Section II: Methodology

Role of Student vs. Mentor

Much of the learning and computational fluid dynamics clarification processes took place with the support and advice of several experts from the Worcester Polytechnic Institute (WPI). These individuals include Dr. Jagannath Jayachandran, Dr. Adriana Hera, and Dr. Aswin Gnanaskandan.

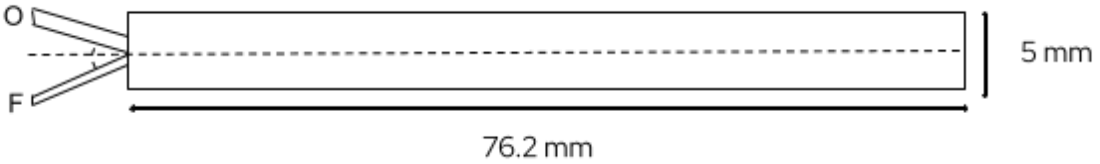
Throughout the course of several meetings with these individuals, feedback and advice were obtained for simulation-specific aspects of this project due to a lack of previous experience in using Ansys Fluent as a computational domain framework. Innovation, project direction, literature review, and experimental analysis have been performed by the student researcher, with academic resources being utilized for clarification and for mapping out effective and timely project plans. Since August of 2023, this project has been pursued at the Massachusetts Academy of Mathematics and Science at Worcester Polytechnic Institute and is planned to face completion on February 15th, 2024.

Equipment and Materials

The planned methodology for this project includes addressing three central objectives: developing a simplified computational model, testing existing injector configurations, and pursuing a short-term iterative adjustment process. Through the three processes of testing, evaluation, and iteration of existing injection schemes, the desired outcome are improved injector schemes and a deeper understanding of the impact of injector geometry on mixture homogeneity. Several models were developed based on the criteria of being inexpensive, simple, and quick to test. Fundamentally, the goal of pursuing a computation-based model is to properly model fluid movement throughout the detonation chamber of a rotating detonation engine. In doing so, the existing Ansys Fluent computational fluid dynamics (CFD) framework was an effective tool for carrying out the planned methodology. Using existing and standardized design parameters from previous works, the created models employ these existing parameters to best align with current propulsion research (Goto et al., 2019; Koo et al., 2023; Bennewitz et al., 2023). In Ansys Fluent, three geometrical domains were developed to simulate mixing processes in pre-tested engines, including axial, radial, and triplet injector schemes. The axial geometrical domain, adopted from Bennewitz et al. (2023), includes a 76.2mm by 5mm chamber “slice”, which predicts particle behavior and could be repeatedly “unrolled” and replicated to model three-dimensional functionality. In Figure 1, the computational geometry produced by gathering previously standardized parameters is expressed graphically. One fuel and one oxidizer injector are present at the inlet end of the chamber. In the present axial injector scheme, each injector sits at an angle of 30 degrees from the chamber’s axial centerline, with a gaseous fuel (CH4) injection orifice of 0.787mm and an oxidizer injection orifice of 1.245mm to maintain the study’s desired injector to annulus ratio of 0.110 (Bennewitz et al., 2023). Both injectors are impinged at a height of 2.16mm from the injector face, with both injecting at a fixed mass flow rate of 0.325 kg/s. As mentioned, these parameters have been found to induce successful experimental detonation results, especially considering their high-pressure injector orifices to avoid flashback and residual backflow to perform at a high ratio of the theoretically optimal Chapman-Jouguet wave parameters.

Figure 1

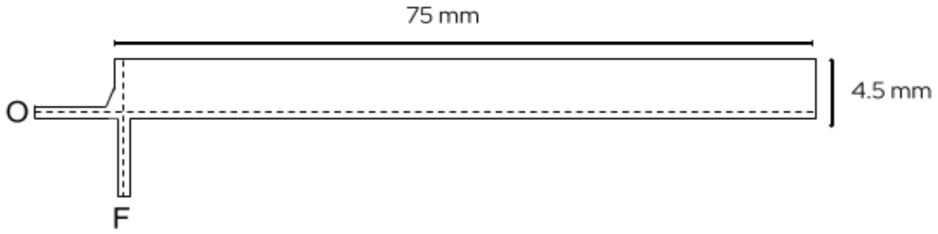
Computational Geometry for Axial Injection Scheme



Note. Figure 1 visually represents the axial injector scheme’s computationally tested injector geometry, including placement of the inlets and general chamber dimensions.

