Minimizing Fuel-Oxidizer Mixture Inhomogeneities in Rotating Detonation Engines

Grant Proposal

Kayla Vallecillo

Massachusetts Academy of Mathematics and Science at Worcester Polytechnic Institute (WPI)

Worcester, MA

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Executive Summary

This project aims to develop a strategy for increasing the efficiency of injecting fuel and oxidizer within a rotating detonation engine (RDE). The rotating detonation engine is an effective yet experimental engine with the ability to advance kinetic propulsion and stationary energy production. Varying the position of injected streams of fuel and oxidizer is often relied on to avoid the flashback phenomenon, which negatively impacts the propagation and sustainability of detonation waves. While alleviating the sustainability of propagated waves, stratified fuel-oxidizer injection methods produce inhomogeneities that create skewed and slow detonation waves and an unsteady exhaust plume. To address the drawbacks of stratified injection within the RDE, numerical and computational fluid dynamics (CFD) simulations through Ansys Fluent will be conducted. Iteratively altering injection-specific variables (injector diameter, distance, and angle), can reduce the impacts of uneven mixture concentration gradients on wave propagation. This project aims to target mixture ratios and measures of homogeneity preceding the incoming detonation wave to maximize wave stability and optimize thrust output. Success will be quantified through the analysis of mixture stratification lengths and equivalence ratios relative to existing injection methods (premixed, axial, stratified, and interval injection). This project will be pursued at the Massachusetts Academy of Mathematics and Science at Worcester Polytechnic.

Minimizing Fuel-Oxidizer Mixture Inhomogeneities in Rotating Detonation Engines

When considering the future of pressure-gain propulsion systems, the rotating detonation engine (RDE) is one of the most promising and interesting areas of modern propulsion research. The RDE is a pressure-gain propulsion system that utilizes rotating detonation waves to compress and ignite a mixture of injected fuel and oxidizer for powerful levels of propulsive thrust. Pressure-gain combustion (PGC) is a promising alternative to conventional combustion methods due to its ability to produce higher levels of propulsive thrust with smaller amounts of fuel input (Rodriguez, 2023). Conventional RDEs are composed of an annular combustion chamber, in which a homogenized fuel-air mixture is injected at the head plane and compressed by a cyclically-moving rotating detonation wave that propagates without the use of any moving parts (Bonanni et al., 2023).

Rotating Detonation 101

Detonation can be characterized as being a chemical reaction in which pressure and temperature rise significantly and immediately. In the RDE, detonation is produced by igniting a specified region of the engine that causes outward movement of pressure, temperature, and material gasses. This outward movement travels at a supersonic speed around the annular detonation chamber and produces significant thrust. Detonation waves propagate within the chamber through the consumption of a reactive fuel mixture. This fuel mixture, which could be hydrogen, methane, or a different reactive gas, is supplemented with oxidizer and air to aid combustion and produce thrust. When injected as a premixed mixture, the flashback phenomenon occurs, which inhibits the engine from achieving optimal thrust production. To avoid this phenomenon, fuel and oxidizer injectors are separated and configured. The injection method used can be adapted based on the drawbacks and benefits of the tested configuration. Generally, separated fuel and oxidizer (or air) injection can cause inhomogeneities in the fuel mixture, which negatively impact detonation wave propagation due to uneven pressure and temperature ratios distributed throughout the detonation chamber. Consider this analogy: within a small swimming pool, your goal is to fill the pool evenly with red blocks and blue blocks. When placing these blocks inside of this swimming pool, it is difficult to ensure that there are no pockets of mostly red or mostly blue blocks, which essentially alludes to the approach to homogeneity. To produce a homogenous distribution of red and blue blocks, the way in which the blocks are placed in the chamber must be adjusted, altered, and iterated, based on previous observations of which adjustments best produce an even distribution. The RDE works in a similar fashion. Fuel and oxidizer must be injected into the chamber in a way that to produces a homogenous distribution of fuel and air, allowing the detonation wave to effectively propagate and produce sufficient thrust.

