasitic combustion occurs within the annulus, two major consequences occur which can drastically inhibit the efficiency of the RDRE [10]. The first effect is heat being released prior to the detonation wave which, in turn, doesn't contribute to sustaining the detonation wave. The second effect concerns the composition of the mixture as the ignition will create intermediate and products species of the reactants as well as increasing the temperature which may lead to a dramatic change in the detonation wavelet. While commensal combustion does not directly impair the detonation wave, its existence points to a non-ideal behavior. In a perfect world, all

reactants that reach the detonation wave would react within the bounds of said detonation wave, releasing all available energy at the highest point of the system. The existence of commensal combustion implies that a form of leakage is occurring, either heat release or mixture. The former is a proposed mechanic which would theoretically occur when chemical reactions do not react fully in the detonation wave due to the detonation wave being a broad region and not an infinitesimally thin zone typically conceptualized. The latter is another hypothesized explanation where some reactants move through the entire detonation wave without reacting, potentially due to stratification or distortion in the wave front. This distortion typically results due to a combination of effects such as

- the density difference between the OF mixture and the background gas,
- lack of fuel sustaining the detonation further from the injector,

which results in both a separation of shock front and reaction front as well as a speed gradient occurring from the point nearest to the injectors to the upper bound as shown in Fig. 1.6 [11]. Given that both forms of secondary combustion can severely inhibit RDRE performance with some studies saying that, in some cases, nearly 50% of all heat release comes from secondary combustion versus the detonation wave, finding methods to reduce this phenomenon can dramatically boost the performance on built/simulated RDREs.

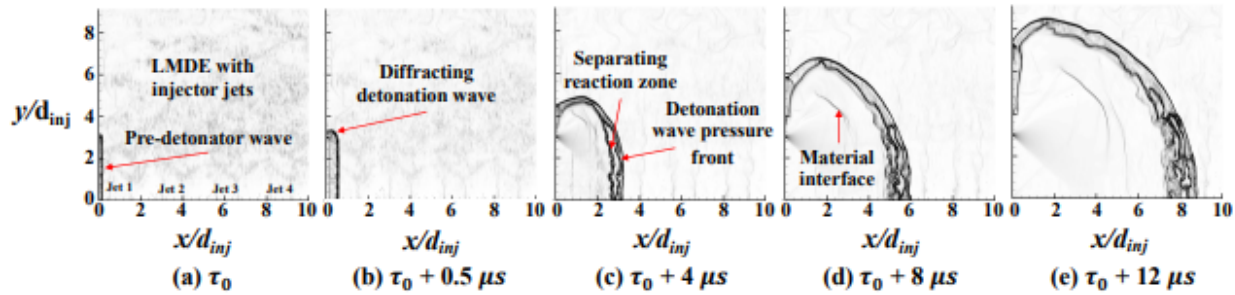


Figure 1.6 Schlieren imaging of a detonation wave moving through a linearized rotating detonation engine [11]

1.2.2.3 Wall Curvature

While not a major contributor such as secondary combustion and stratification, the curvature of the annulus does play a role in understanding potential flaws in RDREs. Due to the racetrack-esque design of the annulus, the detonation wave will experience a degree of flow turning. This flow turning, in turn, leads to the creation of an azimuthal wake shock system forming which affects the flow of the OF mixture during injection recovery [12]. To elaborate, injection recovery is the process where the injectors regain the means to inject new fuel. However, the high-pressure backflow of a shockwave can inhibit the injection recovery process by flowing into the plenum of the injector, making it difficult to reestablish the target pressure necessary to inject more reactants as shown in Fig 1.7 [13]. The presence of these azimuthal shocks can penetrate the injectors, raising local static temperature and pressure which causes

flow losses. As for combating this issue, new designs for the injectors will be necessary to prevent the backflow from drastically interfering with the injectors; certain studies found that decreasing the fuel injector diameter can result in significantly higher CJ velocities.

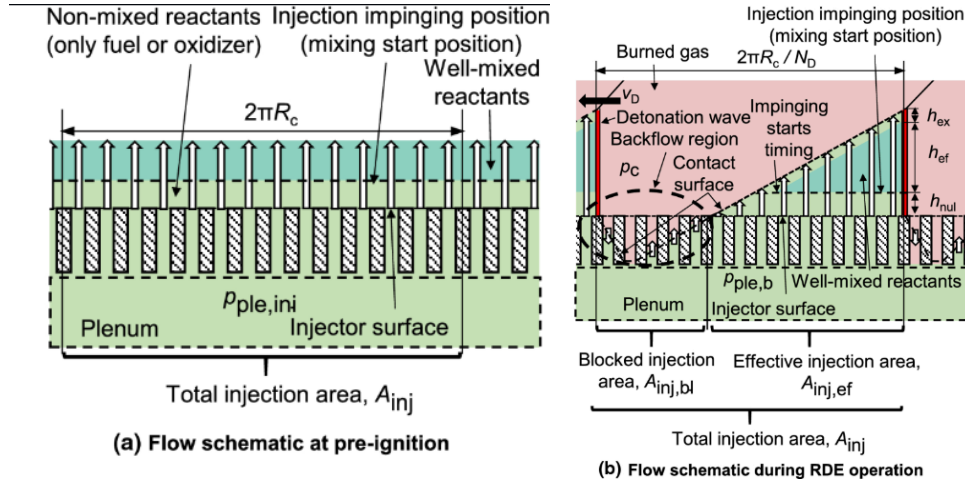


Figure 1.7 - (a) The schematic of the RDRE injectors before the presence of a detonation wave.
(b) The schematic of the injectors during operation [13].

1.2.3 Recent Experimentation on RDREs

With the popularity of RDREs on the rise, many nations and organizations have begun researching and testing potential combinations. These tests were similar to each other in many ways but the major difference between each falls into one of three categories:

- engine type,
- geometry,
- propellant [14].

For rotating detonation engines, there exists two major archetypes: rocket and air-breathing. The difference between the two is that the latter takes oxidizer from the environment for its combustion while the latter requires dedicated oxidizer to operate; for this paper's purpose, the focus will be solely on the rocket engine type. The geometry is another point of difference as while many tests utilize annular geometry or some variation, other tests have disk, hollow, or cone designs. Similar to the engine type, the focus will be on annular geometry. The final category, the propellant, had the most variety from test-to-test as many tests utilized different oxidizers and fuels. The choices made by previous experiments typically utilized the same few fuels and oxidizers but some variety existed, the most common of which are listed in table 1.1.

Table 1.1 - Fuels and oxidizers utilized in RDRE tests [14]

Fuel	Oxidizer
$H_2(l/g)$	$O_2(l/g)$
H_2O_2	N_2O
RP-1	Air
C_2H_4	- - - - -
GCH_4	- - - - -

When it comes to choosing an oxidizer, many organizations opt for the three major choices listed above whereas the fuel has a much larger variety, some of which are used in combination with other fuels such as kerosene. It is for this reason that this paper will focus on testing different combinations of fuels and oxidizers to measure performance while also considering potential drawbacks such as toxicity and cryogenic storage.

1.3 Project Objective

The objective of this project is to launch an investigation into potential OF mixtures for RDRE to determine potentially optimal combinations and ratios to maximize thrust while minimizing negative characteristics. A second objective is to perform research on how rotating detonation rocket engines operate, different types of oxidizers and fuels concerning both the positives and negatives of each choice, and how to properly conduct a trade study. For example, a particular oxidizer-fuel combination may output the highest amount of thrust but potential drawbacks such as the toxicity of the materials and a more complicated pumping system may limit the usefulness of the combination, warranting another OF mixture choice. The goal is to simulate multiple different oxidizer-fuel combinations and ratios moving through a detonation wave, recording the resulting airflow characteristics such as pressure and temperature, and investigate which potential combination can both perform well and help simplify the design process due to lack of complications.

1.4 Methodology

For this project, the first step will be to gather information from relevant sources on both facets of this project: RDREs and how they operate as well as OF combinations and properties such as toxicity and ease of manufacturing. With this data, any necessary calculations will be done to either help verify the authenticity of the future results or expedite the results by preemptively removing unfit OF combinations and mixtures. From here, a combination of NASA's CEARUN and MATLAB's combustion toolbox will be utilized to run several simulations of OF mixtures moving through a detonation wave, altering both the ratio of oxidizer to fuel as well as the combination of the two to test a large range of scenarios. The main purpose is to gather a large sample of data to perform a case study to help determine which OF mixture and ratio is optimal whilst considering the physical restrictions such as the toxicity of the material and potential complexity of the system.

Chapter 2: RDRE Design

The purpose of this chapter is on the design of critical RDRE components, focusing on the design and functionality. The goal is to both better understand the mechanisms behind an RDREs success as well as formulate a baseline for CAD modeling and CFD simulations. These designs will be constructed using Solidworks and will cover particular components in more detail than in previous chapters.

2.1 Annulus

The first major component to examine is the annular combustion chamber. It is here that the oxidizer and fuel typically meet, combine, then react with the detonation wave. The geometry and design play a paramount role in the engine's efficiency as flaws such as a large inner radius can lead to instabilities in the detonation wave.

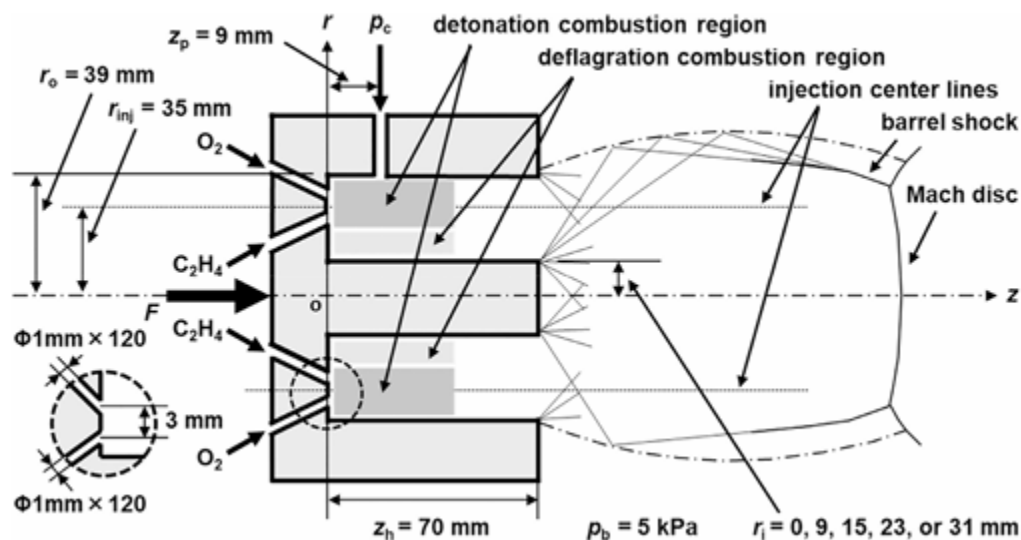


Figure 2.1 - Cross section of a traditional RDRE [6].

While a schematic diagram above shows what a typical RDRE might look like, utilizing two separate injectors for oxidizer and fuel each, an opening for a detonation wave to be incited, and the annular walls. To better illustrate the design, a CAD utilizing measurements similar to the schematic above was created to provide a 3-D model of an annulus.

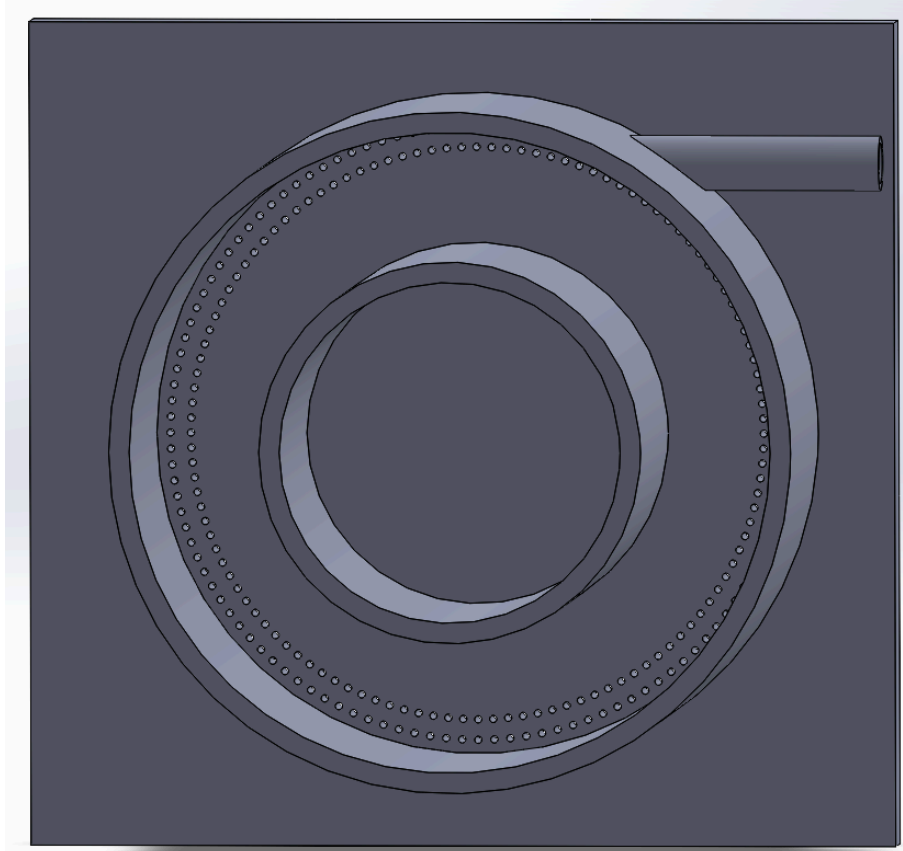


Figure 2.2 - CAD model for RDRE annulus

The design of the annulus has three major facets to focus on:

- the concentric circles,
- the holes,
- and the piping.

The concentric circles are the inner and outer circles which are meant to contain the detonation wave in a circular path while attempting to prevent the wave from being attached to the inner circle. As mentioned above, having the detonation wave attached to the inner radius can cause problems such as acoustic and vibrational complications and additional heating to the inner circle in addition to the innate complications of a detonation wave. Hence, the inner radius is specifically designed such that it balances efficiency with stability. This does propose an interesting conundrum with upscaling the RDRE. The schematic the CAD design was based on was specified millimeters while traditional rockets are on the scale of meters. If the design were to be upscaled to meters, the theory starts to change as different facets begin to play more major roles. A study from the University of Washington examining different sized RDREs utilizing identical parameters supports this as it was determined that mass flux plays a more major role than the geometry when upscaled [15]. This isn't to say that the geometry plays no role but more that having the optimal mass flux will be more beneficial for stabilizing the detonation wave in larger RDREs than in smaller ones.

The holes aligning near the outside circle represent the injectors in which oxidizer and fuel are pumped into the annulus. The particular design above has two rows of holes as it is designed to pump oxidizer and fuel individually into the annulus. To dive into more specifics, there are three approaches to supplying reactant to the RDRE:

- locally mixed reactant,
- premixed reactant,
- and air-breathing.

The last approach, air-breathing, is for engines designed to stay within the atmosphere where the air can act as an oxidizer. Typically these designs have holes near the front of the plane in which air can flow through the internals until it reaches the engine. Given that the focus of this paper concerns rockets which deal with the vacuum of space, air-breathing designs will be left alone. As for the local versus premixed reactants, there exists both pros and cons for both designs.

2.1.1 Premixing Versus Local Mixing

One of the biggest conundrums of rocket fuel is the issue of stratification. As mentioned previously, insufficient mixing of fuel and oxidizer can create fuel-rich and fuel-lean zones which negatively affect the efficiency of the combustion. As a result, proper precautions and design choices are necessary to combat reactant stratification. There are two major ways to mix oxidizer and fuel together: local and premixed. A locally mixed process is typically found for liquid rockets as it entails using injectors to pump fuel and oxidizer separately into the combustion chamber. These injectors are designed to operate at high velocities as is necessary for the fuel and oxidizer to collide at high speeds to properly atomize and mix [16]. However, not every type of injector relies on high-speed collisions to perform localized mixing as some injectors use concentric tubes, splash plates, axial slots, etc. However, for RDREs, it is standard to utilize doublets which operate as explained above: shooting two high speed beams of oxidizer and fuel together; an example of how a doublet injector system works is shown below. Premixing is a process where the fuel and oxidizer are mixed together before entering the combustion chamber. This is traditionally done with solid fuel rockets but the process, in essence, holds up for liquid fuels as well.

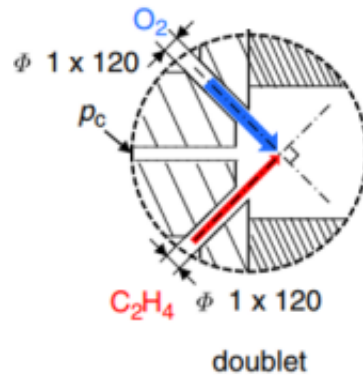


Figure 2.3 - Example of a doublet injection system [17]

When comparing premixed to locally mixed OF mixtures, there is a marked improvement in reducing the stratification of the reaction mixture. However, premixed reactants do have some major complications to contend with before it can be employed in rocket engines. The first issue has to do with the chemistry of the oxidizer and fuel itself. There are a great number of different oxidizers and fuels that agencies use for chemical propulsion. Some of these choices are much harder to handle than others as some are corrosive while others need to be stored cryogenically. Attempting to mix two incompatible reactants can result in ineffective and often more dangerous mixtures than if they were stored separately which drastically reduces the number of viable OF mixtures. This, however, is the least concerning issue with premixing oxidizer and fuel. Unlike solid reactants, combined liquid reactants are far less stable and can easily combust prematurely. By attempting to mix liquid oxidizer and fuel together before the combustion chamber, it creates several more points of failure which will result in catastrophic failure. This alone acts as a deterrent for premixing oxidizers and fuels as the engine is already a complex mechanical system and introducing a premixed OF mixture would further complicate the design. Premixing is not entirely out of the question as it is theoretically possible to engineer a system which focuses on minimizing the potential of a premature and catastrophic combustion but the current technology and practices are unable to design such a system; should a new approach be discovered, premixing may become a potential approach but locally mixing is sufficient for RDREs.

2.1.2 Deflagration-To-Detonation Versus Chemical Incitation

When referencing back to the CAD model, the last major component to discuss is the pipe sticking into the annulus. For RDREs, this is the predetonator which is utilized to initiate the detonation wave; it can be more specifically referred to as the initiation tube. For this type of engine, there exists three different methods of inciting a detonation wave, all of which are shown in the figure below: wall/channel mounted, initiation tube, and timed swirl injections [1].



Figure 2.4 - Three different versions of RDRE detonation initiations. Diaphragm, initiation, and swirl are labeled D, I, and S respectively.

Each of these versions are capable of creating detonation waves with varying success rates with the wall/channel mounted source being the least effective of the three. When comparing the two more effective methods, i.e. the tube and swirl approaches, both have their pros and cons. The tube is the most straightforward of the two approaches but requires specific planning to prevent a second detonation wave forming in the opposite direction than intended. This can be countered by either a diaphragm or ensuring the detonation wave forms within the tube such that, at most, only a weaker reflective shock is formed. Ideally, a diaphragm is not utilized as it complicates restarting the RDRE should the detonation wave dissipate. The swirl design used properly timed reactant injections and spark plugs to incite a detonation wave. Why this design is more complicated than an initiation tube, it can be utilized in scenarios where the alternative is ineffective for any reason.

To incite a detonation wave, there are two main approaches: direct initiation and deflagration-to-detonation [18]. Direct initiation, as the name suggests, creates a detonation wave by releasing a significant amount of energy into a small region containing a combustible gas mixture. If the initiation creates enough energy, the resulting detonation front will climb down towards the CJ detonation propagation velocity. While a potential option, direct initial has two major issues. The first drawback of utilizing direct initiation is how it requires an amount of energy several magnitudes higher than lighting a flame. In addition, the reaction needs to be carefully calibrated as having a massive reaction can cause a catastrophic failure while having too small of a reaction will cause the reaction zone to decouple from the shock front over time. The alternative approach, DTD, works by creating a low energy flame which will be accelerated to the point where miniature explosions of reactants, or hot spots, begin to form which further accelerate the flame until a detonation wave forms in its entirety. Due to the reactants reaching a critical ignition point, the hot spots are characterized as high temperature, high pressure. These hot spots are paramount as their presence allows for the deflagration front to accelerate towards detonation faster. There also exists the added benefit that, due to the fact that self-propagating deflagrations are unstable, the system will nature accelerate towards the CJ detonation velocity; in combination with hot spots, DTD is capable of creating detonation waves while requiring far less energy, making it the ideal choice over a direct initiation [19].

2.2 Injectors

The second major component to discuss is the injectors. While the injectors do not play a direct role in the same manner as the combustion chamber, it is paramount that sufficient research is performed as certain injector configurations may restrict either the effectiveness of the engine or potential fuel and oxidizer choices. The goal is to research different types of injectors, which work best in an RDRE, and any potential imposed restraints. While not extensively researched like other topics of propulsion, there still exists several articles and research papers discussing the intricacies of potential RDRE injectors, focusing on topics such as the spacing scheme as well as different comparisons between topics such as axial slot versus sting, double versus triple pinging, axial versus radial, etc.

2.2.1 Injector Element Scheme

When discussing the injector element scheme whilst taking into account topics previously discussed, it is safe to assume that a more dense scheme would result in a more effective rocket. However, it is still beneficial to analyze different configurations to confirm the assumption. A paper co-headed by the Air Force Research Laboratory was published to specifically tackle this issue by performing hot tests of an RDRE with varying element schemes at a range of different equivalence ratios and mass flow rates [20].

The aforementioned paper experimented with three different injector schemes with conditions ranging from an equivalence ratio between 0.5 and 2.0 as well as different mass flow rates at set equivalence ratios with the flow rate ranging from 0.2 to 1.25 lbm/s [20]. As for the configurations themselves, the three that were utilized are shown below.

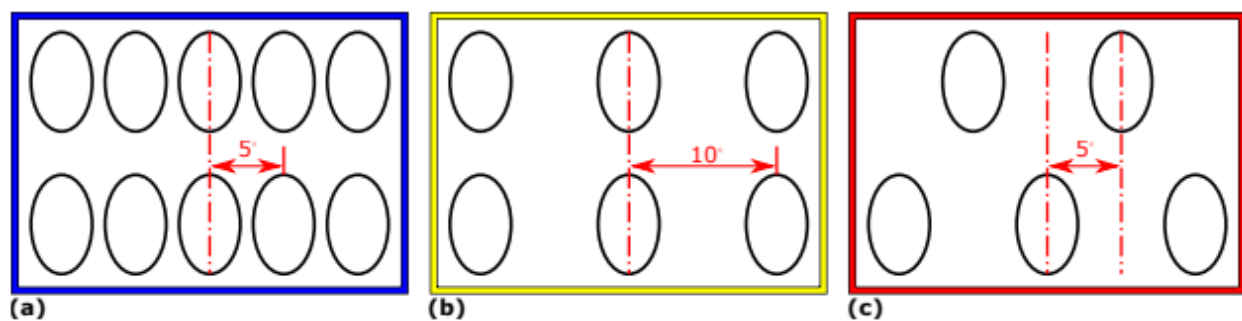


Figure 2.5 - Designs of impinging injector schemes with designs (a) 5 degrees apart, (b) 10 degrees apart, (c) and 5 degrees but misaligned [20]

To further elaborate, the reason why the third design is present is to demonstrate how poor mixing affects engine performance and wave stability. The same can be said for design B as the injector area is doubled in order to maintain the same injection area as design A.

After performing several hot-fire tests, the researchers were able to determine the thrust and specific impulse for all three configurations at different equivalence ratios and mass flow rates, all of which are combined in the following graphs.

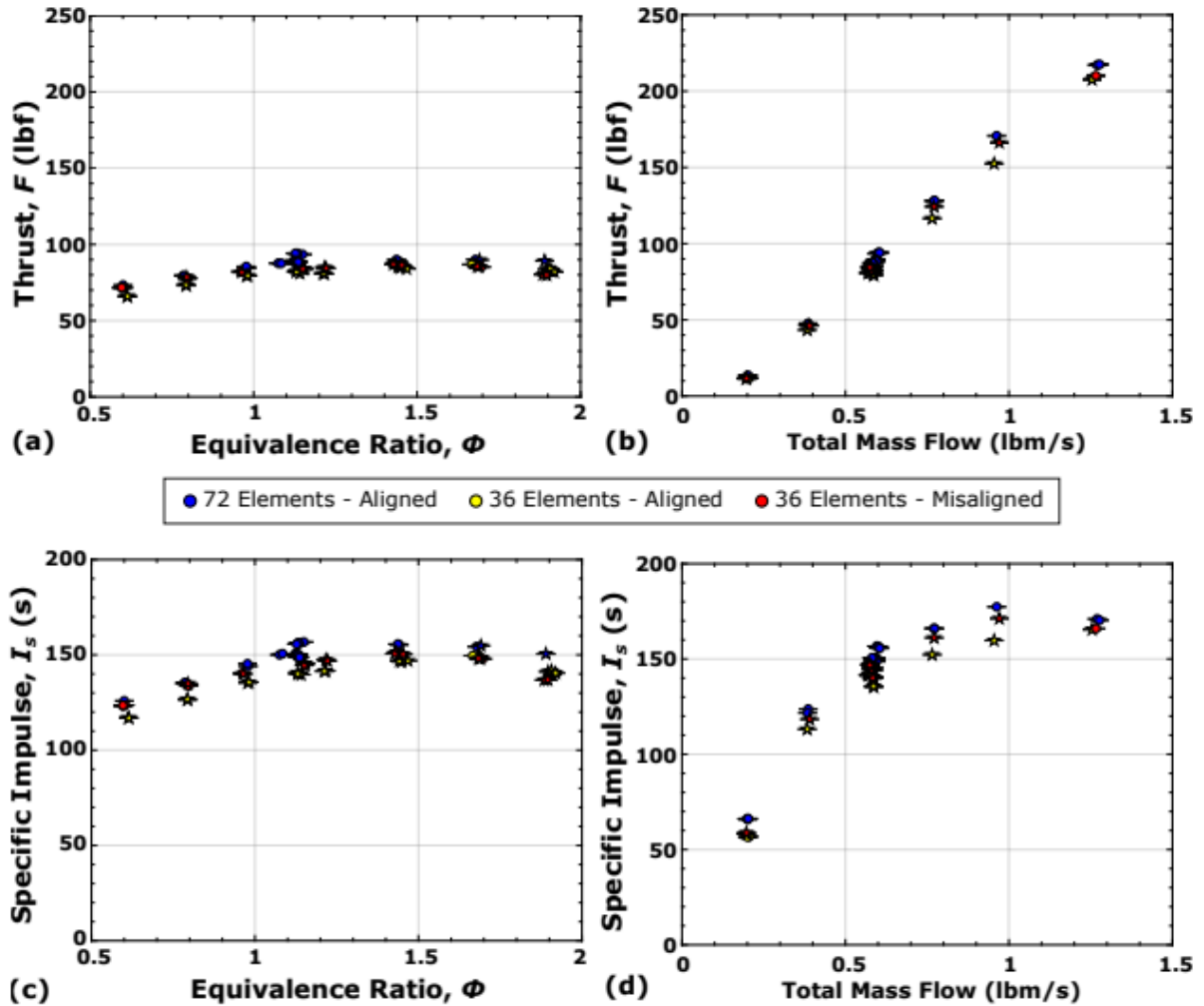


Figure 2.6 - Performances graphs with thrust and specific impulse as functions of equivalence ratio and total mass flow rate [20]

When analyzing Fig. 2.5, a few observations can be made. For starters, it can be seen that increasing the mass flow rate, in general, will produce higher results. However, the equivalence ratio partially follows the same trend but flatlines above a ratio 1 and even begins to decline at ratios above 1.75. Now, when analyzing which configuration produces the best results, it is clear that the 72-injector configuration performs the best while the 36-injector systems, both aligned and not, performed relatively similarly. While it is quite clear that poor mixing, resulting from both 36-injector systems, lowered the rocket's efficiency by 4.5-9.9% depending on the controls,

both injector schemes performed similarly. This lends credibility to the notion that further degradation of the mixing of the oxidizer and fuel may not further decrease performance [20].

