

Injector-Driven High-Frequency Combustion Instability

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by
Jonathan Benjamin Contreras
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approved by
Dr. Periklis Papadopoulos
Faculty Advisor



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ABSTRACT

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A persistent challenge encountered in bipropellant liquid rocket engines since before the Apollo era are combustion instabilities. Combustion instabilities can reduce combustion efficiency and at worst be violently destructive. The contemporary era has sought to ameliorate these instabilities by modeling the behavior by computational means. Whilst expensive computational fluid dynamics (CFD) simulations are capable of predicting most of the instabilities, the cost and time required to do so is prohibitively expensive. The aerospace industry seeks to strike a balance between expensive CFD simulations and less powerful CFD methods capable of predicting the most destructive thermo-acoustic modes. This work seeks to explore the capability of hybrid-LES (Large Eddy Simulations) to predict injector-combustion thermo-acoustic coupling using the Rayleigh criterion.

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Nomenclature

L^*	=	Characteristic Length
L_r	=	Recess Length
c^*	=	Characteristic Velocity
V_c	=	Chamber Volume
$\dot{W}_{tc}$	=	Propellant Mass Flowrate
V	=	Average Specific Volume
t_s	=	Propellant Stay Time
ρ	=	Density
x_i	=	Spatial coordinate
t	=	Time
q	=	Heat Flux
$u_i(x, t)$	=	Instantaneous Velocity
$p(x, t)$	=	pressure
μ	=	Dynamic Viscosity
$f(x, t)$	=	Body Forces
$\boldsymbol{\tau}$	=	Stress Tensor
$\boldsymbol{\tau}^R$	=	Reynolds Stress Tensor
R_{ij}	=	Reynolds Stress Tensor (Index Form)
$\frac{D}{Dt}$	=	Material Derivative
∇	=	Divergence
$\bar{\phi}$	=	Mean (Time-Averaged) Component
$\phi'(x, t), u'_j$	=	Fluctuating Component
k_{KE}	=	Turbulent Kinetic Energy
μ_T	=	Turbulent Eddy Viscosity
δ_{ij}	=	Kronecker Delta
G_ν	=	Turbulent Viscosity
Y_ν	=	Destruction of Turbulent Viscosity
$\sigma_{\bar{\nu}}, C_{b2}$	=	Constants

ν	=	Molecular Kinematic Viscosity
$S_{\bar{\nu}}$	=	User Defined Source Term
μ_t	=	Subgrid-Scale Turbulent Viscosity
τ_{kk}	=	Subgrid-Scale Stresses
$\bar{S}_{ij}$	=	Rate of Strain Tensor
L_s	=	Mixing Length for Subgrid-Scales
k	=	Von Kármán Constant
C_s	=	Smagorinsky Constant
Δ	=	Local Grid Scale
ν_t	=	Eddy viscosity
$\overline{OP}(\vec{x}, t)$	=	Operator Function
h_i	=	Total Specific Enthalpy
$q'(x, t)$	=	Instantaneous Heat Release Fluctuation
C_p	=	Specific Heat Capacity
λ	=	Thermal Conductivity
α	=	Thermal Diffusivity
$\mathcal{D}$	=	Mass Diffusivity
R_i	=	Net Rate of Production of Species i by Chemical Reaction
S_i	=	Rate of Creation by Addition From the Dispersed Phase
Pr	=	Prandtl Number
Sc	=	Schmidt Number
Le	=	Lewis Number
Y_i	=	Mass Fraction of Each Species
$\vec{J}_i$	=	Diffusion Flux of Species i
$\mathcal{R}$	=	Rayleigh Index
T	=	Period of Acoustic Oscillation Cycle
$p'(x, t)$	=	Instantaneous Pressure Fluctuation
A	=	Pre-exponential Factor
β	=	Temperature Exponent
E_a	=	Activation Energy
R_u	=	Universal Gas Constant
C	=	Molar Concentration
A_{mix}	=	Magnussen Constant
Y_F, Y_{ox}	=	Mass Fractions
s	=	Stoichiometric Ratio
Y_{prod}	=	Mass Fraction of the Products
Da	=	Damköhler Number
I	=	Turbulent Intensity

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Chapter 1

Introduction

1.1 Motivation

Combustion instability remains one of the most persistent failure modes in liquid rocket engines. In the 1960's, during the Apollo program, there was a significant effort to ameliorate combustion instabilities; in particular high-frequency transverse combustion instabilities in the F-1 engine[1]. The instabilities encountered during the operation of the F-1 engine hindered combustion efficiency and at worst destroyed the engine. It was due to the rapacious nature of these thermo-acoustic instabilities that the reduction and/or complete removal of it would increase the probability of mission success and subsequently increasing safety for astronauts onboard. High-frequency instabilities are more destructive than low- and medium-frequency instabilities and thus the ability to predict the on start of instabilities allows for attenuation via active and passive controls. With growing computational abilities, Large Eddy Simulations (LES) have become more accessible to researchers and high fidelity simulations are no longer prohibitively computationally expensive for research groups[2][3]. Large LES are still computationally expensive hence, methods that can capture transient phenomena while not being as computationally intensive as LES are preferred. Hybrid-LES are capable of capturing the transient behavior of the system, but do suffer from information loss when compared to LES. In spite of decreasing computational cost, traditional CFD seeks to explore augmentation. However, the highly non-linear nature of combustion requires any algorithm that is applied to be able to understand the complicated behavior. Enter neural networks. Neural networks and by extension machine learning, is a powerful tool that has the capability to model highly non-linear functions, such as those found in flame fronts. The application of machine learning tools is not a novel approach, yet is increasingly popular and beneficial for

predictive modeling.

1.2 Literature Review

1.2.1 Historical Background

Combustion instability date back to the late 1930's with Germany's work on the V-2 rockets[1]. A significant amount of work was contributed toward understanding combustion instabilities during the 40's and 50's in the USA. During these decades there was a focus on studying linear and non-linear instability, both of which result in complex theoretical analyses. Non-linear instabilities could be described as searching for supercritical and subcritical bifurcation or stated in other terms: "determining the conditions for the existence and stability of limit cycles for a linearly unstable system and finding the conditions under which a linearly stable system may become unstable to a sufficiently large disturbance." [1]. In the 1950's there was a heavy reliance on hand calculations to derive the behavior of the system; these hand calculations relied on intimate knowledge of dynamical systems and chaos, in the mathematical sense of the word. Perturbation theory is a rigorous manner in which one may calculate the behavior of a highly non-linear system. There are several methods to solve these systems; however, the discrepancy between the resultant mathematics and the real world phenomena is a mixed result of simplified physical assumptions and the neglecting of higher order terms. Theory could only take you so far. To achieve a high degree of accuracy and certainty regarding thrust chamber behavior, it was imperative to perform real world testing. Real world testing is however, prohibitively expensive especially when it results in the destruction of the engine. The analytical results directed the tests and compare the difference in statements. Despite strong curiosity driving talented researchers to perform the impossible to achieve productive results, this experimental data would be prohibitively expensive, thus leaving several under supplied groups without a testable benchmark. During the Apollo era, there was a great incentive to further the understanding of combustion instabilities, human life. The F-1 engine was the rocket engine that experienced violent results from these instabilities that sometimes resulted in the destruction of the engine. The program tested 108 injectors and over 2,000 full scale engine tests[4]. Thankfully, during this era, the cost prohibitive nature of experimental testing was more of an afterthought. The F-1 engine faced fierce combustion instabilities which, through rigorous testing, were eliminated through the use of baffles. These baffles broke up the combustion regimes and prevented from the instabilities from growing[5]. Despite this success, the amelioration of combustion instabilities from the F-1 engine was an ad-hoc fix

that fails to translate linearly to other engines. The nature of the baffles was a learning point that would influence future design of F-1 inspired rockets such as the SSME. Still, the rigorous experimental testing and elusive nature of combustion instabilities left a desire for a more affordable ubiquitous solution. It wouldn't be until the 1970's when Computational Fluid Dynamics (CFD) simulations would be begin to be popularized by the Rocket Combustor Interactive Design (ROCCID). During this time, the capability of CFD was limited to 1-D and 2-D flows where the chemistry was limited and the grid size was small by today's standards of $< 50K$ cells[6]. ROCCID assisted in performing sensitivity sweeps, determining injector elements and predicting the trends of high-frequency modes. The leveraging of computers to perform engineering work was not novel; however, the 70's was the decade when CFD would never leave the toolbox of the propulsion engineer. With this technology expanding across the desks of researchers across the world, it was only a matter of time before someone developed novel methods to run simulations in a more efficient and detailed manner. In the 90's, one of the first papers to solve for the full 3-D unsteady Euler equations was able to appropriately capture the phase and amplitude of the combustion accurately[7]. This paper helped advance map injector flow fields, coupling injector acoustics to chamber modes and limit cycles. During this period, Reynolds-Averaged Navier-Stokes (RANS) continued to mature and integrate into numerical solvers such as FLUENT. The introduction of Grenda et al. [7] paved the way for other research groups to further hone and develop 3-D models capable of producing the desired increase of fidelity craved by the scientific community. At the turn of the millennia, LES of single injectors and unsteady RANS simulations were of investigative interest. As computational power increase so did the fidelity of RANS. The need for higher fidelity simulations was stated to resolve issues with "...costly, time consuming test, fail, fix development program." [8]. LES investigations explored shear-coaxial injectors in an attempt to achieve a higher degree of accuracy without needing to resort to the computationally intensive Direct Numerical Solutions of Navier-Stokes (DNS) simulations. LES provide the ability to reproduce chamber heat-flux and pressure, locate hot spots and shorten testing life cycles[9]. Simultaneously, the expansion of personal computers and the world wide web helped accelerate the rate at which researchers could share data across continents and encourage further collaboration. The development of the field of propulsion is a direct beneficiary of the digital age and CFD is the undeniable proof. In the modern day, it has become increasingly popular to leverage supercomputers or other High Performance Computing (HPC) clusters to run full-scale LES simulations. In 2021 a team from Japan Aerospace Exploration Agency (JAXA) executed a full-scale 3-D LES with over 500 injectors on the supercomputer JSS3. The mesh for this simulation is in the

billions of cells[10]. The ever increasing integration of computational prowess with the ingenuity of this discipline results in incredible opportunities for the unrelenting pursuit of the perfect simulation at the cost of a dime. The JAXA team is pushing the limits as to what is possible with LES and is providing a road map for other ambitious investigators.

1.2.2 Current State of the Art

Recent work has investigated various aspects of injector-combustion chamber coupling, Hybrid LES and Dynamic Mode Decomposition (DMD) with multiple injectors. Both experimental and simulation work is being done. A paper may begin its investigation by running experiments in a research combustor outfitted with various types of sensors and camera that sufficiently capture the behavior of the desired set up. From here the research group meticulously sets up simulations in an effort to reproduce the results of the test and other simulations that provide further insight to other aspects of the test. Other research groups without the access to an experimental combustor are able to compare their simulations to the established benchmarks of the other groups. Afterward, they can confidently output research and simulations that further the field. Groups may take varied approaches from hybrid simulation models to augmenting an aspect of the simulation to pre-process data "offline" thus streamlining the simulation. Thakur et al. [11] proposed a "compressible flamelet modeling framework for unsteady turbulent combustion ... LES and Hybrid RANS-LES (HRLES) methodologies incorporated in a proven existing solver called Loci-STREAM.". This approach allowed them to create a high-fidelity simulation where the flamelet was capable of handling both ideal gases and real fluids. It was an improvement over the status quo of Loci-STREAM. Guo et al. [12] investigated a single element rocket combustor through the use of a hybrid RANS-LES and DMD. The paper used a 3-D geometry for the simulation and the results reflected an increase of thermo-acoustic combustion instability due to a sudden heat release cause by unburnt reactants combusting upon combustor chamber wall contact. Several papers ape each others hybrid approach to dedicate focus to other related aspects of combustion instability. Whilst there is a desire to discover ever more computationally efficient manner to run higher fidelity simulations there is still much to study with more computationally manageable techniques. Despite the high computational demand of LES, it is still a highly pursued option due to its ability to resolve flow separation, mixing and unsteady behavior than Hybrid-LES. Several researchers have found success in single element LES simulations such as Bee et al. [13]. Bee et al. posits a swirl coaxial injector using liquid oxygen (LOX)/Methane for startup and

subcritical operation. The group investigates the alternative swirl coaxial injector as opposed to shear coaxial injectors and claim better atomization translating to "...improved flame anchoring characteristics...". The results agreed, tests showed " during hot-fire operation and potentially faster propellant mixing, resulting in higher flame intensity closer to the injector exit.". Another work by Philo et al. [14] investigates chamber injector dynamics through an array of seven injectors supplying natural gas and air into a rectangular combustion chamber for two distinct injector lengths. For the configuration given in the paper, it was found that a longer injector length increased the amount of combustion instabilities whereas a shorter injector attenuated the instabilities. Another study used a hybrid-LES method stress-blended eddy simulation (SBES) [15] to validate the experimental results from a rectangular model combustor and benchmark the accuracy of the SBES [16]. Due to the incredibly non-linear nature of combustion instabilities, the current methods of model analysis and prediction leave a desire for greater accuracy. Shadram [17] proposes an architecture where neural networks (NN) replace flamelet tables in single injector LES models. The advantage of incorporating the NN is the increased ability to capture highly non-linear phenomena of the pressure and velocity fields. Opeoluwa et al. [18] explore the insertion of a different neural network, a Mixture of Experts (MoE) approach, to resolve the flamelet tables in a less computationally expensive manner. MoE is an architecture where there are "experts" that help in classifying data that is fed by a gating network [19].

