Investigation of Detonation Theory and the Continuously Rotating Detonation Engine

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By

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ABSTRACT

INVESTIGATION OF DETONATION THEORY AND

THE CONTINUOUSLY ROTATING DETONATION ENGINE

by Samuel Zuniga

The continuous rotating detonation engine (CRDE) has gained attention from researchers across the world due to its high thermal efficiency and simple structure in comparison to other deflagration-detonation based propulsion systems. In this paper, the development of the continuous rotating detonation engine (CRDE) is summarized by providing numerical and experimental work done by various researchers. A background on detonation based combustion theory is established and utilized to benchmark simple detonation wave simulations. The simulation analysis demonstrates that ANSYS Fluent can be used to model ZND (Zeldovich-von Neumann-Döring) and Chapman-Jouguet conditions. A two-dimensional CRDE is then analyzed for a one-step hydrogen-air reaction model. Due to the complexity and importance for stability, both ideal and non-ideal injection conditions are explored.

ACKNOWLEDGEMENTS

I would like to thank Dr. Papadopoulos for all the support and guidance throughout this project. Additionally, I would like to extend my gratitude to a colleague of mine Bhagyashree Nagarkar, for her assistance and support throughout the project. Lastly, I would like to thank my family and friends for being alongside me throughout my educational career.

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Nomenclature

2D = 2-Dimensional

3D = 3-Dimensional

PDE = Pulse Detonation Engine

RDE = Rotational Detonation Engine

CRDE = Continuous Rotating Detonation

RDRE = Rotational Detonation Rocket Engine

= Density

= Velocity

= Total energy per unit mass

= Pressure

= Viscous stress tensor

= Heat flux

K, A = Pre-exponential factors

= Activation energy

= Specific gas constant

= Mass Fraction of the Reactants

= Temperature

= Reactant Species Mass Fraction

= Product Species Mass Fraction

CHAPTER 1: INTRODUCTION

1.1 MOTIVATION

The developing of high performance propulsion systems for commercial and defense applications has sparked an interest in detonation-based propulsion systems because of the difficulty to further improve deflagration-based engines in terms of efficiency and its potential advantages. [1] In a detonation-based propulsion system the detonation wave is sustained by auto-ignition caused by the increased temperature during the adiabatic shock compression of the unburned mixture. The burning and material conversion are so rapid in the detonation that the overall process is thermodynamically close to a constant volume process, compared with a conventional constant pressure process in propulsion systems.[2] Currently, there are several types of detonation-based propulsion systems, including pulsed detonation engines, oblique detonation engines, and rotating detonation engines.

The most studied and developed detonation engine concept is the pulse detonation engine (PDE) due to its simplicity. PDE typically[3] consists of a sufficiently long tube, which is filled with fresh fuel–oxidizer mixture and ignited by a sufficiently strong energy source. The flame initiated by ignition must, in a relatively short time, accelerate to the detonation velocity, such that the transition from deflagration to detonation happens in a relatively small distance. Detonative combustion produces high pressure, which is converted to thrust. After all of the combustible mixture is consumed by detonation, combustion products have to be evacuated from the tube and fresh mixture must be quickly resupplied, and the cycle is repeated as shown in figure 1.

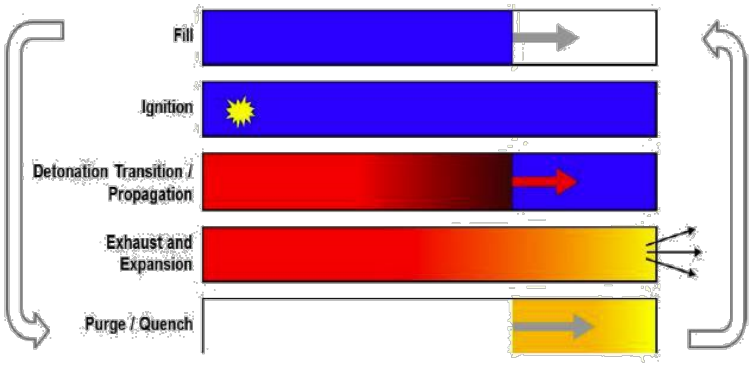

Figure 1: Pulse Detonation Engine Cycle[4]

While the PDE is attractive and successful in many respects, the concept also has many challenges yet to be resolved. These challenges include the[4] complex valving of fresh reactants which adds weight, timing and control of valving for efficient operation, repeated ignition for detonation after each cycle, the length of tube required to achieve deflagration to detonation transition increases the combustor size, and a limiting operating frequency range of 10-100 Hz.

In recent years, the Rotational Detonation Engine (RDE) has gained a lot of attention due to its additional advantages in comparison to the PDE. First off, [4]RDEs continuous valveless injection of reactants is mechanically and aerodynamically superior to the valved PDE, because it reduces weight, complexity, and unsteadiness in upstream components. The RDE has a very simple annular structure that improves its ease of integration with existing components and it only needs to be ignited once. In addition, it can[5] operate under various conditions, such as different altitudes and fuel injection conditions. Furthermore, precise timing and control is generally limited to a single detonation initiation event, and transition to detonation is only required during startup, as a stable detonation can be continuously maintained. Lastly, RDEs generally operate in the kilohertz regime, resulting in exhaust pulsations that are more easily mixed out, reducing the

unsteadiness on downstream components. Therefore, due to considerable advantages the RDE has over the PDE, it has become the favorable candidate for future detonation engine applications.

1.2 BACKGROUND & THEORY

1.2.1 Rotational Detonation Engine Model

The combustor chamber of a RDE is an annular chamber. The inlet end of the combustor is closed but drilled with micro nozzles or slits to inject fuel and oxidizer into the chamber. A basic RDE combustion chamber model is shown in figure 2.

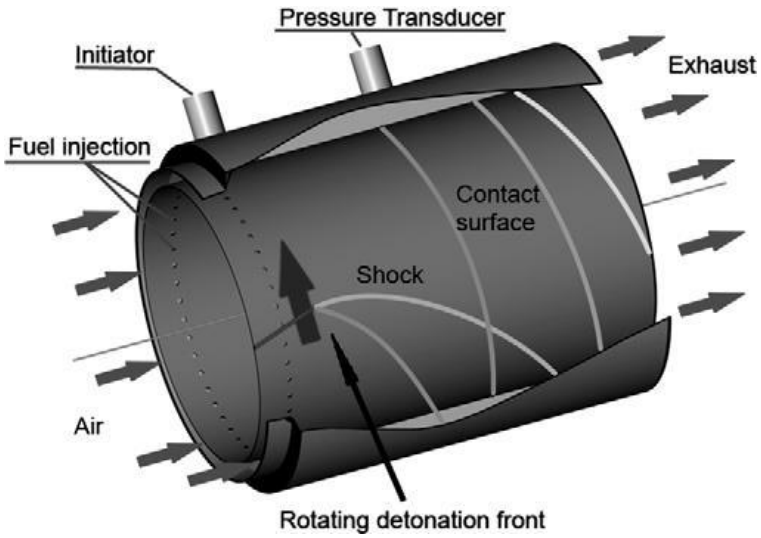

Figure 2: Three-dimensional view of CRDE[3]

An RDE is initiated by a detonation tangentially into an inlet channel that is being continuously filled with the fresh reactants. [6]Since the channel is continuously filled and does not require a purge cycle, the detonation is free to propagate indefinitely in the channel as long as the detonable mixture is supplied. [7]During the operation period, one or more detonation waves lean on the injection end and propagate in the circumferential direction. In front of the detonation wave, there is an area filled with fresh reactants, while behind the detonation wave are burnt products of

high temperature and high pressure. Downstream inside the chamber there are contact surfaces, an oblique shock wave, and expansion waves that enhance the ejection of the burnt product out of the exit almost axially to produce thrust.

1.2.2 Deflagration vs Detonation

There are two models of combustion for a detonative mixture, deflagration and detonation. By definition,[8-10] deflagration is a subsonic wave that is sustained by a chemical reaction, which propagates with a velocity in the order of m/s. Typically, all aircraft turbines are driven by deflagration. In the case of detonation, a combustion wave that is sustained by a chemical reaction, propagates at a supersonic velocity in the order of km/s and result in a higher density and pressure than the initial mixture. During the detonation process, a discontinuous change of velocity can be observed from an initial low speed to the detonation high speed. This occurs when the detonation front has initiated the chemical reaction extremely quickly by compressing the preheated gases, resulting in an increase in temperature and pressure. When comparing the two, detonation is favorable for future application because of its quick heat release, entropy change is smaller, and thermal efficiency is greater.

Shown below in figure 3 are a list of qualitative differences between deflagration and detonation in gases. It can be seen that the Mach, pressure, temperature, and density of a detonation is much higher than that of deflagration, thus making it a topic of interest.

Ratio	Usual magnitude of ratio	
	Detonation	Deflagration
u_u/c_u^a	5–10	0.0001–0.03
u_b/u_u	0.4–0.7	4–16
P_b/P_u	13–55	0.98–0.976
T_b/T_u	8–21	4–16
ρ_b/ρ_u	1.4–2.6	0.06–0.25

[a] c_u is the acoustic velocity in the unburned gases. u_u/c_u is the Mach number of the wave.