The Flashback Phenomenon

Compared with other thrust-producing deflagration systems, the rotating detonation engine produces significant amounts of thrust while maintaining higher levels of thermal efficiency, making this system a high-interest area of research within the field of detonation and propulsive energy-producing systems. Often, fuel and oxidizer injectors are separated to reduce the effect of the flashback phenomenon, an event that occurs when detonation waves propagate inside a premixed fuel injection system, and interrupts systemic injection functions. One way to eliminate the flashback effect would be to While eliminating the flashback effect, separated fuel-oxidizer injectors; however, inhomogeneities in the fuel-oxidizer mixture negatively impact the propagation of the cyclical detonation waves (Bonanni et al., 2023). Spontaneous, disrupted propagation of detonation waves due to structural inhomogeneities in fuel-oxidizer mixtures has led to an unsteady exhaust plume at the combustor exit, significantly reducing the thrust efficiency of the engine (Zhu et al., 2020).

Inhomogeneities in Fuel Mixtures Jeopardize Wave Propagation

Previous research has been centered around the optimization of nozzle geometries, stabilization, alternative configuration, and propagation characteristics to increase the thrust efficiency. With the thrust and denotative efficiencies of RDEs deteriorating due to local pockets of nonhomogenous fuel-air mixings, further research into injection-based variables is needed to minimize this negative effect. Previous investigations on the impact of mixture gradients on the detonation wave structure have found that inhomogeneity results in a skewed detonation wave front and the creation of local zones of deflagration, reducing the overall combustor efficiency. There is evidence to suggest that the fuel-air mixing process has been to be crucial in sustaining continuous detonation for the propagation of supersonic waves, playing a pivotal role in controlling emissions (Prakash et al., 2019). In addition, nozzle integration with the RDE is jeopardized due to uneven exhaust flow at the combustor exit, thus verifying the need to optimize homogenous fuel mixtures for propulsive and non-propulsive purposes (Liu et al., 2022).

In 2022, Ramanujachari et al. designed and tested a rotating detonation engine, performing a simple mixing analysis injection scheme to produce reasonable propulsive performance. An axial injection configuration was pursued, in which hydrogen fuel and air were perpendicularly injected into the detonation chamber through separated injectors. Conducting this pre-detonation wave mixture analysis was useful in obtaining reasonable propulsive performance, due to a visible, and clear relationship between mixture homogeneity and wave propagation characteristics. In optimizing mixture homogeneity preceding the detonation wave, RDE performance can be effectively analyzed through the comparison with other works that highlight mixture homogeneity and its relativity to RDE performance. If the simulation results compare, they can be used to determine whether RDE efficiency could be improved.

Project Approach and Injection Iteration

The common use of stratified injection in modern RDE configurations produces a significant practical need for effective injection methods. This project aims to address this need through iterating injection configurations by altering several injection-specific variables (injector diameter, distance, and angle) to produce a homogenous mixture concentration gradient. In selecting a perpendicular (radial) injection scheme, the initial simulation will be simplified and progressively expanded to enhance the effect of iterative adjustments in following portions of the project. Homogeneity will be quantified through mixture equivalence ratio and particle stratification length prior to the arrival of the detonation wave. Configurations will be recorded and analyzed through several rounds of iteration until a relatively homogenous mixture is achieved. It is expected that this process could minimize inhomogeneities in fuel-oxidizer mixtures within the RDE.

With the potential to improve and reshape the future of energy generation, through stationary and propulsive energy-producing systems, solutions to inefficiencies in the RDE are essential to advance research related to rocket applications of effective rocket propulsion systems. Despite relying on a refined kerosine, ethylene, or hydrogen mixture, RDE capabilities to produce thrust with lower amounts of fuel allows this system to be a central focus in future energy-related endeavors. The present work aims to minimize a functional inefficiency to contribute to the improvement of the greater system through the computational modeling of fuel-oxidizer injection functions.

Section II: Specific Aims

This proposal's objective is to express the direction and goals that this RDE mixing optimization project will pursue. Through the construction of a simple mixing analysis and the development of repeated mixing models, a larger mixing model for the RDE system's injection of hydrogen fuel and air can be developed based on optimized fuel-oxidizer injection variables. In pursuing this strategy, the mixing process within the RDE can be optimized, allowing for optimized thrust and exhaust output.

The long-term goal for this project is to simulate how variations in injection configuration can impact physics experimental applications of RDE testing and performance. In the future, the identified most effective injection configuration can be implemented into a secondary two-dimensional or three-dimensional simulation, where a detonation wave passes through the configuration after the injection process occurs, thus leaving a mixture concentration gradient which can be associated with the performance of rotating detonation wave variables. These characteristics can be utilized to evaluate the effectiveness of the introduced injection method when compared to similar experiments conducted with axial, radial, or stratified injection configurations.