While the above study utilizes a doublet injector scheme, there is research proposing the idea of utilizing a triplet injector scheme with two side fuel injectors and one central oxidizer injector as shown below.

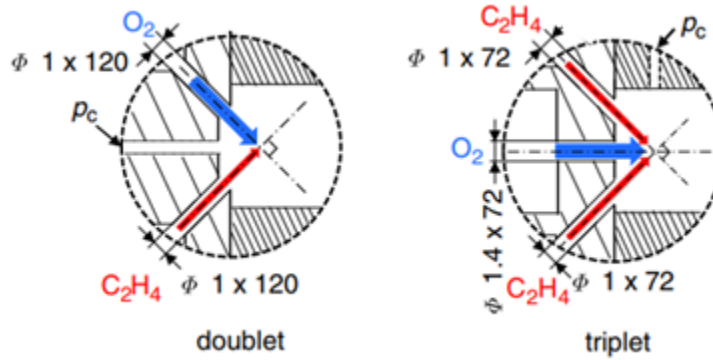


Figure 2.7 - Example of doublet and triplet injector schemes [17]

A study from Japan compared doublet and triplet injector schemes against each other, using a simple slot injector as a control. In addition, three different throat geometries were utilized: a throatless design and two others with area ratios of 2.5 and 8 respectively.

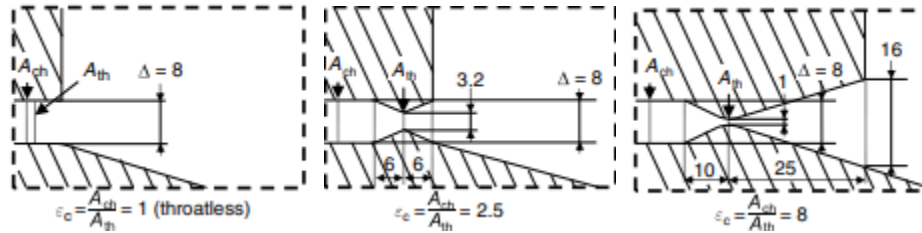


Figure 2.8 - Experimental overview of RDE throat geometries [21]

After testing each configuration, researchers determined two things. Firstly, unsurprisingly, the slot injector performed worse than both the doublet and triplet schemes as well as utilizing a convergence-divergence throat constriction performed higher than a throatless design. As a result, it is safe to imply that throat inclusion will benefit traditional RDRE designs. Secondly, and more shockingly, the characteristic velocity of the doublet and triplet schemes were nearly identical across all tests [21]. However, the benefit of the triplet design was shown after the test and the combustor wall was investigated. It was found that after the doublet tests, the walls of the chamber were found to be damaged while the triplet injectors caused little to no damage.

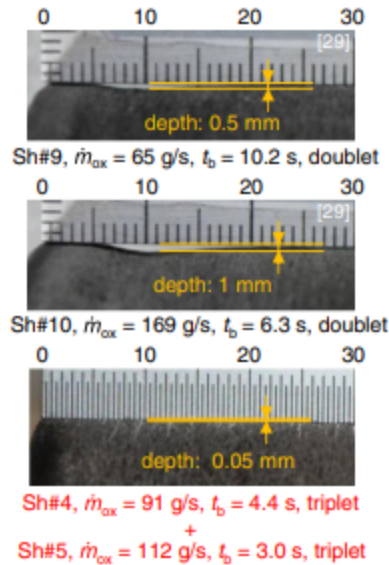


Figure 2.9 - Comparison of combustor wall damage after doublet and triplet experiments [21]

As shown above, the doublet tests caused a divot to form in the carbon-carbon composite walls of the combustion chamber, getting more and more pronounced with higher mass flow rates. Researchers explained this phenomenon using the following schematic.

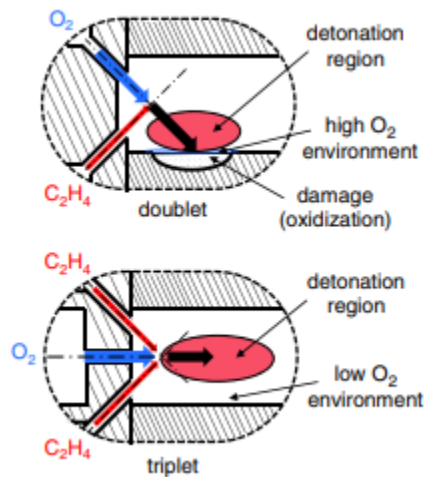


Figure 2.10 - Schematic of resulting detonations from doublet and triplet injectors [21]

Due to the high momentum of the oxygen in the doublet scheme, the detonation region was pushed towards the combustor walls. Funnily enough, it was not the detonation itself that damaged the walls but instead was the excess oxygen and the resulting oxidization that caused the damage. It additionally explains why the triplet injectors did not cause nearly as much damage as the design propels the oxidizer parallel to the walls with the fuel fired from an angle. As a result, the detonation region is centralized in the combustion chamber, creating low oxygen

zones around the walls which minimizes damages. Given that doublet and triplet injectors perform similarly in terms of Isp and thrust, it is safe to assume that a triplet design is better for the longevity of an RDRE.

2.2.2 Injector Type

This section will quickly comment on different types of injectors and their comparative effectiveness. Firstly, there are two major delineations for injectors: axial versus radial and axial versus sting. While there is little information about the use of axial feed injection for RDREs, there have been studies comparing the two. One study compared the corrected thrust obtained from similar chambers using radial and axial injectors, examples of both found below [22].

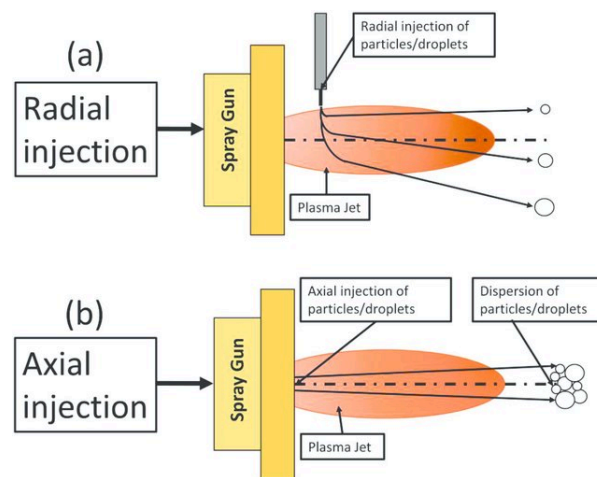


Figure 2.11 - Examples of radial and axial injectors [22]

When testing the two configurations, it was found that there was a 15% increase in corrected thrust when switching from radial to axial injection [23]. This can potentially be explained using conservation of momentum as, unlike the radial version, the axial injection provides momentum down the chamber and out the rocket.

The secondary comparison to make will be between sting versus axial injectors. As mentioned above, axial is more effective than radial but it is still important to compare all possible options rather than settle on the first option that works.

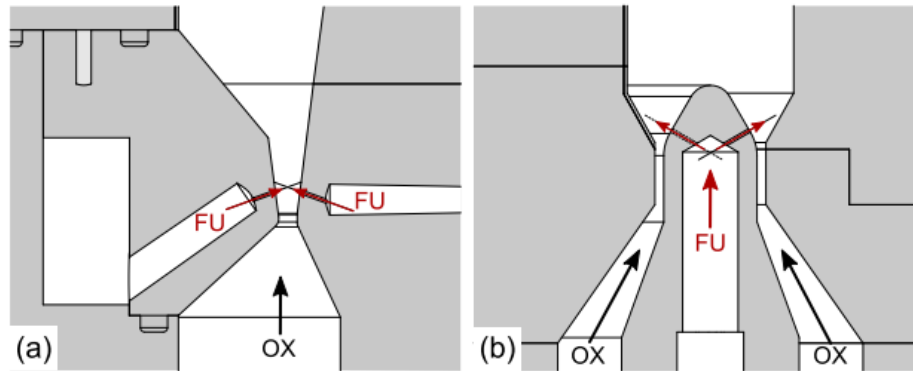


Figure 2.12 - Schematics for (a) axial injectors and (b) sting injectors [24]

The primary difference of sting injectors is how they utilize a singular tube for fuel that shoots out in different directions to react with the oxidizer. Research has been performed to compare the two injection methods in terms of desirable values such as chamber pressure, inlet temperature, wave velocity, etc. [24]. What researchers have found is quite unique: while there existed a one-to-one relationship between the produced thrust and characteristic velocity with the sting injector, the axial injectors had a similar level of efficiency across all tests. It was concluded that axial injectors offer a greater baseline than sting injectors while sting injectors allow for a higher level of efficiency at correct conditions. However, it has yet to be determined what aspect of the design creates this difference; more research is needed.

CHAPTER 3: THEORY AND EQUATIONS

This section will focus on the governing equations and theories that describe the detonation combustion and the resulting fluid flow moving throughout the annulus. As the reactants move into the detonation wave, the resulting reaction is twofold: a combustion process and a dissociation process. The combustion process involves the detonation of reactants into their respective products. However, as mentioned above, there exists commensal combustion which results in dissociation. As a result, after fuel and oxidizer reach the combustion chamber, there will be unreacted reactants, combustion products, and dissociation products.

3.1 Governing Equations

Before discussing any theory, it is paramount to discuss the fundamental equations that several theories are based upon. The first three equations are the conservation equations as many later equations start with manipulating these three. These equations are the conservation of mass, momentum, and energy listed as 3.1-3 respectively.

$$\rho_1 A_1 u_1 = \rho_2 A_2 u_2 \quad (3.1)$$

$$P_1 + \rho_1 u_1^2 = P_2 + \rho_2 u_2^2 \quad (3.2)$$

$$h_1 + \frac{u_1^2}{2} = h_2 + \frac{u_2^2}{2} \quad (3.3)$$

While there exists small addendums for these equations, such as canceling out the areas in Eq.

3.1 in certain scenarios, these equations remain as the fundamental starting point for many other equations as well as being the fundamental equations for the CJ theory.

3.2 Detonation Theory

Before discussing either the governing equations of motion or the detonation reaction itself, it is paramount to review the theories behind detonation and its effectiveness. The study of detonation has many subsections but two of the largest are Chapman-Jouguet theory and ZND theory. Chapman-Jouguet, as mentioned previously, focuses on steady state detonation waves and its propagation. ZND theory, named after its creators, Yakov Zeldovich, John von Neumann, and Werner Döring, provides a one-dimensional model for detonation. It should also be mentioned that gaseous detonations are typically created as unsteady, three-dimensional phenomena which can still be accurately described by ZND theory; for more accurate results, including Wood-Kirkwood theory can better account for realistic detonations.

Detonation, as mentioned previously, is a thermodynamic process in which a strong, supersonic wave front is created followed by a reaction front [25]. As a result, the final products will have higher temperatures, pressures, and densities than the initiation reactants, similarly to traditional deflagration. The difference between deflagration and detonation is twofold: the effectiveness of each thermodynamic cycle and the propagation speed. For propagation speed, deflagration will either create flame fronts in the order of magnitude of cm/s or m/s for laminar and turbulent flames respectively whilst detonation creates fronts with velocities in the km/s range. More importantly, deflagration and detonation have different cycles as deflagration is nearly isobaric while detonation operates using the Fickett-Jacobs cycle whose performance is similar to isochoric reactions. As a result, despite both reactions giving higher product temperatures, detonation performs much better than deflagration as shown in Fig 3.1.

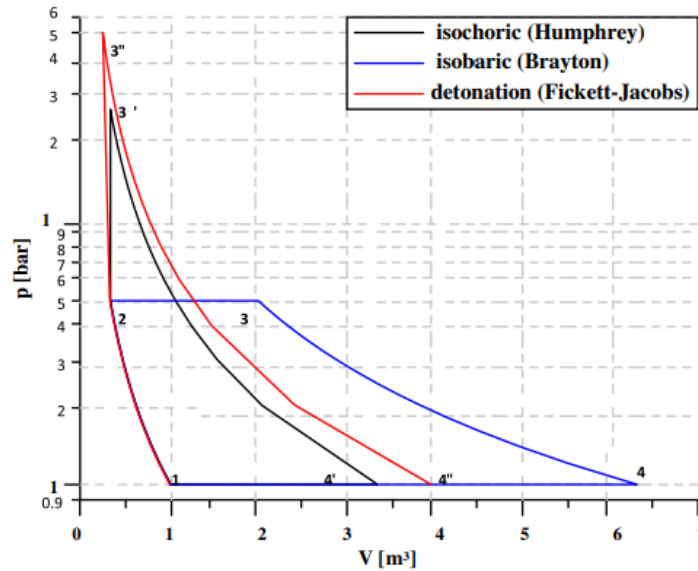


Figure 3.1 - Comparison of isochoric, isobaric, and detonation thermodynamic cycles [25]

As seen from the figure, detonation is capable of reaching higher pressures than both isochoric and isobaric. To provide an alternate approach, the efficiency of each cycle can be calculated using the following equations: for the Brayton-Joule cycle,

$$\eta = 1 - \frac{1}{\left(\frac{p_2}{p_1}\right)^{\frac{\gamma-1}{\gamma}}} \quad (3.4)$$

for the Humphrey cycle,

$$\eta = 1 - \gamma * \frac{T_1}{T_2} * \frac{\left(\frac{T_3}{T_2}\right)^{1/\gamma} - 1}{\left(\frac{T_3}{T_2}\right) - 1} \quad (3.5)$$

and for the Fickett-Jacobs cycle.

$$\eta = 1 - \gamma * \frac{1}{\left(\frac{p_2}{p_1}\right)^{\frac{\gamma-1}{\gamma}}} * \frac{\left(\frac{T_3}{T_2}\right)^{1/\gamma} - 1}{\left(\frac{T_3}{T_2}\right) - 1} \quad (3.6)$$

While not initially visible, when solved for any specific fuel, the Fickett-Jacobs cycle will achieve higher efficiencies than either isobaric and isochoric.

3.2.1 Chapman-Jouguet Theory

Chapman-Jouguet theory means to describe and model steady-state detonations and how they propagate through space. The main focus of the theory is of the reaction zone and the minimum velocity necessary to sustain a propagating detonation wave, also known as the Chapman-Jouguet condition. The CJ condition is directly tied to both the Rayleigh and Hugoniot lines as it means to describe a jump in the P-v graph.

When looking at a wave propagating through space until it reaches gas moving with a velocity u , there are two separate frames of reference: the lab frame and the wave frame as shown below [26].

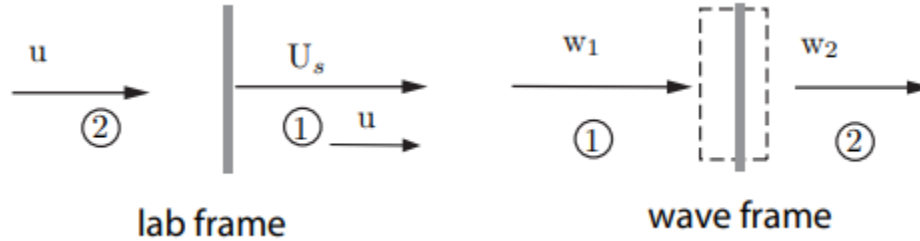


Figure 3.2 - Diagrams for two separate frames of reference for a wave propagating [26]

When looking at the wave frame, in that the wave is treated as stationary, there exists a “jump” in the velocity before and after the wave which, when solved, results in the conservation equations. With these equations, they can be transformed into the equations for the Rayleigh line and the Hugoniot curve. For the former, by combining both the mass and momentum conservation equations, the equation of the Rayleigh line emerges as

$$p_2 = p_1 - \rho^2 u_1^2 (v_2 - v_1) \quad (3.7)$$

which can further be developed into the slope of a line.

$$\frac{p_2 - p_1}{v_2 - v_1} = -\left(\frac{u_1}{v_1}\right)^2 = -\left(\frac{u_2}{v_2}\right)^2 \quad (3.8)$$

As a result, this line must pass through the initial state and final state labelled 1 and 2 respectively. For the Hugoniot curve, by eliminating the velocity post-wave, the energy equation can be written to be purely thermodynamic.

$$h_2 - h_1 = (p_2 - p_1) \frac{(v_2 + v_1)}{2} \quad (3.9)$$

From here, since enthalpy can be written as a function of pressure and volume while energy is a subsequent function of those three variables, Eq. 3.9 can be used to find all possible downstream states as shown in the Hugoniot curve in Fig 3.3.

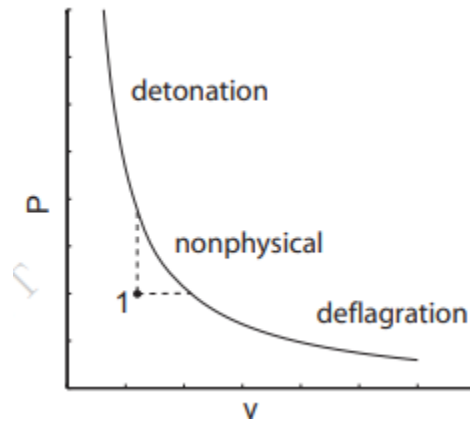


Figure 3.3 - Hugoniot curve for shock wave in a non-frozen mixture [26]

The Hugoniot curve, in combination with a Rayleigh line, displays both the detonation and deflagration regions; in reality, the dotted section depicting the nonphysical region is much larger.

When plotting the Hugoniot curve with two Rayleigh lines, the graph is split into two distinct regions. Focusing on the upper, detonation half, there exists a value known as the Chapman-Jouguet velocity which represents the minimum speed that a wave must possess in order for a solution to the jump condition to exist [26]. When a wave travels at the CJ velocity, the reactants are able to jump to equilibrium products at supersonic velocities. Should the wave travel slower, the Rayleigh line and Hugoniot curve do not intersect meaning no steady-state solution exists. However, should the wave speed be higher than the CJ velocity, there will exist two intersect points resulting in two solutions, referred to as the strong and weak solutions. As for the other point, CV represents the final pressure of a constant state explosion such as a detonation wave.

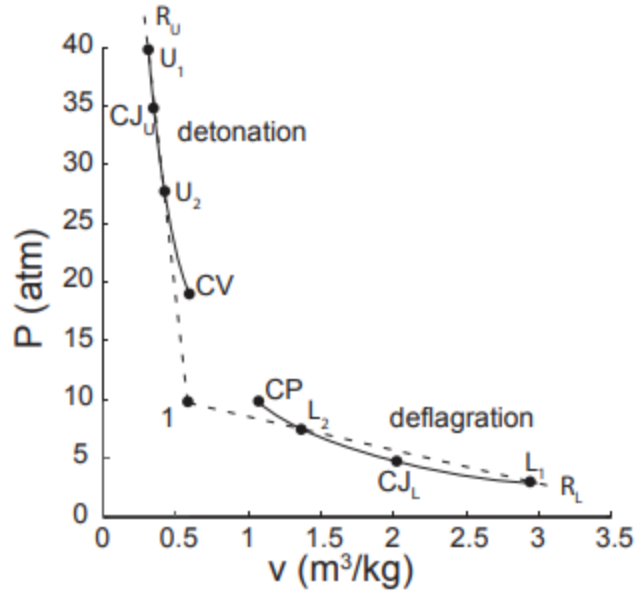


Figure 3.4 - PV diagram depicting Hugoniot curve and two Rayleigh lines for hydrogen-air mixture [26]

When analyzing Fig 3.4, it is evident that the CJ velocity exists where the Rayleigh line and Hugoniot curve are tangential to one another. As a result, this point exists as the solution for what is referred to as the CJ state in which the entropy is at an extreme value. It is possible to prove this mathematically by differentiating the energy version of Eq. 3.9 and combining it with the fundamental equation of thermodynamics to obtain.

$$T \frac{\partial s}{\partial v} \Big|_H = -\frac{\Delta v}{2} \left[\frac{\partial p}{\partial v} \Big|_H - \frac{\Delta p}{\Delta v} \right] \quad (3.10)$$

When solving Eq. 3.10 at several different volumes, it shows that the derivative of entropy with respect to volume is negative when $v < v_{CJ}$, positive when $v > v_{CJ}$, and equal to zero when $v = v_{CJ}$; when derivative twice, the change in entropy is positive at the CJ point, proving that the entropy is a local minimum. When analyzing the slope of the isentrope, it leads to the following equation,

$$\frac{\Delta p}{\Delta v} = -\left(\frac{u_2}{v_2}\right)^2 = \frac{\partial p}{\partial v} \Big|_s = -\left(\frac{a_2}{v_2}\right)^2 \quad (3.11)$$

which shows that the velocity of the products must be moving at the local speed of sound. As a result, the Chapman-Jouguet detonation velocity is reached when the subsequent flow of products is sonic in relationship to the detonation wave.

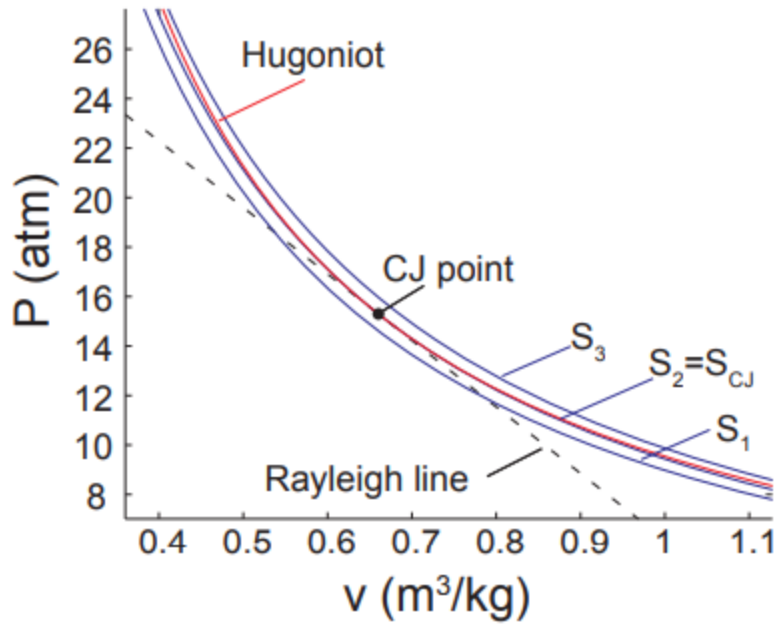


Figure 3.5 - PV diagram plotted alongside the Hugoniot curve, Rayleigh line, and three different isentropes [26]

When looking at the CJ detonation velocity, there are two methods for approximating the value. The first formula is dependent on the heat released by the detonation and is of the form [27].

$$C = \sqrt{2(\gamma^2 - 1)Q} \quad (3.12)$$

However, a better version of Eq. 3.12 exists in the form of

$$C = \sqrt{2\gamma_\infty(\gamma_\infty + 1)\frac{T_\infty R}{W_\infty}} \quad (3.13)$$

where C is more clearly shown to be dependent on the temperature and molecular weight.

The last topic to discuss in detail is the difference between several types of combustion. When looking at a schematic locus containing different burnt-gas states such as in Fig. 3.6, there exists several different types of combustion with some being more prevalent than others. While cluttered, one can separate different positions on the PV diagram and list them into a table concerning the ratio of pressures and volumes.