1.2.3 Gaps Motivating the Present Work

With ever more influence from the application of machine learning (ML) tools, several CFD approaches must be revisited. RANS and LES are seeing a revitalization of approaches and techniques being applied to current curiosities. Shejan et al. [20] perform an incredible survey of tools and practices being applied to reacting flows. With the ever increasing size of simulations and datasets, ML learning becomes increasingly well positioned to integrate itself into CFD studies. In particular large 3-D multi-injector LES simulations such as [10], provide an insight into the future of CFD. These simulations are still prohibitively expensive for several teams; however, the immense amount of resulting data from these types of simulations allow for other groups to run simulations with more confidence, following the paper's setup. The push for the integration of NN into flamelet tables for LES to decrease the computational expense while maintaining if not increasing the fidelity of the simulations has great potential[17][18]. The incorporation of ML approaches should not be limited to flamelet tables in LES, but should expand to predictive capability. The requirements

for a predictive NN would be an immense amount of data and rigorous control to ensure accuracy of the predictive modeling. The potential upside is such that it would reduce the dependency of HPC clusters and increase the fidelity of the simulations while gaining insight into coupled mechanisms.

1.3 Project Proposal

This proposal is dedicated to the feasibility of using a hybrid-LES approach to evaluate L^* and L_r coupled high frequency combustion instabilities in a rectangular model combustor (RMC) using gaseous oxygen (GOX)/Methane at room temperature.

$$L^* = \frac{V_c}{A_t} = \frac{\dot{W}_{tc} V t_s}{A_t} \quad (1.1)$$

L^* is the characteristic length which relates the chamber volume to the nozzle sonic throat area as stated in Eq. 1.1. This parameter is important as its physical meaning is the residence time of the propellant in the combustion chamber relative to acoustic period. Additionally, L_r also holds significant potential for discovering thermo-acoustic combustion instabilities in the RMC. The advantage of the RMC is it decouples the instabilities into transverse and longitudinal modes more so than in a cylindrical combustion chamber. The variation of the L^* and L_r on an RMC should bring clarity on the extent of coupling between transverse and longitudinal modes as a function of L^* and L_r respectively. For validation purposes, the results will be cross referenced with [16]. A simplified geometry, injector setup, species and CFD techniques are used. The reference geometry is an RMC with eleven equally spaced gas-centered shear coaxial (GCSC) injectors in a linear array. The simplified geometry will be a single GCSC. Additionally, to properly capture the physics of the problem without using a large mesh, a 2-D axisymmetric setup will be used. As a consequence, the geometry will be cylindrical not rectangular. The propellant is a GOX/methane mixture at room temperature. For CFD, a hybrid-LES stress-blended eddy simulation (SBES) is used. SBES is a hybrid-LES technique proposed by [15]. As previously stated, the advantage of an RMC is the absence of complex overlapping acoustic modes such as that found in cylindrical combustion chambers. The simplified interactions lead to a simplification of analysis. SBES allows a reduced mesh fidelity away from the injector shear layers while preserving its accuracy in the critical regions. Despite this mesh relaxation, the mesh size is expected to approximate that of an LES in the separating shear layers (SSL). Rigid wall boundary conditions in the RMC enables clear identification of eigenmodes.

The injectors in the publication are arranged in a linear array equidistant from each other thus producing an plane of symmetry about the center injector. This symmetry suppresses odd modes as they would require an asymmetric symmetry for excitation. Due to the changes in geometry discussed previously, there is an expectation of slightly differing results from the paper. The expected behavior should remain the same in the simplified geometry with the expectation that there will now be a tangential mode causing interference with the transverse and longitudinal modes. The selection of SBES is preferred over other hybrid-LES models due to the following: its improved ability to provide a high degree of shielding of RANS boundary layers under mesh refinement, reliable switching from RANS to LES in Separating Shear Layers (SSL) and allowance of the combination of RANS and LES models.

1.4 Methodology

1.4.1 Setup

To most efficiently create the required CAD it is best to create a parametrized geometry. This parameterized geometry allows for rapid L^* variations without needing to manually adjust the CAD. The geometry is simplified to a 2-D planar surface. The motivation behind creating a 2-D surface is to reduce the mesh elements. An axisymmetric simulation can be ran and it will produce results in 3-D. The CAD software used is Solidworks. The CAD is then imported into Ansys Spaceclaim for any geometry repair. After this, the mesh can be created. There are two meshing methods in Ansys, mechanical and fluent. Mechanical meshing is designed for finite element analysis (FEA), but it can still be used for fluid flow analysis given the user understands and adheres to necessary y^+ requirements. Fluent meshing is designed for CFD analysis and preemptively clusters the meshing in physically sensitive areas such as the wall. Once meshing is completed, the mesh file will be imported into Ansys Fluent where the turbulent model and boundary conditions will be defined. After the CFD simulations are complete, post processing will be conducted which will extract values indicative of combustion instability such as the Rayleigh index [21][22].

Chapter 2

Computational Fluid Dynamics Simulation

2.1 Computational Requirements

The software in use for CFD is ANSYS FLUENT. Implementation procedures are curtailed to represent the software environment of Fluent. The expectations for computational requirements are significant, optimally a dedicated workstation will be used to simulate reacting flows. As will become clear in subsequent sections, the computational requirement for unsteady flows are non-trivial. This is due to the inherent complexity in resolving eddy flows and complementary mesh fidelity. As RANS is incapable of capturing instabilities, LES is required. This computational cost could be ameliorated via the use of Hybrid-LES; however, the cost is still more than RANS flows.

2.2 Reynolds-Averaged Navier-Stokes

2.2.1 Theory

$$\nabla \cdot \mathbf{u} = 0 \tag{2.1}$$

$$\frac{D\mathbf{u}}{Dt} = \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} \tag{2.2}$$

Due to the complexity of the Navier-Stokes equation, shown in Eq.(2.2)[23] in convective form for incompressible flow, alternatives for solving for fluid flows have emerged. Bold letters indicate vectors. For the derivation of the Navier-Stokes from component

form to vector form with the incompressibility assumption shown by Eq. (2.1) refer to Appendix A. The direct resolution of Navier-Stokes is known as Direct Numerical Simulation (DNS) and are computationally expensive, more so than LES.

$$\phi(x, t) = \bar{\phi}(x) + \phi'(x, t) \quad (2.3)$$

$$u_i = \bar{u}_i + u'_i \quad (2.4)$$

$$\rho \left(\frac{\partial \bar{\mathbf{u}}}{\partial t} + (\bar{\mathbf{u}} \cdot \nabla) \bar{\mathbf{u}} \right) = -\nabla \bar{p} + \mu \nabla^2 \bar{\mathbf{u}} - \nabla \cdot \boldsymbol{\tau}^R + \rho \bar{\mathbf{f}} \quad (2.5)$$

A solution is to apply Reynolds decomposition and averaging to Eq. (2.2) using Eq. (2.3) and Eq. (2.4), to obtain the incompressible RANS equation Eq. (2.5). The problem with this equation is known as the closure problem[24]. The closure problem is addressed by two general approaches: the Boussinesq hypothesis and the Reynolds stress transport equation modeling (RSM). The Boussinesq hypothesis relates "...the Reynolds stresses to the mean flow velocity gradients via the eddy viscosity concept." An eddy viscosity is used due to the stresses being treated as laminar stress terms, also the turbulence is assumed to be isotropic[24][25].

$$R_{ij} = -\overline{\rho u'_i u'_j} = \mu_T \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} k_{KE} \quad (2.6)$$

$$k_{KE} = \frac{1}{2} \overline{u'_i u'_i} \quad (2.7)$$

For incompressible flow, the Reynolds stress is represented as Eq. (2.6). This reduces the number of unknowns from nine to two: eddy viscosity μ_T , and turbulent kinetic energy k_{KE} Eq. (2.7). This assumes the Reynolds stress is equal to the mean strain which is not true in all flows. Zero equation models are known as algebraic models whilst, one and two equation models are based on the number of turbulence transport equations solved. The Spalart-Allmaras model is a one-equation turbulence model which solves for modified eddy viscosity. The focus will be on the Spalart-Allmaras model due to its later usage; however, it will be explained in the following subsection whilst this subsection will be used to explain other models and approaches. A zero-equation model is an algebraic model such as the Mixing-length model proposed by Prandtl[26]. Its relative simplicity lacks wide application. More widely used models are two-equation models such as: Standard k - ϵ Model and k - ω Model. The former is widespread in turbulence models. The two equations are for: turbulent kinetic energy (k_{KE}) and turbulence dissipation (ϵ)[27]. The turbulence

dissipation rate is the rate at which kinetic energy is converted into thermal energy via viscous dissipation. It excels in prediction when the flows are fully turbulent and far from walls. The limitations of the standard $k-\epsilon$ model are poor predictions when there is strong separation, large streamline curvature and low Reynolds number near wall regions. The $k-\omega$ model also uses turbulence kinetic energy, but differs from the previous model by using specific dissipation rate (ω). The advantages this model boasts are the following: better performance in the near wall region and does not require wall functions. The $k-\omega$ often more accurately predicts boundary layer development and adverse pressure gradients than the $k-\epsilon$ model; however, it is sensitive to freestream conditions[28]. As with many models that capture comparable behavior with contrasting drawbacks, there is a combination of the two. The Shear Stress Transport model (SST) is a two-equation hybrid of the previous $k-$ models. It leverages the advantages of the $k-\omega$ for wall behavior while adapting to the $k-\epsilon$ for freestream behavior[29]. Reynolds Stress Model (RSM) is distinct approach in which solves the transport equations for each component of the Reynolds Stress Tensor (RST) and also the dissipation equation. This totals seven equations, leading to it sometimes being referred to as a seven-model equation[30]. RSM can more accurately model turbulence anisotropy and other interactions than eddy-viscosity models. This comes with an increased computational cost and other issues in implementation, leading to a more general reliance on two-equation models when using RANS.

2.2.2 Implementation

The Spalart-Allmaras (S-A) one-equation model involves solving a single transport equation for a quasi eddy viscosity $\tilde{\nu}$ [31].

$$\frac{\partial}{\partial t}(\rho\tilde{\nu}) + \frac{\partial}{\partial x_i}(\rho\tilde{\nu}u_i) = G_\nu + \frac{1}{\sigma_\nu}((\frac{\partial}{\partial x_j}(\mu + \rho\tilde{\nu})\frac{\partial\tilde{\nu}}{\partial x_j}) + C_{b2}\rho(\frac{\partial\tilde{\nu}}{\partial x_j})^2) - Y_\nu + S_\nu \quad (2.8)$$

When running CFD simulations, the S-A Transport Equation Eq.(2.8) is used for calculations of the species. In ANSYS FLUENT, the setup for RANS simu-



Figure 2.1: Energy button in Ansys fluent

lation is straight forward. Once the desired geometry is imported and a quality

check has been performed, in the physics section of the solver settings, select the "Energy" box in Figure 2.1. The energy button determines whether or not the conservation of energy is used in the solving system [32]. This forces the flow to be non-isothermic and is determined via any temperature independent density model. The following step is to click on the viscous button found in Figure 2.2. Once inside



Figure 2.2: Viscous button in Ansys fluent

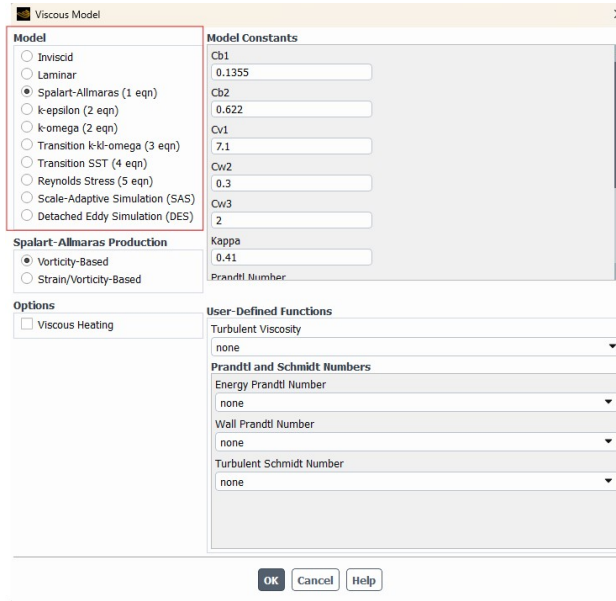


Figure 2.3: Energy transport equation selection in Ansys fluent

that menu, select whichever model desired to be used for the simulation found in Figure 2.3. Two examples of selection are the Spalart-Allmaras and $k-\epsilon$ models. If the Spalart-Allmaras is selected, there will be a selection between vorticity-based and strain/vorticity-based as shown in Figure 2.4. Conversely, if the $k-\epsilon$ selection is chosen there will be two separate selections as shown in figure 2.5. The primary selection will be between: standard, RNG and Realizable. The secondary selection, regarding near wall treatment, are the following: standard wall function, scalable wall

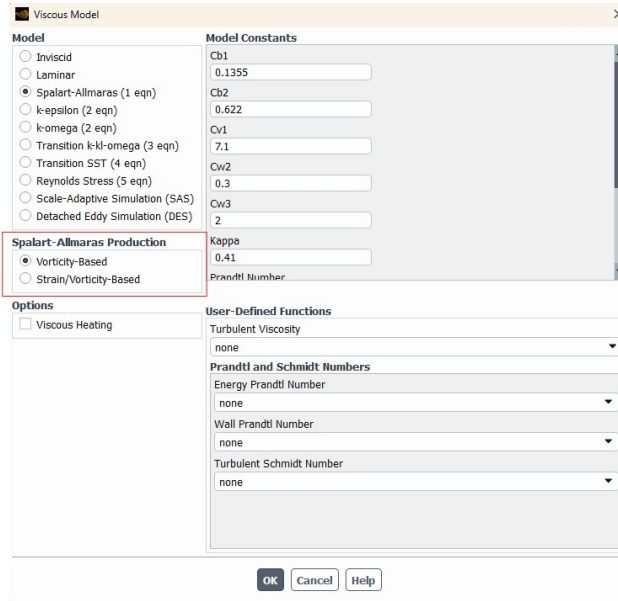


Figure 2.4: Spalart-Allmaras in Ansys fluent

functions, non-equilibrium wall functions, enhanced wall treatment, Menter-Lencher and User-Defined wall functions.