Figure 1

3D to 2D Stratified Injection Model

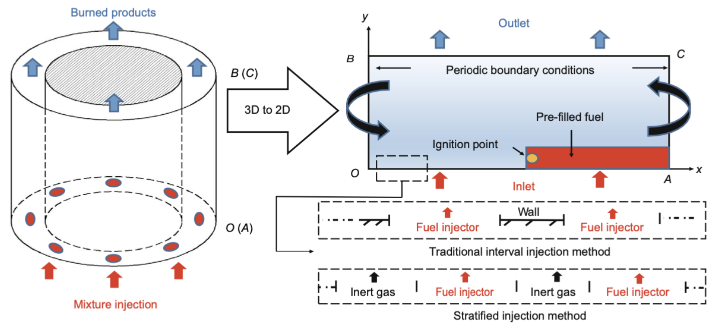


Fig. 1 Combustion chamber and computational domain

Figure 1. Stratified injection model vs traditional interval injection model and three-dimensional to two-dimensional computational domain. Figure from (Lei et al., 2020).

In 2021, Sato et al. demonstrated that detonations can be stabilized when configured with an axial injection configuration, yet recovery of the injectors after the detonation wave passed caused premature deflagration and overall pressure-gain efficiency loss. To combat this loss of engine efficiency, it is predicted that mixing variables or configurational elements must be adjusted. In 2020, Lei et al. tested a novel stratified injection configuration in which air was pushed against a wall perpendicular to the fuel flow, mixing the materials prior to its direct entrance into the chamber, as expressed in Figure 1. The results of this stratified injection test displayed improvement in the proceeding detonation wave's specific impulse, temperature distribution, and fuel consumption. However, fuel distribution became stratified rather than continuous, providing an opportunity for improvement of the existing stratified injection model. As expressed through these previous injection configuration testing schemes, existing injection strategies have shown improvements in RDE performance. Yet, each variation in configuration style, injector diameter, injector distance, and injection angle introduce various drawbacks that could be optimized through an iterative computational approach. In adjusting these values, an analysis of pre-detonation wave fuel concentration gradients can determine the effectiveness of fuel and oxidizer distribution, while an extension of this project can focus on wave behavior (propagation) and deflagration after the injection. Overall, the central aim for this project is to develop a configuration that introduces a strong ability to inject fuel and oxidizer for significant homogeneity levels.

Specific Aim 1: Configure a two-dimensional computational model of the rotating detonation engine.

Specific Aim 2: Construct a simple mixing analysis for a radial, stratified, and axial injection configuration.

Specific Aim 3: Iteratively adjust injection variables to increase fuel-air proportional equivalence.

The expected outcome of this work is that a computational model of the RDE fuel-oxidizer injection sequence can be developed and iterated to produce maximized material concentration homogeneity.

Section III: Project Goals and Methodology

Relevance/Significance

The rotating detonation engine introduces an alternative, high-benefit engine with exciting applications in propulsion sciences and stationary energy systems. The applications of RDE concern high thermodynamic efficiency, emission reduction, high energy conversion rates, and high specific impulse, making this system a competitive, yet experimental engine (Luan et al., 2022). Despite its promising capabilities, the RDE's non-premixed initial fuel and air conditions reduce the efficiency and sustainability of the engine's continuous detonation thrust-producing process. To address this issue, an effective injection configuration must be created and applied to varying engine sizes and configurations. The significance of an optimized injection scheme could allude to its use in future experimental studies where effective pre-detonation injection is analyzed through fuel and air concentration homogeneity and implemented into advanced detonation-introduced simulations.

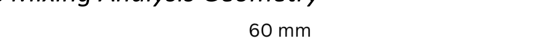
Innovation

This project aims to address the issue currently present in RDE systems regarding mixture homogeneity in non-premixed injection configurations. The RDE is often characterized by its unsteady flow field, the uneven concentration gradient present in fuel-oxidizer mixtures producing uneven exhaust flow, heavy premature deflagration (consumption of residual gasses), and injector interference through the passing detonation wave (Prakash et al., 2020). This project aims to simulate the mixing process through a simple mixing analysis representative of a repeated element of the “rolled out” RDE detonation chamber. In pursuing a simplified model, this problem can be addressed inexpensively, and expanded to three-dimensional or chemistry-based reaction simulations through the introduction of the rotating detonation wave. The current proposed methodology introduces a project that can be easily expanded and can be applied to any RDE configuration as it addresses an elementary, non-specific configuration that can be applied in place of axial, perpendicular, and stratified injection configurations, which are often used in current computational models. This project could verify the effectiveness of simple mixing analysis tools in addressing complex RDE integration and expansion problems.