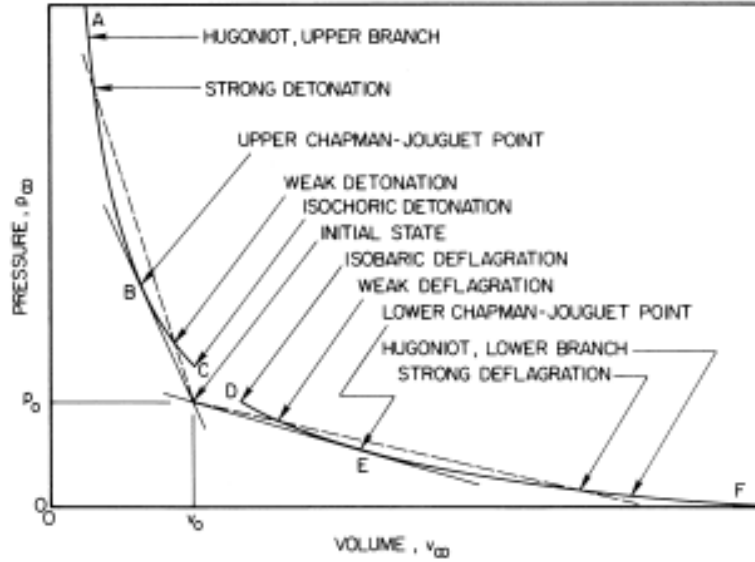


Figure 3.6 - Schematic locus listing the position of several different combustion states on a PV diagram [27]

Table 3.1 Summary of different combustion types and their aspects and relevance [27]

	Section in Fig. 3	Pressure ratio $p = (p_{\infty}/p_0)$	Volume ratio $v = (v_{\infty}/v_0)$	Propagation Mach number M_0	Burnt-gas Mach number M_{∞}	Remarks
Strong detonations	Line A-B	$p_+ < p < \infty$	$v_{\min} < v < v_+$ ($v_{\min} > 0$)	$M_{0+} < M_0 < \infty$	$M_{\infty} < 1$	Seldom observed; requires special experimental arrangement
Upper Chapman- Jouguet point	Point B	$p = p_+$ ($p_+ > 1$)	$v = v_+$ ($v_+ < 1$)	$M_0 = M_{0+}$ ($M_{0+} > 1$)	$M_{\infty} = 1$	Usually observed for waves propagating in tubes
Weak detonations	Line B-C	$p_1 < p < p_+$ ($p_1 > 1$)	$v_+ < v < 1$	$M_{0+} < M_0 < \infty$	$M_{\infty} > 1$	Seldom observed; requires very special gas mixtures
Weak deflagrations	Line D-E	$p_- < p < 1$	$v_1 < v < v_-$ ($v_1 > 1$)	$0 < M_0 < M_{0-}$	$M_{\infty} < 1$	Often observed; $p \approx 1$ in most experiments
Lower Chapman- Jouguet point	Point E	$p = p_-$ ($p_- < 1$)	$v = v_-$ ($v_- > 1$)	$M_0 = M_{0-}$ ($M_{0-} < 1$)	$M_{\infty} = 1$	Not observed
Strong deflagrations	Line E-F	$0 < p < p_-$	$v_- < v < v_{\max}$ ($v_{\max} < \infty$)	$M_{0\min} < M_0 < M_{0-}$ ($M_{0\min} > 0$)	$M_{\infty} > 1$	Not observed; forbidden by considerations of wave structure

As seen in table 3.1, when looking at the upper detonation portion, most laboratory detonations created are placed at the upper CJ point; strong detonations require specific arrangements while weak detonations are only created by particular gas mixtures. Given that many detonations will reside at the upper CJ point, this allows for the existence of RDREs as many gas mixtures will allow for propagating detonation waves to form.

3.2.1.1 Fickett-Jacobs Cycle

The Fickett-Jacobs cycle is used to describe detonations and is based upon the work of Chapman and Jouget; it should also be mentioned that this work was done independently of Zel'dovich as his ideas were not wide spread [28]. The FJ cycle is capable of determining an upper bound of mechanical work obtained from detonating a given mass of explosives. While the cycle itself utilizes the traditional piston-cylinder arrangement, it is capable of describing detonation in pulse and rotating detonation engines.

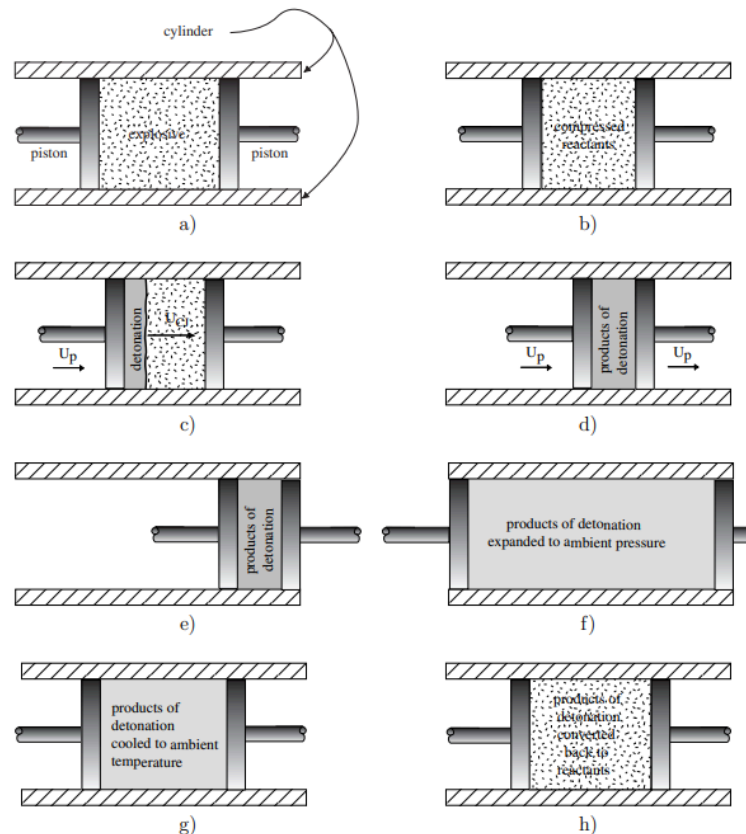


Figure 3.7 - Physical representation of the Fickett-Jacobs cycle. [28]

Fig 3.2 showing the physical process for the FJ cycle. The cycle does operate with some simplifications:

- the reactants and products are contained with the system,
- the cylinder and pistons are both rigid, massless, and adiabatic
- the explosion, pistons, and cylinders are considered a closed system,
- and the pistons can be independently moved.

As for the process itself, the system starts at initial state 1, stage a, where it is then isentropically compressed to state 2, stage b, where the work to make the piston move incites a detonation at stage c. Once the detonation is incited, it moves through the space where it will eventually reach

the second piston, resulting in the entire system moving at velocity U_p as shown in stage d. At this point, the system reaches state 3 where the energy is converted to mechanical motion in stage e where the pistons then adiabatically and reversibly bring the detonation products to state 4, stage f, which results in the products isentropically returning to their original pressure which creates state 5. From here, the system works to return to state one by cooling the products to the original temperature and composition, moving to state 6 or stage h.

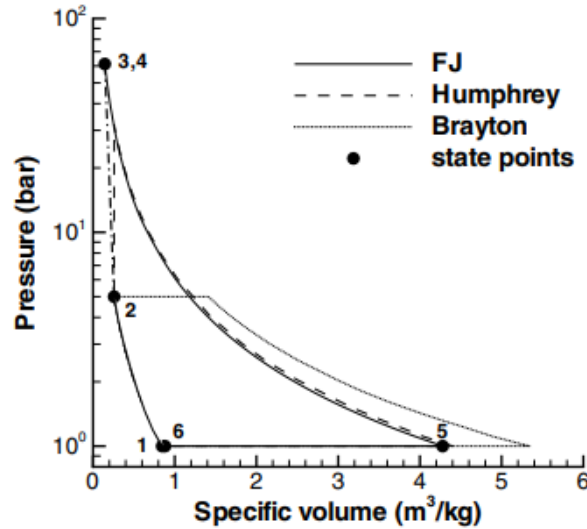


Figure 3.8 - Pressure-specific volume diagram showing the state points of the Fickett-Jacobs cycle [28]

When looking at the pressure-specific volume diagram, there are two points to discuss. Firstly, despite state 1 and 6 in Fig 3.3 occupying the same space, they both have distinct volumes and chemical compositions. Secondly, there exists a dotted line between state 2 and 3 as there is no thermodynamic path between these points as it is here where the detonation is incited; the dotted line is included simply to complete the shape. Despite the detonation causing the system to be temporarily non-uniform, the system is spatially uniform at the beginning and the end [28].

3.2.2 ZND Model

The ZND detonation model was proposed by Yakov Zeldovich, John von Neumann, and Werner Döring independently of one another during World War II and it serves as a means to expand on CJ's theory [29]. The Chapman-Jouguet theory idealizes detonation as a mathematical discontinuity with steady propagation as shown by the gap in Fig. 3.4 [30]. As such, the reaction zone is not included and therefore does not require fluid mechanics and rather just relies on the conservation equations.

The ZND model aims to refine the CJ model by including two new assumptions: the conservation equations still hold true and the heat released from the detonation will be treated as a single forward exothermic rate process rather than an instantaneous heat release [30]. As a result, a steady planar solution to both the shock jump and fluid flow can exist. With the ZND model, the detonation is modeled as a steady reaction zone and flow zone where the former is the typical CJ state and the latter is the ZND reaction zone.

The two zones work together to create a detonation. The initial shockwave will compress the reactants to a high-pressure state even higher than the CJ point referred to as the von Numman spike [30]. At the von Numman spike point, the reactants have yet to actually explode and react. Once the fluid passes the shockwave, it reaches the fluid zone where the gas reacts, explodes, and expands outwards, dropping the pressure until it reaches equilibrium at the CJ point. This adds unto the typical Rayleigh and Hugoniot curve seen with CJ theory as seen in Fig. 3.9

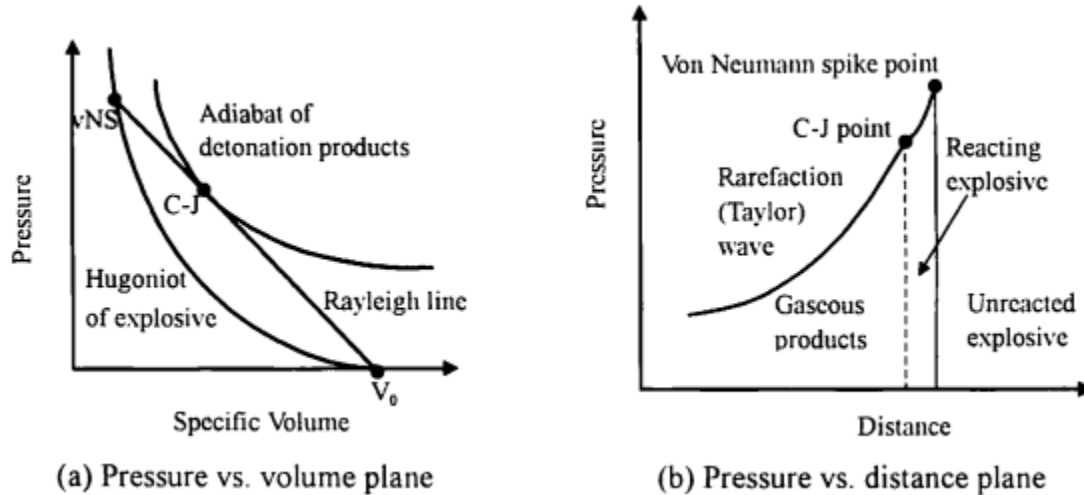


Figure 3.9 PV and PD diagrams for detonations using the ZND model [30]

In addition to the traditional CJ design, the curve extends to show the pressure after the shockwave and how it drops down to the CJ state. This redesigns the CJ state less of a “sweet spot” but more along the lines of the natural state for detonation waves to embody.

However, when considering the ZND model, there exists a possibility that the pressure surpasses even the von Neumann spike. In scenarios where the shock wave’s strength is larger than typical detonations, and overdriven detonation can take place [30]. Here, a detonation is incited in addition to the initial shockwave and detonation. This pushes the pressure farther than the von Neumann state and causes it to settle at equilibrium above the CJ point.

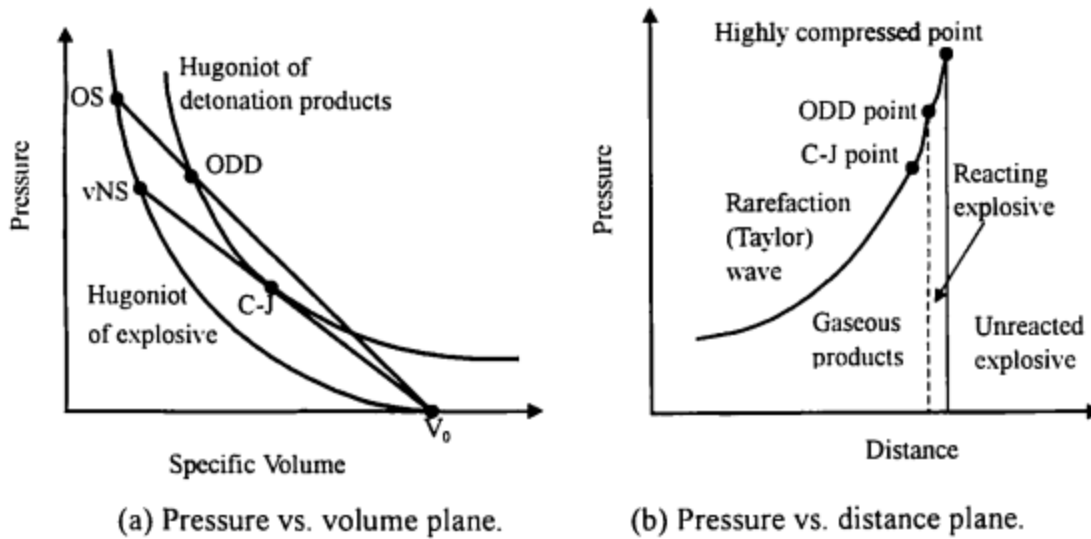


Figure 3.10 - PV and PD graphs of overdriven detonation [30]

While this may seem satisfactory for practical applications given that the pressure is higher than typical detonations in the ZND model, overdriven detonations have one glaring problem. In both the CJ and ZND model, the propagation can be considered to be steady but when a detonation becomes overdriven, the wave becomes unsteady. This comes as a result of the speed of sound being faster than the speed of the wave, meaning any disturbances in the flow field are capable of reaching and interfering with the detonation wave.

3.3 Combustion and Detonation Reactions

When considering what occurs inside the combustion chamber of an RDRE, two major reactions are taking place. The first and most obvious reaction is the detonation of the OF mixture. The second reaction is the result of the commensal combustion which causes dissociation of the mixture. These two effects compose the chemical process within the annulus of an RDRE.

3.3.1 Detonation

When comparing gaseous detonation to detonation propagating through liquids, there exist many logical pitfalls one could fall into: one may assume that a detonation cannot propagate due to the the liquid being unable to react quickly enough or believe that droplets of a certain size are too large for stable detonation waves [31]. However, when a shockwave interacts with fuel droplets, they begin to break up and separate from their parent drops. As seen in Fig. 3.11, after the shockwave passes through droplets, they begin to trail and split into smaller sizes

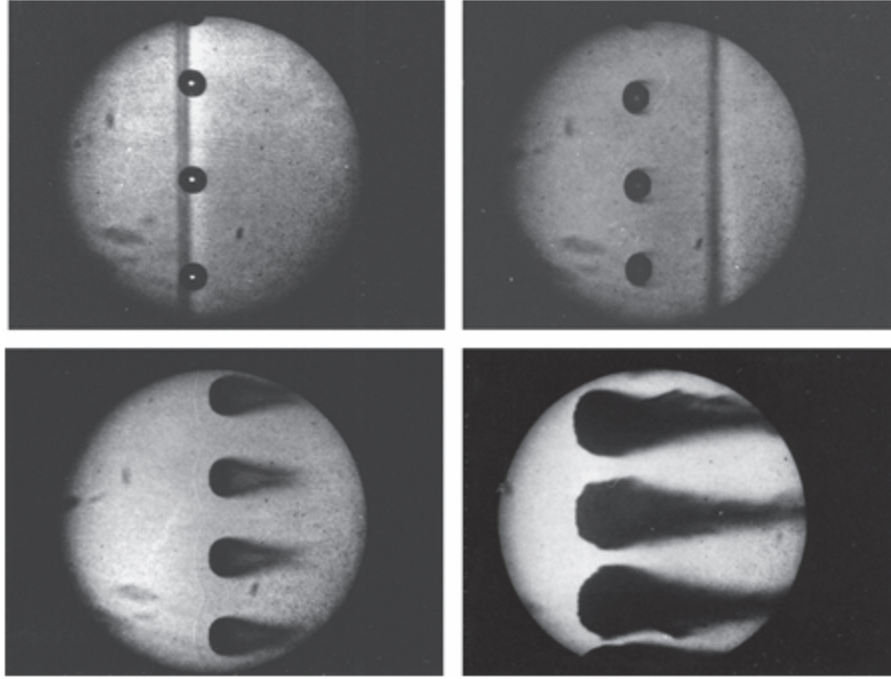


Figure 3.11 - Progression of droplets reacting to a detonation wave starting with undisturbed droplets to just before shockwave, just after shockwave, and a few microseconds after the shockwave [31].

To prove that even large sized droplets can propagate detonations, it is important to consider two aspects: the droplet breakup time and distance [31]. These values describe how long it will take for the droplet to split from the parent and how far after the shockwave it will occur. The first step in determining the two values is with the general equation for the droplet breakup time of

$$t_b = \frac{Kd\sqrt{\rho_l}}{\sqrt{\rho_2 u_2^2/2}} \quad (3.14)$$

where K is a constant. K, in this equation, is loosely dependent on the dynamic pressure but can simply be equated to 7. With Eq. 3.14 put to the side, the next step is to determine the Mach number after the shockwave. The full derivation is in appendix A but for brevity, the equation comes from the conservation equations discussed previously and is as follows.

$$M_2^2 = \frac{(\gamma - 1)M_W^2 + 2}{2\gamma M_W^2 - (\gamma - 1)} \quad (3.15)$$

When dissecting this equation, it shows that when the mach number of the wave is greater than 1, the resulting mach number will always be less than 1. Subsequently, the values for pressure, temperature, and density can all be solved as functions of the initial state, gamma, and the mach number of the wave.

$$\frac{p_2}{p_1} = \frac{2\gamma M_W^2 - (\gamma - 1)}{\gamma + 1} \quad (3.16)$$

$$\frac{T_2}{T_1} = \frac{[2\gamma M_W^2 - (\gamma - 1)][(\gamma - 1)M_W^2 + 2]}{(\gamma - 1)M_W^2 + 2} \quad (3.17)$$

$$\frac{\rho_2}{\rho_1} = \frac{(\gamma + 1)M_W^2}{(\gamma - 1)M_W^2 + 2} \quad (3.18)$$

With the previous equations, it is now possible to recalculate the breakup time as a function of conditions post-shockwave by both converting the Mach numbers into velocities and changing the frame of reference to the laboratory versus wave fixed coordinates. By doing this, Eq. 3.14 transforms into.

$$t_b = \frac{10d}{u_2} \sqrt{\frac{\rho_l}{\rho_1}} \sqrt{\frac{\rho_1}{\rho_2}} \quad (3.19)$$

With the breakup time calculated, the non-dimensional breakup distance can be calculated using the following equation.

$$\tau_b = t_b \frac{u_W}{d} = 10 \left(\frac{\rho_l}{\rho_1} \right)^{1/2} \left(\frac{(\rho_1/\rho_2)^{1/2}}{1 - \rho_1/\rho_2} \right) \quad (3.20)$$

When analyzing Eq 3.19 and 3.20, as the Mach number of the shockwave moves towards infinity, the value of the breakup distance decreases towards 120. When these equations are used to determine the breakup time and distance for physical reactions, the values show that liquids can propagate detonations due to their quick breakup times and short distances. That being said, smaller drops are better as their resulting detonation waves and velocities are closer to the ideal CJ values.

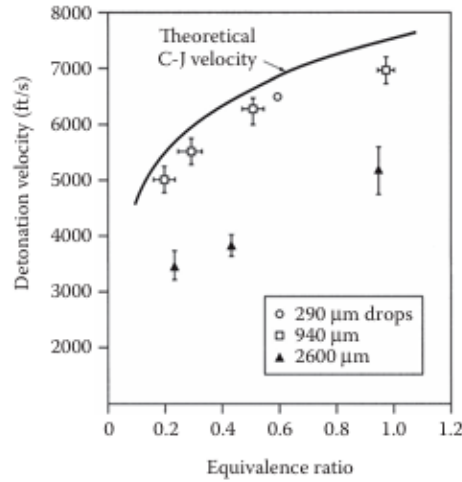


Figure 3.12 - Comparison of different liquid drop sizes to ideal Chapman-Jouguet velocity [31]

When attempting to determine the detonation velocity of the shockwave with liquid fuel, like all good models, it starts with the conservation equations but with an added consideration for drag, heat transfer, and momentum loss due to necessary acceleration of the droplets [31]. Here there exists three states: before shock, after shock, and combustion products. When determining the ratio of pressures and temperatures from state 1 to 3, the following equations are available.

$$\frac{p_3}{p_1} = \frac{\gamma(u_W^2/a_1^2)(1+f)Z}{1+\gamma} \quad (3.21)$$

$$\frac{T_3}{T_1} = \frac{\gamma^2 M_{O_3}(u_W^2/a_1^2)Z^2}{(1+\gamma)^2 M_1} \quad (3.22)$$

Z in these equations is the correction factor that will account for the drag and loss of heat through the walls of the tube/annulus and can be calculated using the following equation.

$$Z = 1 + \frac{1}{\gamma(u_W^2/a_1^2)(1+f)} + \frac{C_h A_R u_2^2}{2(1+f)A_s u_W u_2} \quad (3.23)$$

To better understand the environment and why Z is solved the way it is, the following figure depicts the detonation reaction in its entirety; for this figure, V is equivalent to u in previous equations.

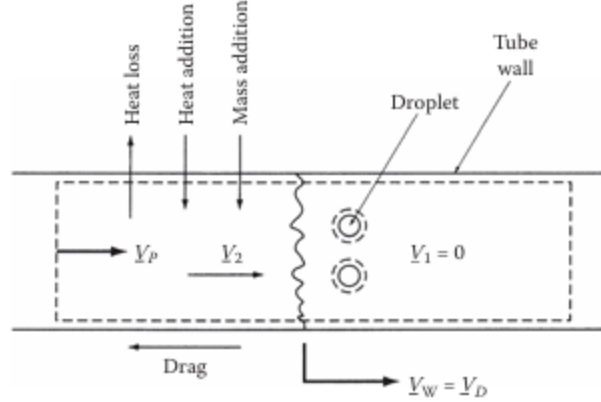


Figure 3.13 - Schematic representation of detonation wave propagation through liquid reactants [31]

For the heat transfer coefficient, it can be solved using the following equation

$$C_h = \frac{\int_2^3 q_{wall} dx}{\rho_2 u_2 (h_2 + u_2^2/2 - h_{wall})} \quad (3.24)$$

where the coefficient is measured to be around 2.5×10^{-3} for liquid spray detonations. With all previous equations, the detonation velocity can be determined utilizing an implicit formula.

$$u_D = \frac{u_{Do}}{\left[1 + \frac{2\gamma^2 C_h A_R u_2^2}{u_D u_2 (1+f) A_s} \right]^{1/2}} \quad (3.25)$$

To eliminate any potential confusion, there is no drag coefficient in Eq. 3.25 as the Reynolds analogy states that the drag coefficient is equal to twice the heat transfer coefficient. Now, given that the equation is implicit, this calls for an iterative solution by calculating the equivalent gas phase detonation parameters and repeating a few times to hone in on the most accurate solution. To help expedite this process, for small droplets i.e. less than a thousand micrometers, the breakup time can replace the area of the reaction zone as the former plays a larger role in smaller droplets.

3.3.2 Combustion and Dissociation

The existence of parasitic and commensal combustion illuminates another reaction occurring within the RDRE's combustion chamber: dissociation. Dissociation occurs when a mixture is exposed to high energy such that the excitement and movement of atoms overpowers the bonds of the molecule and breaks off into its own separate molecule [32]. While there exists many reasons for why this can occur, more often than not, it's a result of high temperature and energy from the environment. Due to the continuous propagation of a detonation wave in the annulus of an RDRE and the heat produced as a result, a portion of the OF mixture does not detonate but rather evaporates and subsequently dissociates.

To determine the amount of dissociation, determining the change of Gibbs free energy at a pressure of 1 atmosphere for the reaction is the first step. To determine the value of Gibbs free energy, a modified version of the traditional equation is used

$$\Delta G^{p=1} = \sum_i^n v_i (H_i - TS_i) \quad (3.26)$$

where n is the number of molecules in the reaction. While the enthalpy and entropy for a specific molecule and temperature, such as N_2 at 3000K, can easily be looked up in a table, the stoichiometric value requires a small bit of nuance. To determine any individual instance of upsilon requires looking at the stoichiometric equation and viewing the coefficient of the specific molecule. When plugging these upsilon values into the summation of Eq. 3.26, it should be noted that the reactants' stoichiometric values should be negative and the products should be positive.

When the Gibbs free energy of the dissociation equation has been calculated, the equilibrium constant for the given reaction can be determined using the solution of Eq. 3.26 [32].

$$K_p = \exp\left(-\frac{\Delta G^{P=1}}{RT}\right) \quad (3.27)$$

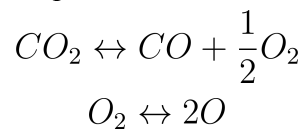
The equilibrium constant is then used to iteratively solve for the arrangement of partial pressures of the mixture. To elaborate, when a mixture is exposed to an environment which promotes dissociation, parts of the mixture begin to break up into smaller molecules which contribute their own pressure on the system. It is through these pressures that allows for determining the mole fractions of each molecule in the system. However, there is no analytical means to find these pressures so an iterative process is used, utilizing various equations to determine the partial pressures; A few of these equations are listed below.

$$K_p = \prod_i P_i^{v_i} \quad (3.28)$$

$$\sum_i P_i = P_{mixture} \quad (3.29)$$

$$\frac{N_i}{N_j} = \frac{\sum_i v_i P_i}{\sum_j v_j P_j} \quad (3.30)$$

To further explain Eq. 3.30, this equation represents the ratio of atoms in a molecule and equates it to the ratio of the atoms in the stoichiometric equations. As an example, take the dissociation of carbon dioxide. Two stoichiometric equations can describe the dissociation of carbon dioxide.



For pure carbon dioxide, the ratio of carbon to oxygen is one-half and when equated to the summation of stoichiometric values and pressures, the following equation emerges.

$$\frac{1}{2} = \frac{P_{CO_2} + P_{CO}}{2P_{O_2} + P_O + 2P_{CO_2} + P_{CO}}$$

The reason determining the partial pressures, and subsequently mole fractions, of dissociated gases is important due to the aforementioned parasitic and commensal combustion reactions. Because these reactions draw reactants away from detonation and instead combust, resulting in dissociation occurring. This dissociation creates losses in the system as pressure and temperature increases from combustion are less than those resulting from detonation with some sources stating that dissociation losses in RDREs are 10% higher than in traditional turbine engines [33].