Figure 3: Qualitative Differences between deflagration and detonation in gases[8]

1.2.3 C-J Condition

A detonation wave can be described by Chapman-Jouguet (C-J) theory. When using C-J theory, the detonation wave is assumed to be one-dimensional, steady, and planar, while the flow behind the supersonic wave are sonic. Figure 4 illustrates the control volume that is used to model a combustion wave:

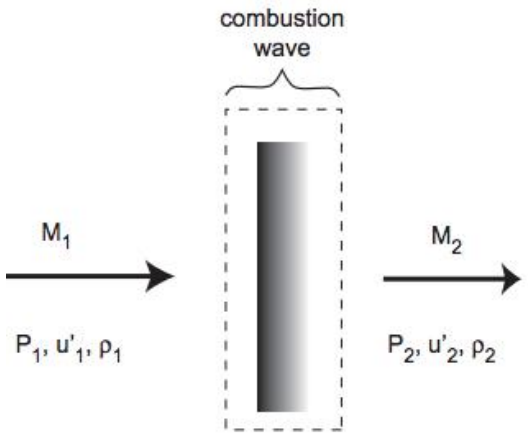

Figure 4: Combustion wave control volume for 1- dimensional analysis[10]

To understand the characteristics of the gas dynamic properties downstream and upstream of the control volume, the governing equations of conservation of mass, momentum, and energy

are applied and manipulated to derive the Hugoniot and Rayleigh relationships. Note,[8] the combustion wave is assumed to be in steady-state, is adiabatic, and remains in chemical and thermodynamic equilibrium.

Coservation of Mass: $\rho_1 u_1 = \rho_2 u_2$ (1.1)

Conservation of Momentum: $P_1 + \rho_1 u_1^2 = P_2 + \rho_2 u_2^2$ (1.2)

Conservation of Energy: $h_1 + \frac{u_1^2}{2} + q = h_2 + \frac{u_2^2}{2}$ (1.3)

Equation of state: $P_1 = \rho_1 R T_1$, $P_2 = \rho_2 R T_2$ (1.4)

where:

R = Specific gas constant

c_p = Specific heat at constant pressure

γ = Ratio of specific heats

q = Energy added due to combustion process

The Hugoniot relation can be derived by substituting the equation of state and $\gamma = \frac{c_p}{c_v}$ into the conservation of energy equation. The[8] Hugoniot relation is used to determine the range of possible solutions for a steady detonation wave.

Hugoniot Relation:

$$\frac{\gamma}{\gamma - 1}\left(\frac{P_2}{\rho_2} - \frac{P_1}{\rho_1}\right) - \frac{1}{2}(P_2 - P_1)\left(\frac{1}{\rho_2} - \frac{1}{\rho_1}\right) = q \quad (1.5)$$

The Rayleigh relation is derived substituting the conservation of mass equation into the conservation of momentum equation.

Rayleigh Relation:

$$u_2 u_2 = \frac{P_2 - P_1}{\frac{1}{\rho_1} - \frac{1}{\rho_2}} \quad (1.6)$$

The Rayleigh relation represents the transition of the reactants from an initial state to a final state, from point A to each of the C-J points. When plotting the two relations, they create the Chapman-Jouguet points at their intersection. The upper C-J point represents the steady detonation velocity solution, lower represents the maximum deflagration point as shown in figure 5. (P-pressure, V-specific volume, A-initial state, U-upper Chapman-Jouguet (C-J) point, L-lower C-J point)

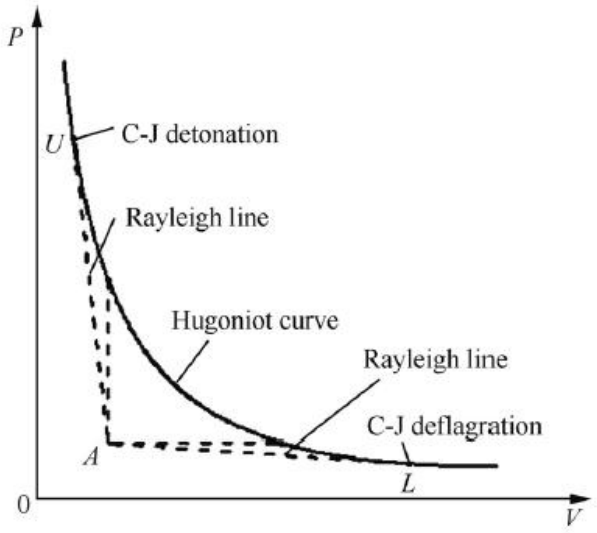

Figure 5: P-V Diagram showing C-J points[9]

The[8] C-J points are obtained by differentiating the Hugoniot relation and using it with the slope of the tangent for each of the two C-J points.

$$\{[\quad]\quad\}=\quad\quad(1.7)$$

By defining the velocity of sound of the burned gas a follows:

$$_2 = (\frac{2}{\quad}) = -\frac{1}{\quad}[\frac{2}{\quad}] \tag{1.8}$$

It can be related to the velocity of the burned gases.

$$[^2] = \frac{1}{\quad}[\frac{^2 - 1}{\quad}] = [^2] \tag{1.9}$$

It can be found that the velocity of the burned gases is equal to the velocity of sound in burned gases.

$$[_2] = [_2] \tag{1.10}$$

Thus, it is proven that the C-J condition yields sonic conditions.

1.2.4 Detonation Wave Structure - ZND Model

Zeldovich, von Neumann, and Döring developed and extension of Chapman-Jouguet theory to describe the structure of a detonation wave. The[8] ZND model stated that a detonation wave consists of a planar shock that propagates at a C-J velocity leaving a heated and compressed gas behind it. In order to evaluate the structure of the detonation wave, the kinetics of the chemical reaction must be incorporated. It is assumed that the flow is one-dimensional, neglecting transport affects, and the wave is assumed to be a discontinuity. A graphical representation of ZND theory for the pressure, temperature, and density are shown as a function of spatial distribution in figure 6.

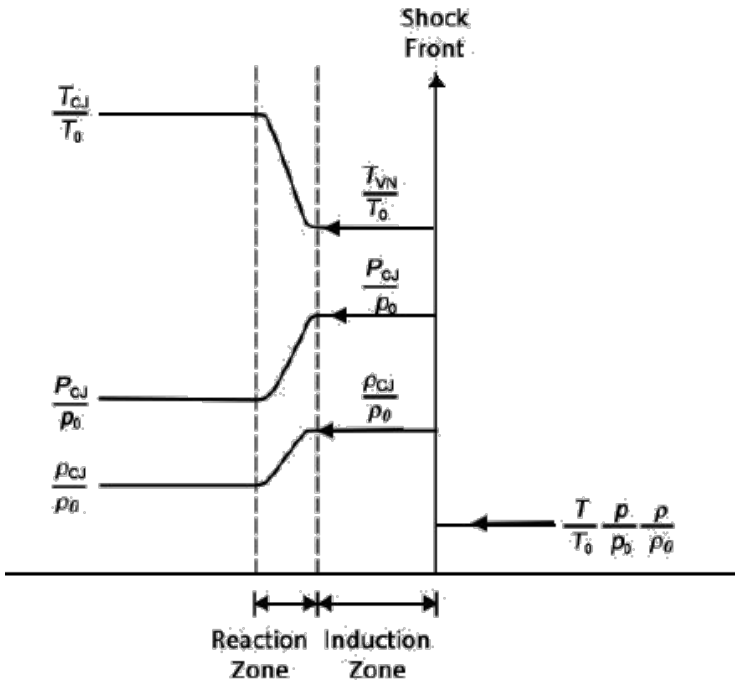

Figure 6: ZND model parameter behavior during detonation[10]

Through the shockwave a large of amount of energy is transferred into the unburned reactants, immediately increasing the pressure, temperature, and density. After the induction period, the chemical reaction begins, causing the temperature to rise and the pressure and density to fall until they reach the C-J values in which the reaction reaches equilibrium.

The structure of a detonation wave can be analyzed by inserting a soot-coated metal foil into a detonation tube. The detonation wave will leave a “fish-scale” pattern imprinted on the foil, as shown below in figure 7.

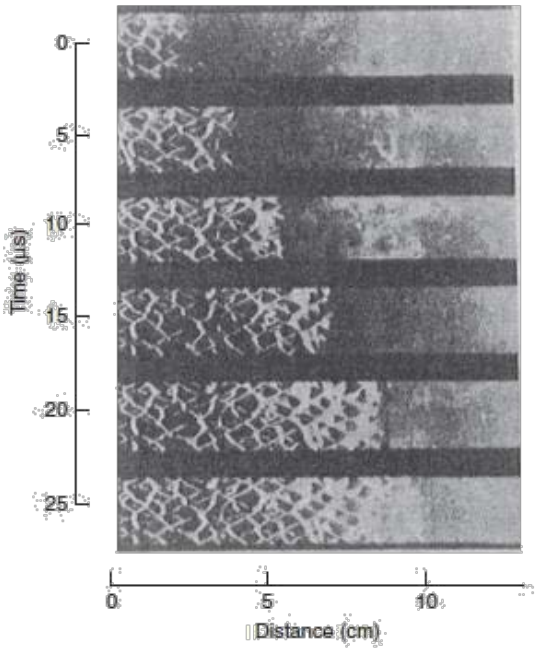

Figure 7: Detonation “Fish-scale” structure

The detonation structure has a complex 3D structure that is a result of transverse waves propagating behind the leading shock wave. At the intersections of the waves are triple points, which enable stability of the detonation, due to their high pressure and high temperature.