Methodology

Figure 2

Rotating Detonation Engine Simulation Configuration and Simple Mixing Analysis Geometry



The planned methodology for this project includes addressing three central aims: development of the model, testing for existing configurations, and a long-term iterative adjustment process. The configuration dimensions and fundamental purposes are based upon an investigation of detonation wave propagation characteristics when introduced to varying concentration gradients of fuel and air pursued by (Prakash et al., 2019), inhomogeneity quantified by the stratification lengths of each respective material. This configuration is heavily inspired by the investigations reviewed in this proposal. In pursuing the represented configuration, these methods aim to focus on mixing prior to the arrival of the detonation wave and introducing the action of injection, rather than pre-injected fuel-air concentrations. To test several injection schemes, a standardized, two-dimensional computational domain will be developed in Ansys Fluent, where the independent placement of varying injection geometries will be placed into a standardized computational domain, of a specified size as recorded in previous literature. Specific injection velocities and quantities are yet to be determined. In Figure 2, the planned, standardized, and interchangeable configuration is expressed. Thoughtful consideration of the design of axial, radial, interval, and stratified injection strategies will be considered during testing and iteration. It is expected that the configuration will be refined and adjusted over the course of the project. Once this configuration is pursued, particle path results from the Ansys Fluent simulation will evaluate homogeneity through density variance levels and fuel-air stratification lengths. This information can be directly compared to the experimental findings of Prakash et al. and the effects of stratification lengths and equivalence ratios on wave propagation can be evaluated without the use of complex detonation wave simulations.

Specific Aim #1: **Configure a two-dimensional computational model of the rotating detonation engine.**

The objective of this aim is to develop a two-dimensional computational model of the rotating detonation engine to develop a low-complexity computational model that accurately represents the RDE's structure and basic configuration.

Justification and Feasibility. To produce an effective model of the mixing process within a three-dimensional RDE chamber, simplifications and assumptions must be made. In various previously completed works, a naturally three-dimensional RDE structure has been converted to two-dimensional simulation configurations to simplify the simulation process (Lei et al., 2020; Prakash & Raman, 2019).

Periodic boundary conditions (PBCs) must be set on the RDE boundaries. PBCs state that any particles leaving the specified boundary will be returned to the opposite side of the boundary, where configuration space is available. In including a set of PBCs, a two-dimensional configuration can be constructed while still modeling the continuity of a cylindrical object. In Figure 1, the use of PBCs can be observed as a method for “rolling out” a three-dimensional cylinder into one strip and taking a small slice out of it. This addition justifies the use of a two-dimensional simulation configuration by first applying to previous, similar work, and additionally avoiding the adjustment and nature of the original cylindrical detonation chamber.

Summary of Preliminary Data. No preliminary data has been gathered for this specific aim’s justification. The decision to not require preliminary data for the creation of the computational model is due to a pre-planned geometric configuration, as described in the methodology section. In developing this geometric configuration with an interchangeable design for fast-paced testing of each scheme, no preliminary data is needed to support this model creation, as it is justified through the adoption of previous works’ parameters.

Expected Outcomes. The overall outcome of this aim is to construct a functional, accurate, and applicable model of the rotating detonation engine without using complex three-dimensional simulation technology. This knowledge will be used to verify the use of a two-dimensional object - as the object itself is unchanged but rather expressed differently while solving and simulating.

Potential Pitfalls and Alternative Strategies. It is expected that due to little experience in computer simulation, computational fluid dynamics, or turbulent and fluid physics, a learning curve in applying Ansys Fluent to express and test ideas will be present. However, confusion and general lack of knowledge can be combated by gaining the advice and guidance of more experienced academic leaders in this subject and learning more about Ansys Fluent outside and prior to simulating.

Specific Aim #2: **Construct a simple mixing analysis for a perpendicular, stratified, interval, and axial injection configuration.**

Justification and Feasibility. While this project will initially simulate perpendicular injection, where air/oxidizer is injected at a perpendicular angle to the injected fuel flow, it is expected that other injection schemes, such as stratified, interval, and axial injection, will be tested and approached similarly. Once determined, an engineering matrix will be developed, and the least optimal injection scheme will be further approached through an iterative process of injection variable adjustment to enhance the resulting homogeneity after injection of the least-homogenous injection scheme. Using this matrix, the choice will be justified through quantitatively comparing specific results (velocity, equivalence ratio, and stratification length). Validity of injection scheme configurations can be justified through the comparison of schemes with existing research, such as axial configuration being compared with (Sato et al., 2020) and interval and stratified injection (Lei et al., 2020). The use of quantitative result-based decision matrices and a proportional significance test can justify the validity of the pursued simulations prior to the iteration stage.