Figure 2

Computational Geometry for Radial Injection Scheme

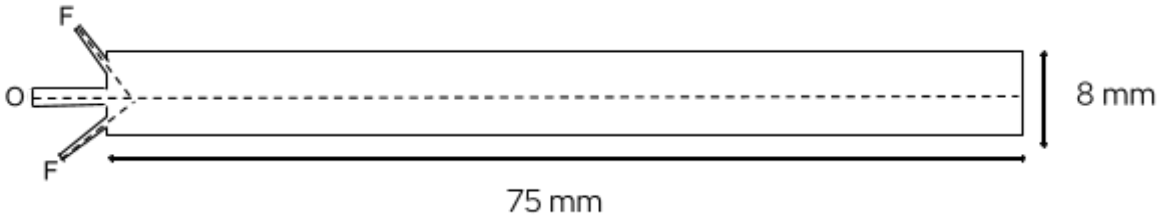


Note. Figure 2 visually represents the radial injector scheme's computationally tested injector geometry, including placement of the inlets and general chamber dimensions.

The second tested injector scheme, which models the radial injector scheme, is expressed visually in Figure 2. This model, based upon parameters identified by Koo et al. (2023), injects gaseous ethylene (C2H4) and gaseous oxygen (O2) into a detonation channel which has a width of 4.5mm and a length of 75mm. The oxidizer is injected from a 0.5 mm slit injector towards the RDE exit direction. In contrast, the gaseous ethylene component is radially injected into the channel in the vertical direction relative to oxidizer injection for mixing. The experiments were originally conducted under three different flow conditions, but the testing within the referenced study was performed at a mass flow rate of 75 g/s due to observations of uncontrolled detonations at high injector mass flow rates (Koo et al., 2023).

Figure 3

Computational Geometry for Triplet Injection Scheme



Note. Figure 3 visually represents the triplet injector scheme's computationally tested injector geometry, including placement of the inlets and general chamber dimensions.

The last existing injector scheme evaluated was an axial-triplet combination injector scheme, which had been reported by Goto et al. (2019). This injector scheme features two fuel injectors, each 1mm in diameter, both of which, when extended, sit at a perpendicular angle, intersecting the chamber axis. In the center of the inlet zone, a single oxidizer injector, being 1.4mm in diameter, is located between both fuel holes. The mass flow rates are 133 g/s for fuel (gaseous ethylene) and 91 g/s for oxidizer injection. For all three tested configurations, a 100µm mesh with an inflation at the inlet boundaries was used to evaluate fluid flow.

Employing a two-dimensional configuration allows for fast-paced testing of each injector scheme without high-fidelity modeling. Determining injector scheme performance using a simplified two-dimensional computational model as a standardized mechanism for performance comparison addresses a deficiency in low-fidelity models for detonation testing, which introduces lengthy testing times and expensive computing resources. This approach combats an ineffective comparison strategy currently existing due to variable detonation kinetic performance. The configuration employs a k-epsilon turbulent flow solver, which breaks down fluid movement within each mesh square to predict how particles will behave throughout the chamber. This solver, often used in CFD as a standard solver, allows the researcher to view and gather information about particle information, including variables such as turbulent kinetic energy, mixture viscosity, temperature, pressure, density, and velocity.

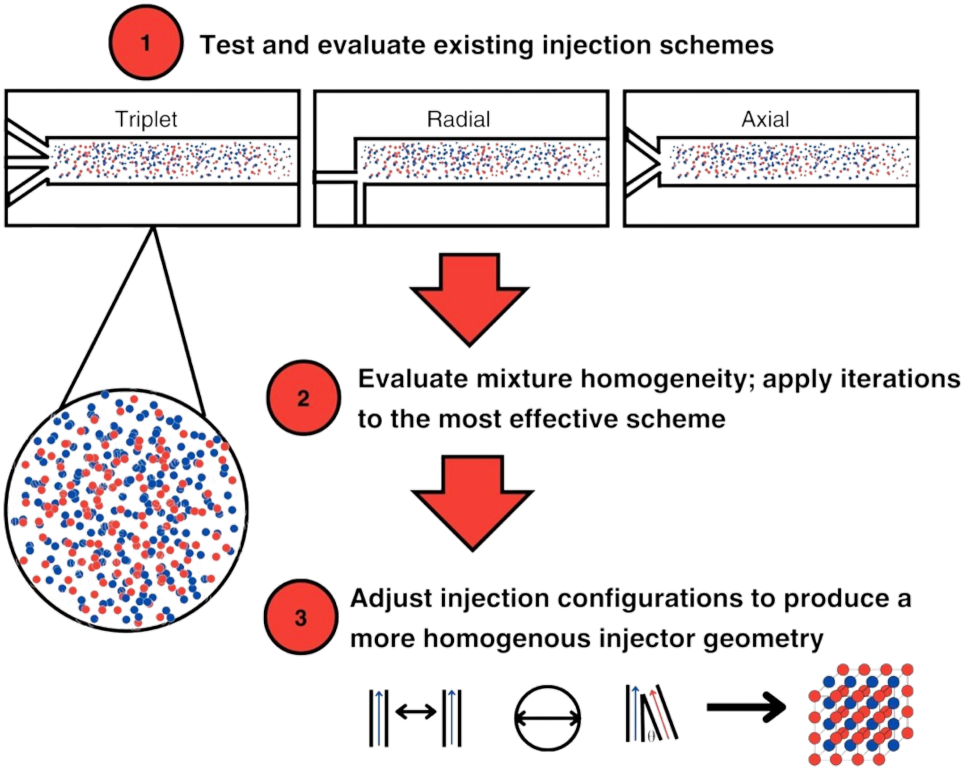
Fundamentally, this transient, density-based turbulent flow model tracks fluid injection and turbulence patterns, providing insight as to how it might impact mixing prior to the arrival of the detonation wave. All results are taken at 750 ms after primary injection, as a standard test consists of 500-750 ms of RDRE combustor operation following ignition, with results being analyzed from output variables stemming from the last 100 ms of injection.