1.2.5 Detonation Initiation

There are two types on initiation,[8,9] direct initiation and deflagration-to-detonation (DDT). Direct initiation generally involves a spark igniter that discharges a large amount of energy that couples with the shock wave and creates a detonation wave. If the critical energy is not met, the blast wave generated will separate from the detonation front and eventually decay. If the required critical energy is too high, then DDT is used since they require less energy to generate a detonation. DDT uses obstacles in the path of the combustion wave to accelerate it to C-J velocities. Under the right conditions the deflagration wave will accelerate to a C-J velocity and transition into a

detonation wave. Both direct initiation and DDT depend on the detonation cell size, initial pressure, initial temperature, and geometric cross-sectional area. When deciding between the two detonation methods further investigation must be done in order to ensure the detonation problem is setup correctly.

1.3 LITERATURE REVIEW

1.3.1 Future Applications

If detonation based propulsion takes over deflagration based, a CRDE could be implemented into different kinds of rockets and aerial vehicles. The simplest engine utilizing continuously rotating detonation is the rocket engine. In a Rotational Detonation Rocket Engine (RDRE),[3] the products from the detonation chamber are flowing out supersonically, therefore there is no need to apply a converging-diverging nozzle and an aerospace nozzle can be attached directly to the detonation chamber, thus simplifying the engine component integration and shortening the rocket. Research on RDRE is already being carried out in many labs across the world. An example of such experiments is presented in figure 8.

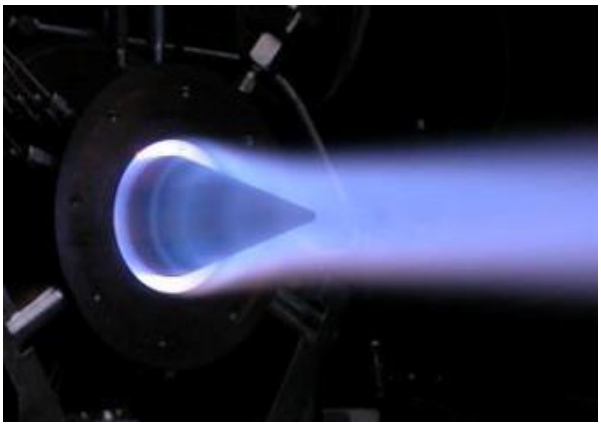

Figure 8: Rotating Detonation Rocket Engine (RDRE)[3]

The continuous rotating detonation could also be directly applied to a[3] ramjet engine; in which it would allow it to be used in a wide range of flight conditions because it is not as sensitive to the inflow. In this case, the length of the ramjet will be shortened also reducing the weight. The schematic example can be seen in figure 9.

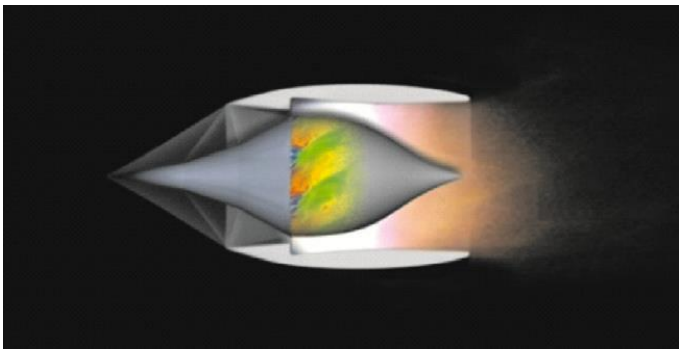

Figure 9: Rotating Detonation Ramjet Engine [11]

The continuous rotation detonation can also be applied in[3,12] turbojet engines, which would reduce the manufacturing process requirements, weight, and number of compressors due to the large effective thrust at low pressure ratio it can produce. The implementation of a CRD chamber into a turbojet engine can be seen in figure 10. The engine would be simpler and more environmentally friendly since lean mixtures can be used in CRDEs.

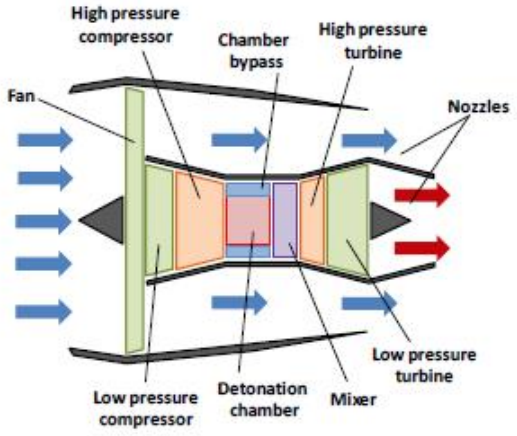

Figure 10: Rotating Detonation Turbojet Engine [13]

1.3.2 Experimental Studies

The concept of the RDE was first introduces by Voitsekhovisky[14,15] in the early 1960's. He was able to experimentally achieve short-lived continuous detonation fueled by oxy-acetylene mixtures at relatively low pressure in a disk-shaped chamber connected to a low-pressure dump chamber. This first experiment conducted at the Institute of Hydrodynamics of the Siberian Division of the Soviet Academy of Sciences in Novosibirsk was considered the first step to developing the RDE. The experimental setup is shown in figure 11.

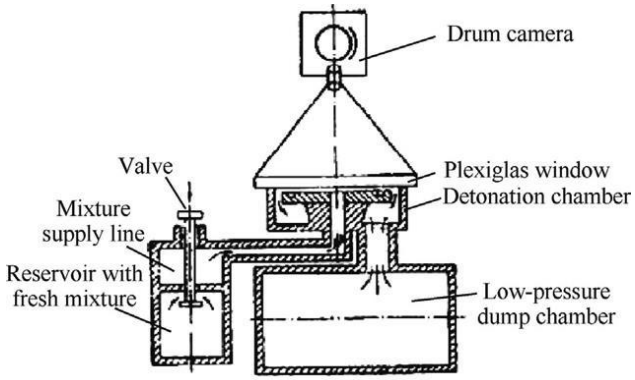

Figure 11: Schematic of the first experimented detonation chamber [14]

In more recent years, extensive experiments have been carried out by different institutions and companies. Bykovskii[16-18] at the Institute of Hydrodynamics in Russia achieved continuous detonations in combustors of different shapes under different injection systems, for various fuels and oxidizers. The fuels tested included hydrogen, acetylene, propane, methane, kerosene, gasoline, benzene, alcohol, acetone, and diesel, with the oxidants being air, gaseous oxygen, or liquid oxygen. The flow of stable detonation waves for a cylindrical chamber are shown in figure 12.

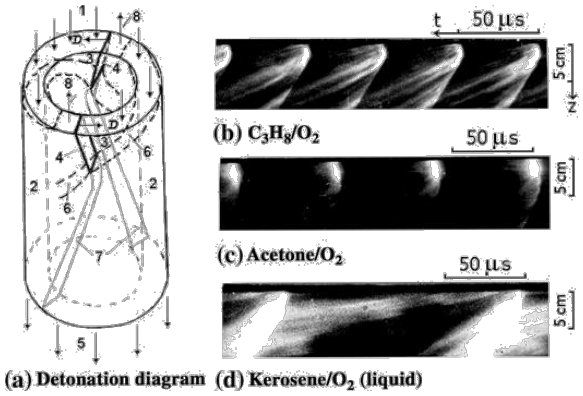

Figure 12: Detonation wave structure for different mixtures [16]

Throughout their research they proposed empirical laws to design a chamber that could achieve stable detonation waves. The[16] critical height of the mixture layer depth h^* ahead of the detonation front was related to the detonation-cell size α as $h^* = (12 \pm 5)\ \alpha$. The minimum length of the chamber was approximated by $L_{min} = 2h^*$. If the chamber length was smaller than L_{min}, then stable detonation waves would not be formed. The radial size could not be smaller than one detonation-cell size. If liquid fuel is used, the radial size should not be smaller than the minimum diameter of droplets.

Wang Jianping's research team at Peking University has done extensive research on CRDE and has progressed rapidly. In[16] 2009, they successfully achieved hydrogen/oxygen rotation detonation waves with a propagating velocity of 2041 m/s. They have also tested several CRDE with a pre-detonation tube, which can be seen in figure 13. Through their research, Wang found that a tangential flow of fresh gas from the pre-detonator would lead to a main detonation wave and a few detonation wavelets, which would slow down the detonation wave.

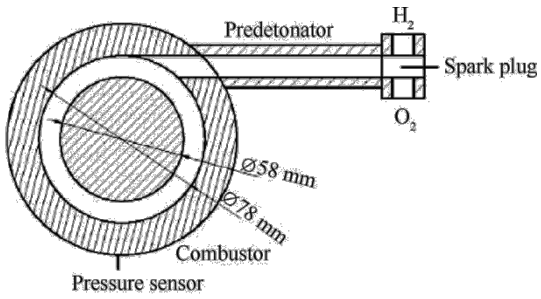

Figure 13: Pre-detonation tube used at Peking University in China [18]

Similarly, to Wang, Liu et al.[20,21], from the National University of Defense Technology in China implement a pre-detonation tube into their CRDE experiments to ignite the engine. They found that there is a small period of time gap between the initiation and formation of stable detonation wave due to the exhaust of the detonation waves. Therefore, more experimenting must be done to establish the stability of detonation waves through the use of a pre-detonator for initiation.