Understanding both detonation and combustion is important for RDREs as it helps to illuminate the reactions occurring within the combustion chamber. In an un-ideal world with non-frozen flow, the resulting flow post detonation wave can be composed of reactants, detonation products, and dissociated reactants. Because of the complex nature of the gas, special considerations must be taken to ensure no adverse reactions occur in the exhaust.

CHAPTER 4: FUEL COMPOSITION

The last topic to discuss before performing detonation simulations will be discussing the possible oxidizer and fuel options. It is paramount to consider all possible combinations and equivalence ratios as each will have different setbacks and benefits. In order to do so, this paper will draw upon OF mixtures utilized in recent detonation tests as well as traditional mixtures to build a table of combinations to test.

4.1 Traditional Reactant Mixtures

While RDREs are the newest experimental mode of propulsion with unique challenges and designs, it is still beneficial to research traditional fuel mixtures to see whether or not they are viable in RDREs. Given the new challenges proposed by RDREs, it would be greatly beneficial to be able to rely on already existing infrastructure around the reactants and reactant storage. Now, this is not to say that it is a priority to use traditional mixtures; if a new mixture is concocted and is vastly more efficient than other mixtures, then it should be utilized across the board. However, it isn't ideal to design a new storage and piping system for a RDRE specific mixture if it is only slightly more efficient than others. As a result, this section will focus on investigating fuels and oxidizers which are widely used before comparing them to newer mixtures in a later chapter to determine whether or not pre-existing infrastructure can be utilized in RDREs.

4.1.1 Cryogenic Reactants

Cryogenic reactants, as the name suggests, are gases condensed down to liquid form. This allows gases such as hydrogen and oxygen to be utilized in new ways; while gaseous propellants can be utilized, much of the recent research on RDRE injectors focus on liquid reactants and as such this paper will too. Before going too in-depth into cryogenic fuel, it is important to differentiate between inert and combustible gases. Theoretically, any gas could be stored cryogenically such as neon and helium but combustible gases are much more efficient for higher Isps and efficiency. As of now, the widely utilized cryogenic fuels and oxidizers are the following: liquid oxygen, liquid hydrogen, liquid methane, and a highly refined version of kerosene named RP-1.

The main benefit of cryogenic fuel is twofold: the expansion of liquid to gas and a reduction of stress in the system. Firstly, because cryogenic liquids have higher densities than their compressed gaseous forms, rockets are able to exploit the liquid-to-gas volume ratios. To elaborate, given that the mass of the reactants is constant, the following relation can be used:

$$\frac{\rho_1}{\rho_2} = \frac{v_2}{v_1} \quad (4.1)$$

And this ratio is not miniscule by any means as the ratio for liquid hydrogen, a popular fuel source, to gaseous hydrogen is 1:848; a single gallon of liquid hydrogen could fill 848 gallons in its gaseous form without compression [34]. As a result, much more propellant can be stored in liquid form. Secondly, given that the fuel and oxidizers are in liquid form, it reduces the strain on most of the system as only the combustion chamber is required to endure high temperatures and pressures in addition to the storage tanks. In addition, is it also possible to utilize regenerative cooling, a process in which the cryogenic liquid is circulated around the nozzles for cooling.

As mentioned above, one of the benefits of cryogenic fuel is listed above as cryogenic fuel and oxidizers are far more dense than their gaseous counterparts which allows for more fuel to be stored than gaseous fuel in the same container. Granted, this behavior is not inherent to all cryogen propellants as subcooled propellants are more efficient than boiling point cryogen in terms of density, vapor pressure, and cooling capacity [35]. These advantages can be furthered by a process known as propellant densification in which a cryogenic heat exchanger, a compressor, and a recirculating pump is utilized in the following setup. This process is capable of more easily bringing fuels and oxidizers to cryogenic levels to take advantage of the benefits.

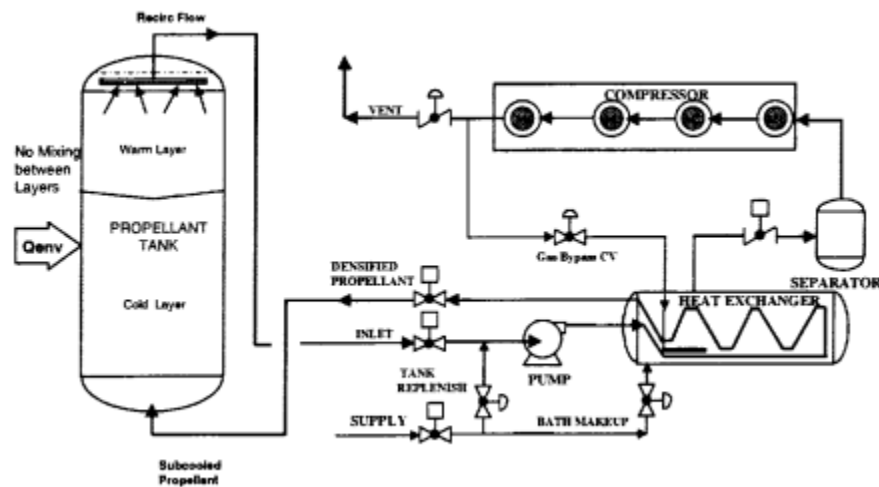


Figure 4.1 - Schematic for a propellant densification system [35]

There are additional benefits to cryogenic propellant besides volume ratios and system strain. The most important of which is that many cryogenic fuels, mostly specifically liquid hydrogen, have better combustion properties, produce higher specific impulses and thrust, and some fuels and oxidizers produce no carbon emissions [36]. Furthermore, due to the fact that the system uses liquid propellant, the system can be turned off and on for thrust control.

While there are many benefits to cryogenic fuel and oxidizers, there are many complications as well, the first of which is the fact that the propellants are cryogenic. As such, great effort must be taken in order to both prevent the supercooled liquids from both heating up as well as to prevent boil-off. As a result, there must be additional components, both passive insulation and active cooling, which adds more weight and complication to the engine already burdened with extra subsystems designed to keep the tank under pressure. There are additional monetary drawbacks as specialty materials are needed to withstand the cold temperatures. Finally, while there is a risk for explosive failure for all propellants, a cryogenic explosion could be even more devastating as shown by a report that investigates these types of failures.

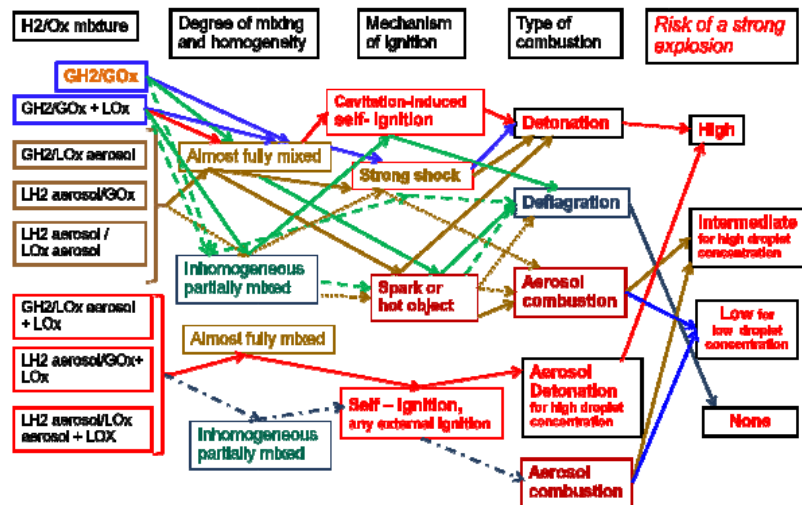


Figure 4.2 - Branching diagram showing possible cryogen explosions [37]

To recap, cryogenic reactants are a fantastic choice for RDREs given how they allow for more propellant storage in addition to providing higher levels of performance. However, there are specific drawbacks that cryogenic propellants have in addition to the already existing drawbacks of liquid propellants. Despite this, cryogenic propellants are one of the better available options as much of the infrastructure for recent rockets are designed for cryogenic fuels and oxidizers so existing supply lines would not be heavily impacted.

4.1.2 Liquid Reactants

Liquid reactants are another potential option for RDREs as they are capable of quickly mixing and share many similar qualities to cryogenic propellants. They have been used in both historical and recent space missions such as the Proton and Briz rockets and have seen great success. While not capable of performing on similar levels to some cryogenic options, liquid propellants can occupy a middle ground between performance and simplicity. Given that these options are capable of maintaining their forms without low temperatures, it removes the need for any cooling systems and a majority of the insulation; there must still be some to prevent evaporation. In addition, they are much easier to store and maintain. A few of the more popular options of liquid propellants are: dinitrogen tetroxide as an oxidizer, hydrogen peroxide, and much of the hydrazine family such as monomethylhydrazine and unsymmetrical dimethylhydrazine. However, many of these options are quite toxic in both exposure and environmentally. While some cryogenic options are toxic, the most popular options, those being LOX and LH2, are not. On the flip side, some of the most popular, non-cryogenic options are toxic, corrosive, and even carcinogenic [38]. There are other potential options for liquid propellants such as chlorine trifluoride and pentafluoride but these are rather unstable and are not yet viable. There is also the aspect that harmful byproducts would be created as a result of the nitrogens and carbons that are a part of the propellants' molecules.

While liquid propellants can create excellent OF mixtures for traditional rockets, there exists an aspect of some combinations that renders them unviable in RDREs: hypergolic. Hypergolic mixtures, such as hydrazine hydrate and high-test peroxide, are mixtures that spontaneously combust when mixed together [39]. Historically, these mixtures were valuable as rockets using hypergolic mixtures did not require ignition systems, saving on weight. Unfortunately, this independent combustion will clash with the detonation waves in an RDRE. As mentioned above, parasitic combustion is a major problem in terms of efficiency for RDREs as the fuel deflagrating produces less thrust than fuel that detonates. By using a hypergolic combination, the parasitic combustion could stall the engine as the OF mixture combusting would starve the detonation wave of valuable oxygen and fuel. As a result, several liquid OF mixtures are rendered invalid for use in RDREs. This does not mean that liquid propellant cannot be used in an RDRE, it simply means that great effort must be taken to avoid any mixtures that are hypergolic.

4.1.3 Alternate Traditional Reactants

Before moving on to other topics, it is important to discuss the last major choice when it comes to rocket propulsion: solid fuel, and subsequently hybrid rockets. Plain and simple, any form of propellant that contains solid fuel will not suffice, not even with a liquid oxidizer. While solid rockets have the advantages of being easy to store and can produce large amounts of thrust, RDREs require rapid mixing to function. While solid chemical propellants have oxidizer mixed in the fuel, that loops back to the problems of pre-mixing as the possibility of backflow can cause the propellant to combust. On the other hand, hybrid mixtures have a similar issue in that the liquid oxidizer and solid propellant would have to sufficiently mix together in the combustion chamber before the detonation wave reaches their position. Otherwise, the OF mixture would have to be mixed together before the combustion chamber which creates the same problem with solid propellants.

With all that being said, there is a potential for solid propellant to be used in RDREs as researchers at Purdue are attempting to identify a fuel that can be adapted. The research focuses on creating a substance that can be burned with the goal of “producing something that can then burn again in an RDE [40].” This would allow for RDRE rockets to take advantage of the safety and stability of solid fuels. In addition, engineers could more specifically tailor the fuel to an RDRE with the inclusion of additional additives. However, this is still a recent endeavour so any tests have yet to be undertaken. There also exists the issue of having to effectively have two combustion chambers: one for the solid fuel and another for a detonation wave to react with the first combustions’ byproducts. For all intensive purposes of this paper, solid fuels will not be considered that may potentially change in the future.

4.2 Recent Experimented Mixtures

This section is, more or less, an addendum to the previous section as the focus will be on recent experiments and drawing any potential connections to traditional OF mixtures. While table 1.1 does slightly cover this topic, this portion of the paper will reference more specific cases and their benefits and detriments.

Recent NASA experiments on RDREs use a variety of different oxidizer and fuel choices and have found for several of them to be viable and are, but not limited to: methane, kerosene, and hydrogen for fuels and oxygen, air, and hydrogen peroxide for oxidizers [41]. While the paper does specifically note liquid hydrogen, there are other hydrocarbon options available, some of which are capable of sustaining liquid form at room temperature such as pentane, heptane, and octane.

During experiments, several different combinations were tested and both comparisons and conclusions were drawn. When comparing kerosene to methane with both using oxygen, a similar amount of waves were formed but with slightly different wave speeds, with the author associated this difference due to injector mixing properties and combustion kinematics [41]. However, hydrogen had a unique issue as it both created a vastly different number of waves at low pressure while also producing pure deflagration at pressures above 250 psia CTAP. While this is a call for concern, the leading theory of the author is that either the annulus or injector design compromised the OF mixture's efficiency; it is mentioned earlier that larger annuluses can create deflagration zones. That being said, when comparing the results to traditional rockets at similar conditions, the hydrogen/oxygen mixture had similar efficiency and Isp values, concluding that hydrogen can function in an RDRE but may require a unique design/approach versus other fuels like methane and kerosene.

Before moving on towards the detonation simulations, there are three more topics to discuss. Firstly, a secondary project report talks about oxidizer cooling in RDREs as it mentions "it was identified that fuel cooling alone is insufficient and oxygen cooling is a prerequisite for any RDRE design [42]." This may be in part to the heat and pressure tolerance needed to maintain detonation waves, especially those whose expected thrust output is below 15,000 lbf. Interestingly, higher thrust classes may not require oxidizer cooling due to design choices made to withstand the harsh conditions. The second point, and arguably the most interesting one, is about the idea that multiple detonation waves may be more ideal than a singular wave. The previously mentioned experiment determined that single waves create a substantial vibration on the RDRE, an environment not found when the mode is transitioned higher i.e. more detonation waves [41]. This may need to be taken into consideration as to what is considered an optimal OF mixture for RDREs as there should be multiple, stable detonations rather than one singular, powerful one. The last point capstones the concerns about detonation waves and strength as there is a current concern about manufacturability confidence and scaling for higher thrust classes. While not entirely validated, there is evidence pointing towards the conclusion that with higher and higher thrust classes, the ability to properly scale and manufacture as shown by the following two graphs.

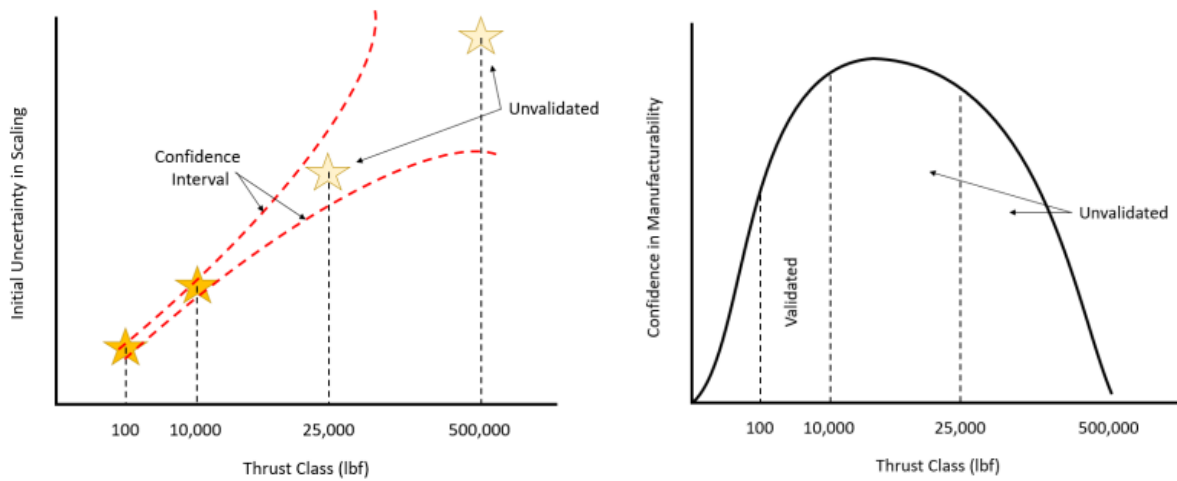


Figure 4.3 - Representations of uncertainty in scaling (left) and manufacturing (right) is terms of rising thrust class [41]

This *may* present a concern for some OF combinations and RDRE designs as producing large amounts of thrust may not be optimal due to the potential for failure as well as the difficulty in machine components with sufficient enough factors of safety.

CHAPTER 5: DETONATION SIMULATIONS

In order to compare the efficiency of different OF mixtures, NASA's CEARUN program will be utilized to perform CEA analysis, or chemical equilibrium with applications. This program allows for a series of inputs in order to run a variety of different options. For the purpose of this paper, the focus will be on simulating Chapman-Jouguet detonation which provides the following inputs: oxidizer and fuel choice, mixture ratio, and a temperature and pressure schedule. The output of the CEA analysis will provide the characteristics of both the unburnt and burnt gas as well as the detonation properties; it will be these properties that will be used to compare the effectiveness of each mixture.

5.1 Input Options

The first two inputs can be lumped together as one as CEARUN is capable of simulating a diverse amount of fuels and oxidizers while taking into account the mixture ratio, temperature of the reactants, and purity, with the latter not being taken into account for this paper. The temperature and pressure schedules represent the range of initial conditions for the reaction taking place. For the purposes of this paper, a singular initial condition will be established in order to more easily compare different mixtures. As for the initial conditions of the combustion chamber, they will be established to be 1 bar and 300K to simulate recent tests [43].

The detonation simulations will focus on combining several different compatible oxidizers and fuels at three different mixture ratios to provide a wide array of different scenarios to pick from. For the oxidizer and fuel choices, these will be drawn from both traditional rockets as well as more recent RDRE tests, the collection of which are listed below.

Table 5.1 - List of each simulated fuel and oxidizer

Fuel	Oxidizer
N_2H_4	Air
H_2	O_2
C_4H_{10} (n-butane)	NO_2
CH_4	N_2O_4

Before moving on, it is important to note that C_4H_{10} is n-butane and not isobutane; while they possess identical formulas, their structures vary with n-butane having a linear structure versus a branched chain like isobutane. As for the mixture ratios, the three options will be 0.8, 1.2, and 1.0 to simulate a fuel-lean, a fuel-rich, and a balanced split respectively. It should be noted that these values represent the global equivalence based on the OF weight ratio. This is important to state as there are two ways to describe equivalence ratios: valence electrons and weight ratio. While these two values are typically identical for stoichiometric conditions as fuels possess positive valence electrons and oxidizers contain negative valences, these are specific cases in which the valence electrons are reversed, resulting in different calculatable equivalence ratios [44]. As a result, for the purpose of continuity, all equivalence ratios will be based on the OF weight ratio. This will result in circumstances in which OF may be upwards of 16 to account for vastly more hydrogen atoms; an alternate approach in which both ratios can be tested could be considered for future work.

With the chosen oxidizers, fuels, and equivalence ratios, there will be 48 different simulations of Chapman-Jouguet detonation. Unfortunately, at the time of writing, CEARUN is unable to run detonation simulations with liquids due to the subroutine HCALC which requires gaseous reactants to function. As a result, the selection of reactants is greatly limited. However, this can be rectified in future work using more powerful softwares such as CFD.

In order to determine efficiency, three characteristics will be examined: the detonation pressure ratio, the detonation temperature ratio, and the sonic velocity. These values have been chosen for two major reasons. Firstly, higher pressure and temperature values resulting from higher ratios allows for greater thrust generation. Secondly, as mentioned previously, the minimum Chapman-Jouguet velocity is the speed in which the resulting flow of products is sonic relative to the wave [26]. When analyzing the ZND model, the reactants hit the detonation wave, slow down due to the shock, then re-accelerates back to the local sonic velocity [8]. Therefore, having a higher local sonic velocity is better as it grants a stronger “jumping-off” point for the eventual flow manipulation through a convergence-divergence nozzle.

5.2 Chapman-Jouguet Simulations

Before any relevant simulations can be done, it is paramount to establish a benchmark. Many institutions use widely different methods and softwares to simulate their detonation reactions and by being able to replicate their results through CEARUN will show that CEA analysis is valid for Chapman-Jouguet detonation simulations. To do this, a comparison is made between a CEARUN simulation and published calculations of detonation parameters from ARS Journal [45]. In this publication, the detonation parameters are derived from the Hugoniot equation for a hydrogen-oxygen mixture and is solved based on the Chapman-Jouguet point. In addition, several assumptions are made to be more idealized such as assuming that only the neutral species

of the byproducts are created from the detonation. To properly compare both the calculations to the simulations, the environment will be set such that both detonations are solved in an environment of 313.16K, 1 atmosphere, and with a molar percentage of fuel of 30%. Under these circumstances, CEARUN calculated a post-detonation gas at 2910.06K and 14.67 atm while the calculations got a result of 2860K and 14.38 atm. While not precisely exact, the percent error is less than 3% for each value which can be accounted for by CEARUN possibly considering a slightly less ideal detonation than the calculations. All in all, given the closeness of the two methods, it is safe to assume that CEARUN can provide accurate data of Chapman-Jouguet detonations. However, before moving on to the simulations themselves, it must be noted that the values provided are the theoretical ratios and speeds and not experimental values and as such, there will be some amount of disparity but not enough to discredit the simulations.

5.3 Simulation Results

After simulating all variations of the Chapman-Jouguet detonations, the following results are provided.

Table 5.2 - Results from CEARUN Chapman-Jouguet detonation simulations

CHAPMAN-JOUGUET DETONATION SIMULATIONS										
FUEL	OXIDIZER	$\phi = 0.8$			$\phi = 1.0$			$\phi = 1.2$		
		Pressure Ratio	Temperature Ratio	Sonic Velocity (m/s)	Pressure Ratio	Temperature Ratio	Sonic Velocity (m/s)	Pressure Ratio	Temperature Ratio	Sonic Velocity (m/s)
N2H4	Air	20.103	9.629	1058.4	22.307	10.173	1101.0	23.606	10.320	1132.8
	O2	37.927	12.445	1346.6	40.839	12.587	1397.8	42.951	12.585	1,435.2
	NO2									
	N2O4									
H2	Air	14.543	9.214	1041.1	15.487	9.810	1089.0	15.599	9.901	1125.4
	O2	18.451	12.134	1444.1	18.648	12.244	1542.1	18.672	12.211	1626.0
	NO2	22.567	12.060	1351.2	22.261	12.176	1429.9	21.863	12.149	1497.9
	N2O4	27.216	11.935	1331.4	26.131	12.085	1411.8	25.116	12.059	1480.7
C4H10 : N-butane	Air	16.496	8.805	958.9	18.277	9.414	991.1	18.946	9.496	1015.1
	O2	33.450	12.504	1208.1	37.246	12.782	1264.7	40.640	12.911	1312.1
	NO2	43.017	12.362	1177.2	46.749	12.645	1224.5	49.988	12.776	1264.6
	N2O4	75.673	12.337	1160.5	80.903	12.674	1210.3	84.981	12.814	1251.7
CH4	Air	15.510	8.638	962.2	17.073	9.262	996.7	17.375	9.272	1021.6
	O2	27.245	12.179	1228.6	29.123	12.395	1288.7	30.564	12.448	1338.5
	NO2	34.832	12.066	1190.6	36.336	12.288	1240.3	37.371	12.346	1281.9
	N2O4	52.680	11.963	1171.5	53.232	12.228	1223.3	53.161	12.286	1265.8

Firstly, to address the elephant in the chart, half of the hydrazine simulations were discounted due to the fact that mixtures containing hydrazine and either N_2O_4 or NO_2 are hypergolic which inherently causes them to be suboptimal for operation in RDREs. The other two versions are still considered as hydrazine is still an effective fuel source.

When analyzing table 5.2, some notable trends appear. Firstly, for a majority of the simulations, the measured variables increase in value at higher and higher equivalence ratios with a notable exception being hydrogen gas mixed with either NO_2 or N_2O_4 . This can be beneficial for some injector schemes as having an oxidizer-rich environment can damage the combustion chamber walls. Secondly, air, while usable as an oxidizing agent, regularly underperforms versus any other oxidizer simply due to the multitude of other elements that provide nothing to the reaction. It may have value in air-breathing designs for missiles and jets but is generally not recommended for rockets; its inclusion acts more as a baseline for other oxidizers. Lastly, and perhaps most importantly, N_2O_4 regularly delivered the best performance against all other options. Granted, in some cases, it produced a slightly lower temperature and sonic velocity than other combinations but the difference in pressure ratios more than makes the difference.

When comparing the most prominent OF mixtures, the following chart appears; the sonic velocity is listed in hectometers for the express purpose to ensure the graph remains legible.

Prominent OF Mixtures' Results

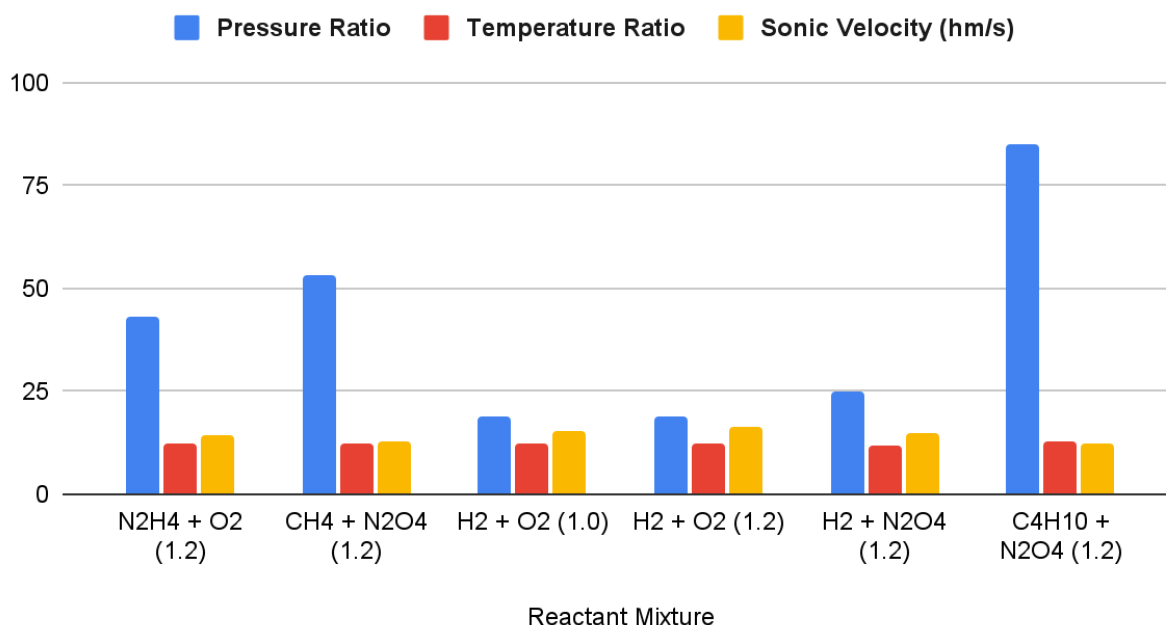


Figure 5.1 - Chart comparing the detonation parameters of prominent Chapman-Jouguet detonation simulations

Before discussing the different OF mixtures, an interesting point should be made about the two mixtures of hydrogen and oxygen.