This project consists of three major phases: testing, evaluation, and iteration. During the testing phase, existing injection schemes, including axial, radial, and axial-triplet, will be computationally modeled. Through testing each scheme, comparisons can be made between injector scheme performance to evaluate the ability of an injector scheme to produce a homogeneous mixture of fuel and oxidizer. In evaluating homogeneity and observing particle behavior, each tested configuration can be compared, with one injection scheme being deemed as the “most effective” currently existing model. To effectively compare injector schemes, the standardized computational parameters will be employed, with independently varying injector schemes being implemented to determine their impact on mixture quality.

In determining the most effective injection scheme, the next phase includes pursuing a short-term iterative adjustment process. The purpose of this process is to adjust injection variables, including injector diameter, distance and angle of injection to determine how these variables alter mixture homogeneity levels. This testing methodology allows relationships between injector variables and injector performance to be effectively compared. In addition, this methodology incorporates the use of an iterative improvement process, which alters the stated variables for a specified number of trials to identify which adjustments best improved mixture homogeneity. To further understand these fundamental project methods, see Figure 4.

Figure 4

Fundamental Project Methodology



Note. Figure 4 visually represents the planned fundamental project methodology which was developed with the intention of addressing the need of enhanced injection in RDEs.

Techniques

The techniques utilized through the testing and modeling phase of this project follow no traditional path; rather they employ parameters including density distribution to effectively and accurately model homogeneity, a previously unquantified concept, in a mixture following fuel and oxidizer injection through a simple computational domain. To quantify homogeneity, the technique of employing a density level comparison between the inlet and chamber body is determined as being sufficient.

Statistical Tests

Homogeneity in a mixture can be quantified in various ways, including stratification length, coefficient of variation, observations of turbulent kinetic energy contours, and comparing parameters to ensure that mass fractions throughout the chamber are equal to inflow mass fractions. During the initial phases of this project, a turbulent kinetic energy contour was adopted to evaluate the magnitude and location of mixing turbulence in the computational domain following a steady, pressure-based injection. However, due to its indirect quantification of homogeneity, this evaluation technique was altered. The chosen method of quantification involves comparing the average density at all inlet locations to the chamber body. Considering the higher density of oxidizer, density contours can also be applied to reinforce predictions of particle movement and the homogeneity quantification methods.

Student's Homogeneity Formulas

The following equations were developed to effectively quantify homogeneity and inlet-to-chamber density ratios following injection. These values were processed and stored utilizing the Ansys Fluent CFD-Post program. The homogeneity quantification method is composed of three parts: inlet density, channel density, and comparison values. In Equation 1, the average density at all inlets is recorded. This value provides an averaged density value which factors the density of two density-varying materials, throughout the chamber in a homogenous mixture. The inclusion of the last Z-inlet calculation is dependent on the number of inlets in the tested configuration.

densityInlet = (ave (Density)@inlet_X + ave (Density)@inlet_Y + ave (Density)@inlet_Z)/3 (1)

The second equation calculates the average density value throughout the entire detonation channel.

densitySurfaceBody = ave(Density)@surface_body (2)

The third equation, and last phase of the homogeneity quantification, evaluates the ratio between inlet and channel density.

densityFactor = densityInlet/densitySurfaceBody (3)

If the input parameters are the same as the parameters in the detonation channel, the densityFactor would equal 1, representing an equal ratio and similar inlet-chamber mixture composition. Each tested configuration can be evaluated using these formulas and compared to the optimal density factor by finding a difference. Deviation from the optimal density factor value of 1 determines how homogenous the mixture within the chamber is. The lowest deviation value is correlated with homogeneity, meaning that the most effective injection scheme will be determined as the one with the lowest relative deviation value.