Also in China, Nanjing University of Science and Technology performed research on CRDEs which resulted in promising data. Zheng et al.[22], at the university achieved hydrogen-air rotating detonation waves with an equivalence ratio of 0.93, and detonation wave velocity ranging from 1518.5 to 1606.1 m/s. Peng et al.[23], also at the university experimented with slot-orifices impinging injection method during ignition with an automotive spark plug. It was found that the success rate of rotating detonation wave initiation was up to 94%.

Extensive CRDE experiments have been performed by Wolanski's research group at Warsaw University in Poland. They experimented with a[24] variety of cylindrical chambers, ranging from 50 mm to 200 mm in diameter, were tested with fuels of acetylene, hydrogen, methane, ethane, propane, and kerosene with air, oxygen-enriched air, and oxygen under different injection

stagnation conditions. Stable detonation waves were developed for long durations. An experimental cylindrical chamber is shown in figure 14.

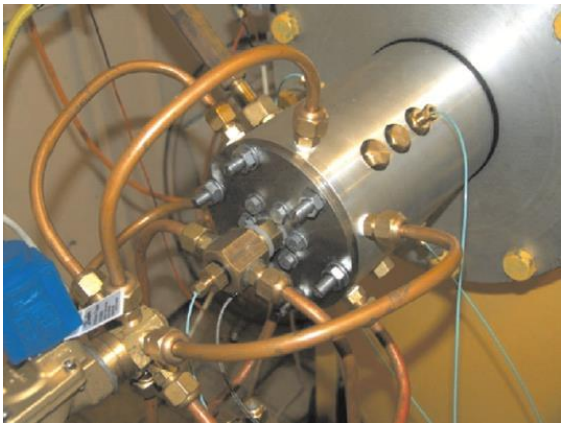

Figure 14: Experimental Cylindrical Chamber in Wolanski's Lab [24]

Wolanski et al.[3], built a small model rocket engine and achieved rotating detonation for a variety of gaseous oxygen-fuel mixtures. As fuel, gaseous hydrogen, methane, ethane, and propane were used. It was found that the values of specific impulse for a RDRE are higher than those obtained from conventional rocket engines.

More recently, Wolanski with the Polish Aviation Institute[3] have begun to research a rotating detonation turbojet engine, by replacing a GTD-350 turbojet engine combustor with a continuous detonation wave combustor as seen in figure 15. They built a research facility for CRD combustion chamber research and are now working on optimizing the chamber under different operating conditions.

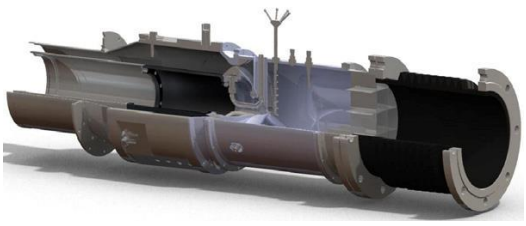

Figure 15: Continuous detonation wave combustor integrated into a GTD-350 turbojet [3]

MBDA-France[25] developed a full-size model of the engine for a supersonic missile and performed ground tests. They[26] claimed that the new continuous detonation engine would greatly reduce the mass and decrease the body length of the missile.

In the United Stated there are several research teams running experimental studies of CRDE. [27]Pratt & Whitney Rocketdyne have been investigating CRDE behavior by using modular hardware. Continuous detonation was achieved for multiple propellants and engines geometries. Their experimental setup can be seen in figure 16.

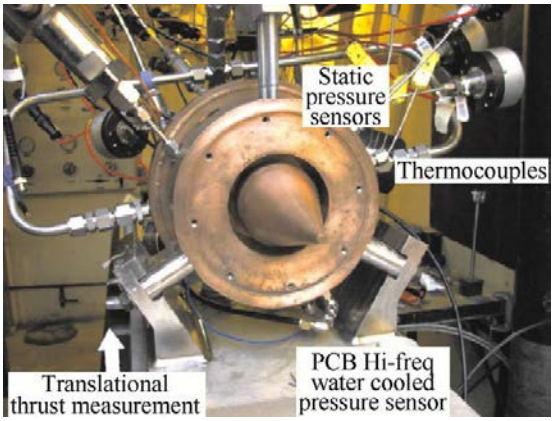

Figure 16:CRDE at Pratt & Whitney facility [27]

Since[27] 2010, Aerojet Rocketdyne have been developing and testing modular RDE hardware. They have run over 400 tests with the longest being about 7 seconds (35,000) cycles. In their experiments, they have used hydrogen, methane, and ethane as fuels for various exhaust configurations. A test RDE is shown below in figure 17.

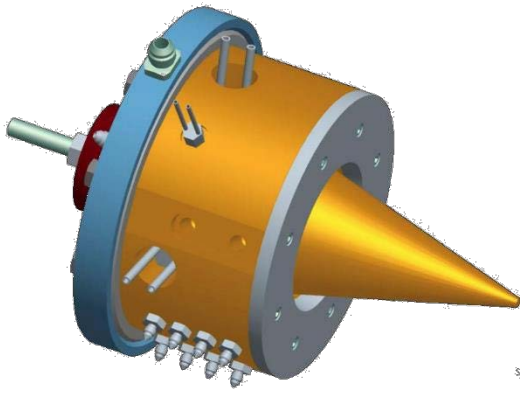

Figure 17: Aerojet Rocketdyne test RDE [27]

The Air Force Research Laboratory (AFRL) works with a few Universities to research CRDE. They[28-30] performed experiments in different chamber sizes for a wide range of flow rates and equivalence ratios for hydrogen-air and ethylene-air mixtures. In their experiments a high-speed camera was used that captured the basic flow of multi-detonation waves in the combustion channel. One of the universities AFRL is currently working with is the University of Cincinnati. At Cincinatti[4] they are experimenting with an air-breathing CRDE. They have successfully sustained stable detonation waves for hydrogen-air mixtures, which can be seen in figure 18.

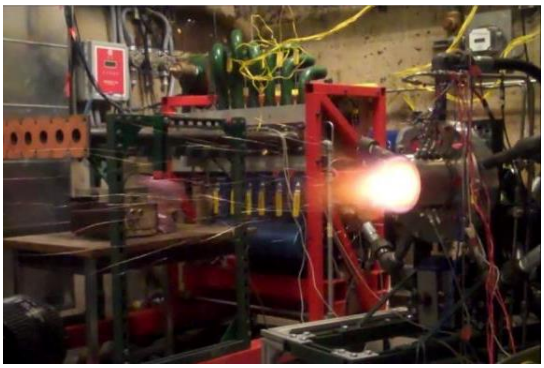

Figure 18: Successful detonation at the University of Cincinnati [4]

1.3.3 Numerical studies

Numerical simulations are used for a variety of applications and offer a very good tool to better understand different physical phenomena without actually building a prototype and conducting experimental research. In recent years,[11] detailed simulations of the flow field structure in the combustion chamber of a CRDE have been performed for a variety of different initial conditions and geometries. Numerical simulation has become a very powerful tool to assist in optimizing experimental research.

At Peking University in China,[31-40] Wang Jianping's research team have been performing 2D and 3D CRDE simulations on many levels since 2007. They have researched CRDE fuel injections limits, nozzle effects, viscous effects, self-ignition, particle path, thermodynamic and propulsive performance, shock reflections near the head end, and the propagation process of multi-detonation waves. They are recognized as the first to perform 2D and 3D simulations of CRDE to validate RDEs feasibility and explore its physical characteristics.

Many other researchers at Peking University in China have also contributed to numerical CRDE studies. Shao et al.[31], verified that rotating detonation waves are feasible for a range of subsonic to hypersonic injection. Zhou et al.[37,38] found that the combustion products flow out almost axially by using a tracking method he proposed in the flow field. Tang et al.[34] proposed and verified the feasibility of a CRDE model without an inner cylinder that would reduce difficulties with engine cooling. Liu et al.[34,35] captured the phenomenon of spontaneous formation of multi-front detonation waves in a CRDEs combustion chamber, which can be seen in figure 19.

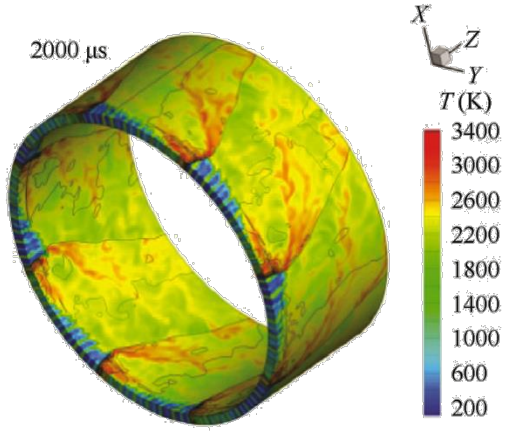

Figure 19: Multi-head rotating detonation waves [35]

In Japan, several researchers have conducted numerical simulations using different reaction chemical models to simulate higher fidelity flow fields of small combustion chambers. Hishida et al.[41] used a two-step reaction chemical model and assumed a 3D cylindrical chamber to be a 2D plane with periodic boundary conditions in the circumferential direction and without variation in the radial direction. They obtained detail structure of the detonation flow field as shown in figure 20.