2.3 Large Eddy Simulation

2.3.1 Theory

LES is a suitable middle ground between RANS and DNS. It provides a higher fidelity than RANS by resolving the large eddies while modeling the small eddies. This technique is preferred over RANS when the fidelity desired is higher, turbulent, high Reynolds flow and computational restricted from leveraging DNS. LES reduces computational cost compared to DNS by requiring a coarser mesh and larger timestep; however, LES still requires a finer mesh than RANS. There are two types of approaches to applying LES. There are subgrid-scale models and inlet boundary conditions for scale resolving simulations. Within subgrid-scale (SGS) models are there are several flavors used in Fluent such as: Smagorinsky-Lilly model, Dynamic Smagorinsky-Lilly model, Wall Adapting Local Eddy Viscosity (WALE) model and

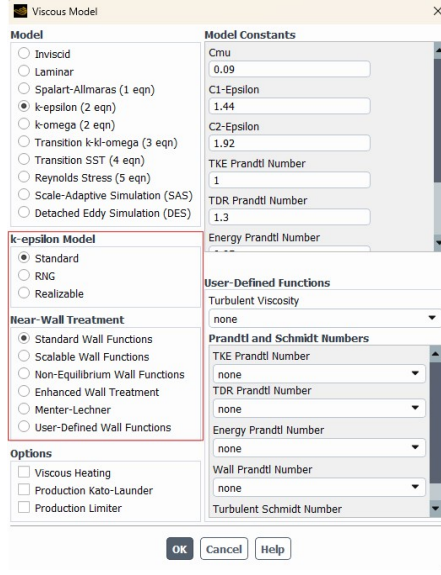


Figure 2.5: k - ϵ model in Ansys fluent

Dynamic Kinetic Energy Subgrid-Scale model.

$$\tau_{ij} - \frac{1}{2}\tau_{kk}\delta_{ij} = -2\mu_t\bar{S}_{ij} \quad (2.9)$$

$$\bar{S}_{ij} \equiv \frac{1}{2}\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i}\right) \quad (2.10)$$

The SGS turbulent stresses Eq.(2.9) are used to compute the SGS turbulence models in Ansys Fluent[32]. The rate of strain tensor is given by Eq.(2.10).

$$\mu_t = \rho L_s^2 |\bar{S}| \quad (2.11)$$

$$|\bar{S}| \equiv \sqrt{2\bar{S}_{ij}\bar{S}_{ij}} \quad (2.12)$$

$$L_s = \min(kd, C_s\Delta) \quad (2.13)$$

$$\Delta = V^{\frac{1}{3}} \quad (2.14)$$

In Fluent, the eddy viscosity of the Smargorinsky-Lilly model[33][34] is computed via Eqs. (2.11)-(2.14)[32]. This model represents the resolved turbulent kinetic energy as heat dissipation which is what is expected. The limitations of this adoption is the

eddies near the boundary regions does not properly represent the expected behavior near the wall where a no-slip condition is expected.

$$\nu_t = C_m \Delta^2 \overline{OP}(\vec{x}, t) \quad (2.15)$$

WALE seeks to remedy the inaccuracy in near wall behavior via a novel operator function, shown in Eq. (2.15) exhibiting the following properties: "invariant to any coordinate translation to rotation, can be easily assessed on any kind of computational grid, is a function of both the strain and the rotation rates...concerning the contribution of turbulent structure to the global dissipation, and it goes naturally to zero at the wall so that neither damping function nor dynamic procedure are needed to reproduce the effect of the no-slip condition.". This novel operator produces the desired wall behavior in Eq. (2.16)[35].

$$\nu_t = O(y^3) \quad (2.16)$$

Germano et al. [36] proposed an approach to the Smagorinsky-Lilly which involved a dynamic Smagorinsky coefficient which models the subgrid scales based on the smallest resolved scales allowing it to account for backscatter. Backscatter, also known as negative eddy viscosity, is the transfer of energy from small grid scale to large grid scale, the opposite of forward scatter[37]. The Dynamic Kinetic Energy Subgrid-Scale Model leverages an adaptive C_k constant to avoid overly dissipative and non-adaptive behavior exhibited by a static constant.

$$k_{sgs} = \frac{1}{2}(\overline{u_k u_k} - \bar{u}_k \bar{u}_k) \quad (2.17)$$

$$\frac{\partial k_{sgs}}{\partial t} + \tilde{u}_i \frac{\partial k_{sgs}}{\partial x_i} = -\tau_{ij} \frac{\partial \bar{u}_i}{\partial x_j} - \epsilon_{sgs} + \frac{\partial}{\partial x_i} (\nu_T \frac{\partial k_{sgs}}{\partial x_i}) \quad (2.18)$$

$$\tau_{ij} - \frac{1}{3} \delta_{ij} \tau_{kk} = -2C_k \Delta \sqrt{k_{sgs}} \bar{S}_{ij} \quad (2.19)$$

Additionally, the deviatoric SGS stress Eq. (2.19) [38] achieves the desired modeling behaviors by utilizing Eq. (2.17) which is obtained by solving the transport equation Eq. (2.18)[39, 40]. This approach allows for a more accurate representation of backscatter at the cost of induced numerical instability.

2.4 Hybrid RANS/LES

2.4.1 Theory

Whilst RANS excels at minimizing computational cost it fails to properly capture unsteady behavior. On the contrary, LES excels at capturing unsteady transient

behavior yet suffers from significant computational cost requirements. A hybridization of these methods known as Hybrid RANS/LES is a comprise which allows the capture of unsteady regimes yet manages to reduce the computational requirement of an LES simulation. One example is the Detached-Eddy Simulation (DES) proposed by Spalart et al. [41]. The mechanism of DES is to use RANS to simulate the attached eddy layers near the wall while using LES to simulate the eddies in the detached layers far from the wall. Since RANS is used in the boundary layer and RANS uses the assumption of the Boussinesq hypothesis, the information lost in the boundary layer is the energy backscatter. This is a key piece of information to maintain since this is a major difference from WALE which is capable of modeling backscatter. There are several different hybrid-LES models to select from such as: scale adaptive simulation (SAS), delayed DES (DDES), shear layer adapted (SLA) DDES (DDES-SLA), improved DDES (IDDES), shielded detached eddy simulation (SDDES) and stress-blended eddy stimulation (SBES)[42, 43, 44, 15].

$$d_{DES} = \min(d, C_{DES}\Delta_{max}) \quad (2.20)$$

In S-A based DES the length scale shown by Eq. 2.20 dictates the RANS-LES switching behavior. As an unwanted consequence this leads to grid induces separation (GIS), which is when the model determines the grid is sufficiently fine to switch to LES, but the grid lacks the granularity to resolve the eddies directly using LES [45]. This forces the user to be purposeful in mesh creation and ensure the mesh meets RANS standard, but does not exceed that level of fidelity too much that the model switches to LES.

$$\tau_{ij}^{SBES} = f_{shield} \cdot \tau_{ij}^{RANS} + (1 - f_{shield}) \cdot \tau_{ij}^{LES} \quad (2.21)$$

Contrary to other hybrid-LES approaches, the SBES is not properly defined as a turbulence model but rather as an approach to the RANS-LES switching problem. SBES uses existing RANS and LES turbulence models and instead of relying on Eq. 2.20 to determine when to switch between RANS and LES, it relies on Eq. 2.21. The former is mesh dependent while the latter is stress dependent.

2.4.2 Implementation

The implementation of a hybrid-LES model in ANSYS is straightforward. Follow exactly as done in §2.2.2 when selecting the turbulence model with the only difference of selecting the box next to the "Stress blending (SBES)/ Shielded DES" and selcting the appropriate radio button for the hybrid-LES desired. Fig 2.6 shows the selection

area. It is important to note SBES will use LES in the SSL and as such requires a higher mesh fidelity and smaller time steps.

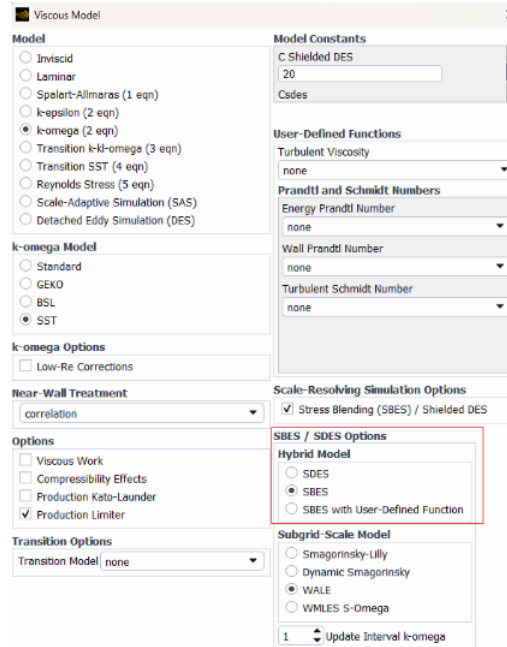


Figure 2.6: SBES turbulence model selection

Chapter 3

Implementation

3.1 CFD Initial and Boundary Conditions



Figure 3.1: Geometry

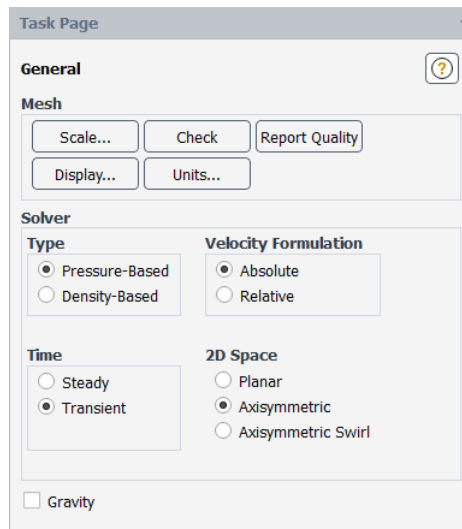


Figure 3.2: Solver type selection

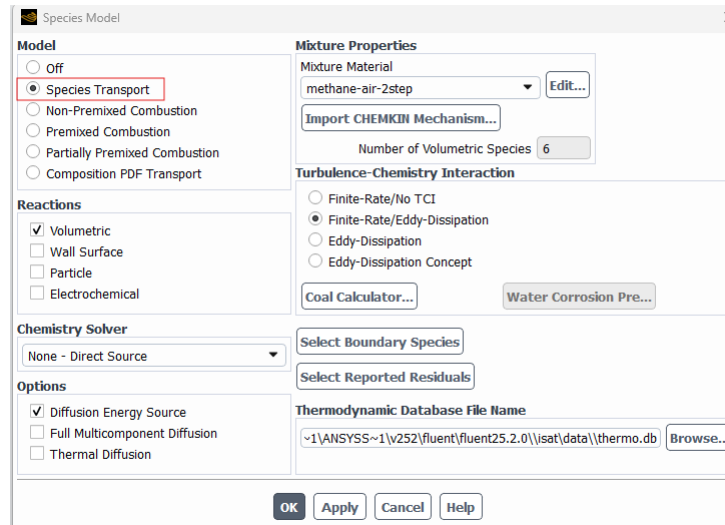


Figure 3.3: Species model selection

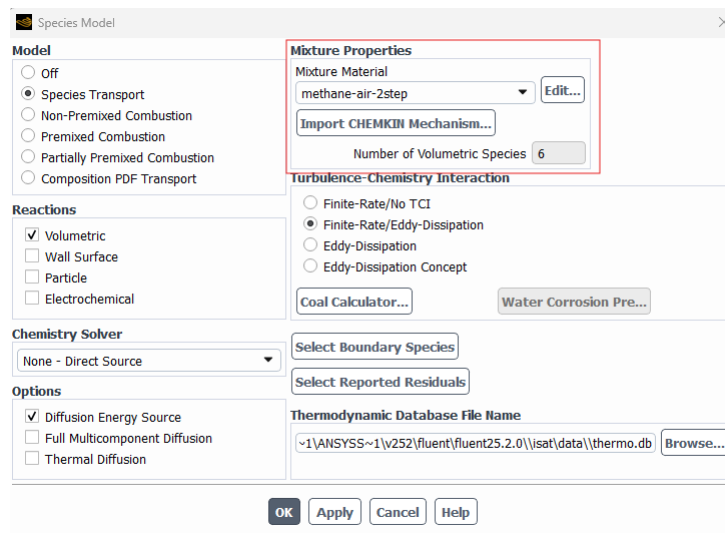


Figure 3.4: Species mixture properties

3.1.1 Initial Conditions

The setup of the simulations were done using the Ansys software package. The CAD models were created in Ansys Spaceclaim. Meshing was completed in Ansys Mechanical. CFD was completed using Ansys Fluent. There were three unique geometries used and for one geometry there were two meshing grids to determine