Table 5.3 - Comparison of hydrogen and oxygen mixture at two different equivalence ratios

$H_2 + O_2$ at $\phi = 1$	$H_2 + O_2$ at $\phi = 1.2$
Pressure Ratio: 18.648	Pressure Ratio: 18.672
Temperature Ratio: 12.244	Temperature Ratio: 12.211
Sonic Velocity: 1542.1	Sonic Velocity: 1626.0

These two mixtures are intriguing as they illuminate a greater trend with hydrogen as a fuel: when moving from an equivalence ratio of 1 to 1.2, the temperature ratio decreases but the sonic velocity increases. Even more strangely, when looking at hydrogen with both nitrogen oxidizers, the pressure decreases as well unlike with pure oxygen where the pressure increases slightly. This trend can be explained by the ratio of specific heats γ . At higher equivalence ratios, there is a larger percentage of hydrogen in the reactant mixture which, combined with the high temperature of the detonation, dissociates much more easily than oxygen. By dissociating from a diatomic molecule into a monoatomic molecule, the rotational energy can be simplified to zero. And, since the rotational energy of the molecule can be neglected, this shifts the specific heat at both constant pressure and volume downwards which then increases γ which finally increases the speed of sound. This should be considered as a potential benefit of reactants such as hydrogen as dissociation will help to increase the sonic velocity of the exhaust gases.

Returning to the other four prominent reactant mixtures, some clear points are made by the simulations:

- N_2O_4 provides the highest values versus all other simulated oxidizers,
- higher equivalence ratios boast the higher detonation parameters.

As a result, the most prominent reactant mixtures abide by the above points with the exception of hydrazine due to the avoidance of hypergolic mixtures. When analyzing each OF mixture against one another, a clear outlier is present with n-butane and its remarkably high pressure ratio which can make it a viable propellant option. As for hydrazine and methane, they both manage to output viable pressures and sonic velocities. Hydrogen, however, does fall behind the alternate options which will be discussed later.

CHAPTER 6: FUEL CASE STUDY

After selecting several viable RDRE propellant mixtures, the logical next step would be to analyze the major components' pros and cons to determine practicality beyond just detonation viability. It is also important to circle back to why certain choices were made, why some were excluded, and how future work will be shaped.

6.1 N_2O_4 Versus O_2

As seen in table 5.2, when comparing N_2O_4 and O_2 , N_2O_4 regularly outputs higher pressure values with only slightly lower temperature ratios. This can be attributed to the fact that, at STP, N_2O_4 has three times the density than O_2 which contributes more oxygen for the reaction and subsequently a higher pressure. However, it is unfair to use O_2 when LOX is a much more viable option as its density impulse is higher than N_2O_4 when both options are liquid due to the closer density values.

LOX and $N_2O_4(l)$ are both viable options as each contributes their own pros and cons. Starting with LOX, it will generate a higher specific impulse when combined with common fuels such as kerosene and LH2 and isn't inherently toxic. However, LOX is cryogenic which requires specialized tanks and piping, special handling to avoid cryogenic injuries, and a complex cooling system to keep LOX cold and operational. This also plays poorly with LOX's lower density requiring larger, heavier tanks which in some cases offset the Isp bonus when choosing LOX. On the flip side, $N_2O_4(l)$ will output lower Isps than LOX while being storable at room temperature and more dense than LOX, not requiring a complex cooling system and larger tanks for storage. Nonetheless, $N_2O_4(l)$ is a highly toxic and corrosive substance which can even create trace amounts of nitrous acid when combusted as well as limiting several fuel choices for RDRE use as some mixtures are hypergolic.

When considering LOX versus $N_2O_4(l)$, there is much ambiguity regarding optimality as each option is suitable for different scenarios. Unfortunately, this conversation must be shelved for the time being as considering liquid reactants in Chapman-Jouguet detonation simulations is beyond this paper's capabilities at the moment. Should this topic be revisited again in the future, more rigorous simulations can be undertaken which allows for liquid components to be considered, potentially using CFD or alternate simulation software. As for the gaseous alternatives, N_2O_4 is superior to O_2 given the disparity between detonation parameters. While this opinion may not hold against future testing, it will still serve to act as a baseline.

6.2 Butane and Alternate Heavy Hydrocarbons

Butane may be seen as a solid “shoo-in” for optimal RDRE mixtures given the drastic disparity of pressure ratios between alternate fuel sources. There is some support to this idea as hydrocarbons such as methane have been used as rocket fuel in the past. In addition, the CEARUN simulations showed that post-detonation, a butane and N_2O_4 mixture manages to output the highest temperature ratios in addition to the pressure ratios. While appealing on paper, butane does have a good few complications that arise from its use. Firstly, n-butane has both a remarkably low boiling point and high vapor pressure, resulting in either having to store the butane cryogenically before vaporising in later in the problem, using pressure to maintain the butane as a liquid at ambient temperature, or having to adapt the feed system to sustain high pressures, all of which adds extra weight and complication to the RDRE. In addition, coking/sooting becomes an issue with any heavy hydrocarbon which can damage injectors, turbopumps, and the combustion chamber itself.

Why butane may not be ideal as a singular fuel source, there is some basis to work with as heavy hydrocarbons have been used as RDRE fuel such as RP-1. RP-1, or more generally, kerosene, is simply just a well-curated mixture of heavy hydrocarbons that contains some of the same issues as butane when it comes to coking yet has seen widespread use as its heritage is well known and studied [46]. This is not to say that butane cannot be used in RDREs as it is a relatively new technology which may challenge traditional rocket mixtures. Should butane provide comparable values to traditional choices, an argument can be made to begin studying n-butane as a fuel choice. As such, butane can be considered as an RDRE fuel option but it must be compared to traditional heavy hydrocarbon options like RP-1 and LPG, a limitation of this paper.

6.3 Hydrazine Versus Methane

Out of the prominent propellant mixtures, hydrazine with oxygen and methane with dinitrogen tetroxide are the two optimal amongst the simulations. Each combination outputs roughly similar with methane outputting higher pressure and hydrazine with the higher sonic velocity. Each of these attributes can be attributed to methane’s higher vapor pressure and hydrazine having more monoatomic molecules than the methane reaction. Given that both mixtures are viable in Chapman-Jouguet detonations, it must come down to the physical properties of the two mixtures.

The main drawback from hydrazine as a fuel source is the toxic byproducts created by the detonation. When performing the CEARUN simulations, mass fractions are output showing the burnt gas composition and are listed alongside the simulations in appendix B. Comparing the two mixtures, the hydrazine mixture produces more toxic byproducts at higher mass fractions than the methane mixture such as nitrous acid, nitrogen oxides, and ammonia, each of which are either toxic to humans, bad for the environment, or both. Methane, on the other hand, has both less toxic byproducts as it produces less nitrogen-based gases as it produces more carbon-based gases; while carbon dioxide is not safe, it has less of an impact as a greenhouse gas than nitrogen dioxide. However, if environmental impact is of utmost concern, one can replace the nitrogen oxide and run methane and oxygen to remove nitrogen products. While there will be a notable drop in the pressure ratio of the detonation, it can be considered viable as it produces results comparable to methane and hydrazine. Finally, as a hydrocarbon, methane does have a coking issue but nowhere near the same level as butane would. Additionally, given methane's history as a rocket propellant, its sooting patterns are well known and researched with anti-coking procedures in place to ensure carbon deposits do not form.

There exists different points of comparison between hydrazine and methane, the first of which is cost. The Department of Defense has a list for propellant and oxidizer prices for aerospace uses; unfortunately methane is not listed on more recent documents so one from 2017 will act as the basis [47]. To determine these prices, a bit of trickery is required as methane is sold in cubic yards while hydrazine is sold in pounds. As a result, a conversion of both pounds of hydrazine to cubic yards and cubic yards of methane to pounds is necessary to find ample points of comparison. Taking into account the densities, molecular weights, and conversion ratios, a cubic yard of methane gas is equal to around 2.25 pounds of hydrazine, assuming the hydrazine is kept at 25 C and is vaporized purely in hydrazine gas. Looking at the cost of each, a cubic yard of methane is around \$430.65 while 2.25 pounds of hydrazine costs around \$400. It should be noted that the methane is considered to be at industry standard which is 60 degrees F and 14.7 psia. Ironically enough, the cost disparity between each propellant is around \$30 per pound; this can rack up quickly for massive scale projects but the difference is not substantial.

Tying into the previous topic, the density of each propellant does play a role as less dense options require a larger tank and therefore adds additional weight to the entire assembly. The density of methane gas at STP is 0.717 kg/m^3 while hydrazine gas has a vapor density slightly above that of air at around 1.1. As a result, when looking at equal masses of methane and hydrazine, a tank designed to store methane will be much larger than the hydrazine tank, requiring much more weight to be added to a potential rocket. However, a very important detail about this entire idea is that hydrazine is a liquid at room temperature. Liquids, on principle, are far more dense than their gaseous versions which could allow for an even smaller tank if hydrazine is still in liquid form. Given how the simulations were conducted around gaseous propellants, it is necessary to consider the implications.

It is possible to convert hydrazine from a liquid to gas with multiple different methods, each of which having their own pros and cons. Firstly, the obvious is heat: add heat until the hydrazine molecules have enough energy to break their bonds and turn into vapor. While simple, it does promote issues as there needs to be a heating element added somewhere in the assembly, adding more weight and complexity, in addition to the fact that there will be a source of abundant energy near the propellants as well as potential the oxidizer. As mentioned above with the premixing concept, there should be little potential sources of error before the combustion chamber; a small gas leak that potentially reaches the heat causes a *large* problem due to hydrazine's propensity for explosive decompositions [48]. The other method is much safer and takes advantage of the unstable nature of hydrazine by utilizing low pressures to safely encourage vaporization. While this method is safer by not necessitating heat, the complexity of adding a near-vacuum chamber in order to turn liquid hydrazine into gaseous hydrazine would be astronomical; To turn a stored liquid into a gas quickly enough to be consistently pumped into a combustion chamber may not even be possible. The idea could work if the RDRE was designed to only fire for short periods of time over a long period of time to allow for the hydrazine to vaporize in stages but it is not applicable for surface-to-space launches. Unfortunately, as it stands, gaseous hydrazine must be stored as a gas and not in its more efficient liquid form due to the complexity and dangers it imposes.

When considering all aspects of each fuel and oxidizer, it is of this paper's opinion that methane and dinitrogen tetroxide is the most optimal choice amongst the options simulated as it provides above average results while not possessing the more detrimental aspects of other mixtures. While hydrazine can be considered more cost-efficient and effective in terms of temperature and sonic velocity, the complications it brings along makes it less than ideal. Hydrazine is highly unstable, toxic to both humans and the environment, and is prone to explode when given an inch. Unfortunately, as the saying goes, there is no limit to complexity. With that being said, methane, while highly reactive in the presence of both energy and catalysts, remains a far more simple fuel source than hydrazine and in an engine as complicated as an RDRE, simplicity is ideal. All in all, methane in combination with a powerful oxidizer like dinitrogen tetroxide is a stand out choice for use in future RDRE designs.

Chapter 7: Conclusion

Utilizing detonation waves for propulsion is an idea that was conceived in the 50s given how they provide greater outputs than traditional deflagration engines. Up until recently, detonation engines were shelved until more powerful computational methods were devised to solve the intricacies of detonation engines. As a result of modern technology and techniques, multiple variations of detonation engines are currently being researched such as the RDRE. With simulations of complex fluid dynamics being possible, it is paramount to now focus on the finer details such as potential fuel-oxidizer mixtures.

When analyzing different fuel and oxidizer choices, in combination with RDRE schematics and design, it shows that traditional fuel and oxidizer options are still viable when undergoing a Chapman-Jouguet detonation. As for the specifics, more dense fuels and powerful oxidizers like methane and dinitrogen tetroxide are prominent choices as they balance both excellent detonation parameters with less severe drawbacks. Methane and N_2O_4 is capable of producing high pressures and temperatures while not suffering from severe coking and is less toxic in both exposure and environmental impact. While there may be more specifics that can only be seen with alternate simulations, a traditional, well-researched mixture may be an optimal OF mixture for extended use in RDREs.

7.1 Future Work

This paper focused more on gaseous reactants for Chapman-Jouguet detonations as this was a limitation imposed by the CEARUN software. This, unfortunately, prevents many prominent liquid options such as LOX, LH2, and hydrogen peroxide from being considered. Should this topic be revisited at a later point, a different software such as StarCCM, MATLAB, or Ansys should be considered in order to allow for more diverse options. By performing these new simulations, it will allow for a comparison to the simulations of this paper to help as a baseline. In addition, it may be beneficial to consider alternate options such as mixture ratios based on weight instead of equivalence or adding an additional stage in which the most prominent choices are more closely observed and calibrated.

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Appendix A: Derivation of Mach Downstream as Function of Detonation Wave

As shown previously, much of the work determining the droplet breakup time and heat transfer of gaseous detonations relies on the fundamental Eq. 3.15. The purpose of this appendix is to illuminate the process in which this equation was calculated: as a point of reference, Eq. 3.15 is shown as.

$$M_2^2 = \frac{(\gamma - 1)M_W^2 + 2}{2\gamma M_W^2 - (\gamma - 1)} \quad (\text{A.1})$$

In order to calculate the above equation, one must start with the 1-D model for propagation velocity and subsequently pressure and temperature changes; for this derivation, the steps will be in line with those provided by Ragland and Bryden [31].

Like all good derivations, it is essential to start with a diagram to understand what precisely is occurring in the annulus. However, attempting to analyze the system as it is found, as a fixed position model, will promote an unsteady problem due to the reactants having no translational velocity. As such, the problem must be translated into a fixed-wave scenario such that a steady flow is created as seen in Fig. A.1; do note that the diagram uses a capital V to denote velocity but moving forward, u will represent velocity.

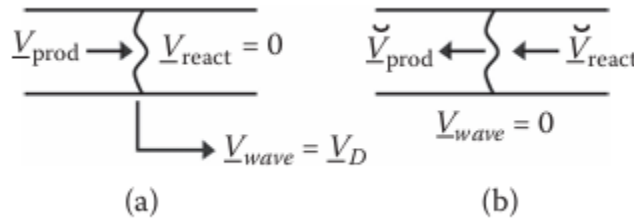


Figure A.1 - Models for a traveling wave system (a) and a standing wave system (b)

When the moving wave transforms into a standing wave, the velocity is then applied onto the products and reactants, changing them as such; for simplicity's sake, the small v will represent the velocity before the transformation.

$$u_{\text{react}} = u_D \quad (\text{A.2})$$

$$u_{\text{prod}} = u_D - v_{\text{prod}} \quad (\text{A.3})$$

Using Eq. A.1 and A.2, the conservation equations can be adapted to this new coordinate system. However, when establishing our equations, the speed of sound needs to be adjusted as the speed of sound of a reacting mixture is different from normal. For our mixture, the speed of sound of the products is.

$$a_{prod} = \sqrt{\left(\frac{\partial p_{prod}}{\partial \rho_{prod}}\right)_s} \quad (A.4)$$

This solution can be taken further by including variable molecular weights and specific heats by rewriting the conservation equations in the Rankine-Hugoniot form but the changes are minor and as such, it is safe to assume constant values. Moving from here, the mach speed can be rewritten using this new speed of sound to be

$$M^2 = \frac{u^2}{\gamma RT} = \frac{\rho u^2}{\gamma p} \quad (A.5)$$

which can be rewritten to solve for either the velocity or density.

$$\rho = \frac{\gamma p(M^2)}{u^2} \quad (A.6)$$

$$u^2 = \gamma RT M^2 \quad (A.7)$$

Using these new values for the conservation equations, the conservation equations can be rewritten as such.

$$\frac{p_{react}^2 M_{react}^2}{T_{react}} = \frac{p_{prod}^2 M_{prod}^2}{T_{prod}} \quad (A.8)$$

$$p_{react}(1 + \gamma M_{react}^2) = p_{prod}(1 + \gamma M_{prod}^2) \quad (A.9)$$

From here, it is possible to combine the energy and continuity equations to get an equation for the heat of reaction per unit mass.

$$\left[c_{p,prod} T_{prod} + \frac{u_{prod}^2}{2} \right] - \left[c_{p,react} T_{react} + \frac{u_{react}^2}{2} \right] = \frac{q}{\dot{m}} \quad (A.10)$$

Before any more steps are taken, it's important to adapt this equation as the steps taken are adapted for detonations of gaseous mixtures and not liquid mixtures; this can be amended by taking q to be 0.

Eq. A.9 can be further simplified by utilizing the aforementioned change and by dividing the equation by the specific heat capacity of the reactants, using the long-form version with γ and R .

$$T_{react} \left[1 + \frac{\gamma - 1}{2} M_{react}^2 \right] = T_{prod} \left[1 + \frac{\gamma - 1}{2} M_{prod}^2 \right] \quad (A.11)$$

Finally, from this point, the equation can solve for the pressure ratio in terms of Mach and γ , combined with Eq. A.7 to find the temperature ratio across the detonation, and rearrange Eq. A.10 in order to achieve Eq. 3.15.

Appendix B: CEARUN Chapman-Jouguet Detonation Simulation Outputs

NASA-GLENN CHEMICAL
EQUILIBRIUM PROGRAM CEA2,
FEBRUARY 5, 2004
BY BONNIE MCBRIDE AND
SANFORD GORDON
REFS: NASA RP-1311, PART I, 1994
AND NASA RP-1311, PART II, 1996

Pressure (1 value):
p,bar= 1
Temperature (1 value):
t,k= 300

Equivalence based on Fuel/Oxid. wt ratio
(Eq 9.19*) (3 values):
phi = .8, 1, 1.2

You selected the following fuels and
oxidizers:

reac
fuel N2H4 wt%=100.0000
oxid Air wt%=100.0000

REACTANT		WT
FRACTION	ENERGY	TEMP
KJ/KG-MOL	K	
FUEL	N2H4	1.0000000
0.000	0.000	
OXIDANT	Air	
1.0000000	0.000	0.000

O/F= 5.39372 %FUEL= 15.640342
R,EQ.RATIO= 0.800304 PHI,EQ.RATIO=
0.800000

UNBURNED GAS

P1, BAR 1.0000
T1, K 300.00
H1, KJ/KG 462.90
M1, (1/n) 29.407
GAMMA1 1.3525
SON VEL1,M/SEC 338.7

BURNED GAS

P, BAR 20.103
T, K 2888.62
RHO, KG/CU M 2.1250 0
H, KJ/KG 1722.57
U, KJ/KG 776.53
G, KJ/KG -26913.6
S, KJ/(KG)(K) 9.9134

M, (1/n) 25.387
(dLV/dLP)t -1.00542
(dLV/dLT)p 1.1194
Cp, KJ/(KG)(K) 2.5493
GAMMA_s 1.1842
SON VEL,M/SEC 1058.4

DETONATION PARAMETERS

P/P1 20.103
T/T1 9.629
M/M1 0.8633
RHO/RHO1 1.8024
DET MACH NUMBER 5.6326
DET VEL,M/SEC 1907.8

MASS FRACTIONS

*Ar	0.01090
*CO	0.00006
*CO2	0.00031
*H	0.00010
HO2	0.00003
*H2	0.00079
H2O	0.16132
*NO	0.01556
NO2	0.00002
*N2	0.76652
N2O	0.00001
*O	0.00166
*OH	0.01248
*O2	0.03024

* THERMODYNAMIC PROPERTIES
FITTED TO 20000.K

NOTE. WEIGHT FRACTION OF FUEL
IN TOTAL FUELS AND OF OXIDANT IN
TOTAL OXIDANTS

REACTANT FRACTION	WT TEMP	WT TEMP
KJ/KG-MOL	K	
FUEL	N2H4	1.0000000
0.000	0.000	
OXIDANT	Air	
1.0000000	0.000	0.000

O/F= 4.31498 %FUEL= 18.814754
R,EQ.RATIO= 1.000000 PHI,EQ.RATIO=
1.000000

UNBURNED GAS

P1, BAR	1.0000
T1, K	300.00
H1, KJ/KG	557.35
M1, (1/n)	29.499
GAMMA1	1.3441
SON VEL1,M/SEC	337.1

BURNED GAS

P, BAR	22.307
T, K	3051.99
RHO, KG/CU M	2.1497 0
H, KJ/KG	1953.81
U, KJ/KG	916.10
G, KJ/KG	-29424.6
S, KJ/(KG)(K)	10.2813
M, (1/n)	24.454
(dLV/dLP)t	-1.01015
(dLV/dLT)p	1.2114
Cp, KJ/(KG)(K)	3.2391
GAMMA s	1.1681
SON VEL,M/SEC	1101.0

DETONATION PARAMETERS

P/P1	22.307
T/T1	10.173
M/M1	0.8290
RHO/RHO1	1.8177
DET MACH NUMBER	5.9363
DET VEL,M/SEC	2001.3

MASS FRACTIONS

*Ar	0.01049
*CO	0.00012
*CO2	0.00020
*H	0.00029
HO2	0.00002
*H2	0.00264
H2O	0.17812
*NO	0.01071
NO2	0.00001
*N2	0.77256
*O	0.00159
*OH	0.01377
*O2	0.00948

* THERMODYNAMIC PROPERTIES
FITTED TO 20000.K

NOTE. WEIGHT FRACTION OF FUEL
IN TOTAL FUELS AND OF OXIDANT IN
TOTAL OXIDANTS

REACTANT	WT FRACTION
ENERGY TEMP	
KJ/KG-MOL K	
FUEL N2H4	1.0000000
0.000 0.000	
OXIDANT Air	
1.0000000 0.000 0.000	

O/F= 3.59581 %FUEL= 21.758928
R, EQ. RATIO= 1.199696 PHI, EQ. RATIO=
1.200000

UNBURNED GAS

P1, BAR 1.0000
T1, K 300.00
H1, KJ/KG 644.95
M1, (1/n) 29.584
GAMMA1 1.3365
SON VEL1, M/SEC 335.7

BURNED GAS

P, BAR 23.606
T, K 3095.91
RHO, KG/CU M 2.1554 0
H, KJ/KG 2122.39
U, KJ/KG 1027.16
G, KJ/KG -30699.7
S, KJ/(KG)(K) 10.6018

M, (1/n) 23.503
(dLV/dLP)t -1.00990
(dLV/dLT)p 1.2033
Cp, KJ/(KG)(K) 3.2740
GAMMA s 1.1717
SON VEL, M/SEC 1132.8

DETONATION PARAMETERS

P/P1 23.606
T/T1 10.320
M/M1 0.7944
RHO/RHO1 1.8173
DET MACH NUMBER 6.1326
DET VEL, M/SEC 2058.7

MASS FRACTIONS

*Ar 0.01011
*CO 0.00016
*CO2 0.00012
*H 0.00048
HO2 0.00001
*H2 0.00565
H2O 0.18391
*NO 0.00622
*N2 0.77816
*O 0.00100
*OH 0.01129
*O2 0.00287

* THERMODYNAMIC PROPERTIES
FITTED TO 20000.K

NOTE. WEIGHT FRACTION OF FUEL
IN TOTAL FUELS AND OF OXIDANT IN
TOTAL OXIDANTS

NASA-GLENN CHEMICAL
EQUILIBRIUM PROGRAM CEA2,
FEBRUARY 5, 2004
BY BONNIE MCBRIDE AND
SANFORD GORDON
REFS: NASA RP-1311, PART I, 1994
AND NASA RP-1311, PART II, 1996

Pressure (1 value):

p,bar= 1

Temperature (1 value):

t,k= 300

Equivalence based on Fuel/Oxid. wt ratio
(Eq 9.19*) (3 values):

phi = .8, 1, 1.2

You selected the following fuels and
oxidizers:

reac

fuel N2H4 wt%=100.0000

oxid O2 wt%=100.0000

REACTANT	WT
FRACTION	ENERGY TEMP

KJ/KG-MOL K

FUEL	N2H4	1.0000000
------	------	-----------

0.000	0.000
-------	-------

OXIDANT	O2
---------	----

1.0000000	0.000	0.000
-----------	-------	-------

O/F= 1.24819 %FUEL= 44.480194

R,Eq.RATIO= 0.800000 PHI,Eq.RATIO=
0.800000

UNBURNED GAS

P1, BAR 1.0000

T1, K 300.00

H1, KJ/KG 1323.33

M1, (1/n) 32.019

GAMMA1 1.2808

SON VEL1,M/SEC 315.9

BURNED GAS

P, BAR 37.927

T, K 3733.55

RHO, KG/CU M 2.3814 0

H, KJ/KG 3536.98

U, KJ/KG 1944.35

G, KJ/KG -45630.7

S, KJ/(KG)(K) 13.1691

M, (1/n) 19.491

(dLV/dLP)t -1.05319

(dLV/dLT)p 1.8745

Cp, KJ/(KG)(K) 8.5706

GAMMA_s 1.1386

SON VEL,M/SEC 1346.6

DETONATION PARAMETERS

P/P1 37.927

T/T1 12.445

M/M1 0.6087

RHO/RHO1 1.8551

DET MACH NUMBER 7.9086

DET VEL,M/SEC 2498.1

MASS FRACTIONS

*H 0.00234

HNO 0.00005

HNO2 0.00001

HO2 0.00040

*H2 0.00850

H2O 0.34980

H2O2 0.00004

*N 0.00004

*NH 0.00001

*NO 0.04540

NO2 0.00009

*N2 0.36753

N2O 0.00001

*O 0.02780

*OH 0.10057

*O2 0.09739

* THERMODYNAMIC PROPERTIES
FITTED TO 20000.K

NOTE. WEIGHT FRACTION OF FUEL
IN TOTAL FUELS AND OF OXIDANT IN
TOTAL OXIDANTS

REACTANT	WT FRACTION
ENERGY TEMP	
KJ/KG-MOL K	
FUEL N2H4	1.0000000
0.000 0.000	
OXIDANT O2	
1.0000000 0.000 0.000	

O/F= 0.99855 %FUEL= 50.036194
R,EQ.RATIO= 1.000000 PHI,EQ.RATIO=
1.000000

UNBURNED GAS

P1, BAR 1.0000
T1, K 300.00
H1, KJ/KG 1488.42
M1, (1/n) 32.022
GAMMA1 1.2710
SON VEL1,M/SEC 314.7

BURNED GAS

P, BAR 40.839
T, K 3775.95
RHO, KG/CU M 2.3825 0
H, KJ/KG 3876.16
U, KJ/KG 2162.00
G, KJ/KG -48066.3
S, KJ/(KG)(K) 13.7561