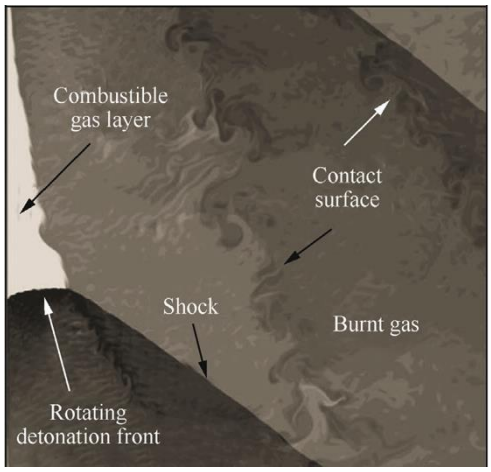

Figure 20: Temperature Distribution in CRDE flow field [41]

Tsuboi et al.[42] used a detailed reaction model for hydrogen-oxygen that resulted in to very similar specific impulse and thrust when conduction 2D and 3D simulations under the same conditions without a contracting tail nozzle. However, when the contraction tail nozzle was added, 3D simulations yielded a higher specific impulse and thrust. Uemura et al.[43] also used a detailed reaction model, but they discovered that there is an interaction point between the detonation front and the oblique shock wave, that an unreacted gas pocket appears and ignites periodically to generate transverse waves. The generated transverse waves propagate towards the inlet wall and then bounces back to the interaction point to maintain detonation propagation.

Yi et al.[44,45] in Singapore used a one-step reaction model of hydrogen-air to perform 2D and 3D CRDE simulations to estimate various design parameters on the propulsive performance of CRDE. They found that the propulsive performance was strongly dependent on the injection conditions, but weakly dependent on the axial chamber length effects and number of detonation waves.

In France, Davidenko et al.[46,47] performed 2D and 3D CRDE simulations, which proved that CRDE has a significant advantage over a conventional rocket engine when comparing their work cycle and specific impulse. Their 3D simulations were different than many other researchers because they used the adaptive mesh refinement method to increase computational efficiency. When comparing their 2D and 3D simulation results they yielded to be very similar.

Wolanski et al.[3] at Warsaw University of Technology in Poland used a one-step Arrhenius model for a hydrogen-air mixture to perform a 2D and 3D one-wave and two-waved CDRE simulation. They found that the thrust of the one-wave and two-waved detonation engine converged to very similar values once stabilized, as seen in figure 21.

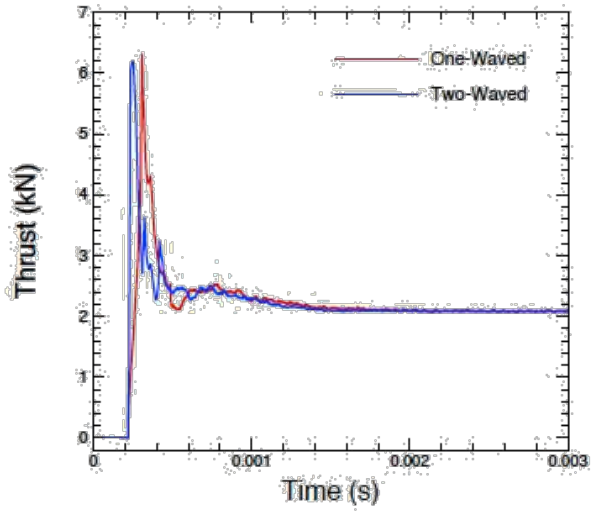

Figure 21: One-waved and two-waved CRDE thrust comparison [3]

In the United States there are a few institutions and companies who have performed 2D and 3D CRDE simulations. At the University of Texas in Arlington, Lu et al.[48,49], developed an air-breathing CRDE model and analyzed the effects of Mach number on its propulsive performance. The model yielded a specific impulse of 3800 s when using hydrogen as the fuel and 1500 s when using propane. At the University of Cincinnati, Gutmark's[50] research team performed 3D simulations of a centerbodiless CRDE. They are using the program Fluent by ANSYS and a Spalart-Allmaras turbulence model to simulate the mixing of the hydrogen and air. They proved the feasibility of a CRDE without an inner wall under non premixed injection.

Since 2011, Schwer and Kailasanath, from the U.S. Naval Research Laboratory have been performing numerical simulations of CRDE. They have obtained [51-56] the typical flow field of rotating detonation waves and have investigated the effects of stagnation pressure, back pressure, different fuels, injection fill region, combustor size, exhaust plenum on the flow field, and different injector configurations. Simulation results when using different injectors can be seen in figure 22.

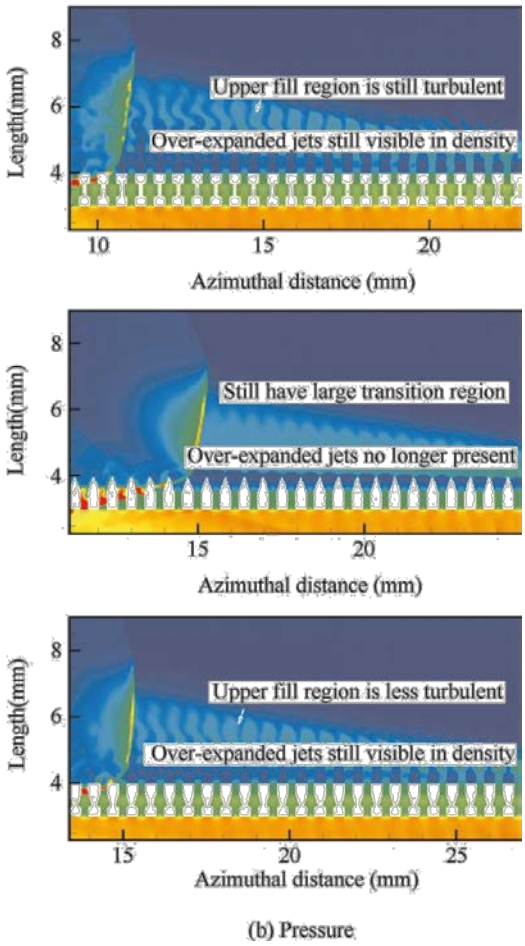

Figure 22: Pressure gradient for different injector conditions [55]

1.3.4 Challenges

There have been significant advancements in the development of CRDE since it was initially proposed in the 1960's. However, there are still many challenges that need further investigation numerically and experimentally. During CDRE[3] operation there is intense heat transfer in the walls by intense turbulence and shock waves associated with the detonation process. Therefore, the walls of the combustion chamber must be able to withstand extreme hot temperatures and cooling must be implemented in order to successfully operate the engine for long periods.

Another challenge involves the pressure losses in the feeding system. The[3] gain from the detonative combustion must be sufficient enough to compensate the feeding losses or the engine will stop running. This problem isn't as critical when using liquid rocket engine systems because the required power to supply both propellants to the detonation chamber is not as high in comparison to gaseous systems.

During combustion,[11] sufficient mixing must happen rapidly and in a short distance to sustain detonation waves. Currently, most numerical simulations are based on the ideal injection model, meaning the combustion mixtures are stoichiometric premixed. During future simulations researchers should focus on providing a more accurate model of the detonation combustion process by analyzing different equivalence ratios and non-premixed combustible mixtures. Usually in simulations, gaseous hydrogen is mainly used, but gaseous mixtures are unrealistic in practical application. Therefore, research on different fuels and oxidants that can sustain stable detonation waves must be done.

1.4 PROPOSAL

The study of this project will be focused on modeling and creating a simulation of a continuous rotating detonation engine combustion chamber by using a single-step hydrogen-air mechanism. A detailed review of the concepts leading to the CRDE will be conducted. Once the project has been outlined, it will be divided into multiple segments in order to gain experience with integrating chemistry and fluid dynamics in the ANSYS fluent software. Afterwards, the CRDE approach will be split into several categories including geometry, grid dependence, required schemes, and initiation of the problem due to its complexity. The geometry of the combustion chamber as well as most of the requirements will be established by researching previously conducted simulations other researchers have done. This project will be focused on two-dimensional analysis in order to

reduce the computational power required for a three-dimensional analysis. The two-dimensional simulations will be analyzed with ideal and non-ideal injector conditions. Afterwards, different injector conditions such as fuels, oxidizer, and injector parameters will be studied to understand their affect in the CRDE.

1.5 METHODOLOGY

For this study to be successful, analytical studies need to be conducted by using the two-dimensional unsteady Euler equations with source terms due to chemical reactions. Therefore, this study will be performed using computational fluid dynamics (CFD). During the computational study,[3] the transport properties such as viscosity, thermal conduction, and mass diffusion will be ignored since the effect of transport phenomena is usually small in detonation propagating in a straight duct.