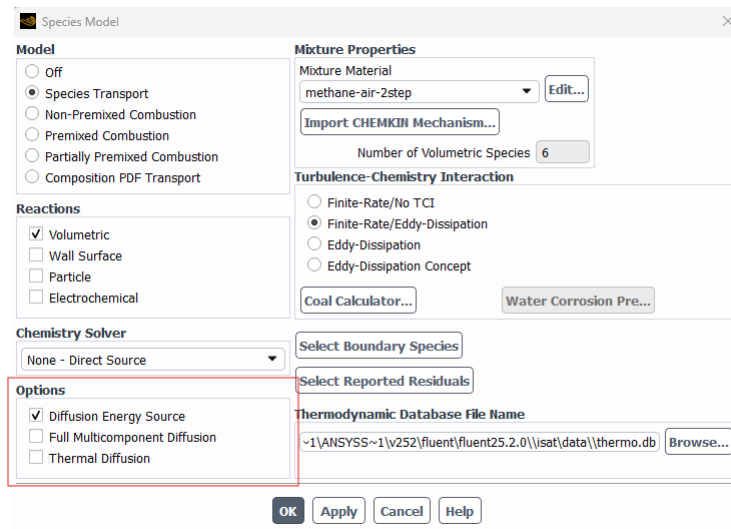


Figure 3.5: Species transport options

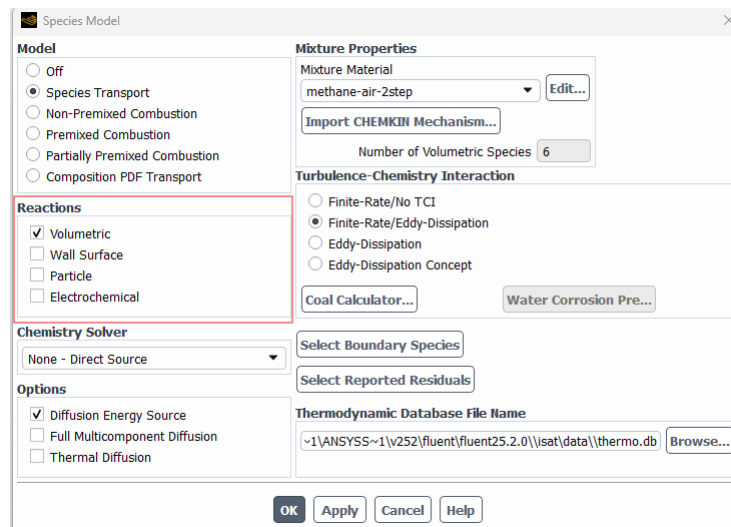


Figure 3.6: Species reaction mechanisms

mesh independence. The geometry was created in Ansys Spaceclaim as seen in Fig. 3.1. There were 3 separate geometries created with dimensions listed in Table 3.1 varying the recess lengths.

After creating the geometry it is meshed in Ansys Mechanical. Due to the limitation on the number of nodes available for the student version of the software, inflation

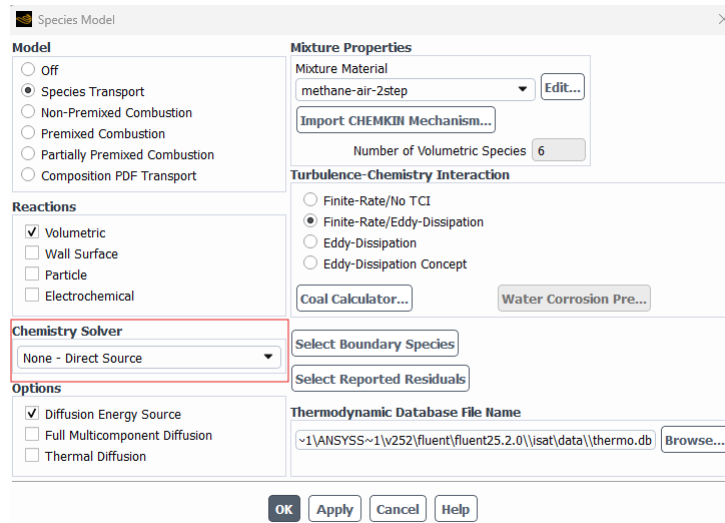


Figure 3.7: Species chemistry solver settings

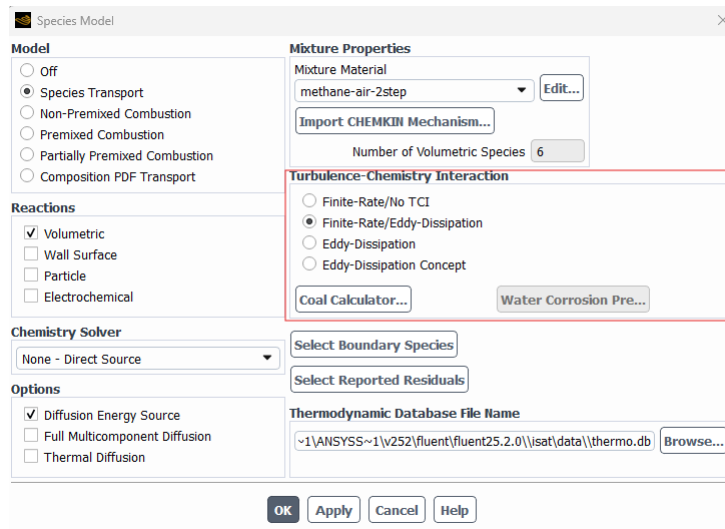


Figure 3.8: Species turbulence–chemistry interaction model

layers at the wall were not in use. Instead the cell count was concentrated in the separating shear layers (SSL) where the combustion is expected to occur. Once the meshing is completed the mesh is imported into Ansys Fluent. Fig. 3.2 shows the selections made for the simulation. A pressure-based solver was selected as it was determined there would not be a significant gain compared to density-based solver

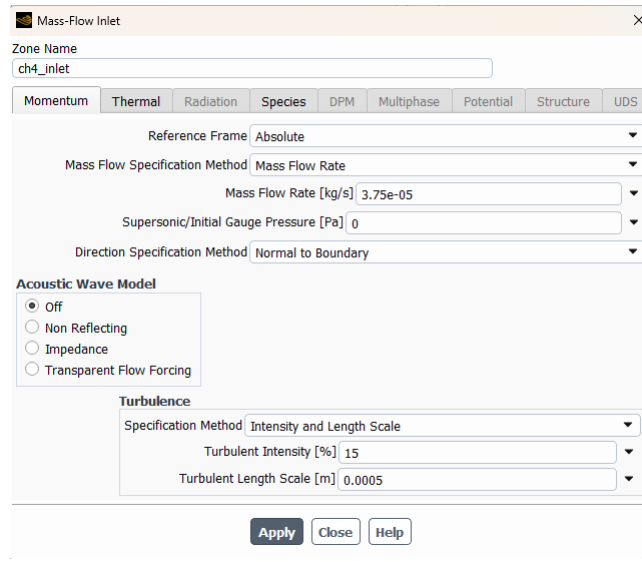


Figure 3.9: CH₄ mass flow rate – momentum equation

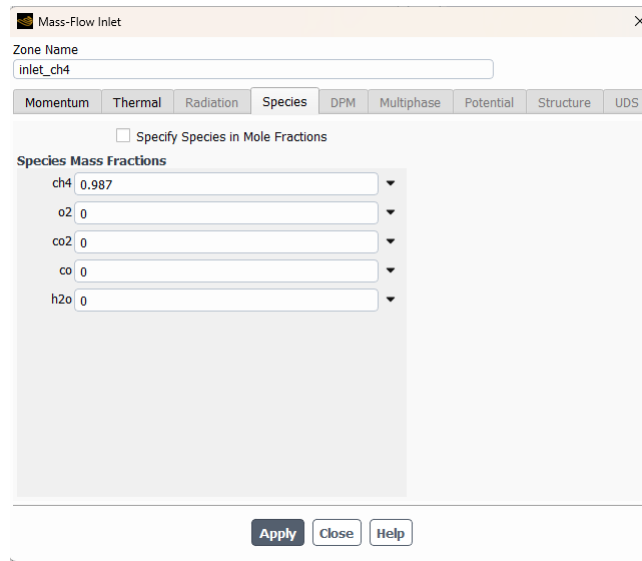


Figure 3.10: CH₄ mass flow rate – species transport

given the added computational time. A transient time was selected given the problem type of engine startup, a non-steady state problem. The case was a 2D axisymmetric case due to the desire to model a 3D case given the computational constraints. The species model selection was species transport as highlighted in Fig. 3.3. Partially

Mass-Flow Inlet

Zone Name
inlet_o2

Momentum Thermal Radiation Species DPM Multiphase Potential Structure UDS

Reference Frame Absolute

Mass Flow Specification Method Mass Flow Rate

Mass Flow Rate [kg/s] 0.00015

Supersonic/Initial Gauge Pressure [Pa] 0

Direction Specification Method Normal to Boundary

Acoustic Wave Model

☒ Off
☐ Non Reflecting
☐ Impedance
☐ Transparent Flow Forcing

Turbulence

Specification Method Intensity and Length Scale

Turbulent Intensity [%] 15

Turbulent Length Scale [m] 0.0005

Apply Close Help

Figure 3.11: O₂ mass flow rate – momentum equation

Mass-Flow Inlet

Zone Name
inlet_o2

Momentum Thermal Radiation Species DPM Multiphase Potential Structure UDS

☐ Specify Species in Mole Fractions

Species Mass Fractions

ch4	0
o2	0.987
co2	0
co	0
h2o	0

Apply Close Help

Figure 3.12: O₂ mass flow rate – species transport

premixed combustion would be a more accurate model; however, due to time constraints this was forgone. Fig. 3.4 shows the mixture selected, methane-air-2step. The two step methane mixture was selected over its greater ability to accurately model combustion dynamics over the single step mixture while still avoiding further

Pressure Outlet

Zone Name: outlet

Momentum Thermal Radiation **Species** DPM Multiphase Potential Structure UDS

Backflow Reference Frame: Absolute

Gauge Pressure [Pa]: 0

Pressure Profile Multiplier: 1

Backflow Direction Specification Method: Normal to Boundary

Backflow Pressure Specification: Total Pressure

☐ Prevent Reverse Flow

☐ Average Pressure Specification

☐ Target Mass Flow Rate

Turbulence

Specification Method: Intensity and Length Scale

Backflow Turbulent Intensity [%]: 15

Backflow Turbulent Length Scale [m]: 0.0005

Acoustic Wave Model

☒ Off

☐ Non Reflecting

☐ Impedance

☐ Transparent Flow Forcing

Apply Close Help

Figure 3.13: Outlet boundary condition setup

Wall

Zone Name: wall

Adjacent Cell Zone: fff_surface

Momentum Thermal Radiation **Species** DPM Multiphase UDS Potential Structure Ablation

Wall Motion

☒ Stationary Wall ☒ Relative to Adjacent Cell Zone

☐ Moving Wall

Shear Condition

☒ No Slip

☐ Specified Shear

☐ Specularity Coefficient

☐ Marangoni Stress

Wall Roughness

Roughness Models

☒ Standard

☐ High Roughness (Icing)

Sand-Grain Roughness

Roughness Height [m]: 0

Roughness Constant: 0.5

Apply Close Help

Figure 3.14: Wall momentum boundary condition

complexity. Figs. 3.5—3.8 show the rest of the species model selections.