Summary of Preliminary Data.

Preliminary data has been gathered for this aim to evaluate the difference in homogeneity levels for various injection configurations. Considering the complexity of homogeneity analysis, the simple mixing analysis featured for both interval and radial injection configurations utilizes a turbulent kinetic energy contour to express the greatest magnitude and area of mixing between two fluid injections of hydrogen fuel and oxidizer. In comparing both injection scheme results, the radial injection scheme produces a lower area of turbulence, yet at a greater magnitude than that of the interval injection scheme. This relationship clearly expresses that the axial injection scheme is more effective at injection due to its ability to promote greater mixing reactions, evident by the magnitude of turbulent kinetic energy beyond the injector inlet. This result clearly justifies the use of computational models to model fluid interaction and can be adjusted and improved to better quantify homogeneity at a more direct level.

Figure 3

Simple Mixing Analysis for Interval Injection Scheme

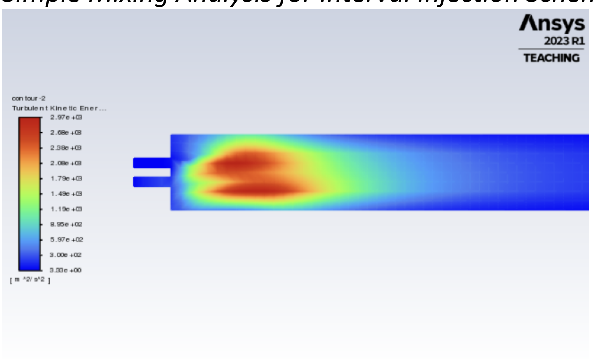
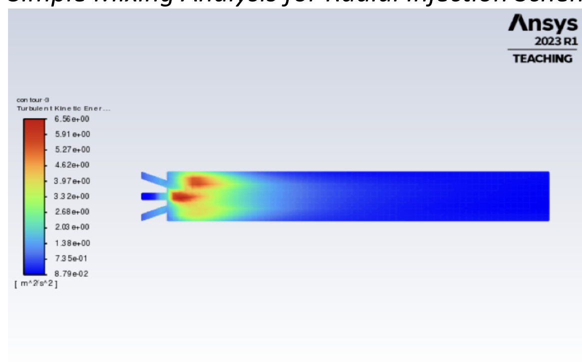


Figure 4

Simple Mixing Analysis for Radial Injection Scheme



Expected Outcomes.

The overall outcome of this aim is to justify the constructed models through the comparative analysis with existing research. This knowledge will be used for quantifying homogeneity and success. The final scheme produced after the iteration process can be compared with previous data to effectively evaluate the success of the introduced injection scheme.

Potential Pitfalls and Alternative Strategies. Similarly to the potential pitfalls in specific aim #1, this aim is heavily CFD-based and will involve analyzing, testing, and compiling data to understand the physical process. Due to limited experience, this process will likely be complex but can be combated through direct simplification and assumptions, as well as gaining the advice of professionals and academic leaders at the Worcester Polytechnic Institute.

***Specific Aim #3:* Iteratively adjust injection variables to increase fuel-air proportional equivalence.**

Justification and Feasibility. As detailed in the work by (Prakash & Raman, 2019), quantitative analysis through equivalence and mixture homogeneity data can further guide the analysis of success and the next steps taken in the iteration phases. Figure 3 clearly expresses this acquisition process by visually representing the process of stratification of fuel concentrations to evaluate the homogeneity of the fuel-air mixture. This value, along with equivalence ratios, can be used to quantify success in an injection scheme. Injection schemes that are less successful can be approached more critically in the iteration phase. There will be at least two iteration phases in which several injection-specific variables, such as injector diameter, distance, and angle of injection, can be altered to produce a more homogenous mixture.

Figure 3

Visual representation of homogeneity measurement acquisition.