Before performing the simulation, a CAD model will be designed. CRDE's are represented as an annular cylinder as seen in most of the research currently being conducted. However, since this study focuses on two-dimensional approach, it will be assumed that the distance between the two ducts is infinitesimally small. The next step will be to generate a mesh for the CAD model. A structured mesh will be generated in ANSYS Fluent. The grid size will rely heavily on grid sizes from previously conducted research on CRDE's. The boundary conditions necessary for the model include setting the walls as periodic conditions, a pressure outlet at the exit end, and the injector conditions vary depending on the ideal or non-ideal approach. When using the ideal approach, the injector is modeled using a user defined function (UDF), which can be complicated without the proper experience. When using the non-ideal approach, the injectors are modeled individually throughout the inlet wall region. The project's success will rely heavily on understanding how to model the injector conditions correctly and how to implement them in ANSYS fluent correctly.

When beginning the simulation process, the chemistry and fluid mechanics must be confirmed by benchmarking a detonation tube simulation. A one-dimensional detonation tube will be used to confirm the mathematical formulation and physical characteristics of a combustion wave resulting from detonation. After confirming the model setup is correct, the solution will be used to initiate the detonation in the CRDE model.

CHAPTER 2: MATHEMATICAL FORMULATION

2.1 GOVERNING EQUATIONS

The following three-dimensional Navier Stokes equations in integral form are the governing equations for a single-component fluid in an arbitrary control volume in ANSYS Fluent.

$$\frac{\partial}{\partial t}\int_{V} \; + \oint [\; - \;]\,dA = \int \qquad (2.1)$$

Where vectors , , are defined as

$$0 \qquad (2.2)$$

( ) (+) (τ +)

= Source terms (body forces and energy sources)

, , , , , = density, velocity, total energy per unit mass, pressure, viscous stress tensor, and heat flux, respectively.

When applying the assumptions made for the CRDE from 3D to 2D, the governing equations simplify to the unsteady Euler equations. It[31,37] is assumed that the effects of transport properties such as the viscosity, thermal conduction, and mass diffusion can be ignored, resulting in **G**=0. Turbulence is also neglected in order to focus on the effects of the chemical reaction. The setup involves a one-step, irreversible Arrhenius kinetics, resulting in source terms being added due to the chemical reactions involved. This results in the following equations expressed in vector form in Cartesian coordinates:

$$\frac{\partial}{\partial t} + \frac{\partial}{\partial x} + \frac{\partial}{\partial y} = \qquad (2.3)$$

Where vectors , , , are defined as:

The total enthalpy H is defined as:

$$= + \quad (2.5)$$

Where the total energy is the sum of the kinetic and internal energy. In the following equation q is the total chemical energy release, and is the ratio of specific heats.

$$= + + \quad (2.6)$$

The first-order Arrhenius equation defines the mass production rate as follows.

$$= \quad (2.7)$$

Where

K, A = Pre-exponential factors

= Activation energy
= Specific gas constant
= Mass Fraction of the Reactants
= Temperature

The thermodynamic properties for the one-step hydrogen-air reaction model are considered to be constant. The one-step reaction model is used to simplify the chemical kinetics and reduce the computational time.

CHAPTER 3: VERIFICATION OF CODE AND CHEMICAL KINEMATICS

3.1 VALIDATION CASE: 1D DETIONATION

3.1.1 Setup: Grid & Boundary Conditions

The simulation for a one-dimensional detonation in an open tube is conducted in order to verify that ANSYS Fluent can accurately calculate the ZND and CJ conditions while using a one-step stoichiometric hydrogen-air mechanism. The results of the following simulation will serve as a validation study for detonation based studies. The solution to the one-dimensional detonation wave will also serve as the initiation to the CRDE. The grid setup is a uniform structured mesh with 0.1 mm spacing,[10,31] which were shown to capture the physical parameters of interest in several studies. The boundary conditions were all set to adiabatic walls, except for the bottom boundary which was set to symmetry, and the pressure outlet. The pressure outlet was set to standard atmospheric conditions.

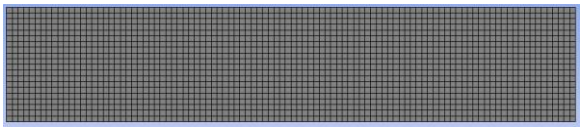

Figure 23: Grid setup of tube analyzed

3.1.2 Chemical Formulation & Initialization

In order to initialize the problem correctly, the mass fractions for each of the species in the chemical mechanism was to be calculated. For this simulation a stoichiometric hydrogen-air mixture ($= 1.0$) as shown below was used.

$$_2 + 0.5\,(\,_2 + 3.76\,_2) \rightarrow \,_2 + 0.5(3.76\,\,_2) \tag{3.1}$$

The mass fraction for the reactants and for the products were calculated as follows:

$$= \frac{2}{} = 0.02852 \quad (3.2)$$

$$= \frac{0.5\ 2}{} = 0.22640 \quad (3.3)$$

$$= \frac{0.5(3.76\ 2)}{} = 0.74510 \quad (3.4)$$

$$= \frac{2}{} = 0.25480 \quad (3.5)$$

$$= \frac{0.5(3.76\ 2)}{} = 0.74520 \quad (3.6)$$

An initial thin region of reacted gases (burned) is patched in the left closed end of the tube to initiate the detonation. In the other region, stoichiometric (unburned) gases are patched. The setup can be seen in Figure 24, and table 3.1.

Figure 24: Patching sections for the tube. (Red = burned gas, Blue=unburned gas)

Table 3.1: Initial conditions for each of the patching sections

Initial Conditions (Burned Gas)		
	90 [atm]	Initial Pressure
	3500 [K]	Initial Temperature
	0.25480	
	0.74520	
Initial Conditions (Unburned Gas)		
	1 [atm]	Initial Pressure
	300 [K]	Initial Temperature
	0.02852	
	0.22640	
	0.74510	

3.1.3 Solver

The simulation was carried out using the density based solver, which is known to capture flow discontinuities such as shockwaves. The model was axis-symmetric, laminar, transient with a constant time step of $1x10^{-7}$ [s], and limited to a Courant number of 0.5 to impose stability on the solution. Second order upwind scheme is used for spatial discretization with second order implicit formulation for temporal discretization. The numerical flux's were calculated using ROE's flux difference splitting scheme.

3.1.4 Results

3.1.4.1 Pressure and Temperature

The solution fully develops after the combustion wave has propagated sufficiently along the tube. Shown below is the combustion wave propagating through the tube once the detonation occurs.

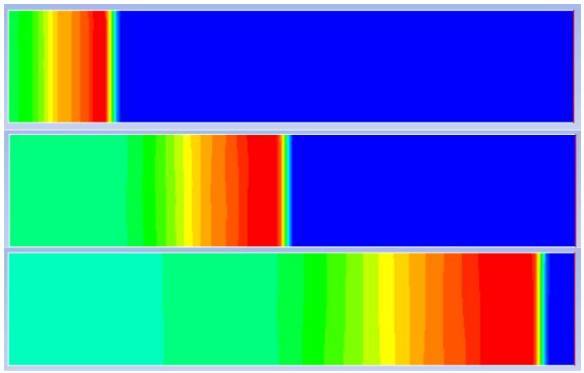

Figure 25:Combustion wave propagating through the tube after detonation

The C-J pressure and temperature was measured at different locations for the detonation wave, as shown in table 3.2. The pressure peaks varied depending on the location analyzed as the wave traveled. As it can be seen, the pressure peak can be analyzed almost instantaneously after

the detonation has occurred. Throughout each of the measurements the pressure and temperature remained within a constant range as expected from theory.

Table 3.2: C-J Condition Measurements

Distance [m]	Pressure [Pa]	Temperature [K]
0.032	1.53e6	2974
0.088	1.52e6	2750
0.144	1.43e6	2626
0.200	1.44e6	2630
0.286	1.51e6	2686
0.455	1.54e6	3032
Average	1.49e6	2783

The following figures display the distribution of pressure and temperature. Both the temperature and pressure distribution yielded ZND model characteristics. It can clearly be seen where the shock front dramatically impacts the pressure and temperature, then where the induction and reaction zones take place. Therefore, the one-step stoichiometric hydrogen-air model can be used to simulate ZND model behavior.