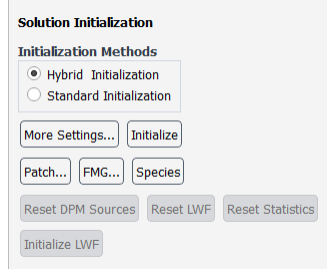


Figure 3.15: Solution initialization settings

Table 3.1: Geometric parameters for injector configurations

Parameter	Case 1	Case 2	Case 3
Recess length (mm)	0 mm	6 mm	10 mm
Axis length (mm)	110 mm	110 mm	110 mm
Outlet radius (mm)	1 mm	1 mm	1 mm
O ₂ inlet radius (mm)	2.35 mm	2.35 mm	2.35 mm
CH ₄ inlet inner radius (mm)	2.85 mm	2.85 mm	2.85 mm
CH ₄ inlet outer radius (mm)	3.35 mm	3.35 mm	3.35 mm
Chamber radius (mm)	5 mm	5 mm	5 mm
Chamber length (mm)	55 mm	55 mm	55 mm
Converging nozzle angle (deg)	135	135	135

$$Sc \equiv \frac{\nu}{\mathcal{D}} = \frac{\text{rate of momentum transport}}{\text{rate of mass transport}} \quad (3.1)$$

$$Pr \equiv \frac{C_p \mu}{\lambda} = \frac{C_p \rho \frac{\mu}{\rho}}{\lambda} = \frac{\nu}{\alpha} = \frac{\text{rate of momentum transport}}{\text{rate of energy transport}} \quad (3.2)$$

$$Le \equiv \frac{\lambda}{\rho C_p \mathcal{D}} = \frac{\alpha}{\mathcal{D}} = \frac{\text{rate of energy transport}}{\text{rate of mass transport}} \quad (3.3)$$

$$Le \equiv \frac{Sc}{Pr} \quad (3.4)$$

The motivation for the diffusion term to be selected is to more accurately model how the heat, mass and momentum propagate in the simulation. Diffusivity is de-

Solution Methods

Pressure-Velocity Coupling

Scheme: PISO

Skewness Correction: 1

Neighbor Correction: 1

☒ Skewness-Neighbor Coupling

Flux Type: Rhie-Chow: momentum based ☒ Auto Select

Spatial Discretization

Gradient: Least Squares Cell Based

Pressure: Second Order

Density: Second Order Upwind

Momentum: Bounded Central Differencing

Turbulent Kinetic Energy: Second Order Upwind

Specific Dissipation Rate: Second Order Upwind

ch4: Second Order Upwind

o2: Second Order Upwind

co2: Second Order Upwind

co: Second Order Upwind

h2o: Second Order Upwind

Energy: Second Order Upwind

Spatial Discretization Parameters

Bounded Central Diff. Boundedness: 1

Pseudo Time Method: Off

Transient Formulation: Bounded Second Order Implicit

Figure 3.16: Solution methods configuration

terminated by assuming the Unity Lewis Number $L = 1$. Embedded in the Lewis Number are the Prandtl and Schmidt number which are defined by Eqs. 3.2 & 3.1. Pr and Sc represent whether the velocity boundary layer is thicker or thinner than the thermal boundary layer and whether momentum diffuses faster than the chemical species [46]. The Lewis Number is the ratio of these non-dimensional parameters as stated by Eqs. 3.3 & 3.4.

$$\frac{\partial(\rho Y_i)}{\partial t} + \nabla \cdot (\rho \nu Y_i) = -\nabla \cdot J_i + R_i + S_i \quad (3.5)$$

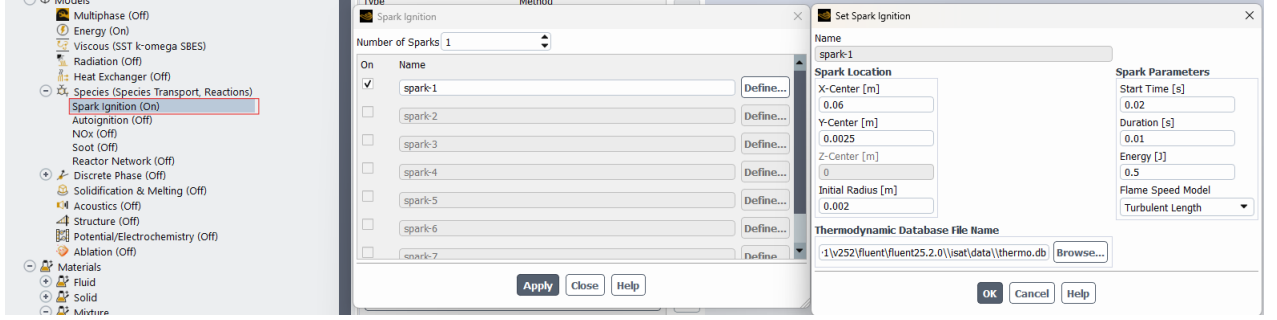


Figure 3.17: Spark ignition configuration

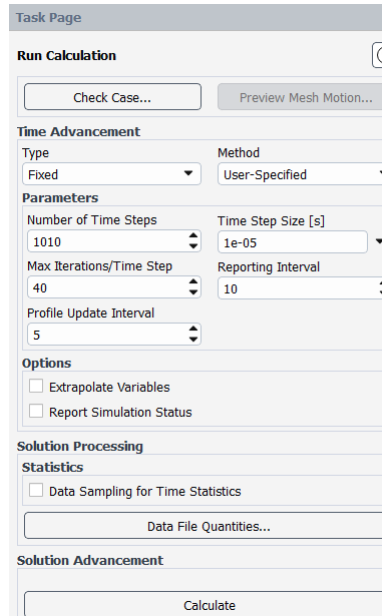


Figure 3.18: Timestep and transient stepping parameters

$$q' = \sum_{i=1}^N h_i R_i \quad (3.6)$$

$$\mathcal{R} = \frac{1}{T} \int_0^T \int_V p'(x, t) \cdot q'(x, t) dV dt \quad (3.7)$$

Fig. 3.6 shows volumetric selected under reactions. Volumetric is essential to the setup because its selection enables a non-zero R_i in Eq. 3.5[32][47]. When evaluating

the Rayleigh Criterion in Eq. 3.7 the heat release term cannot equal zero. Thus when evaluating Eq. 3.6 neither contributing term can be zero. When determining the selection of the chemistry solver, the direct source is the suitable choice for the chemical mixture selected. The Ansys Fluent theory guide suggest to select direct source for simple mechanisms to avoid the overhead of a lookup table [32]. When determining which turbulence-chemistry interaction model to select as shown by Fig. 3.8, the Ansys Fluent theory guide provides guidance. When comparing the pure eddy dissipation to the finite-rate/eddy dissipation for selection it is important to consider the assumptions.

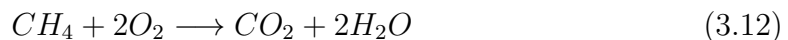
$$\dot{\omega}_{Eddy} = A_{mix} \cdot \rho \frac{\epsilon}{k} \cdot \min(Y_F, \frac{Y_{ox}}{s}, \frac{Y_{prod}}{1+s}) \quad (3.8)$$

$$\dot{\omega}_{Arrhenius} = A \cdot T^\beta \cdot e^{-\frac{E_a}{RuT}} \cdot [C_{fuel}]^n [C_{ox}^m] \quad (3.9)$$

$$\dot{\omega}_{net} = \min(\dot{\omega}_{Arrhenius}, \dot{\omega}_{Eddy}) \quad (3.10)$$

$$Da = \frac{\tau_{flow}}{\tau_{chem}} \quad (3.11)$$

Pure dissipation assumes instantaneous reactions upon mixing basing reaction purely off of Eq. 3.8[47]. Finite rate mixing assumes perfect mixing and is governed by Eq. 3.9[48]. Finite-Rate/Eddy Dissipation takes advantage of both mechanisms and seeks to implement Eq. 3.10 which then is dictated by the limiting factor of both equations [49]. This is key when implementing sensitive systems such as combustion instability. This model switching can also be understood through the use of the Damköhler Number (Da). When $Da \gg 1$ the eddy dissipation dominates, meaning the chemistry is faster than the flow. When $Da \ll 1$ the Arrhenius expression dominates, meaning the flow is faster than the chemistry [50]. Figs. 3.9—3.12 show the inlet conditions for both the methane and oxygen.



To create the most unstable conditions, the methane/oxygen mixture must be stoichiometric. Since the molar masses of $CH_4 = 16.04g/mol$ and $2O_2 = 64.00g/mol$ the stoichiometric mass ratio is $\frac{O}{F} = 4.0$. The goal during these simulations is to achieve a velocity ratio, between the fuel and oxidizer, that creates vortices and mixing.

$$\dot{m} = \rho v A = 1.31 \frac{kg}{m^3} (5.73 \times 10^{-6} m^2) 20 \frac{m}{s} \approx 0.00015 \frac{kg}{s} \quad (3.13)$$

$$\dot{m} = \frac{0.00015}{4} = 3.75 \times 10^{-5} \frac{kg}{s} \quad (3.14)$$

Selecting a velocity of 20 m/s for O_2 and using the geometry from Table 3.1, we can calculate the expected mass flow rate as shown in Eqs. 3.13 & 3.14.

$$I = 0.16Re^{-\frac{1}{8}} \quad (3.15)$$

$$Re = \frac{\rho v D}{\mu} \quad (3.16)$$

When determining the turbulence intensity, values between 3% and 5% are typical; however, the desire is to accelerate turbulence intensity Eq. 3.15 in the injectors. The Reynolds number can be calculated using Eq. 3.16, since the Reynolds number fell in the transitional turbulence region 15% was selected [32]. The turbulent length scale was selected to be smaller than the diameter of the injectors. Regarding, the species mass fraction in Figs. 3.10 & 3.12, the quantities were selected based on [16]. Fig. 3.13 showing the selections regarding the outlet, follow the same justifications. Fig. 3.14 assumes a no-slip condition and adiabatic walls. Hybrid initialization was selected adhering to Ansys Fluent theory guide[32]. The two parameters changed in Fig. 3.16 were the Pressure-velocity coupling scheme and the transient formulation. For the Pressure-velocity couples scheme PISO (Pressure-Implicit with Splitting of Operators) was selected due to its greater ability to handle transient simulations than SIMPLE assuming a proper selecting of a sufficiently small timestep [51][52]. The Bounded Second Order Implicit serves to better capture the numerical behavior for transient cases [32]. Fig. 3.17 shows details regarding a spark ignition used in the simulation. The location of the spark ignition is placed in the separating shear layers (SSL) to invigorate combustion. The selected start time gives the gases sufficient time to travel down the injectors and mix together. The duration of the spark is set to 1 ms to minimize the chance of the flame being extinguished. The amount of energy selected to increase the temperature of the mixture past the auto-ignition temperature of ~ 900 K [53].

Given the chemistry of the model as methane/Gox at room temperature, the flow will not self ignite. This is advantageous given the ability to model the mixing before ignition using a RANS model, $k - \omega$. This allows the simulation to run as a RANS model while the fuel and oxidizer propagate and mix before ignition. This saves computational time at a slight loss of information. The information lost are the eddies that form in the injector posts. This is acceptable. During this initial time stepping phase before ignition, the timestep size is 1×10^{-4} seconds. The exact

number of time steps vary on the recess geometry. The max iterations per timestep is set to 40 to allow the residuals to converge. Once mixing has begun and before the spark ignites, the timestep is changed to 1×10^{-5} seconds and the number of time steps is set to a minimum of 1000. Additionally, the turbulence model is switched to SBES with $k - \omega$ set as the RANS model and WALE set as the LES model.

Chapter 4

Results

4.1 CFD Results

Fig. 4.1a compares contour maps of the heat of the reaction based on varying injector recess lengths. Fig. 4.2 compares contour maps of the mass fraction of CH_4 based on varying injector recess lengths. Fig. 4.3 compares contour maps of the mass fraction of CO based on varying injector recess lengths. Fig. 4.4 compares contour maps of the mass fraction of CO_2 based on varying injector recess lengths. Fig. 4.5 compares contour maps of the mass fraction of H_2O based on varying injector recess lengths. Fig. 4.6 compares contour maps of the mass fraction of O_2 based on varying injector recess lengths. Fig. 4.7 compares contour maps of the static pressure based on varying injector recess lengths. Fig. 4.8 compares contour maps of the static temperature based on varying injector recess lengths.

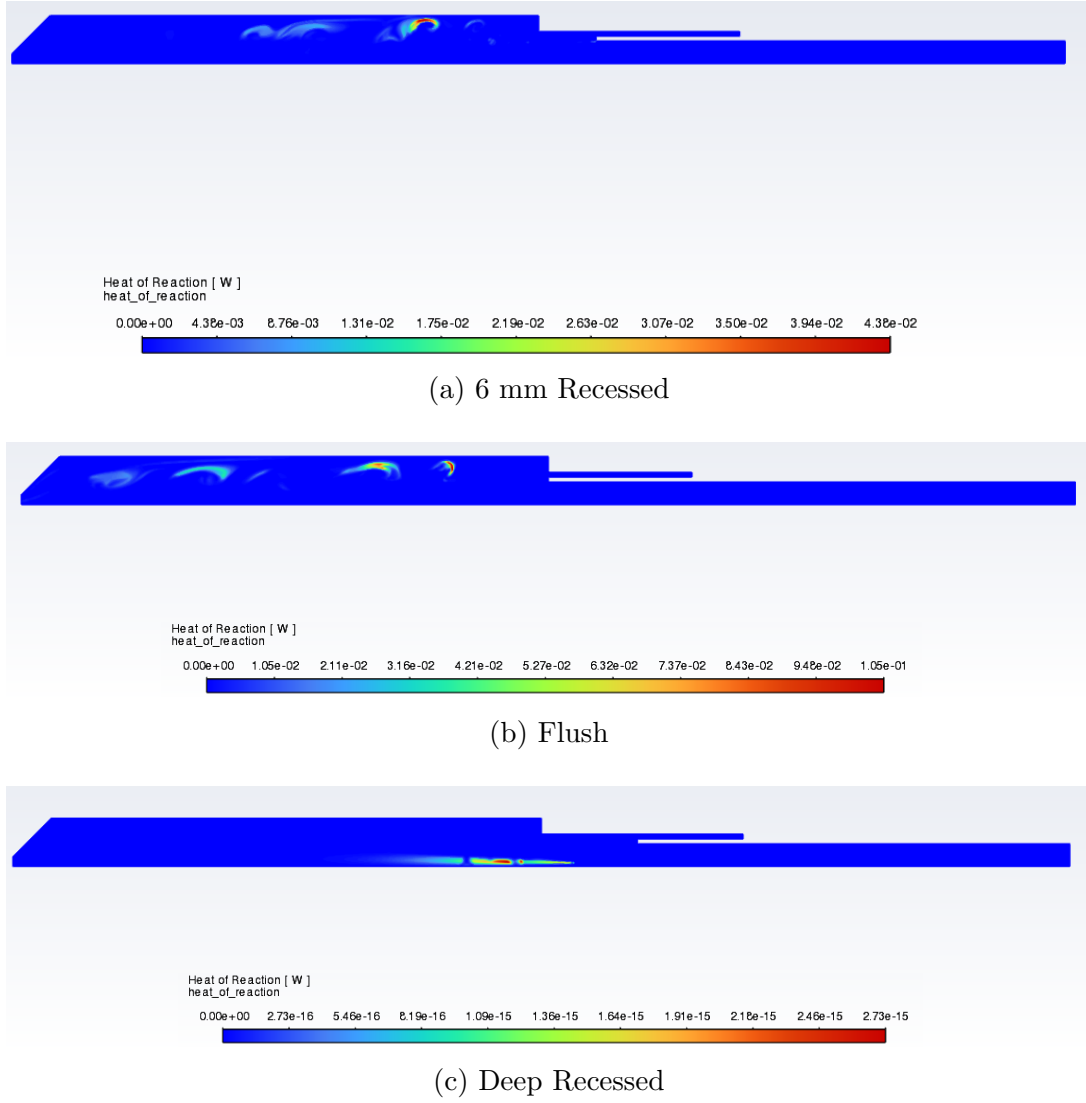
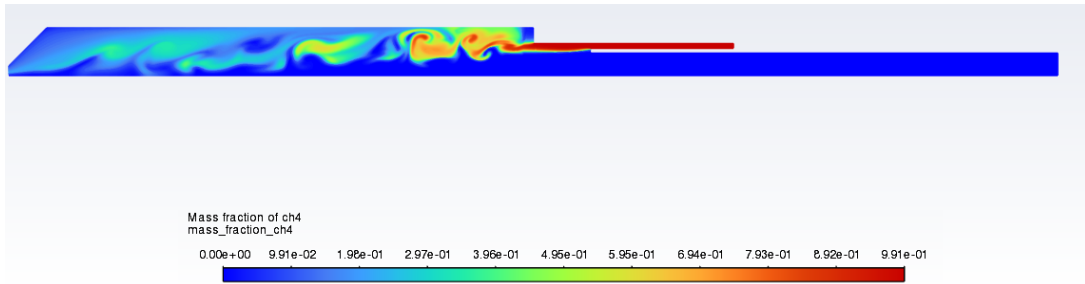
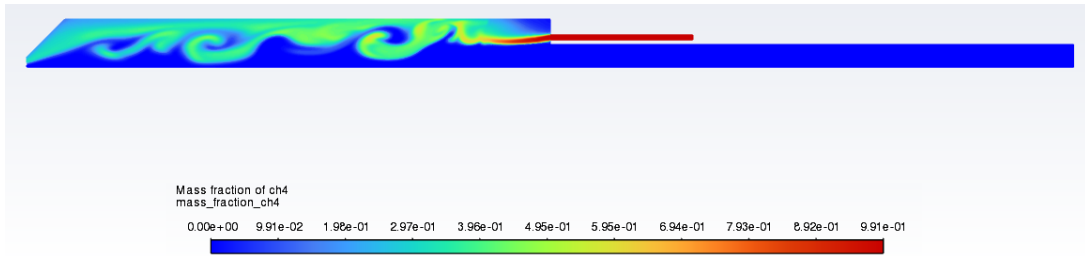