M, (1/n) 18.315
(dLV/dLP)t -1.05669
(dLV/dLT)p 1.9222
Cp, KJ/(KG)(K) 9.3510
GAMMA_s 1.1398
SON VEL,M/SEC 1397.8

DETONATION PARAMETERS

P/P1 40.839
T/T1 12.587
M/M1 0.5720
RHO/RHO1 1.8558
DET MACH NUMBER 8.2443
DET VEL,M/SEC 2594.1

MASS FRACTIONS

*H 0.00319
HNO 0.00005
HNO2 0.00001
HO2 0.00026
*H2 0.01357
H2O 0.36429
H2O2 0.00003
*N 0.00005
*NH 0.00002
NH2 0.00001
*NO 0.03567
NO2 0.00005
*N2 0.42064
N2O 0.00001
*O 0.02157
*OH 0.09137
*O2 0.04922

* THERMODYNAMIC PROPERTIES
FITTED TO 20000.K

NOTE. WEIGHT FRACTION OF FUEL
IN TOTAL FUELS AND OF OXIDANT IN
TOTAL OXIDANTS

REACTANT	WT
FRACTION ENERGY TEMP	
KJ/KG-MOL K	
FUEL N2H4	1.0000000
0.000 0.000	
OXIDANT O2	
1.0000000 0.000 0.000	

O/F= 0.83213 %FUEL= 54.581347
 R,EQ.RATIO= 1.200000 PHI,EQ.RATIO=
 1.200000

UNBURNED GAS

P1, BAR 1.0000
 T1, K 300.00
 H1, KJ/KG 1623.47
 M1, (1/n) 32.024
 GAMMA1 1.2635
 SON VEL1,M/SEC 313.7

BURNED GAS

P, BAR 42.951
 T, K 3775.37
 RHO, KG/CU M 2.3817 0
 H, KJ/KG 4137.94
 U, KJ/KG 2334.55
 G, KJ/KG -49533.7
 S, KJ/(KG)(K) 14.2163

M, (1/n) 17.406
 (dLV/dLP)t -1.05284
 (dLV/dLT)p 1.8607
 Cp, KJ/(KG)(K) 9.3236
 GAMMA_s 1.1423
 SON VEL,M/SEC 1435.2

DETONATION PARAMETERS

P/P1 42.951
 T/T1 12.585
 M/M1 0.5435
 RHO/RHO1 1.8551
 DET MACH NUMBER 8.4870
 DET VEL,M/SEC 2662.5

MASS FRACTIONS

*H 0.00379
 HNO 0.00004
 HNO2 0.00001
 HO2 0.00016
 *H2 0.01915

H2O 0.36749
 H2O2 0.00002
 *N 0.00005
 *NH 0.00002
 NH2 0.00001
 NH3 0.00001
 *NO 0.02674
 NO2 0.00003
 *N2 0.46454
 N2O 0.00001
 *O 0.01538
 *OH 0.07748
 *O2 0.02507

* THERMODYNAMIC PROPERTIES
 FITTED TO 20000.K

NOTE. WEIGHT FRACTION OF FUEL
 IN TOTAL FUELS AND OF OXIDANT IN
 TOTAL OXIDANTS

NASA-GLENN CHEMICAL
 EQUILIBRIUM PROGRAM CEA2,
 FEBRUARY 5, 2004
 BY BONNIE MCBRIDE AND
 SANFORD GORDON

REFS: NASA RP-1311, PART I, 1994
 AND NASA RP-1311, PART II, 1996

Pressure (1 value):
 p,bar= 1
 # Temperature (1 value):
 t,k= 300

Equivalence based on Fuel/Oxid. wt ratio
 (Eq 9.19*) (3 values):
 phi = .8, 1, 1.2

You selected the following fuels and oxidizers:

reac
fuel H2 wt%=100.0000
oxid Air wt%=100.0000

REACTANT FRACTION	ENERGY	WT TEMP
----------------------	--------	------------

KJ/KG-MOL	K	
FUEL H2		1.0000000
0.000	0.000	
OXIDANT Air		
1.0000000	0.000	0.000

O/F= 42.87028 %FUEL= 2.279447
R,EQ.RATIO= 0.800304 PHI,EQ.RATIO=
0.800000

UNBURNED GAS

P1, BAR 1.0000
T1, K 300.00
H1, KJ/KG -1.82
M1, (1/n) 22.200
GAMMA1 1.4012
SON VEL1,M/SEC 396.8

BURNED GAS

P, BAR 14.543
T, K 2764.13
RHO, KG/CU M 1.5896 0
H, KJ/KG 1184.96
U, KJ/KG 270.10
G, KJ/KG -26741.2
S, KJ/(KG)(K) 10.1031

M, (1/n) 25.121
(dLV/dLP)t -1.00434
(dLV/dLT)p 1.1005
Cp, KJ/(KG)(K) 2.5010
GAMMA_s 1.1847
SON VEL,M/SEC 1041.1

DETONATION PARAMETERS

P/P1 14.543
T/T1 9.214
M/M1 1.1316
RHO/RHO1 1.7860
DET MACH NUMBER 4.6863
DET VEL,M/SEC 1859.4

MASS FRACTIONS

*Ar 0.01262
*CO 0.00005
*CO2 0.00039
*H 0.00007
HO2 0.00003
*H2 0.00063
H2O 0.19142
*NO 0.01408
NO2 0.00002
*N2 0.73139
*O 0.00133
*OH 0.01147
*O2 0.03650

* THERMODYNAMIC PROPERTIES
FITTED TO 20000.K

NOTE. WEIGHT FRACTION OF FUEL
IN TOTAL FUELS AND OF OXIDANT IN
TOTAL OXIDANTS

REACTANT FRACTION	ENERGY	WT TEMP
----------------------	--------	------------

KJ/KG-MOL	K	
FUEL H2		1.0000000
0.000	0.000	
OXIDANT Air		
1.0000000	0.000	0.000

O/F= 34.29623 %FUEL= 2.833164
R,EQ.RATIO= 1.000000 PHI,EQ.RATIO=
1.000000

UNBURNED GAS

P1, BAR 1.0000
T1, K 300.00
H1, KJ/KG -1.65
M1, (1/n) 21.008
GAMMA1 1.4014
SON VEL1,M/SEC 407.9

BURNED GAS

P, BAR 15.487
T, K 2942.91
RHO, KG/CU M 1.5194 0
H, KJ/KG 1335.14
U, KJ/KG 315.82
G, KJ/KG -29846.5
S, KJ/(KG)(K) 10.5955

M, (1/n) 24.005
(dLV/dLP)t -1.00960
(dLV/dLT)p 1.2075
Cp, KJ/(KG)(K) 3.3637
GAMMA_s 1.1635
SON VEL,M/SEC 1089.0

DETONATION PARAMETERS

P/P1 15.487
T/T1 9.810
M/M1 1.1427
RHO/RHO1 1.8040
DET MACH NUMBER 4.8162
DET VEL,M/SEC 1964.6

MASS FRACTIONS

*Ar 0.01255
*CO 0.00013
*CO2 0.00026
*H 0.00025
HO2 0.00002
*H2 0.00264
H2O 0.22019
*NO 0.00944
NO2 0.00001

*N2 0.72937
*O 0.00137
*OH 0.01358
*O2 0.01017

* THERMODYNAMIC PROPERTIES
FITTED TO 20000.K

NOTE. WEIGHT FRACTION OF FUEL
IN TOTAL FUELS AND OF OXIDANT IN
TOTAL OXIDANTS

REACTANT	WT FRACTION
ENERGY TEMP	
KJ/KG-MOL K	
FUEL H2	1.0000000
0.000 0.000	
OXIDANT Air	
1.0000000 0.000	0.000

O/F= 28.58019 %FUEL= 3.380641
R, EQ.RATIO= 1.199696 PHI, EQ.RATIO=
1.200000

UNBURNED GAS

P1, BAR 1.0000
T1, K 300.00
H1, KJ/KG -1.50
M1, (1/n) 19.949
GAMMA1 1.4016
SON VEL1,M/SEC 418.6

BURNED GAS

P, BAR 15.599
T, K 2970.23
RHO, KG/CU M 1.4400 0
H, KJ/KG 1418.14
U, KJ/KG 334.86
G, KJ/KG -31412.2
S, KJ/(KG)(K) 11.0531

M, (1/n) 22.797
(dLV/dLP)t -1.00871

(dLV/dLT)p 1.1864
 Cp, KJ/(KG)(K) 3.3474
 GAMMA_s 1.1691
 SON VEL,M/SEC 1125.4

DETONATION PARAMETERS

P/P1 15.599
 T/T1 9.901
 M/M1 1.1428
 RHO/RHO1 1.8005
 DET MACH NUMBER 4.8403
 DET VEL,M/SEC 2026.3

MASS FRACTIONS

*Ar 0.01248
 *CO 0.00019
 *CO2 0.00017
 *H 0.00044
 HO2 0.00001
 *H2 0.00652
 H2O 0.23442
 *NO 0.00472
 *N2 0.72744
 *O 0.00075
 *OH 0.01047
 *O2 0.00238

* THERMODYNAMIC PROPERTIES
 FITTED TO 20000.K

NOTE. WEIGHT FRACTION OF FUEL
 IN TOTAL FUELS AND OF OXIDANT IN
 TOTAL OXIDANTS

NASA-GLENN CHEMICAL
 EQUILIBRIUM PROGRAM CEA2,
 FEBRUARY 5, 2004

BY BONNIE MCBRIDE AND
 SANFORD GORDON

REFS: NASA RP-1311, PART I, 1994
 AND NASA RP-1311, PART II, 1996

Pressure (1 value):

p,bar= 1

Temperature (1 value):

t,k= 300

Equivalence based on Fuel/Oxid. wt ratio
 (Eq 9.19*) (3 values):

phi = .8, 1, 1.2

You selected the following fuels and
 oxidizers:

reac

fuel H2 wt%=100.0000

oxid O2 wt%=100.0000

REACTANT	WT
FRACTION	TEMP

KJ/KG-MOL	K
FUEL H2	1.0000000
0.000 0.000	
OXIDANT O2	
1.0000000 0.000 0.000	

O/F= 9.92085 %FUEL= 9.156794
 R,EQ.RATIO= 0.800000 PHI,EQ.RATIO=
 0.800000

UNBURNED GAS

P1, BAR 1.0000
T1, K 300.00
H1, KJ/KG 3.97
M1, (1/n) 13.548
GAMMA1 1.4009
SON VEL1,M/SEC 507.9

BURNED GAS

P, BAR 18.451
T, K 3640.17
RHO, KG/CU M 9.9837-1
H, KJ/KG 2484.46
U, KJ/KG 636.34
G, KJ/KG -54918.9
S, KJ/(KG)(K) 15.7694

M, (1/n) 16.377
(dLV/dLP)t -1.07419
(dLV/dLT)p 2.2468
Cp, KJ/(KG)(K) 13.6337
GAMMA1 1.1284
SON VEL,M/SEC 1444.1

DETONATION PARAMETERS

P/P1 18.451
T/T1 12.134
M/M1 1.2088
RHO/RHO1 1.8382
DET MACH NUMBER 5.2268
DET VEL,M/SEC 2654.5

MASS FRACTIONS

*H 0.00373
HO2 0.00060
*H2 0.01295
H2O 0.58049
H2O2 0.00006
*O 0.04864
*OH 0.16716
*O2 0.18637

* THERMODYNAMIC PROPERTIES FITTED TO 20000.K

NOTE. WEIGHT FRACTION OF FUEL
IN TOTAL FUELS AND OF OXIDANT IN
TOTAL OXIDANTS

REACTANT	WT
FRACTION	ENERGY
	TEMP
KJ/KG-MOL	K
FUEL H2	1.0000000
0.000 0.000	
OXIDANT O2	
1.0000000 0.000 0.000	

O/F= 7.93668 %FUEL= 11.189834
R,EQ.RATIO= 1.000000 PHI,EQ.RATIO=
1.000000

UNBURNED GAS

P1, BAR 1.0000
T1, K 300.00
H1, KJ/KG 4.47
M1, (1/n) 12.010
GAMMA1 1.4014
SON VEL1,M/SEC 539.5

BURNED GAS

P, BAR 18.648
T, K 3673.33
RHO, KG/CU M 8.8518-1
H, KJ/KG 2834.01
U, KJ/KG 727.29
G, KJ/KG -61191.3
S, KJ/(KG)(K) 17.4298

M, (1/n) 14.497
(dLV/dLP)t -1.08202
(dLV/dLT)p 2.3596
Cp, KJ/(KG)(K) 16.2840
GAMMA1 1.1288
SON VEL,M/SEC 1542.1

DETONATION PARAMETERS

P/P1 18.648
T/T1 12.244
M/M1 1.2071
RHO/RHO1 1.8384
DET MACH NUMBER 5.2548
DET VEL,M/SEC 2834.9

MASS FRACTIONS

*H 0.00558
HO2 0.00042
*H2 0.02255
H2O 0.66063
H2O2 0.00005
*O 0.04137
*OH 0.16594
*O2 0.10347

* THERMODYNAMIC PROPERTIES
FITTED TO 20000.K

NOTE. WEIGHT FRACTION OF FUEL
IN TOTAL FUELS AND OF OXIDANT IN
TOTAL OXIDANTS

REACTANT	WT
FRACTION	ENERGY TEMP
KJ/KG-MOL K	
FUEL H2	1.0000000
0.000 0.000	
OXIDANT O2	
1.0000000 0.000 0.000	

O/F= 6.61390 %FUEL= 13.133870
R,EQ.RATIO= 1.200000 PHI,EQ.RATIO=
1.200000

UNBURNED GAS

P1, BAR 1.0000
T1, K 300.00
H1, KJ/KG 4.95
M1, (1/n) 10.834

GAMMA1 1.4018
SON VEL1,M/SEC 568.1

BURNED GAS

P, BAR 18.672
T, K 3663.45
RHO, KG/CU M 7.9812-1
H, KJ/KG 3146.30
U, KJ/KG 806.83
G, KJ/KG -66396.0
S, KJ/(KG)(K) 18.9827

M, (1/n) 13.020
(dLV/dLP)t -1.07732
(dLV/dLT)p 2.2834
Cp, KJ/(KG)(K) 17.3022
GAMMA_s 1.1301
SON VEL,M/SEC 1626.0

DETONATION PARAMETERS

P/P1 18.672
T/T1 12.211
M/M1 1.2017
RHO/RHO1 1.8375
DET MACH NUMBER 5.2592
DET VEL,M/SEC 2987.7

MASS FRACTIONS

*H 0.00714
HO2 0.00026
*H2 0.03462
H2O 0.72084
H2O2 0.00004
*O 0.03125
*OH 0.15027
*O2 0.05557

* THERMODYNAMIC PROPERTIES
FITTED TO 20000.K

NOTE. WEIGHT FRACTION OF FUEL
IN TOTAL FUELS AND OF OXIDANT IN
TOTAL OXIDANTS

NASA-GLENN CHEMICAL
EQUILIBRIUM PROGRAM CEA2,
FEBRUARY 5, 2004
BY BONNIE MCBRIDE AND
SANFORD GORDON

REFS: NASA RP-1311, PART I, 1994
AND NASA RP-1311, PART II, 1996

Pressure (1 value):

p,bar= 1

Temperature (1 value):

t,k= 300

Equivalence based on Fuel/Oxid. wt ratio
(Eq 9.19*) (3 values):

phi = .8, 1, 1.2

You selected the following fuels and
oxidizers:

reac

fuel H2 wt%=100.0000

oxid NO2 wt%=100.0000

REACTANT	WT
FRACTION	ENERGY TEMP

KJ/KG-MOL K

FUEL	H2	1.0000000
------	----	-----------

0.000	0.000
-------	-------

OXIDANT	NO2
---------	-----

1.0000000	0.000	0.000
-----------	-------	-------

O/F= 14.26347 %FUEL= 6.551592

R,EQ.RATIO= 0.800000 PHI,EQ.RATIO=
0.800000

UNBURNED GAS

P1, BAR 1.0000

T1, K 300.00

H1, KJ/KG 697.68

M1, (1/n) 18.935

GAMMA1 1.3499

SON VEL1,M/SEC 421.7

BURNED GAS

P, BAR 22.567

T, K 3617.94

RHO, KG/CU M 1.3997 0

H, KJ/KG 2888.68

U, KJ/KG 1276.40

G, KJ/KG -47539.8

S, KJ/(KG)(K) 13.9385

M, (1/n) 18.658

(dLV/dLP)t -1.05730

(dLV/dLT)p 1.9719

Cp, KJ/(KG)(K) 9.9424

GAMMA s 1.1325

SON VEL,M/SEC 1351.2

DETONATION PARAMETERS

P/P1 22.567

T/T1 12.060

M/M1 0.9854

RHO/RHO1 1.8439

DET MACH NUMBER 5.9082

DET VEL,M/SEC 2491.5

MASS FRACTIONS

*H 0.00257

HNO 0.00003

HNO2 0.00001

HO2 0.00039

*H2 0.00939

H2O 0.41851

H2O2 0.00004

*N 0.00003

*NH 0.00001

*NO	0.03898
NO2	0.00007
*N2	0.26624
N2O	0.00001
*O	0.03129
*OH	0.11315
*O2	0.11929

* THERMODYNAMIC PROPERTIES
FITTED TO 20000.K

NOTE. WEIGHT FRACTION OF FUEL
IN TOTAL FUELS AND OF OXIDANT IN
TOTAL OXIDANTS

REACTANT FRACTION	WT TEMP	ENERGY
KJ/KG-MOL	K	
FUEL H2	1.0000000	
0.000 0.000		
OXIDANT NO2		
1.0000000 0.000	0.000	

O/F= 11.41077 %FUEL= 8.057516
R,EQ.RATIO= 1.000000 PHI,EQ.RATIO=
1.000000

UNBURNED GAS

P1, BAR	1.0000
T1, K	300.00
H1, KJ/KG	686.86
M1, (1/n)	16.679
GAMMA1	1.3564
SON VEL1,M/SEC	450.4

BURNED GAS

P, BAR	22.261
T, K	3652.92
RHO, KG/CU M	1.2327 0
H, KJ/KG	3139.09
U, KJ/KG	1333.24
G, KJ/KG	-52288.5
S, KJ/(KG)(K)	15.1735

M, (1/n)	16.819
(dLV/dLP)t	-1.06509
(dLV/dLT)p	2.0916
Cp, KJ/(KG)(K)	11.8954
GAMMA _s	1.1322
SON VEL,M/SEC	1429.9

DETONATION PARAMETERS

P/P1	22.261
T/T1	12.176
M/M1	1.0084
RHO/RHO1	1.8435
DET MACH NUMBER	5.8528
DET VEL,M/SEC	2636.0

MASS FRACTIONS

*H	0.00389
HNO	0.00003
HNO2	0.00001
HO2	0.00027
*H2	0.01655
H2O	0.47751
H2O2	0.00003
*N	0.00003
*NH	0.00001
*NO	0.02984
NO2	0.00004
*N2	0.26592
N2O	0.00001
*O	0.02681
*OH	0.11295
*O2	0.06611

* THERMODYNAMIC PROPERTIES
FITTED TO 20000.K

NOTE. WEIGHT FRACTION OF FUEL
IN TOTAL FUELS AND OF OXIDANT IN
TOTAL OXIDANTS

REACTANT FRACTION	ENERGY	WT TEMP
KJ/KG-MOL	K	
FUEL H2		1.0000000
0.000	0.000	
OXIDANT NO2		
1.0000000	0.000	0.000
O/F= 9.50898 %FUEL= 9.515673		
R,EQ.RATIO= 1.200000 PHI,EQ.RATIO= 1.200000		

UNBURNED GAS

P1, BAR	1.0000
T1, K	300.00
H1, KJ/KG	676.39
M1, (1/n)	14.954
GAMMA1	1.3615
SON VEL1,M/SEC	476.5

BURNED GAS

P, BAR	21.863
T, K	3644.79
RHO, KG/CU M	1.1043 0
H, KJ/KG	3361.08
U, KJ/KG	1381.27
G, KJ/KG	-56203.8
S, KJ/(KG)(K)	16.3425

M, (1/n)	15.307
(dLV/dLP)t	-1.06279
(dLV/dLT)p	2.0552
Cp, KJ/(KG)(K)	12.7188
GAMMA _s	1.1333
SON VEL,M/SEC	1497.9

DETONATION PARAMETERS

P/P1	21.863
T/T1	12.149
M/M1	1.0236
RHO/RHO1	1.8420
DET MACH NUMBER	5.7898

DET VEL,M/SEC 2759.1

MASS FRACTIONS

*H	0.00503
HNO	0.00003
HO2	0.00017
*H2	0.02553
H2O	0.52265
H2O2	0.00002
*N	0.00003
*NH	0.00001
NH2	0.00001
*NO	0.02181
NO2	0.00002
*N2	0.26523
*O	0.02050
*OH	0.10309
*O2	0.03587

* THERMODYNAMIC PROPERTIES
FITTED TO 20000.K

NOTE. WEIGHT FRACTION OF FUEL
IN TOTAL FUELS AND OF OXIDANT IN
TOTAL OXIDANTS

NASA-GLENN CHEMICAL
EQUILIBRIUM PROGRAM CEA2,
FEBRUARY 5, 2004

BY BONNIE MCBRIDE AND
SANFORD GORDON

REFS: NASA RP-1311, PART I, 1994
AND NASA RP-1311, PART II, 1996

Pressure (1 value):
p,bar= 1
Temperature (1 value):
t,k= 300

Equivalence based on Fuel/Oxid. wt ratio
(Eq 9.19*) (3 values):
phi = .8, 1, 1.2

You selected the following fuels and oxidizers:

reac	
fuel H2	wt%=100.0000
oxid N2O4	wt%=100.0000

REACTANT FRACTION	ENERGY KJ/KG-MOL	WT TEMP (SEE NOTE) K
FUEL H2	0.000	1.0000000
OXIDANT N2O4	0.000	0.000

O/F= 14.26347 %FUEL= 6.551592
R, EQ. RATIO= 0.800000 PHI, EQ. RATIO= 0.800000

UNBURNED GAS

P1, BAR	1.0000
T1, K	300.00
H1, KJ/KG	116.07
M1, (1/n)	23.443
GAMMA1	1.2553
SON VEL1, M/SEC	365.5

BURNED GAS

P, BAR	27.216
T, K	3580.60
RHO, KG/CU M	1.7391 0
H, KJ/KG	2264.65
U, KJ/KG	699.70
G, KJ/KG	-46726.6
S, KJ/(KG)(K)	13.6824

M, (1/n)	19.024
(dLV/dLP)t	-1.04938
(dLV/dLT)p	1.8506
Cp, KJ/(KG)(K)	8.9907

GAMMA	1.1326
SON VEL, M/SEC	1331.4

DETONATION PARAMETERS

P/P1	27.216
T/T1	11.935
M/M1	0.8115
RHO/RHO1	1.8504
DET MACH NUMBER	6.7409
DET VEL, M/SEC	2463.5

MASS FRACTIONS

*H	0.00200
HNO	0.00003
HNO2	0.00001
HO2	0.00039
*H2	0.00823
H2O	0.43902
H2O2	0.00004
*N	0.00002
*NH	0.00001
*NO	0.03741
NO2	0.00007
*N2	0.26697
N2O	0.00001
*O	0.02552
*OH	0.10358
*O2	0.11668

* THERMODYNAMIC PROPERTIES
FITTED TO 20000.K

NOTE. WEIGHT FRACTION OF FUEL
IN TOTAL FUELS AND OF OXIDANT IN
TOTAL OXIDANTS

REACTANT FRACTION	ENERGY KJ/KG-MOL	WT TEMP K
FUEL H2	0.000	1.0000000
OXIDANT N2O4	0.000	0.000

O/F= 11.41077 %FUEL= 8.057516
R, EQ. RATIO= 1.000000 PHI, EQ. RATIO= 1.000000

UNBURNED GAS

P1, BAR 1.0000
T1, K 300.00
H1, KJ/KG 114.62
M1, (1/n) 20.015
GAMMA1 1.2713
SON VEL1, M/SEC 398.0

BURNED GAS

P, BAR 26.131
T, K 3625.44
RHO, KG/CU M 1.4841 0
H, KJ/KG 2527.44
U, KJ/KG 766.68
G, KJ/KG -51589.3
S, KJ/(KG)(K) 14.9269

M, (1/n) 17.120
(dLV/dLP)t -1.05837
(dLV/dLT)p 1.9906
Cp, KJ/(KG)(K) 10.9987
GAMMA_s 1.1320
SON VEL, M/SEC 1411.8

DETONATION PARAMETERS

P/P1 26.131
T/T1 12.085
M/M1 0.8554
RHO/RHO1 1.8495
DET MACH NUMBER 6.5599
DET VEL, M/SEC 2611.1

MASS FRACTIONS

*H 0.00324
HNO 0.00003
HNO2 0.00001
HO2 0.00026

*H2 0.01539
H2O 0.49833
H2O2 0.00003
*N 0.00003
*NH 0.00001
*NO 0.02817
NO2 0.00004
*N2 0.26671
N2O 0.00001
*O 0.02217
*OH 0.10415
*O2 0.06143