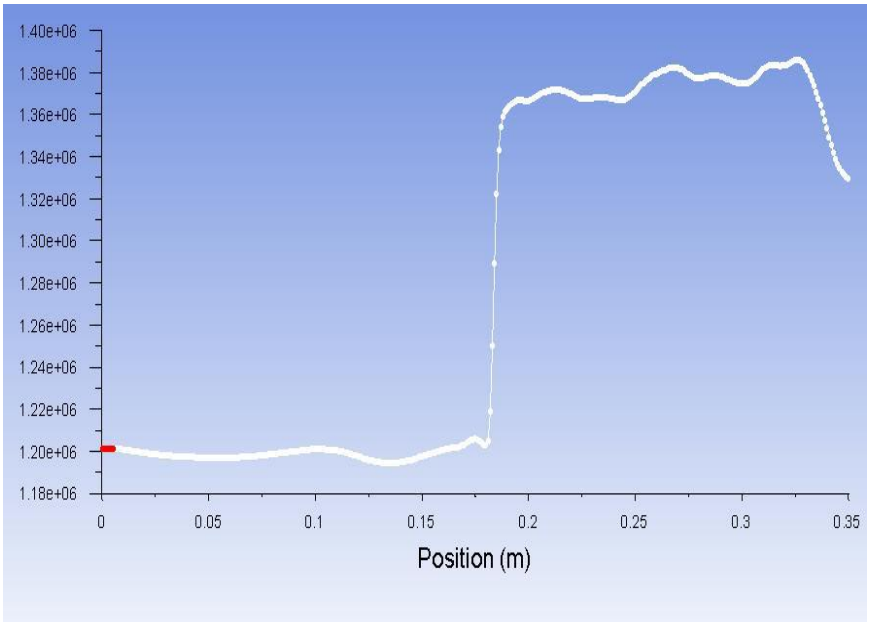

Figure 26: Pressure distribution of detonation in tube [Pa]

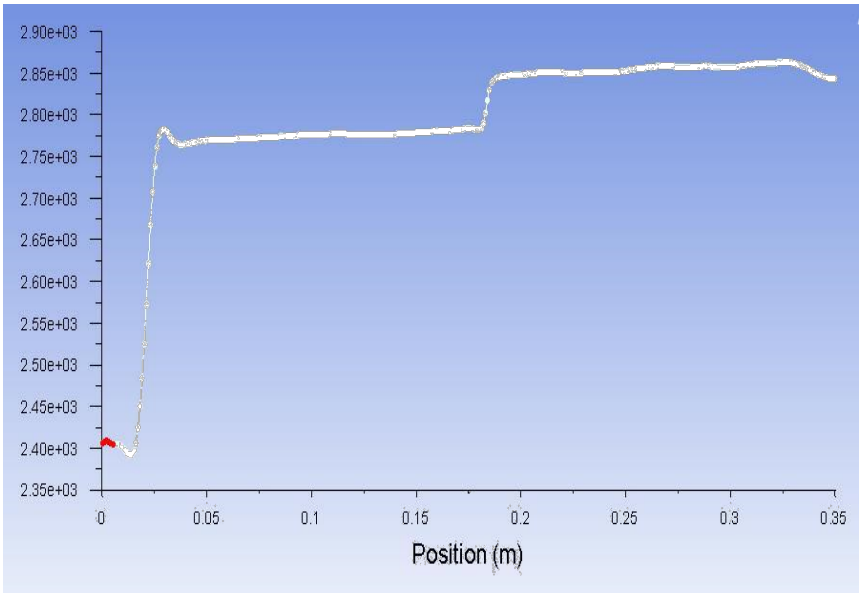

Figure 27: Temperature distribution of detonation in tube [K]

3.1.4.2 Velocity

The velocity of the wave was calculated by analyzing the peak pressure wave at different locations and time steps as it propagated through the tube as shown in the table 3.3.

Table 3.3: Velocity Measurements

Distance [m]	Time [s]	Velocity [m/s]
0.028	0.0000144	1944
0.084	0.0000431	1949
0.140	0.0000718	1950
0.197	0.0001005	1960
0.283	0.0001290	2190
0.452	0.0002152	2102
Average		2015

3.1.4.3 Detonation Benchmark

In order to benchmark the results for the detonation wave, the stoichiometric hydrogen-air mixture was analyzed using NASA's Chemical Equilibrium with Applications (CEA) program. The results for the mixture with the equivalence ratio of 1 are shown in the following table.

Table 3.4: C-J Conditions (CEA Benchmark)

	1.59e6 [Pa]
	2947 [K]
	1968 [m/s]
,	15.507
,	9.823

When comparing the averaged C-J parameters from the simulation to the values from CEA, they yielded to be very similar. When comparing the values from both of the analysis, a 6.49 % difference for pressure, 5.72 % difference for temperature, and a 2.36% difference for detonation velocity. Therefore, it is determined that ANSYS Fluent can accurately simulate both the ZND model and C-J Conditions using a stoichiometric one-step hydrogen-air chemical mechanism.

CHAPTER 4: CRDE COMPUTATIONAL SETUP

4.1 PHYSICAL & COMPUTATIONAL MODEL

The continuous rotational detonation engine is modeled as a three-dimensional annular chamber. However, if the [3,26,39] distance between the inner and outer walls is assumed to be infinitely small, the domain can be modeled as a two-dimensional chamber as shown in Figure 28.

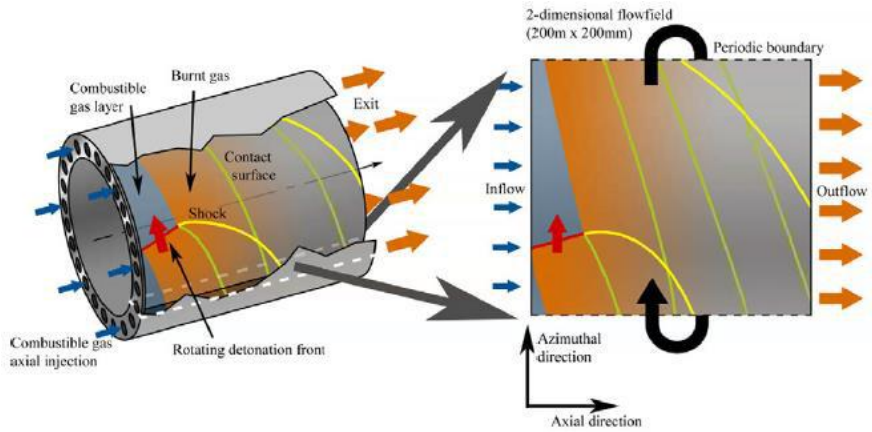

Figure 28: 2d simplification of CRDE [3]

In past computational CRDE research, it has been proven that the solution to the two-dimensional and three-dimensional solutions yield to be very similar. Therefore, the domain is simplified to reduce the computational time and required for the simulation.

The flow field is initially filled with stoichiometric hydrogen and oxygen mixture. The hydrogen-oxygen mixture is modeled by using the one-step mechanism to generate a steady state approximation without complicating the chemistry involved with the hydrogen-air mixture. Note, that viscosity, thermal conduction, and mass diffusion are ignored in this study. To simulate the tangential detonation, a[31,39] one-dimensional C-J detonation is artificially patched in the domain for a short distance from the head left-end, with a strong tangential velocity to ignite the flow into a detonation in one direction. The head end has a slip rigid wall boundary condition imposed, while the combustion chamber exit has a pressure outlet boundary condition applied. The lower and upper boundaries of the domain have periodic boundary conditions imposed due to the nature of CRDE's.

4.2 INJECTION BOUNDARY CONDITIONS

4.2.1 Non-Ideal Injection Condition Approach

The non-ideal injection condition approach for a CRDE involves modeling many injectors across the combustion chamber with a mixture plenum. For this approach, the model generated by Kailasanath et al[57], was implemented in order to have a benchmark for the solution. The injectors had the following dimensions: W=5.65486 [mm], T= 10 [mm], R=2.5 [mm], and =1.131 [mm]. The mixture plenum was 30 [mm] in axial length, and included 50 injectors.

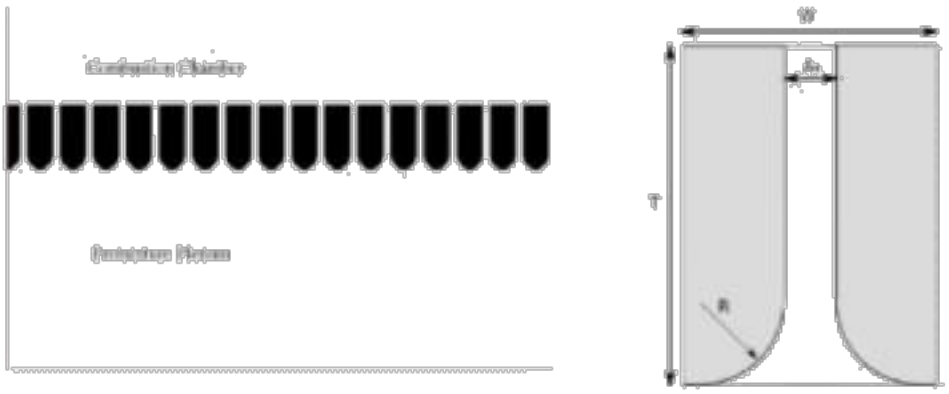

Figure 29:Modeling injectors for the non-ideal approach

4.2.2 Ideal-Injection Condition Approach

Generally, an oxidizer and fuel are injected into the combustion chamber. It is assumed that fresh fuel and oxidizer is supplied through many small injectors mounted on the closed end of the combustion chamber to create a detonable mixture for the initiator, however they are not actually physically modeled as in the non-ideal injection model. It is[3] critical that the detonable mixture is generated continuously in order to sustain a continuous and steady rotating detonation wave. There are three types of injection conditions that must be taken into account when setting up the computational model. In[45] the first condition the detonation wave is in front of the injector, so the wall pressure will be greater than the injection pressure. The flow properties are obtained using the isentropic relations.

= . = (, ,and = 0 (4.1)

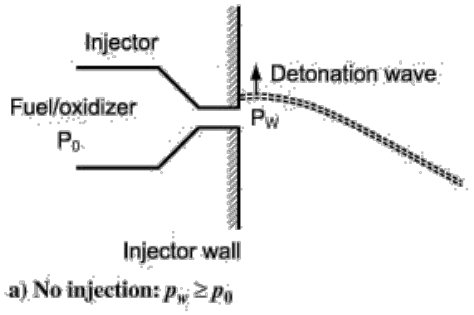

Figure 30: 1st injection condition, no flow supplied.