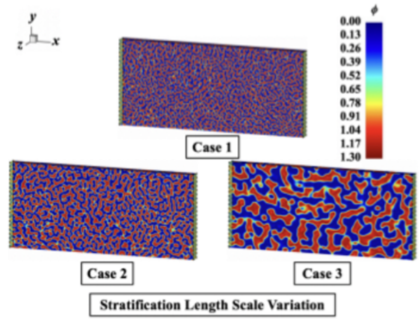


Figure 3. Visual representation of the stratification of a fuel mixture to evaluate homogeneity of the fuel mixture. Figure gathered from (Prakash & Raman, 2019).

Summary of Preliminary Data. No preliminary data has been gathered for this specific aim's justification. Testing data will be used to evaluate success and high-need iteration opportunities. Further research must be conducted to understand the relationship between injection variables and mixture homogeneity. It is expected that through physics and fluid motion analysis, this relationship can be better defined. It is a matter of knowing which values to find that will be approached during the iteration phases.

Expected Outcomes. The overall outcome of this aim is to improve the homogeneity values of an injection scheme to produce the most homogenous fuel-air mixture to enhance the efficiency and thrust output of the RDE. This knowledge will be used for understanding the relationship between injection variables and homogeneity and can be employed in future RDE-related works if found successful.

Potential Pitfalls and Alternative Strategies. It is expected that the iteration phase will be most challenging, as it is difficult to know which values to change to produce a more homogenous mixture. However, these challenges can be addressed through asking questions, testing, and adjusting/making assumptions if needed.

Section IV: Resources/Equipment

This project consists of two components: simulation and analysis. For this simulation, Ansys Fluent will be used to configure, implement, and test for raw data and data visualizations. Analysis will likely be conducted in Ansys Fluent or using other data analysis tools. Any WPI-affiliated computer can simulate the described configuration, making this project inexpensive. Ansys Fluent is a computational fluid dynamics (CFD) software that can model fluid flow, heat and mass transfer, chemical reactions, mixing schemes, and more. By constructing a two-dimensional simple mixing analysis in Ansys Fluent, velocity and distribution data can be gathered when introducing two materials perpendicularly within a rotating detonation chamber. It is expected that initial simulations will be oversimplified due to the Ansys Fluent learning process but will progressively advance as the project develops.

Section V: Ethical Considerations

Considering that the nature of this project is computational, there are no risks to any living organisms. The rotating detonation engine introduces applications in energy production and propulsion/kinetic applications, including defense technologies. The methods used in this project are aimed to optimize mixing strategies in the RDE and are not motivated for use of the RDE in defense.

Section VI: Timeline

Date/Time Frame	Objective(s)	Action Steps
December 4th, 2023	Obtain preliminary data to justify methodology.	● Highlight 2-3 similar works that could be mimicked/related to this project methodology. ● Construct an Engineering Matrix to justify choice and functionality/similarity of model results to other peer-reviewed works. ● Justify the use of a two-dimensional simulation and compare mixture equivalence ratio/stratification length results to other works.
December 8th, 2023	Complete evaluation of preliminary data	● Evaluate configuration data and test one injection scheme. ● Find equivalence ratio and stratification length (quantify mixture homogeneity). ● Predict detonation wave success through comparison with previous works. ● Quantify success of the presented injection scheme.
December 12th, 2023	Present preliminary data to technical audiences at December Fair.	● Present findings to a general and technical audience. ● Improve presentation skills and refine research focus. ● Utilize feedback and suggestions in future aspects of this project.
January 2nd, 2024 - January 12th,	First Iteration Phase - Includes Testing and Analysis	● Adjust injection-specific variables in the most inefficient

2024		configuration to produce more homogenous mixture concentrations. ● Evaluate success, as described in preliminary data analysis.
January 15th, 2024 - January 26th, 2024	Second Iteration Phase - Includes Testing and Analysis	● Continue adjustments. ● Adjust injection-specific variables in the most inefficient configuration to produce more homogenous mixture concentrations. ● Evaluate success, as described in preliminary data analysis. ● Determine best course of action (such as continued iteration phase or conclusion and analysis of the project). ● Additionally, consider next steps, remaining questions, and extensions.

Section VII: Appendix

While this project requires little/no funding for resources or materials, it's possible extensions, such as the fabrication of a detonation engine, testing, and detonation wave production after physically mixing the injection scheme would require funding. A potential granting organization is the Department of Defense and their recent Multidisciplinary University Research Initiative (MURI). While this project aims to advance the future of rocket propulsion, this granting organization offers extensive opportunities for development and advanced research. In addition, the National Aeronautics and Space Administration (NASA) funds research projects related to rockets, space advancement, and explorative sciences. This organization could act as a primary sponsor due to their previous affiliated work with the RDE.

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