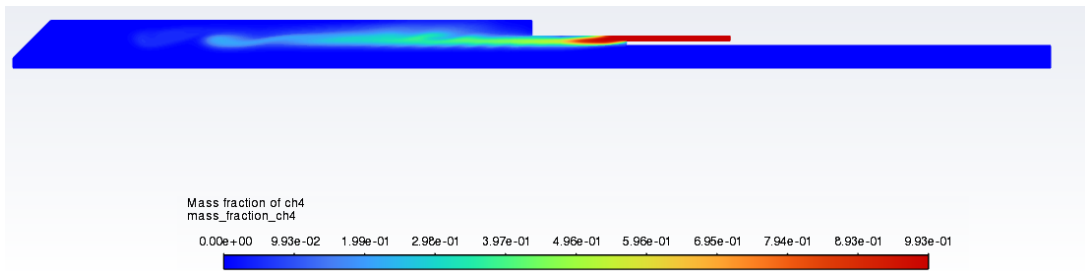
Figure 4.1: Comparison of heat of reaction contours across injector recess configurations.



(a) 6 mm Recessed

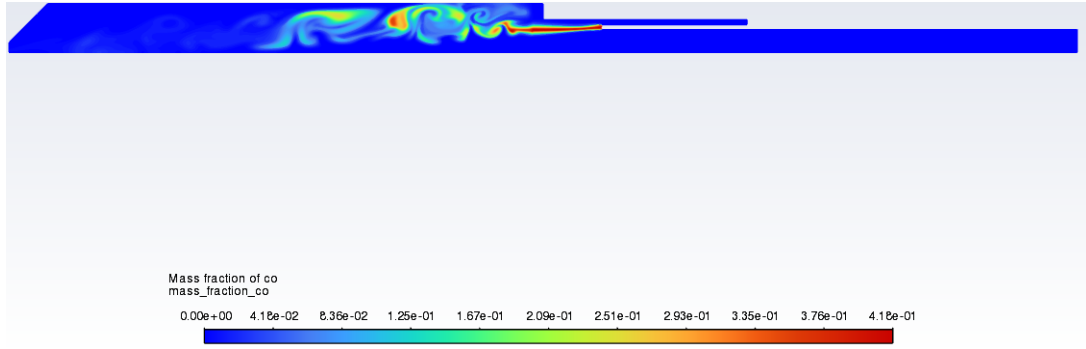


(b) Flush

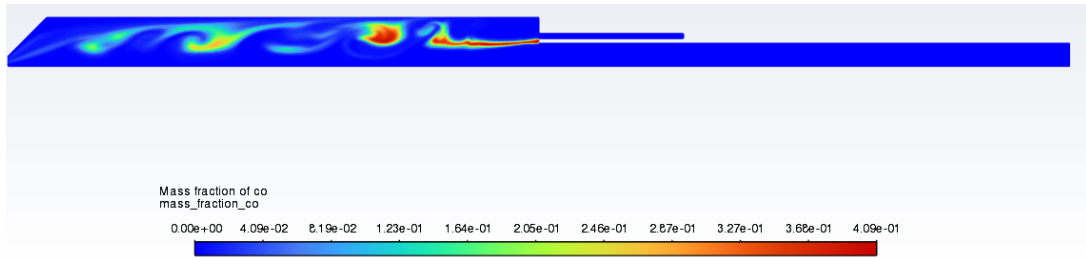


(c) Deep Recessed

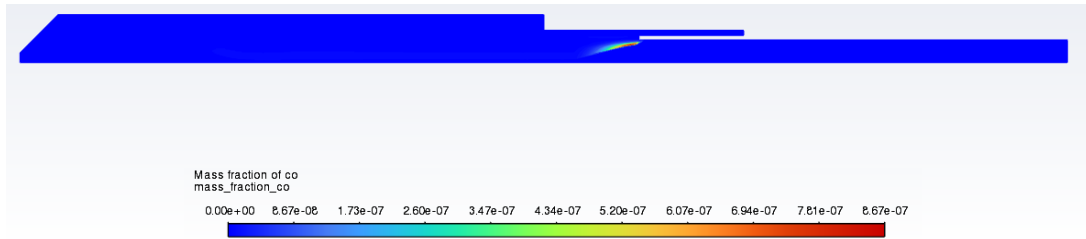
Figure 4.2: Comparison of CH_4 mass fraction contours across injector recess configurations.



(a) 6 mm Recessed

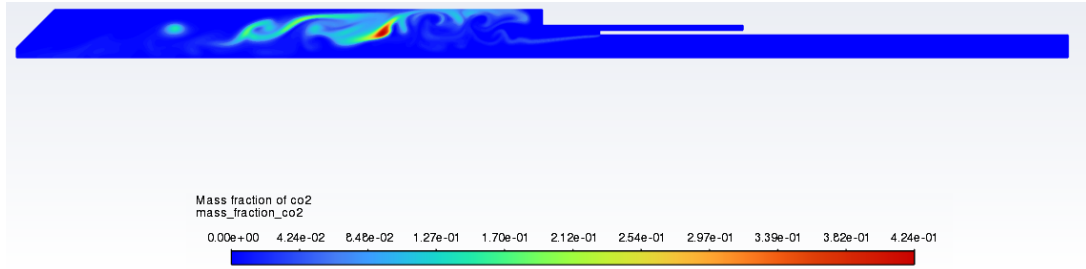


(b) Flush

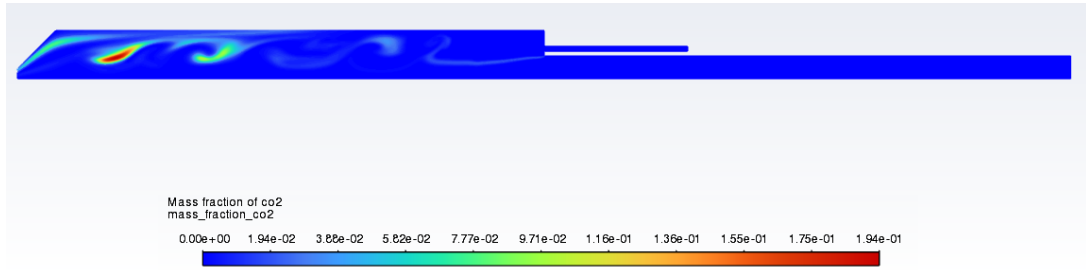


(c) Deep Recessed

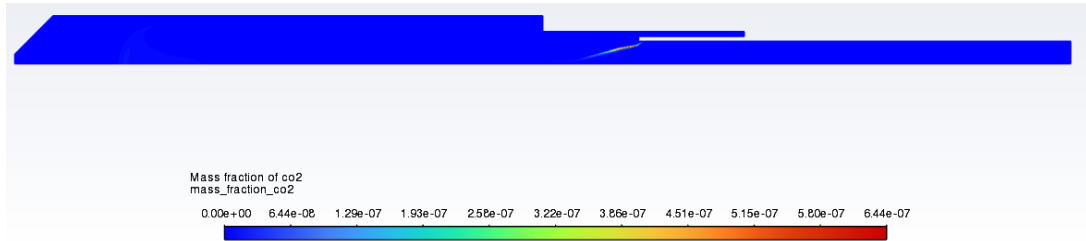
Figure 4.3: Comparison of CO mass fraction contours across injector recess configurations.



(a) 6 mm Recessed

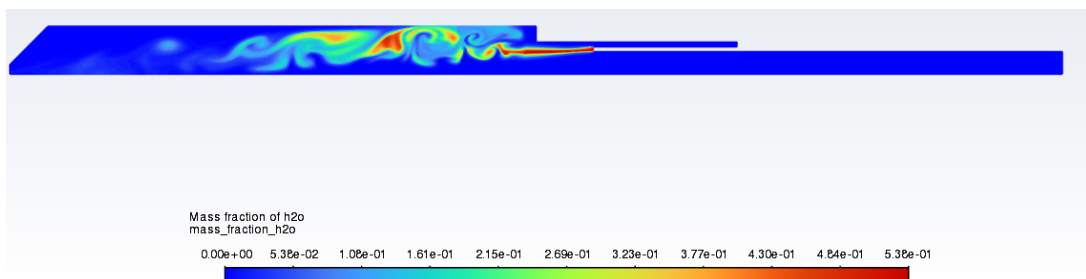


(b) Flush

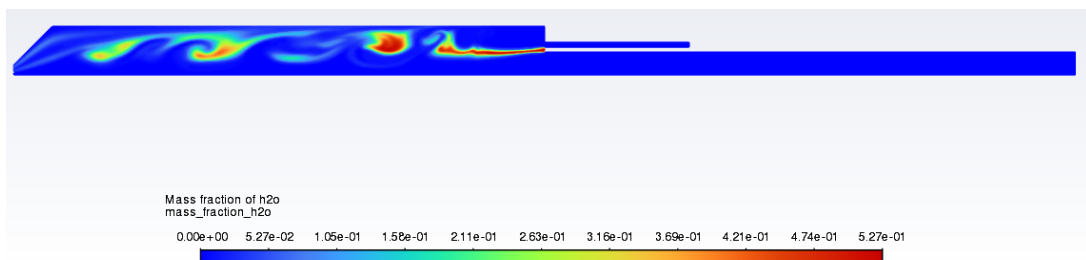


(c) Deep Recessed

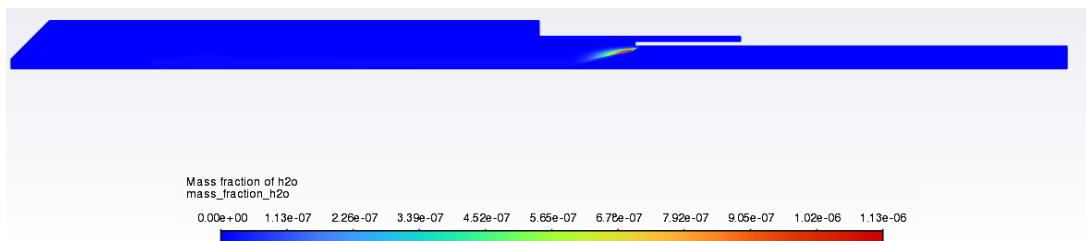
Figure 4.4: Comparison of CO₂ mass fraction contours across injector recess configurations.