In the second condition, the wall pressure is less than the injection total pressure, but greater than the critical pressure, as shown in figure 31.

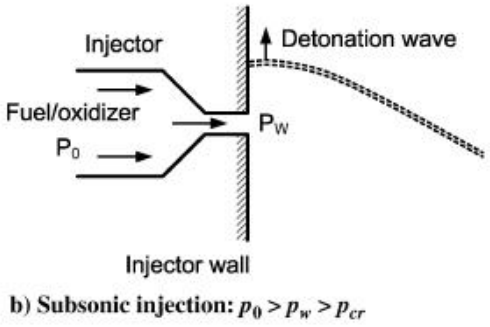

Figure 31: 2nd injection condition, subsonic injection.

The flow properties are thus modeled by:

(4.2)

(4.3)

$$= \left(\frac{}{}\right)^{\frac{-1}{}}, \quad \text{and} \quad = \sqrt{\left(\frac{2}{-1}\right)\left[1-\left(\frac{}{}\right)^{\frac{(-1)}{}}\right]}$$

Where the critical pressure is defined as:

$$= {}_0\left(\frac{2}{+1}\right)^{\frac{}{-1}}$$

In the last condition, the detonation wave is propagating towards the injector, as shown in figure 32. The wall pressure is less than the critical pressure, and the flow properties are calculated as follows:

$$= \quad = \left(\right) \quad , \quad \text{and} \quad = \sqrt{\left(\right)} \qquad (4.4)$$

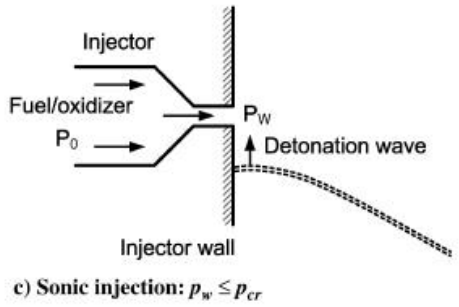

Figure 32: 3rd injection condition, supersonic injection

4.3 SETUP, GRID, & BOUNDARY CONDITIONS

When setting up the CRDE, both ideal and non-ideal injector models had the same boundary conditions and mesh sizing. The models had a pressure outlet with atmospheric conditions, and the left and right walls were set to translational periodic. To ignite the and create the combustion wave a separate surface was generated in order to patch the solution to the one-dimensional detonation wave. Note, the C-J velocity was patched in the tangential direction in order for the combustion wave to propagate in the correct direction. The grid setup remained the same as in the one-dimensional analysis performed, with 0.1 mm spacing. However, the mesh was set to be adaptive in order for the mesh to capture the shockwaves accurately as the combustion wave propagates through the combustion chamber of the CRDE.

In the non-ideal injector case, shown in figure 33, the mixture plenum area was initialized to be have stoichiometric hydrogen-air at P = 10 atm and T = 300 k. The area in the combustion

chamber was set to air at atmospheric conditions, and the inlet condition was set to a velocity inlet.

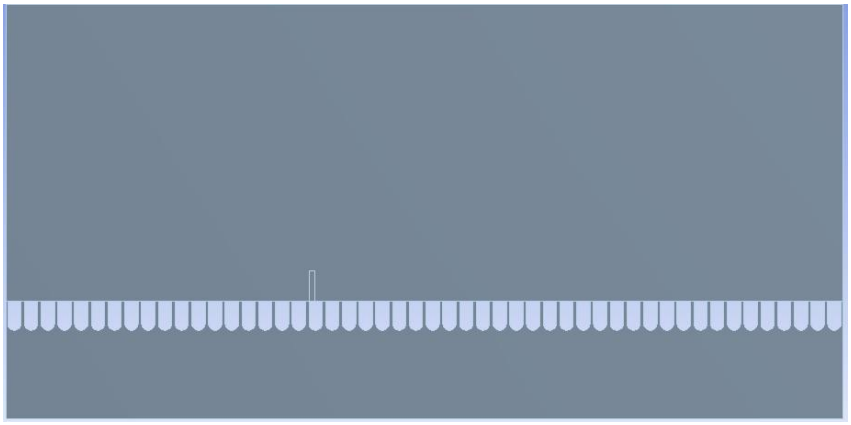

Figure 33: Non-ideal injector model

For the ideal-injector case, the combustion chamber zone was initialized with stoichiometric hydrogen-air. The bottom boundary zone had to be approached differently, since it is defined by three different injections conditions. Therefore, a user-defined function (UDF) profile was required to be generated in order to define the inlet boundary condition. The UDF allows the user to create their own code to manipulate the conditions imposed on a boundary when setting up a problem.

Figure 34: Ideal injector model

4.4 BENCHMARK & RESULTS

For both injector models, the solutions should have been nearly identical. The expected results can be seen in figure 35. It was expected that the detonation wave would sustain itself as it propagates from left to right in the combustion chamber. The detonation wave, shock wave, mixture layer, and contact surface is clearly defined throughout the domain as expected.

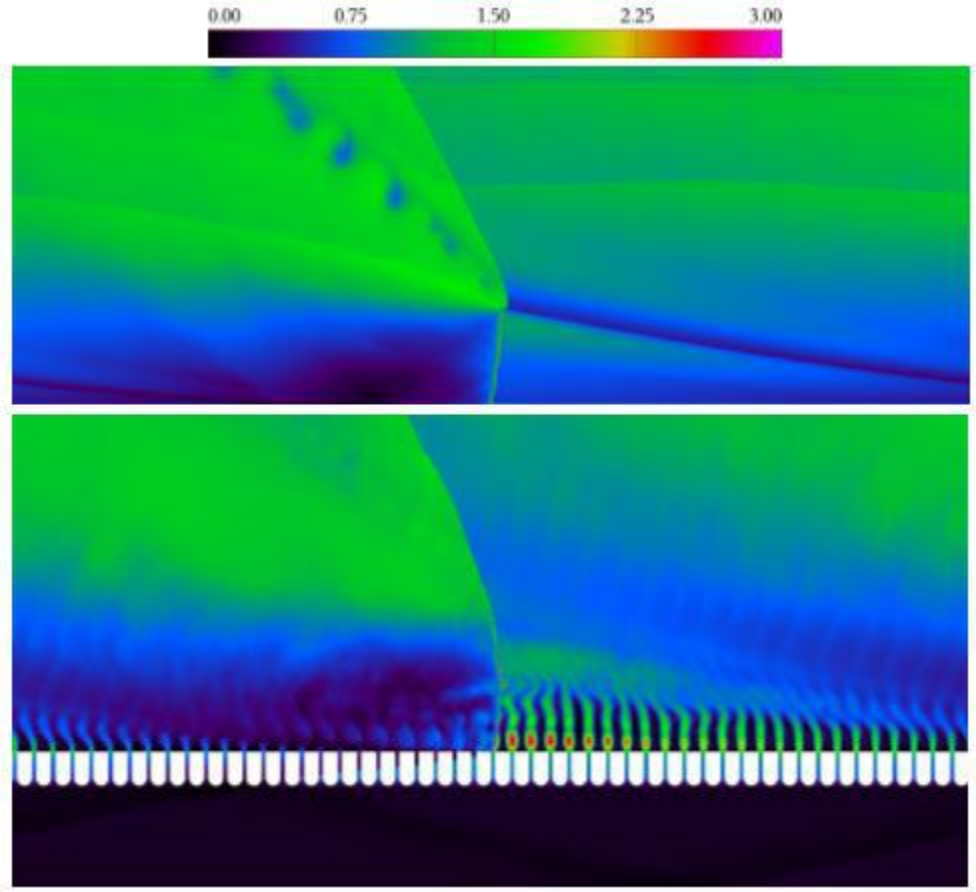

Figure 35: Expected Mach number results for ideal model (top) and non-ideal model (bottom)

When running the non-ideal injector case in ANSYS fluent, the results would not converge to the solution that was expected. During the detonation, as the wave propagated forward, behind the wave there was a large back pressure affecting the injectors. Eventually, the

solver would diverge and the simulation would crash. This led to focusing on the UDF approach, since it was clear that the non-ideal injector case could not be solved without imposing every injection condition required. The UDF boundary condition approach was researched thoroughly. However, the code required for the conditions to be imposed in ANSYS fluent could not be debugged to work as expected.

CHAPTER 5: CONCLUSION & FUTURE RECOMMENDATIONS

The theory behind detonations and continuous rotating detonation engines was investigated. It was proven that both the ZND model and C-J conditions could be successfully and accurately simulated using ASNSY Fluent. The C-J temperature, pressure, and velocity were all within a 10% difference, when benchmarking the solutions to NASA's CEA results. The solution to the one-dimensional model was then used to initialize the detonation in the CRDE. The CRDE's approach and setup was researched thoroughly, unfortunately the simulations ran did not yield the expected solution.

It is known that most computational studies on the CRDE have been conducted with in-house solvers, not ANSYS Fluent. Therefore, it is recommended that future researchers who want to simulate the CRDE problem on ANSYS Fluent should be experts with the program. Creating and writing a user-defined function to be implemented into ANSYS fluent is very complicated, especially for someone figuring out the program through a project. If experienced enough in the program, a variety of analysis could be conducted using the proposed model.

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