* THERMODYNAMIC PROPERTIES
FITTED TO 20000.K

NOTE. WEIGHT FRACTION OF FUEL
IN TOTAL FUELS AND OF OXIDANT IN
TOTAL OXIDANTS

REACTANT		WT
FRACTION	ENERGY	TEMP
KJ/KG-MOL	K	
FUEL H2		1.0000000
0.000 0.000		
OXIDANT N2O4		
1.0000000 0.000 0.000		

O/F= 9.50898 %FUEL= 9.515673
R, EQ. RATIO= 1.200000 PHI, EQ. RATIO= 1.200000

UNBURNED GAS

P1, BAR 1.0000
T1, K 300.00
H1, KJ/KG 113.23
M1, (1/n) 17.532
GAMMA1 1.2843
SON VEL1, M/SEC 427.4

BURNED GAS

P, BAR 25.116
T, K 3617.81
RHO, KG/CU M 1.2983 0
H, KJ/KG 2757.66
U, KJ/KG 823.18
G, KJ/KG -55494.6
S, KJ/(KG)(K) 16.1015

M, (1/n) 15.550
(dLV/dLP)t -1.05633
(dLV/dLT)p 1.9576
Cp, KJ/(KG)(K) 11.7787
GAMMA_s 1.1333
SON VEL,M/SEC 1480.7

DETONATION PARAMETERS

P/P1 25.116
T/T1 12.059
M/M1 0.8869
RHO/RHO1 1.8472
DET MACH NUMBER 6.3985
DET VEL,M/SEC 2735.1

MASS FRACTIONS

*H 0.00431
HNO 0.00002
HO2 0.00016
*H2 0.02457
H2O 0.54236
H2O2 0.00002
*N 0.00003
*NH 0.00001
NH2 0.00001
*NO 0.02004
NO2 0.00002
*N2 0.26606
*O 0.01671
*OH 0.09411
*O2 0.03156

* THERMODYNAMIC PROPERTIES
FITTED TO 20000.K

NOTE. WEIGHT FRACTION OF FUEL
IN TOTAL FUELS AND OF OXIDANT IN
TOTAL OXIDANTS

NASA-GLENN CHEMICAL
EQUILIBRIUM PROGRAM CEA2,
FEBRUARY 5, 2004
BY BONNIE MCBRIDE AND
SANFORD GORDON
REFS: NASA RP-1311, PART I, 1994
AND NASA RP-1311, PART II, 1996

Pressure (1 value):

p,bar= 1

Temperature (1 value):

t,k= 300

Equivalence based on Fuel/Oxid. wt ratio
(Eq 9.19*) (3 values):
phi = .8, 1, 1.2

You selected the following fuels and
oxidizers:

reac

fuel C4H10,n-butane wt%=100.0000

oxid Air wt%=100.0000

REACTANT	WT
FRACTION	ENERGY TEMP

KJ/KG-MOL	K
FUEL C4H10,n-butane	
1.0000000	0.000 0.000
OXIDANT Air	
1.0000000	0.000 0.000

O/F= 19.32958 %FUEL= 4.918942
R,EQ.RATIO= 0.800304 PHI,EQ.RATIO=
0.800000

UNBURNED GAS

P1, BAR 1.0000
T1, K 300.00
H1, KJ/KG -108.66
M1, (1/n) 29.698
GAMMA1 1.3687
SON VEL1,M/SEC 339.1

BURNED GAS

P, BAR 16.496
T, K 2641.65
RHO, KG/CU M 2.1319 0
H, KJ/KG 905.54
U, KJ/KG 131.76
G, KJ/KG -22827.5
S, KJ/(KG)(K) 8.9842

M, (1/n) 28.386
(dLV/dLP)t -1.00339
(dLV/dLT)p 1.0853
Cp, KJ/(KG)(K) 2.1328
GAMMA_s 1.1882
SON VEL,M/SEC 958.9

DETONATION PARAMETERS

P/P1 16.496
T/T1 8.805
M/M1 0.9558
RHO/RHO1 1.7906
DET MACH NUMBER 5.0638
DET VEL,M/SEC 1716.9

MASS FRACTIONS

*Ar 0.01228
*CO 0.00843
*CO2 0.13619
*H 0.00002
HO2 0.00001

*H2 0.00012
H2O 0.07240
*NO 0.01215
NO2 0.00002
*N2 0.71235
*O 0.00074
*OH 0.00492
*O2 0.04034

* THERMODYNAMIC PROPERTIES
FITTED TO 20000.K

NOTE. WEIGHT FRACTION OF FUEL
IN TOTAL FUELS AND OF OXIDANT IN
TOTAL OXIDANTS

REACTANT	WT
FRACTION	ENERGY TEMP
	(SEE NOTE)
KJ/KG-MOL	K
FUEL C4H10,n-butane	
1.0000000	0.000 0.000
OXIDANT Air	
1.0000000	0.000 0.000

O/F= 15.46366 %FUEL= 6.073983
R,EQ.RATIO= 1.000000 PHI,EQ.RATIO=
1.000000

UNBURNED GAS

P1, BAR 1.0000
T1, K 300.00
H1, KJ/KG -133.59
M1, (1/n) 29.875
GAMMA1 1.3619
SON VEL1,M/SEC 337.2

BURNED GAS

P, BAR 18.277
T, K 2824.06
RHO, KG/CU M 2.1690 0
H, KJ/KG 985.92
U, KJ/KG 143.29
G, KJ/KG -25040.1

S, KJ/(KG)(K) 9.2158

M, (1/n) 27.866
(dLV/dLP)t -1.00730
(dLV/dLT)p 1.1728
Cp, KJ/(KG)(K) 2.7470
GAMMA_s 1.1656
SON VEL,M/SEC 991.1

DETONATION PARAMETERS

P/P1 18.277
T/T1 9.414
M/M1 0.9327
RHO/RHO1 1.8110
DET MACH NUMBER 5.3225
DET VEL,M/SEC 1794.8

MASS FRACTIONS

*Ar 0.01213
*CO 0.03117
*CO2 0.13545
*H 0.00006
HO2 0.00001
*H2 0.00049
H2O 0.08577
*NO 0.00913
NO2 0.00001
*N2 0.70504
*O 0.00087
*OH 0.00639
*O2 0.01347

* THERMODYNAMIC PROPERTIES
FITTED TO 20000.K

NOTE. WEIGHT FRACTION OF FUEL
IN TOTAL FUELS AND OF OXIDANT IN
TOTAL OXIDANTS

REACTANT	WT
FRACTION	ENERGY TEMP

KJ/KG-MOL K
FUEL C4H10,n-butane
1.0000000 0.000 0.000
OXIDANT Air
1.0000000 0.000 0.000

O/F= 12.88638 %FUEL= 7.201299
R,EQ.RATIO= 1.199696 PHI,EQ.RATIO=
1.200000

UNBURNED GAS

P1, BAR 1.0000
T1, K 300.00
H1, KJ/KG -157.92
M1, (1/n) 30.051
GAMMA1 1.3554
SON VEL1,M/SEC 335.4

BURNED GAS

P, BAR 18.946
T, K 2848.69
RHO, KG/CU M 2.1712 0
H, KJ/KG 1000.18
U, KJ/KG 127.55
G, KJ/KG -25819.9
S, KJ/(KG)(K) 9.4149

M, (1/n) 27.143
(dLV/dLP)t -1.00533
(dLV/dLT)p 1.1257
Cp, KJ/(KG)(K) 2.4499
GAMMA_s 1.1808
SON VEL,M/SEC 1015.1

DETONATION PARAMETERS

P/P1 18.946
T/T1 9.496
M/M1 0.9032
RHO/RHO1 1.8022
DET MACH NUMBER 5.4541
DET VEL,M/SEC 1829.4

MASS FRACTIONS

```

*Ar      0.01199
*CO      0.06687
*CO2     0.11350
*H       0.00011
*H2      0.00140
H2O      0.09560
*NO      0.00404
*N2      0.69891
*O       0.00041
*OH      0.00468
*O2      0.00249
    
```

* THERMODYNAMIC PROPERTIES
FITTED TO 20000.K

NOTE. WEIGHT FRACTION OF FUEL
IN TOTAL FUELS AND OF OXIDANT IN
TOTAL OXIDANTS

NASA-GLENN CHEMICAL
EQUILIBRIUM PROGRAM CEA2,
FEBRUARY 5, 2004

BY BONNIE MCBRIDE AND
SANFORD GORDON

REFS: NASA RP-1311, PART I, 1994
AND NASA RP-1311, PART II, 1996

Pressure (1 value):

p,bar= 1

Temperature (1 value):

t,k= 300

Equivalence based on Fuel/Oxid. wt ratio
(Eq 9.19*) (3 values):

phi = .8, 1, 1.2

You selected the following fuels and
oxidizers:

```

reac
fuel C4H10,n-butane  wt%=100.0000
oxid O2              wt%=100.0000
    
```

REACTANT	WT
FRACTION	ENERGY

KJ/KG-MOL	K
FUEL	C4H10,n-butane
1.0000000	0.000 0.000
OXIDANT	O2
1.0000000	0.000 0.000

O/F= 4.47317 %FUEL= 18.270960
R,EQ.RATIO= 0.800000 PHI,EQ.RATIO=
0.800000

UNBURNED GAS

```

P1, BAR      1.0000
T1, K        300.00
H1, KJ/KG    -393.46
M1, (1/n)    34.862
GAMMA1       1.2895
SON VEL1,M/SEC 303.8
    
```

BURNED GAS

```

P, BAR      33.450
T, K        3751.18
RHO, KG/CU M 2.5950 0
H, KJ/KG    1392.66
U, KJ/KG    103.66
G, KJ/KG    -40685.4
S, KJ/(KG)(K) 11.2173
    
```

```

M, (1/n)    24.196
(dLV/dLP)t  -1.06834
(dLV/dLT)p  2.1420
Cp, KJ/(KG)(K) 8.5131
GAMMAAs     1.1323
SON VEL,M/SEC 1208.1
    
```

DETONATION PARAMETERS

P/P1 33.450
T/T1 12.504
M/M1 0.6941
RHO/RHO1 1.8567
DET MACH NUMBER 7.3848
DET VEL,M/SEC 2243.2

MASS FRACTIONS

*CO 0.19397
*CO2 0.24859
COOH 0.00002
*H 0.00140
HCO 0.00001
HO2 0.00058
*H2 0.00309
H2O 0.19400
H2O2 0.00004
*O 0.04190
*OH 0.09236
*O2 0.22404

* THERMODYNAMIC PROPERTIES
FITTED TO 20000.K

NOTE. WEIGHT FRACTION OF FUEL
IN TOTAL FUELS AND OF OXIDANT IN
TOTAL OXIDANTS

REACTANT	WT
FRACTION	TEMP

KJ/KG-MOL	K
FUEL	C4H10,n-butane
1.0000000	0.000 0.000
OXIDANT	O2
1.0000000	0.000 0.000

O/F= 3.57853 %FUEL= 21.841058
R,EQ.RATIO= 1.000000 PHI,EQ.RATIO=
1.000000

UNBURNED GAS

P1, BAR 1.0000
T1, K 300.00
H1, KJ/KG -470.68
M1, (1/n) 35.482
GAMMA1 1.2738
SON VEL1,M/SEC 299.2

BURNED GAS

P, BAR 37.246
T, K 3834.65
RHO, KG/CU M 2.6424 0
H, KJ/KG 1489.18
U, KJ/KG 79.659
G, KJ/KG -43807.6
S, KJ/(KG)(K) 11.8125

M, (1/n) 22.620
(dLV/dLP)t -1.07457
(dLV/dLT)p 2.2092
Cp, KJ/(KG)(K) 9.2801
GAMMA_s 1.1347
SON VEL,M/SEC 1264.7

DETONATION PARAMETERS

P/P1 37.246
T/T1 12.782
M/M1 0.6375
RHO/RHO1 1.8576
DET MACH NUMBER 7.8509
DET VEL,M/SEC 2349.3

MASS FRACTIONS

*CO 0.27491
*CO2 0.22952
COOH 0.00003
*H 0.00211
HCO 0.00002
HO2 0.00047
*H2 0.00534
H2O 0.22107
H2O2 0.00004

*O 0.03786
 *OH 0.09569
 *O2 0.13295

Cp, KJ/(KG)(K) 9.4114
 GAMMA_s 1.1378
 SON VEL,M/SEC 1312.1

* THERMODYNAMIC PROPERTIES
 FITTED TO 20000.K

DETONATION PARAMETERS

NOTE. WEIGHT FRACTION OF FUEL
 IN TOTAL FUELS AND OF OXIDANT IN
 TOTAL OXIDANTS

P/P1 40.640
 T/T1 12.911
 M/M1 0.5900
 RHO/RHO1 1.8573
 DET MACH NUMBER 8.2548
 DET VEL,M/SEC 2437.0

REACTANT WT
 FRACTION ENERGY TEMP

MASS FRACTIONS

KJ/KG-MOL K
 FUEL C4H10,n-butane
 1.0000000 0.000 0.000
 OXIDANT O2
 1.0000000 0.000 0.000

*CO 0.35532
 *CO2 0.20223
 COOH 0.00003
 *H 0.00283
 HCO 0.00003
 HO2 0.00032
 *H2 0.00848
 H2O 0.24078
 H2O2 0.00003
 *O 0.02962
 *OH 0.08916
 *O2 0.07116

O/F= 2.98211 %FUEL= 25.112311
 R,EQ.RATIO= 1.200000 PHI,EQ.RATIO=
 1.200000

UNBURNED GAS

* THERMODYNAMIC PROPERTIES
 FITTED TO 20000.K

NOTE. WEIGHT FRACTION OF FUEL
 IN TOTAL FUELS AND OF OXIDANT IN
 TOTAL OXIDANTS

BURNED GAS

P, BAR 40.640
 T, K 3873.18
 RHO, KG/CU M 2.6858 0
 H, KJ/KG 1567.16
 U, KJ/KG 53.993
 G, KJ/KG -46184.3
 S, KJ/(KG)(K) 12.3288

M, (1/n) 21.282
 (dLV/dLP)_t -1.07281
 (dLV/dLT)_p 2.1612

NASA-GLENN CHEMICAL
EQUILIBRIUM PROGRAM CEA2,
FEBRUARY 5, 2004
BY BONNIE MCBRIDE AND
SANFORD GORDON
REFS: NASA RP-1311, PART I, 1994
AND NASA RP-1311, PART II, 1996

Pressure (1 value):
p,bar= 1
Temperature (1 value):
t,k= 300

Equivalence based on Fuel/Oxid. wt ratio
(Eq 9.19*) (3 values):
phi = .8, 1, 1.2

You selected the following fuels and
oxidizers:
reac
fuel C4H10,n-butane wt%=100.0000
oxid NO2 wt%=100.0000

REACTANT	WT
FRACTION	ENERGY TEMP
KJ/KG-MOL	K
FUEL	C4H10,n-butane
1.0000000	0.000 0.000
OXIDANT	NO2
1.0000000	0.000 0.000

O/F= 6.43119 %FUEL= 13.456802
R,EQ.RATIO= 0.800000 PHI,EQ.RATIO=
0.800000

UNBURNED GAS

P1, BAR 1.0000
T1, K 300.00
H1, KJ/KG 353.70
M1, (1/n) 47.333
GAMMA1 1.2329
SON VEL1,M/SEC 254.9

BURNED GAS

P, BAR 43.017
T, K 3708.69
RHO, KG/CU M 3.5284 0
H, KJ/KG 2056.24
U, KJ/KG 837.05
G, KJ/KG -37473.0
S, KJ/(KG)(K) 10.6586

M, (1/n) 25.292
(dLV/dLP)t -1.04857
(dLV/dLT)p 1.8251
Cp, KJ/(KG)(K) 6.4889
GAMMA1 1.1366
SON VEL,M/SEC 1177.2

DETONATION PARAMETERS

P/P1 43.017
T/T1 12.362
M/M1 0.5343
RHO/RHO1 1.8594
DET MACH NUMBER 8.5871
DET VEL,M/SEC 2188.8

MASS FRACTIONS

*CO 0.14075
*CO2 0.18641
COOH 0.00001
*H 0.00095
HCO 0.00001
HNO 0.00003
HNO2 0.00001
HO2 0.00038
*H2 0.00227

H2O	0.14626
H2O2	0.00003
*N	0.00002
*NO	0.04431
NO2	0.00013
*N2	0.24271
N2O	0.00001
*O	0.02655
*OH	0.06314
*O2	0.14603

* THERMODYNAMIC PROPERTIES
FITTED TO 20000.K

NOTE. WEIGHT FRACTION OF FUEL
IN TOTAL FUELS AND OF OXIDANT IN
TOTAL OXIDANTS

REACTANT	WT
FRACTION	ENERGY TEMP
KJ/KG-MOL	K
FUEL	C4H10,n-butane
1.0000000	0.000 0.000
OXIDANT	NO2
1.0000000	0.000 0.000

O/F= 5.14495 %FUEL= 16.273528
R,EQ.RATIO= 1.000000 PHI,EQ.RATIO=
1.000000

UNBURNED GAS

P1, BAR	1.0000
T1, K	300.00
H1, KJ/KG	271.85
M1, (1/n)	47.621
GAMMA1	1.2237
SON VEL1,M/SEC	253.2

BURNED GAS

P, BAR	46.749
T, K	3793.41
RHO, KG/CU M	3.5501 0
H, KJ/KG	2114.35
U, KJ/KG	797.50
G, KJ/KG	-40073.5
S, KJ/(KG)(K)	11.1213

M, (1/n)	23.951
(dLV/dLP)t	-1.05445
(dLV/dLT)p	1.8995
Cp, KJ/(KG)(K)	7.1103
GAMMA _s	1.1386
SON VEL,M/SEC	1224.5

DETONATION PARAMETERS

P/P1	46.749
T/T1	12.645
M/M1	0.5030
RHO/RHO1	1.8595
DET MACH NUMBER	8.9936
DET VEL,M/SEC	2276.9

MASS FRACTIONS

*CO	0.20388
*CO2	0.17251
COOH	0.00002
*H	0.00147
HCO	0.00001
HNO	0.00003
HNO2	0.00001
HO2	0.00030
*H2	0.00403
H2O	0.16804
H2O2	0.00002
*N	0.00003
*NH	0.00001
*NO	0.03585
NO2	0.00008
*N2	0.23809
N2O	0.00001
*O	0.02413

*OH 0.06593
 *O2 0.08554

* THERMODYNAMIC PROPERTIES
 FITTED TO 20000.K

NOTE. WEIGHT FRACTION OF FUEL
 IN TOTAL FUELS AND OF OXIDANT IN
 TOTAL OXIDANTS

REACTANT	WT
FRACTION	TEMP

KJ/KG-MOL	K
FUEL C4H10,n-butane	
1.0000000	0.000 0.000
OXIDANT NO2	
1.0000000	0.000 0.000

O/F= 4.28746 %FUEL= 18.912682
 R,EQ.RATIO= 1.200000 PHI,EQ.RATIO=
 1.200000

UNBURNED GAS

P1, BAR 1.0000
 T1, K 300.00
 H1, KJ/KG 195.17
 M1, (1/n) 47.894
 GAMMA1 1.2156
 SON VEL1,M/SEC 251.6

BURNED GAS

P, BAR 49.988
 T, K 3832.76
 RHO, KG/CU M 3.5684 0
 H, KJ/KG 2157.25
 U, KJ/KG 756.40
 G, KJ/KG -42042.5
 S, KJ/(KG)(K) 11.5321

M, (1/n) 22.749
 (dLV/dLP)t -1.05419
 (dLV/dLT)p 1.8824
 Cp, KJ/(KG)(K) 7.2679

GAMMA1 1.1416
 SON VEL,M/SEC 1264.6

DETONATION PARAMETERS

P/P1 49.988
 T/T1 12.776
 M/M1 0.4750
 RHO/RHO1 1.8585
 DET MACH NUMBER 9.3404
 DET VEL,M/SEC 2350.2

MASS FRACTIONS

*CO	0.26763
*CO2	0.15226
COOH	0.00002
*H	0.00200
HCO	0.00002
HNO	0.00003
HNO2	0.00001
HO2	0.00020
*H2	0.00652
H2O	0.18408
H2O2	0.00002
*N	0.00004
*NH	0.00001
*NO	0.02667
NO2	0.00004
*N2	0.23434
N2O	0.00001
*O	0.01896
*OH	0.06176
*O2	0.04536

* THERMODYNAMIC PROPERTIES
 FITTED TO 20000.K

NOTE. WEIGHT FRACTION OF FUEL
 IN TOTAL FUELS AND OF OXIDANT IN
 TOTAL OXIDANTS

NASA-GLENN CHEMICAL
EQUILIBRIUM PROGRAM CEA2,
FEBRUARY 5, 2004
BY BONNIE MCBRIDE AND
SANFORD GORDON
REFS: NASA RP-1311, PART I, 1994
AND NASA RP-1311, PART II, 1996

Pressure (1 value):

p,bar= 1

Temperature (1 value):

t,k= 300

Equivalence based on Fuel/Oxid. wt ratio
(Eq 9.19*) (3 values):

phi = .8, 1, 1.2

You selected the following fuels and
oxidizers:

reac

fuel C4H10,n-butane wt%=100.0000

oxid N2O4 wt%=100.0000

REACTANT	WT
FRACTION	ENERGY TEMP

KJ/KG-MOL K

FUEL C4H10,n-butane

1.0000000 0.000 0.000

OXIDANT N2O4

1.0000000 0.000 0.000

O/F= 6.43119 %FUEL= 13.456802

R,EQ.RATIO= 0.800000 PHI,EQ.RATIO=
0.800000

UNBURNED GAS

P1, BAR 1.0000

T1, K 300.00

H1, KJ/KG -184.93

M1, (1/n) 85.317

GAMMA1 1.1109

SON VEL1,M/SEC 180.2

BURNED GAS

P, BAR 75.673

T, K 3700.97

RHO, KG/CU M 6.3887 0

H, KJ/KG 1491.07

U, KJ/KG 306.59

G, KJ/KG -36713.6

S, KJ/(KG)(K) 10.3229

M, (1/n) 25.979

(dLV/dLP)t -1.04093

(dLV/dLT)p 1.7042

Cp, KJ/(KG)(K) 5.7564

GAMMA1 1.1371

SON VEL,M/SEC 1160.5

DETONATION PARAMETERS

P/P1 75.673

T/T1 12.337

M/M1 0.3045

RHO/RHO1 1.8678

DET MACH NUMBER 12.0281

DET VEL,M/SEC 2167.7

MASS FRACTIONS

*CO 0.12165

*CO2 0.21641

COOH 0.00002

*H 0.00062

HCO 0.00001

HNO 0.00003

HNO2 0.00002

HO2 0.00044

*H2 0.00182

H2O	0.15729
H2O2	0.00004
*N	0.00002
*NO	0.04326
NO2	0.00017
*N2	0.24319
N2O	0.00002
*O	0.01905
*OH	0.05535
*O2	0.14061

U, KJ/KG	285.59
G, KJ/KG	-39454.7
S, KJ/(KG)(K)	10.7906

M, (1/n)	24.580
(dLV/dLP) _t	-1.04725
(dLV/dLT) _p	1.7872
C _p , KJ/(KG)(K)	6.3849
GAMMA _s	1.1389
SON VEL,M/SEC	1210.3

* THERMODYNAMIC PROPERTIES
FITTED TO 20000.K

NOTE. WEIGHT FRACTION OF FUEL
IN TOTAL FUELS AND OF OXIDANT IN
TOTAL OXIDANTS

REACTANT	WT
FRACTION	ENERGY

KJ/KG-MOL	K
FUEL	C4H10,n-butane
1.0000000	0.000 0.000
OXIDANT	N2O4
1.0000000	0.000 0.000

O/F= 5.14495 %FUEL= 16.273528
R,EQ.RATIO= 1.000000 PHI,EQ.RATIO=
1.000000

UNBURNED GAS

P1, BAR	1.0000
T1, K	300.00
H1, KJ/KG	-249.25
M1, (1/n)	84.037
GAMMA1	1.1098
SON VEL1,M/SEC	181.5

BURNED GAS

P, BAR	80.903
T, K	3802.06
RHO, KG/CU M	6.2907 0
H, KJ/KG	1571.68

DETONATION PARAMETERS

P/P1	80.903
T/T1	12.674
M/M1	0.2925
RHO/RHO1	1.8672
DET MACH NUMBER	12.4509
DET VEL,M/SEC	2259.8

MASS FRACTIONS

*CO	0.18730
*CO2	0.19855
COOH	0.00003
*H	0.00104
HCO	0.00002
HNO	0.00004
HNO2	0.00001
HO2	0.00034
*H2	0.00345
H2O	0.18083
H2O2	0.00003
*N	0.00002
*NH	0.00001
*NO	0.03462
NO2	0.00010
*N2	0.23865
N2O	0.00001
*O	0.01768
*OH	0.05867
*O2	0.07858

* THERMODYNAMIC PROPERTIES
FITTED TO 20000.K

NOTE. WEIGHT FRACTION OF FUEL
IN TOTAL FUELS AND OF OXIDANT IN
TOTAL OXIDANTS

REACTANT	WT
FRACTION	ENERGY TEMP

KJ/KG-MOL	K
FUEL	C4H10,n-butane
1.0000000	0.000 0.000
OXIDANT	N2O4
1.0000000	0.000 0.000

O/F= 4.28746 %FUEL= 18.912682
R, EQ. RATIO= 1.200000 PHI, EQ. RATIO=
1.200000

UNBURNED GAS

P1, BAR	1.0000
T1, K	300.00
H1, KJ/KG	-309.51
M1, (1/n)	82.872
GAMMA1	1.1088
SON VEL1, M/SEC	182.7

BURNED GAS

P, BAR	84.981
T, K	3844.30
RHO, KG/CU M	6.1964 0
H, KJ/KG	1632.01
U, KJ/KG	260.55
G, KJ/KG	-41438.3
S, KJ/(KG)(K)	11.2037