(a) 6 mm Recessed

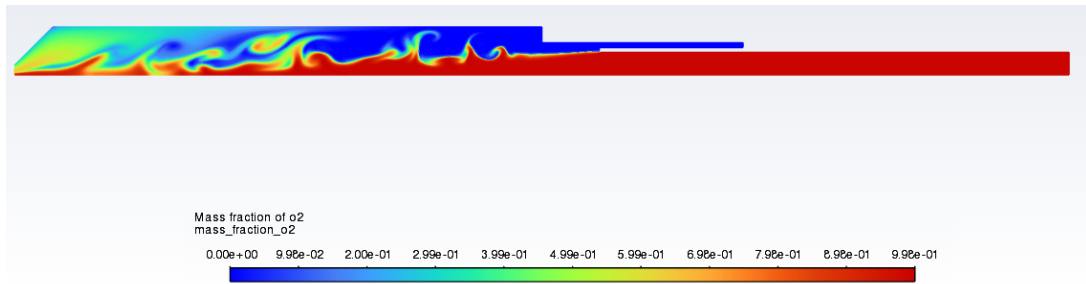


(b) Flush

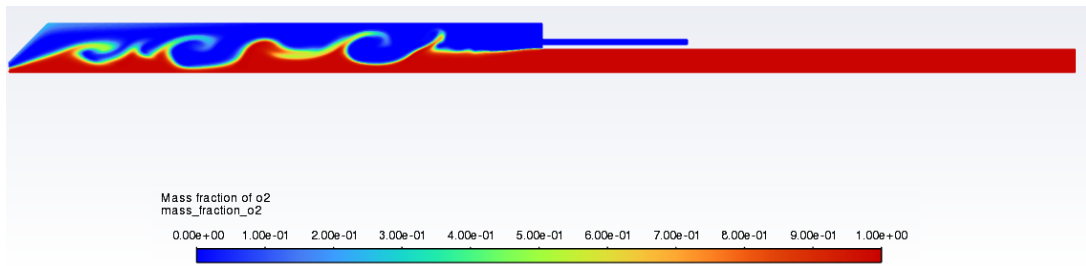


(c) Deep Recessed

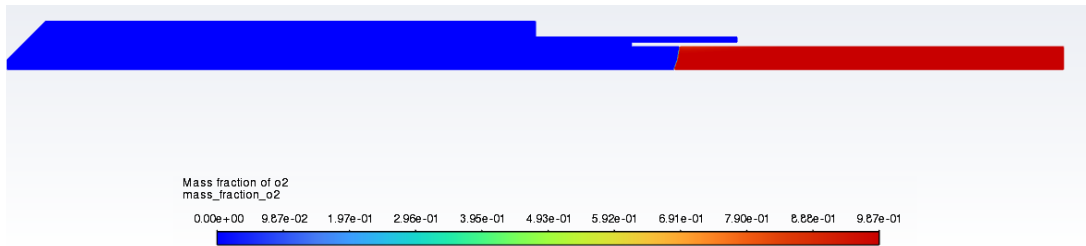
Figure 4.5: Comparison of H_2O mass fraction contours across injector recess configurations.



(a) 6 mm Recessed

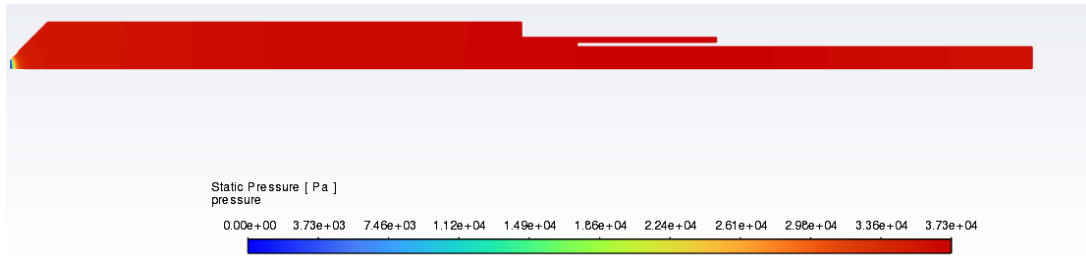


(b) Flush

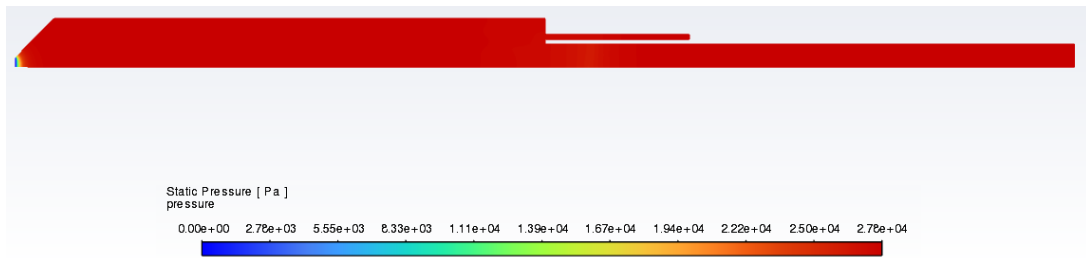


(c) Deep Recessed

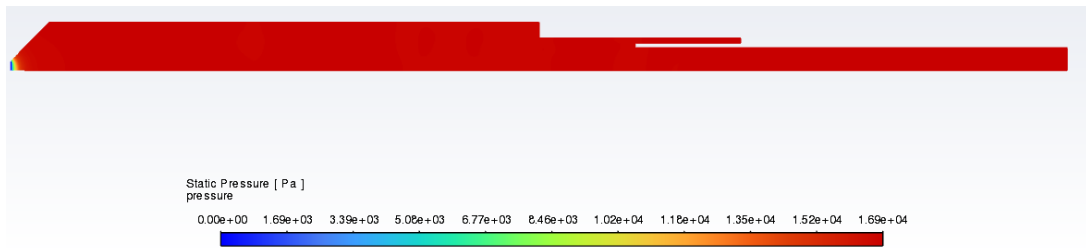
Figure 4.6: Comparison of O₂ mass fraction contours across injector recess configurations.



(a) 6 mm Recessed

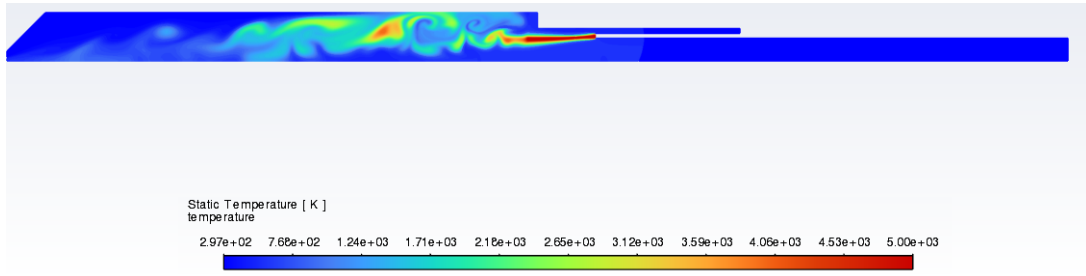


(b) Flush

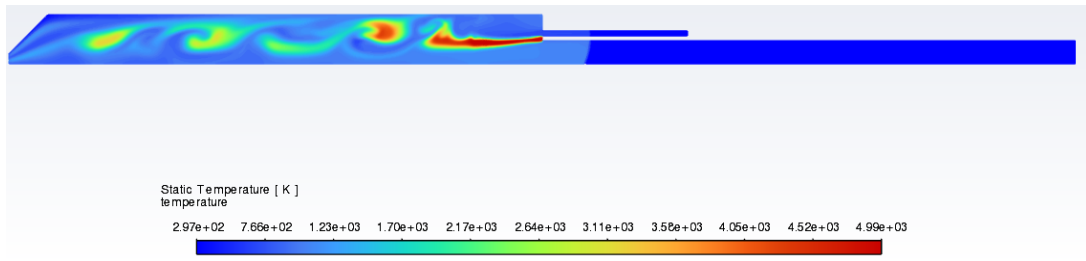


(c) Deep Recessed

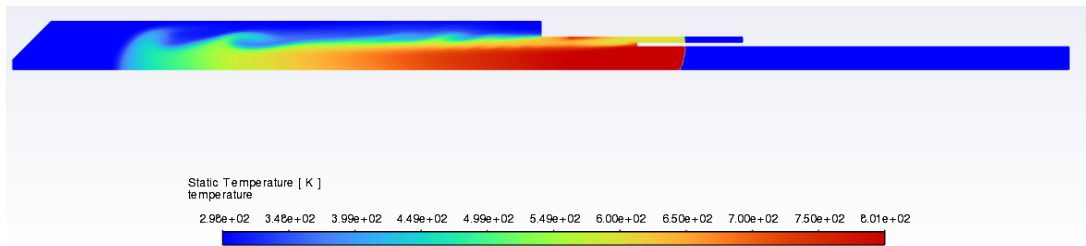
Figure 4.7: Comparison of static pressure contours across injector recess configurations.



(a) 6 mm Recessed



(b) Flush



(c) Deep Recessed

Figure 4.8: Comparison of static temperature contours across injector recess configurations.

4.2 Modal Acoustics Results

4.2.1 Acoustics Contours

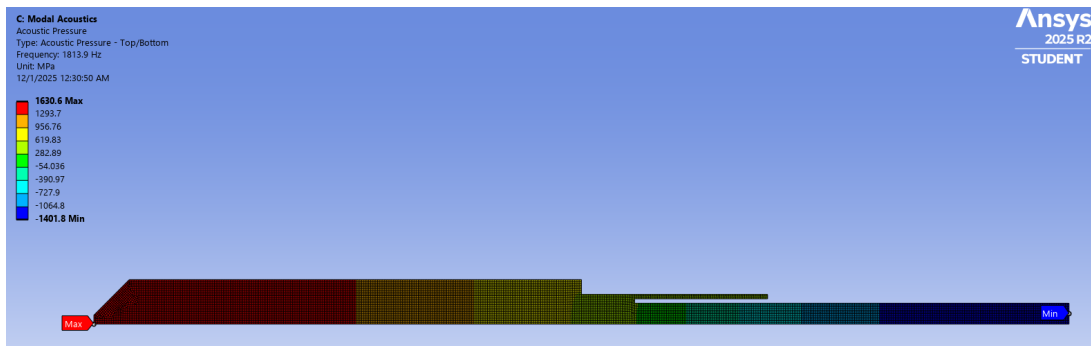
Fig. 4.9 compares the frequency contours of the first mode across different recess lengths. Fig. 4.10 compares the frequency contours of the second mode across different recess lengths. Fig. 4.11 compares the frequency contours of the third mode across different recess lengths. Fig. 4.12 compares the frequency contours of the fourth mode across different recess lengths. Fig. 4.13 compares the frequency contours of the fifth mode across different recess lengths. Fig. 4.14 compares the frequency contours of the sixth mode across different recess lengths. Fig. 4.15 is the data pulled from [16] for comparison.

4.2.2 Frequencies

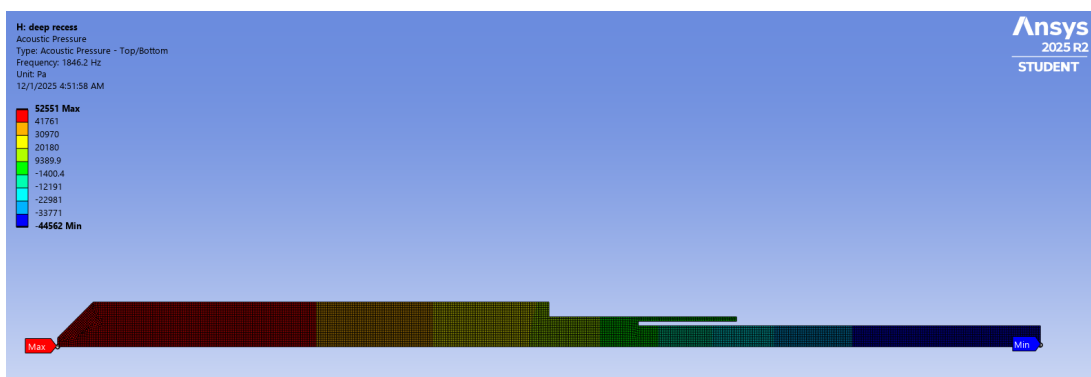
Table 4.1 showcases how the natural frequencies of the geometry vary with the differing geometries.

Table 4.1: Modal frequencies (Hz) for each injector recess configuration.