M, (1/n)	23.306
(dLV/dLP)t	-1.04652
(dLV/dLT)p	1.7637
Cp, KJ/(KG)(K)	6.4822
GAMMA s	1.1424
SON VEL, M/SEC	1251.7

DETONATION PARAMETERS

P/P1	84.981
T/T1	12.814
M/M1	0.2812
RHO/RHO1	1.8650
DET MACH NUMBER	12.7787
DET VEL, M/SEC	2334.5

MASS FRACTIONS

*CO	0.25485
*CO2	0.17231
COOH	0.00003
*H	0.00148
HCO	0.00003
HNO	0.00004
HNO2	0.00001
HO2	0.00022
*H2	0.00590
H2O	0.19823
H2O2	0.00003
*N	0.00003
*NH	0.00001
*NO	0.02488
NO2	0.00005
*N2	0.23517
N2O	0.00001
*O	0.01359
*OH	0.05442
*O2	0.03869

* THERMODYNAMIC PROPERTIES
FITTED TO 20000.K

NOTE. WEIGHT FRACTION OF FUEL
IN TOTAL FUELS AND OF OXIDANT IN
TOTAL OXIDANTS

NASA-GLENN CHEMICAL
EQUILIBRIUM PROGRAM CEA2,
FEBRUARY 5, 2004
BY BONNIE MCBRIDE AND
SANFORD GORDON
REFS: NASA RP-1311, PART I, 1994
AND NASA RP-1311, PART II, 1996

Pressure (1 value):
p,bar= 1
Temperature (1 value):
t,k= 300

Equivalence based on Fuel/Oxid. wt ratio
(Eq 9.19*) (3 values):
phi = .8, 1, 1.2

You selected the following fuels and
oxidizers:
reac
fuel CH4 wt%=100.0000
oxid Air wt%=100.0000

REACTANT	WT
FRACTION	ENERGY TEMP
KJ/KG-MOL K	
FUEL CH4	1.0000000
0.000 0.000	
OXIDANT Air	
1.0000000 0.000 0.000	

O/F= 21.54815 %FUEL= 4.434953
R,EQ.RATIO= 0.800304 PHI,EQ.RATIO=
0.800000

UNBURNED GAS

P1, BAR 1.0000
T1, K 300.00
H1, KJ/KG -208.41
M1, (1/n) 27.966
GAMMA1 1.3903
SON VEL1,M/SEC 352.1

BURNED GAS

P, BAR 15.510
T, K 2591.33
RHO, KG/CU M 1.9998 0
H, KJ/KG 801.45
U, KJ/KG 25.878
G, KJ/KG -22910.4
S, KJ/(KG)(K) 9.1505

M, (1/n) 27.780
(dLV/dLP)t -1.00274
(dLV/dLT)p 1.0702
Cp, KJ/(KG)(K) 2.0768
GAMMAs 1.1938
SON VEL,M/SEC 962.2

DETONATION PARAMETERS

P/P1 15.510
T/T1 8.638
M/M1 0.9934
RHO/RHO1 1.7837
DET MACH NUMBER 4.8739
DET VEL,M/SEC 1716.3

MASS FRACTIONS

*Ar 0.01234
*CO 0.00577
*CO2 0.11307
*H 0.00001
HO2 0.00001
*H2 0.00013
H2O 0.09563
*NO 0.01116
NO2 0.00002

*N2 0.71647
 *O 0.00061
 *OH 0.00500
 *O2 0.03976

(dLV/dLT)p 1.1553
 Cp, KJ/(KG)(K) 2.7105
 GAMMA_s 1.1685
 SON VEL,M/SEC 996.7

* THERMODYNAMIC PROPERTIES
 FITTED TO 20000.K

DETONATION PARAMETERS

NOTE. WEIGHT FRACTION OF FUEL
 IN TOTAL FUELS AND OF OXIDANT IN
 TOTAL OXIDANTS

P/P1 17.073
 T/T1 9.262
 M/M1 0.9795
 RHO/RHO1 1.8057
 DET MACH NUMBER 5.0941
 DET VEL,M/SEC 1799.7

REACTANT WT
 FRACTION ENERGY TEMP

MASS FRACTIONS

KJ/KG-MOL K
 FUEL CH4 1.0000000
 0.000 0.000
 OXIDANT Air
 1.0000000 0.000 0.000

*Ar 0.01221
 *CO 0.02436
 *CO2 0.11259
 *H 0.00006
 HO2 0.00001
 *H2 0.00063
 H2O 0.11358
 *NO 0.00791
 NO2 0.00001
 *N2 0.71008
 *O 0.00070
 *OH 0.00645
 *O2 0.01141

O/F= 17.23852 %FUEL= 5.482900
 R, EQ.RATIO= 1.000000 PHI, EQ.RATIO=
 1.000000

* THERMODYNAMIC PROPERTIES
 FITTED TO 20000.K

UNBURNED GAS

NOTE. WEIGHT FRACTION OF FUEL
 IN TOTAL FUELS AND OF OXIDANT IN
 TOTAL OXIDANTS

P1, BAR 1.0000
 T1, K 300.00
 H1, KJ/KG -257.08
 M1, (1/n) 27.740
 GAMMA1 1.3881
 SON VEL1,M/SEC 353.3

BURNED GAS

REACTANT WT
 FRACTION ENERGY TEMP

P, BAR 17.073
 T, K 2778.45
 RHO, KG/CU M 2.0081 0
 H, KJ/KG 865.73
 U, KJ/KG 15.553
 G, KJ/KG -25319.1
 S, KJ/(KG)(K) 9.4243

KJ/KG-MOL K
 FUEL CH4 1.0000000
 0.000 0.000
 OXIDANT Air
 1.0000000 0.000 0.000

M, (1/n) 27.172
 (dLV/dLP)_t -1.00648

O/F= 14.36544 %FUEL= 6.508114
 R,EQ.RATIO= 1.199696 PHI,EQ.RATIO=
 1.200000

UNBURNED GAS

P1, BAR 1.0000
 T1, K 300.00
 H1, KJ/KG -304.68
 M1, (1/n) 27.522
 GAMMA1 1.3861
 SON VEL1,M/SEC 354.4

BURNED GAS

P, BAR 17.375
 T, K 2781.52
 RHO, KG/CU M 1.9785 0
 H, KJ/KG 851.15
 U, KJ/KG -27.035
 G, KJ/KG -26021.5
 S, KJ/(KG)(K) 9.6611

M, (1/n) 26.335
 (dLV/dLP)t -1.00412
 (dLV/dLT)p 1.0987
 Cp, KJ/(KG)(K) 2.3438
 GAMMAs 1.1883
 SON VEL,M/SEC 1021.6

DETONATION PARAMETERS

P/P1 17.375
 T/T1 9.272
 M/M1 0.9569
 RHO/RHO1 1.7931
 DET MACH NUMBER 5.1680
 DET VEL,M/SEC 1831.7

MASS FRACTIONS

*Ar 0.01208
 *CO 0.05599
 *CO2 0.09101
 *H 0.00011
 *H2 0.00196

H2O 0.12546
 *NO 0.00284
 *N2 0.70471
 *O 0.00026
 *OH 0.00411
 *O2 0.00147

* THERMODYNAMIC PROPERTIES
 FITTED TO 20000.K

NOTE. WEIGHT FRACTION OF FUEL
 IN TOTAL FUELS AND OF OXIDANT IN
 TOTAL OXIDANTS

NASA-GLENN CHEMICAL
 EQUILIBRIUM PROGRAM CEA2,
 FEBRUARY 5, 2004
 BY BONNIE MCBRIDE AND
 SANFORD GORDON

REFS: NASA RP-1311, PART I, 1994
 AND NASA RP-1311, PART II, 1996

Pressure (1 value):

p,bar= 1

Temperature (1 value):

t,k= 300

Equivalence based on Fuel/Oxid. wt ratio
 (Eq 9.19*) (3 values):
 phi = .8, 1, 1.2

You selected the following fuels and
 oxidizers:

reac

fuel CH4 wt%=100.0000

oxid O2 wt%=100.0000

REACTANT		WT
FRACTION	ENERGY	TEMP
KJ/KG-MOL	K	
FUEL CH4		1.0000000
0.000	0.000	
OXIDANT O2		
1.0000000	0.000	0.000
O/F= 4.98658 %FUEL= 16.704030		
R,EQ.RATIO= 0.800000 PHI,EQ.RATIO= 0.800000		

UNBURNED GAS

P1, BAR 1.0000
 T1, K 300.00
 H1, KJ/KG -774.66
 M1, (1/n) 27.440
 GAMMA1 1.3632
 SON VEL1,M/SEC 352.0

BURNED GAS

P, BAR 27.245
 T, K 3653.66
 RHO, KG/CU M 2.0384 0
 H, KJ/KG 1061.94
 U, KJ/KG -274.62
 G, KJ/KG -42483.2
 S, KJ/(KG)(K) 11.9182

M, (1/n) 22.729
 (dLV/dLP)t -1.06411
 (dLV/dLT)p 2.0990
 Cp, KJ/(KG)(K) 9.0229
 GAMMA1 1.1293
 SON VEL,M/SEC 1228.6

DETONATION PARAMETERS

P/P1 27.245
 T/T1 12.179
 M/M1 0.8283
 RHO/RHO1 1.8530
 DET MACH NUMBER 6.4671

DET VEL,M/SEC 2276.5

MASS FRACTIONS

*CO	0.15527
*CO2	0.21426
COOH	0.00001
*H	0.00150
HCO	0.00001
HO2	0.00056
*H2	0.00407
H2O	0.27170
H2O2	0.00004
*O	0.03758
*OH	0.10089
*O2	0.21410

* THERMODYNAMIC PROPERTIES
FITTED TO 20000.K

NOTE. WEIGHT FRACTION OF FUEL
IN TOTAL FUELS AND OF OXIDANT IN
TOTAL OXIDANTS

REACTANT		WT
FRACTION	ENERGY	TEMP
KJ/KG-MOL	K	
FUEL CH4		1.0000000
0.000	0.000	
OXIDANT O2		
1.0000000	0.000	0.000

O/F= 3.98926 %FUEL= 20.043038
 R,EQ.RATIO= 1.000000 PHI,EQ.RATIO= 1.000000

UNBURNED GAS

P1, BAR 1.0000
 T1, K 300.00
 H1, KJ/KG -929.85
 M1, (1/n) 26.680
 GAMMA1 1.3584
 SON VEL1,M/SEC 356.4

BURNED GAS

P, BAR 29.123
T, K 3718.48
RHO, KG/CU M 1.9830 0
H, KJ/KG 1093.87
U, KJ/KG -374.75
G, KJ/KG -46012.5
S, KJ/(KG)(K) 12.6682

M, (1/n) 21.052
(dLV/dLP)t -1.07079
(dLV/dLT)p 2.1824
Cp, KJ/(KG)(K) 10.0867
GAMMA_s 1.1308
SON VEL,M/SEC 1288.7

DETONATION PARAMETERS

P/P1 29.123
T/T1 12.395
M/M1 0.7890
RHO/RHO1 1.8539
DET MACH NUMBER 6.7042
DET VEL,M/SEC 2389.2

MASS FRACTIONS

*CO 0.22376
*CO2 0.19823
COOH 0.00002
*H 0.00229
HCO 0.00001
HO2 0.00042
*H2 0.00719
H2O 0.31083
H2O2 0.00004
*O 0.03296
*OH 0.10282
*O2 0.12142

* THERMODYNAMIC PROPERTIES
FITTED TO 20000.K

NOTE. WEIGHT FRACTION OF FUEL
IN TOTAL FUELS AND OF OXIDANT IN
TOTAL OXIDANTS

REACTANT		WT
FRACTION	ENERGY	TEMP
KJ/KG-MOL	K	
FUEL CH4		1.0000000
0.000	0.000	
OXIDANT O2		
1.0000000	0.000	0.000

O/F= 3.32439 %FUEL= 23.124669
R,EQ.RATIO= 1.200000 PHI,EQ.RATIO=
1.200000

UNBURNED GAS

P1, BAR 1.0000
T1, K 300.00
H1, KJ/KG -1073.08
M1, (1/n) 26.015
GAMMA1 1.3544
SON VEL1,M/SEC 360.4

BURNED GAS

P, BAR 30.564
T, K 3734.39
RHO, KG/CU M 1.9332 0
H, KJ/KG 1108.90
U, KJ/KG -472.13
G, KJ/KG -48668.9
S, KJ/(KG)(K) 13.3296

M, (1/n) 19.639
(dLV/dLP)t -1.06810
(dLV/dLT)p 2.1260
Cp, KJ/(KG)(K) 10.3063
GAMMA_s 1.1332
SON VEL,M/SEC 1338.5

DETONATION PARAMETERS

P/P1 30.564
T/T1 12.448
M/M1 0.7549
RHO/RHO1 1.8536
DET MACH NUMBER 6.8850
DET VEL,M/SEC 2481.1

MASS FRACTIONS

*CO 0.29235
*CO2 0.17498
COOH 0.00002
*H 0.00304
HCO 0.00002
HO2 0.00026
*H2 0.01159
H2O 0.33934
H2O2 0.00003
*O 0.02446
*OH 0.09293
*O2 0.06097

* THERMODYNAMIC PROPERTIES
FITTED TO 20000.K

NOTE. WEIGHT FRACTION OF FUEL
IN TOTAL FUELS AND OF OXIDANT IN
TOTAL OXIDANTS

NASA-GLENN CHEMICAL
EQUILIBRIUM PROGRAM CEA2,
FEBRUARY 5, 2004
BY BONNIE MCBRIDE AND
SANFORD GORDON
REFS: NASA RP-1311, PART I, 1994
AND NASA RP-1311, PART II, 1996

Pressure (1 value):

p,bar= 1

Temperature (1 value):

t,k= 300

Equivalence based on Fuel/Oxid. wt ratio
(Eq 9.19*) (3 values):

phi = .8, 1, 1.2

You selected the following fuels and
oxidizers:

reac

fuel CH4 wt%=100.0000

oxid NO2 wt%=100.0000

DETONATION PROPERTIES
OF AN IDEAL REACTING GAS

CASE = _____

REACTANT	WT
FRACTION	ENERGY TEMP
	(SEE NOTE)
KJ/KG-MOL K	
FUEL CH4	1.0000000
0.000 0.000	
OXIDANT NO2	
1.0000000 0.000 0.000	

O/F= 7.16933 %FUEL= 12.240900
R,EQ.RATIO= 0.800000 PHI,EQ.RATIO=
0.800000

UNBURNED GAS

P1, BAR 1.0000
T1, K 300.00
H1, KJ/KG 84.85
M1, (1/n) 37.445
GAMMA1 1.2917
SON VEL1,M/SEC 293.3

BURNED GAS

P, BAR 34.832
T, K 3619.92
RHO, KG/CU M 2.7868 0
H, KJ/KG 1818.71
U, KJ/KG 568.82
G, KJ/KG -38651.0
S, KJ/(KG)(K) 11.1797

M, (1/n) 24.080
(dLV/dLP)t -1.04641
(dLV/dLT)p 1.8066
Cp, KJ/(KG)(K) 6.8435
GAMMA_s 1.1341
SON VEL,M/SEC 1190.6

DETONATION PARAMETERS

P/P1 34.832
T/T1 12.066
M/M1 0.6431
RHO/RHO1 1.8564
DET MACH NUMBER 7.5348
DET VEL,M/SEC 2210.3

MASS FRACTIONS

*CO 0.11267
*CO2 0.15875
COOH 0.00001
*H 0.00103
HNO 0.00003
HNO2 0.00001
HO2 0.00036
*H2 0.00299
H2O 0.20230
H2O2 0.00003
*N 0.00002
*NO 0.04078
NO2 0.00011
*N2 0.24808
N2O 0.00001
*O 0.02410
*OH 0.06907
*O2 0.13964

* THERMODYNAMIC PROPERTIES
FITTED TO 20000.K

NOTE. WEIGHT FRACTION OF FUEL
IN TOTAL FUELS AND OF OXIDANT IN
TOTAL OXIDANTS

REACTANT	WT	
FRACTION	ENERGY	TEMP
KJ/KG-MOL	K	
FUEL	CH4	1.0000000
0.000	0.000	
OXIDANT	NO2	
1.0000000	0.000	0.000

O/F= 5.73547 %FUEL= 14.846780
R,EQ.RATIO= 1.000000 PHI,EQ.RATIO=
1.000000

UNBURNED GAS

P1, BAR 1.0000
T1, K 300.00
H1, KJ/KG -55.62
M1, (1/n) 36.018
GAMMA1 1.2925
SON VEL1,M/SEC 299.2

BURNED GAS

P, BAR 36.336
T, K 3686.51
RHO, KG/CU M 2.6810 0
H, KJ/KG 1826.96
U, KJ/KG 471.66
G, KJ/KG -41530.6
S, KJ/(KG)(K) 11.7611

M, (1/n) 22.616
(dLV/dLP)t -1.05269
(dLV/dLT)p 1.8943
Cp, KJ/(KG)(K) 7.6821
GAMMA_s 1.1351
SON VEL,M/SEC 1240.3

DETONATION PARAMETERS

P/P1 36.336
T/T1 12.288
M/M1 0.6279
RHO/RHO1 1.8567
DET MACH NUMBER 7.6976
DET VEL,M/SEC 2303.0

MASS FRACTIONS

*CO 0.16559
*CO2 0.14709
COOH 0.00001
*H 0.00161
HCO 0.00001
HNO 0.00003
HNO2 0.00001
HO2 0.00027
*H2 0.00540
H2O 0.23311
H2O2 0.00003
*N 0.00002
*NH 0.00001
*NO 0.03198
NO2 0.00006
*N2 0.24426
N2O 0.00001
*O 0.02127
*OH 0.07093
*O2 0.07830

* THERMODYNAMIC PROPERTIES
FITTED TO 20000.K

NOTE. WEIGHT FRACTION OF FUEL
IN TOTAL FUELS AND OF OXIDANT IN
TOTAL OXIDANTS

REACTANT	WT
FRACTION ENERGY	TEMP
KJ/KG-MOL K	
FUEL CH4	1.0000000
0.000 0.000	
OXIDANT NO2	
1.0000000 0.000	0.000

O/F= 4.77956 %FUEL= 17.302368
R,EQ.RATIO= 1.200000 PHI,EQ.RATIO= 1.200000

UNBURNED GAS

P1, BAR 1.0000
T1, K 300.00
H1, KJ/KG -188.00
M1, (1/n) 34.769
GAMMA1 1.2931
SON VEL1,M/SEC 304.6

BURNED GAS

P, BAR 37.371
T, K 3703.88
RHO, KG/CU M 2.5866 0
H, KJ/KG 1819.68
U, KJ/KG 374.90
G, KJ/KG -43681.9
S, KJ/(KG)(K) 12.2849

M, (1/n) 21.315
(dLV/dLP)t -1.05173
(dLV/dLT)p 1.8711
Cp, KJ/(KG)(K) 7.9131
GAMMA s 1.1375
SON VEL,M/SEC 1281.9

DETONATION PARAMETERS

P/P1 37.371
T/T1 12.346
M/M1 0.6130
RHO/RHO1 1.8556
DET MACH NUMBER 7.8102
DET VEL,M/SEC 2378.8

MASS FRACTIONS

*CO 0.21926
*CO2 0.13011
COOH 0.00002
*H 0.00217
HCO 0.00002

HNO	0.00002
HO2	0.00017
*H2	0.00885
H2O	0.25585
H2O2	0.00002
*N	0.00003
*NH	0.00001
*NO	0.02278
NO2	0.00003
*N2	0.24108
N2O	0.00001
*O	0.01589
*OH	0.06453
*O2	0.03915

* THERMODYNAMIC PROPERTIES
FITTED TO 20000.K

NOTE. WEIGHT FRACTION OF FUEL
IN TOTAL FUELS AND OF OXIDANT IN
TOTAL OXIDANTS

NASA-GLENN CHEMICAL
EQUILIBRIUM PROGRAM CEA2,
FEBRUARY 5, 2004

BY BONNIE MCBRIDE AND
SANFORD GORDON

REFS: NASA RP-1311, PART I, 1994
AND NASA RP-1311, PART II, 1996

Pressure (1 value):

p,bar= 1

Temperature (1 value):

t,k= 300

Equivalence based on Fuel/Oxid. wt ratio
(Eq 9.19*) (3 values):

phi = .8, 1, 1.2

You selected the following fuels and
oxidizers:

reac

fuel CH4

wt%=100.0000

oxid N2O4

wt%=100.0000

REACTANT	WT
FRACTION	ENERGY
TEMP	
KJ/KG-MOL	K
FUEL	CH4
0.000	0.000
OXIDANT	N2O4
1.0000000	0.000
	0.000
	1.0000000

O/F= 7.16933 %FUEL= 12.240900
R,Eq.RATIO= 0.800000 PHI,Eq.RATIO=
0.800000

UNBURNED GAS

P1, BAR 1.0000
T1, K 300.00
H1, KJ/KG -461.34
M1, (1/n) 58.247
GAMMA1 1.1609
SON VEL1,M/SEC 223.0

BURNED GAS

P, BAR 52.680
T, K 3588.91
RHO, KG/CU M 4.3545 0
H, KJ/KG 1238.62
U, KJ/KG 28.851
G, KJ/KG -37800.5
S, KJ/(KG)(K) 10.8777

M, (1/n) 24.666
(dLV/dLP)t -1.03889
(dLV/dLT)p 1.6885
Cp, KJ/(KG)(K) 6.1067
GAMMA s 1.1344
SON VEL,M/SEC 1171.5

DETONATION PARAMETERS

P/P1 52.680
T/T1 11.963
M/M1 0.4235
RHO/RHO1 1.8648
DET MACH NUMBER 9.7979
DET VEL,M/SEC 2184.6

MASS FRACTIONS

*CO 0.09774
*CO2 0.18221
COOH 0.00001
*H 0.00070
HNO 0.00003
HNO2 0.00001
HO2 0.00039
*H2 0.00241
H2O 0.21497
H2O2 0.00003
*N 0.00001
*NO 0.03915
NO2 0.00013
*N2 0.24883
N2O 0.00001
*O 0.01769
*OH 0.06049
*O2 0.13516

* THERMODYNAMIC PROPERTIES
FITTED TO 20000.K

NOTE. WEIGHT FRACTION OF FUEL
IN TOTAL FUELS AND OF OXIDANT IN
TOTAL OXIDANTS

REACTANT	WT
FRACTION ENERGY	TEMP
KJ/KG-MOL K	
FUEL CH4	1.0000000
0.000 0.000	
OXIDANT N2O4	
1.0000000 0.000 0.000	

O/F= 5.73547 %FUEL= 14.846780
R,EQ.RATIO= 1.000000 PHI,EQ.RATIO= 1.000000

UNBURNED GAS

P1, BAR 1.0000
T1, K 300.00
H1, KJ/KG -585.60
M1, (1/n) 54.027
GAMMA1 1.1688
SON VEL1,M/SEC 232.3

BURNED GAS

P, BAR 53.232
T, K 3668.52
RHO, KG/CU M 4.0382 0
H, KJ/KG 1266.85
U, KJ/KG -51.351
G, KJ/KG -40811.4
S, KJ/(KG)(K) 11.4701

M, (1/n) 23.139
(dLV/dLP)t -1.04573
(dLV/dLT)p 1.7873
Cp, KJ/(KG)(K) 6.9654
GAMMA s 1.1352
SON VEL,M/SEC 1223.3

DETONATION PARAMETERS

P/P1 53.232
T/T1 12.228
M/M1 0.4283
RHO/RHO1 1.8644
DET MACH NUMBER 9.8178
DET VEL,M/SEC 2280.6

MASS FRACTIONS

*CO 0.15310
*CO2 0.16670
COOH 0.00002
*H 0.00118
HCO 0.00001

HNO	0.00003
HNO2	0.00001
HO2	0.00028
*H2	0.00469
H2O	0.24745
H2O2	0.00003
*N	0.00002
*NH	0.00001
*NO	0.03028
NO2	0.00007
*N2	0.24505
N2O	0.00001
*O	0.01599
*OH	0.06306
*O2	0.07200

* THERMODYNAMIC PROPERTIES
FITTED TO 20000.K

NOTE. WEIGHT FRACTION OF FUEL
IN TOTAL FUELS AND OF OXIDANT IN
TOTAL OXIDANTS

REACTANT	WT
FRACTION	ENERGY
KJ/KG-MOL	K
FUEL	CH4
0.000	0.000
OXIDANT	N2O4
1.0000000	0.000
	0.000

O/F= 4.77956 %FUEL= 17.302368
R,EQ.RATIO= 1.200000 PHI,EQ.RATIO=
1.200000

UNBURNED GAS

P1, BAR	1.0000
T1, K	300.00
H1, KJ/KG	-702.69
M1, (1/n)	50.574
GAMMA1	1.1758
SON VEL1,M/SEC	240.8

BURNED GAS

P, BAR	53.161
T, K	3685.76
RHO, KG/CU M	3.7757 0
H, KJ/KG	1274.36
U, KJ/KG	-133.60
G, KJ/KG	-42959.5
S, KJ/(KG)(K)	12.0013
M, (1/n)	21.766
(dLV/dLP)t	-1.04446
(dLV/dLT)p	1.7591
Cp, KJ/(KG)(K)	7.1340
GAMMA _s	1.1380
SON VEL,M/SEC	1265.8

DETONATION PARAMETERS

P/P1	53.161
T/T1	12.286
M/M1	0.4304
RHO/RHO1	1.8622
DET MACH NUMBER	9.7881
DET VEL,M/SEC	2357.2

MASS FRACTIONS

*CO	0.21014
*CO2	0.14444
COOH	0.00002
*H	0.00166
HCO	0.00002
HNO	0.00003
HNO2	0.00001
HO2	0.00017
*H2	0.00812
H2O	0.27112
H2O2	0.00002
*N	0.00002
*NH	0.00001
*NO	0.02071
NO2	0.00003
*N2	0.24205
N2O	0.00001
*O	0.01165

*OH 0.05660
*O2 0.03318

NOTE. WEIGHT FRACTION OF FUEL IN
TOTAL FUELS AND OF OXIDANT IN
TOTAL OXIDANT

* THERMODYNAMIC PROPERTIES
FITTED TO 20000.K