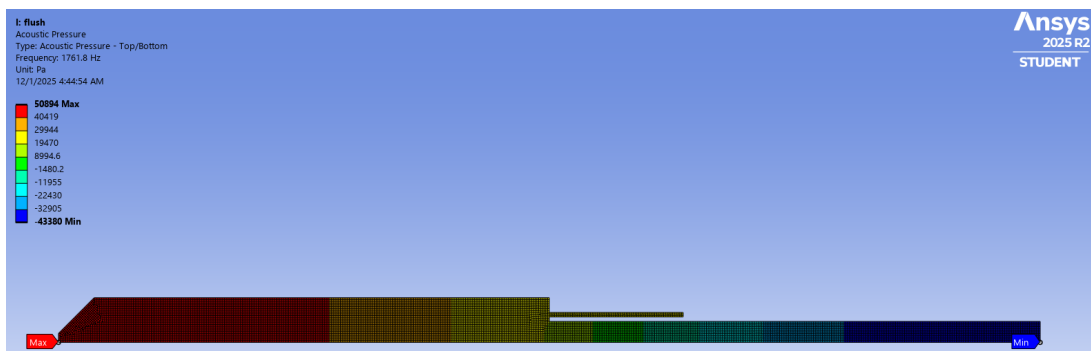
Geometry	Mode 1	Mode 2	Mode 3	Mode 4	Mode 5	Mode 6
Case 01 Flush	1761.8	3627.9	4957.6	5591.8	7124.5	8331.5
Case Coarse Mesh 6 mm Recess	1815.7	3550.7	5163.0	5433.0	7086.0	8512.4
Case 02 6 mm Recessed	1813.9	3548.6	5158.1	5399.9	7078.3	8497.6
Case 03 Deep Recessed	1846.2	3565.4	5158.3	6535.3	7508.8	8760.5



(a) 6 mm Recessed

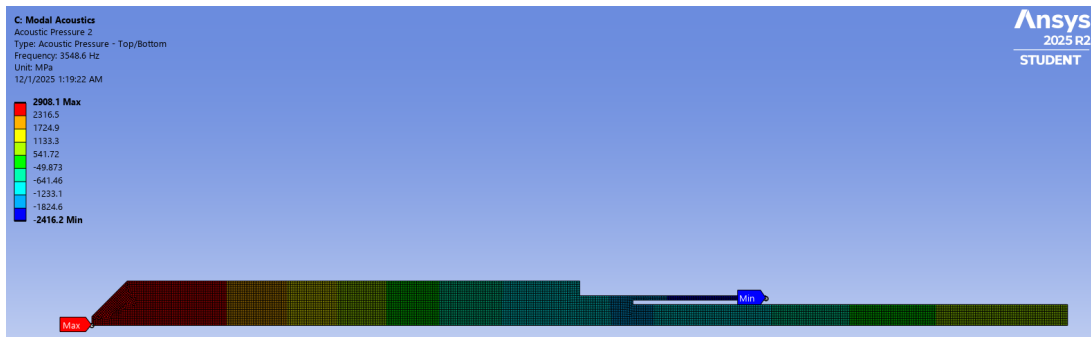


(b) Deep Recessed

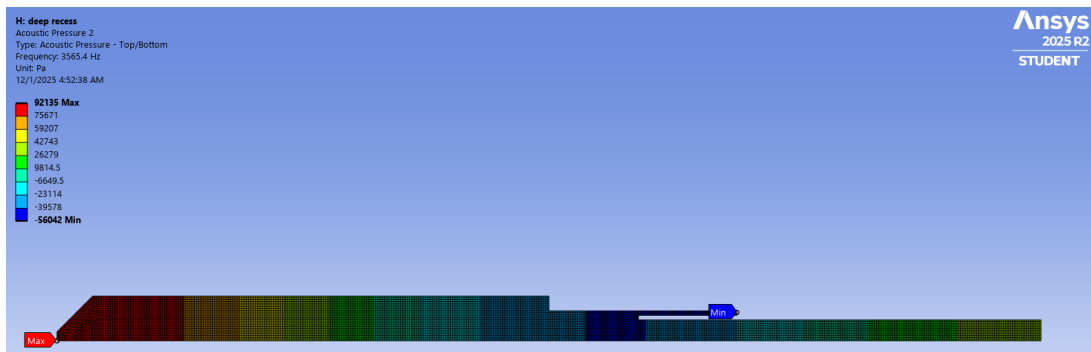


(c) Flush

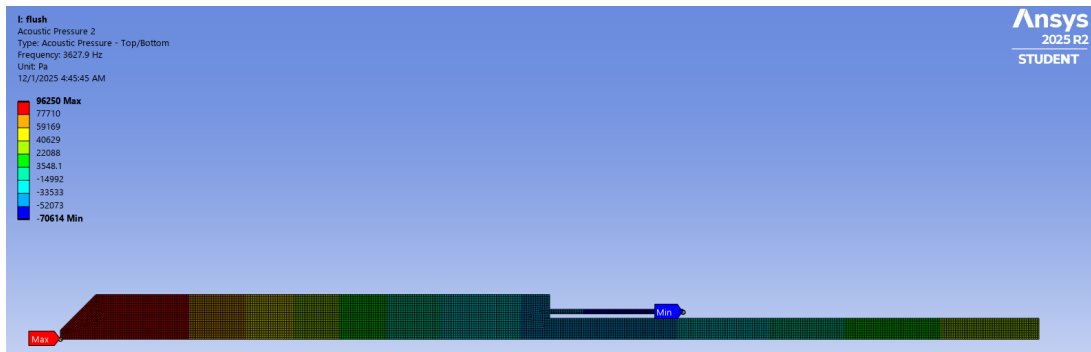
Figure 4.9: Comparison of acoustic mode 1 contours across injector recess configurations.



(a) 6 mm Recessed

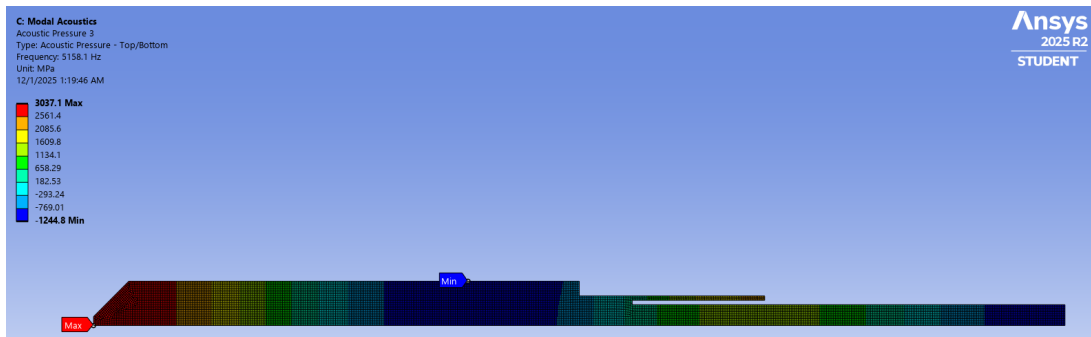


(b) Deep Recessed

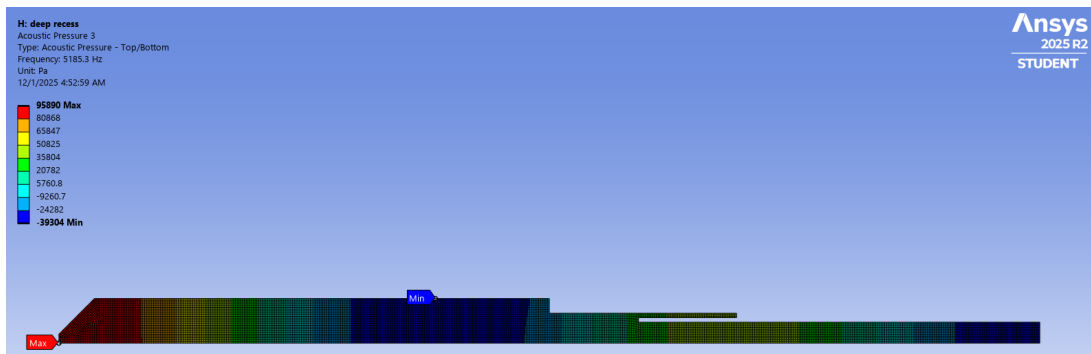


(c) Flush

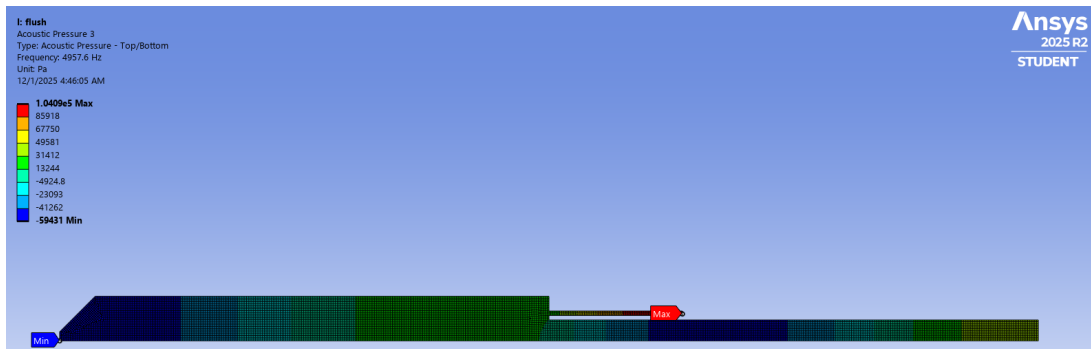
Figure 4.10: Comparison of acoustic mode 2 contours across injector recess configurations.



(a) 6 mm Recessed

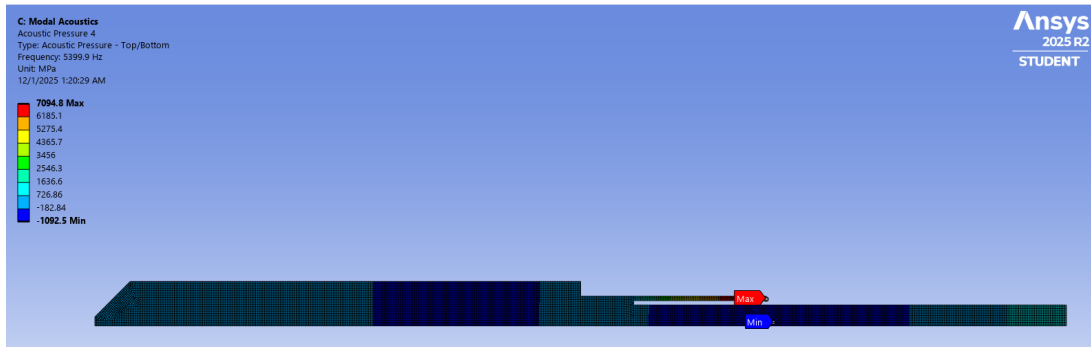


(b) Deep Recessed

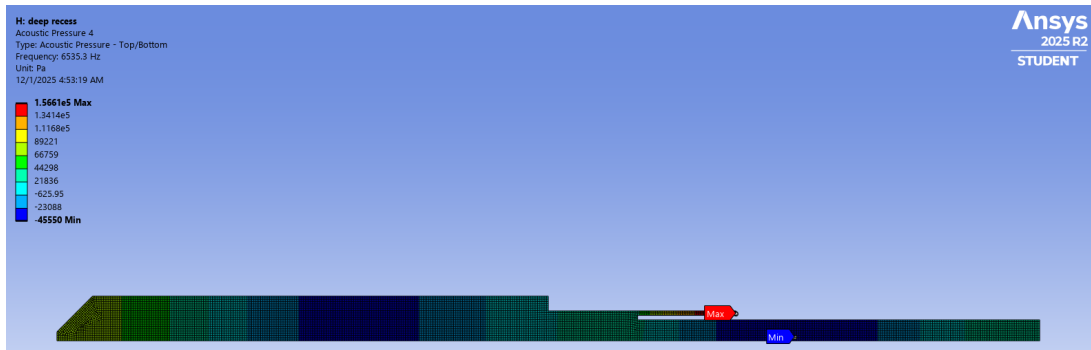


(c) Flush

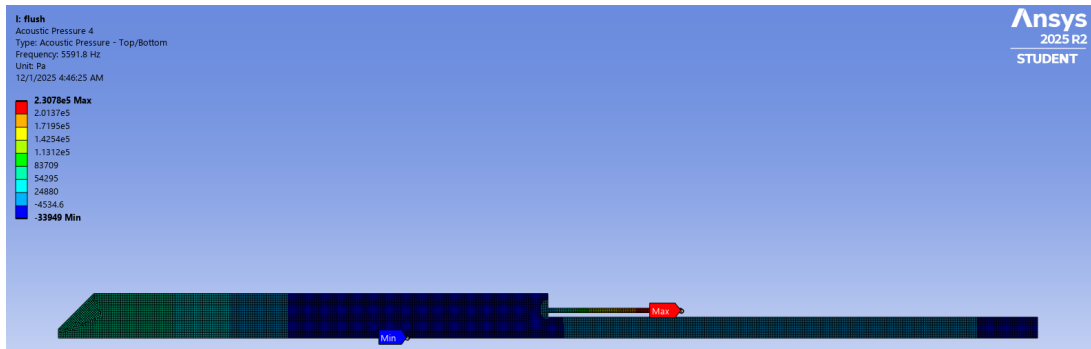
Figure 4.11: Comparison of acoustic mode 3 contours across injector recess configurations.



(a) 6 mm Recessed

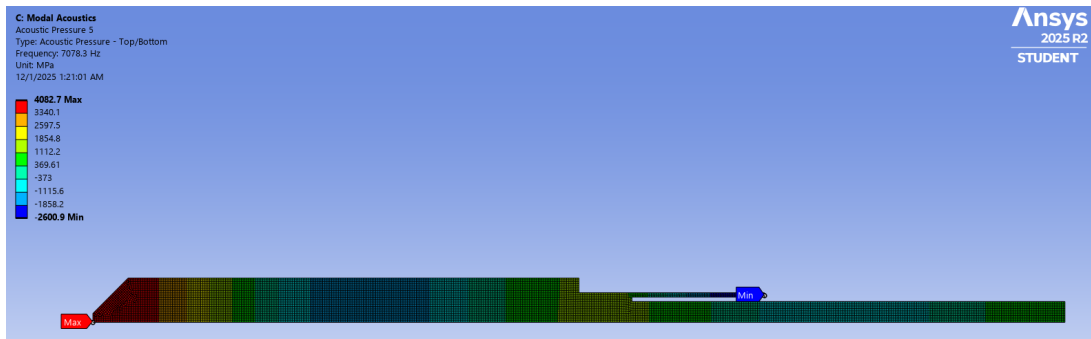


(b) Deep Recessed

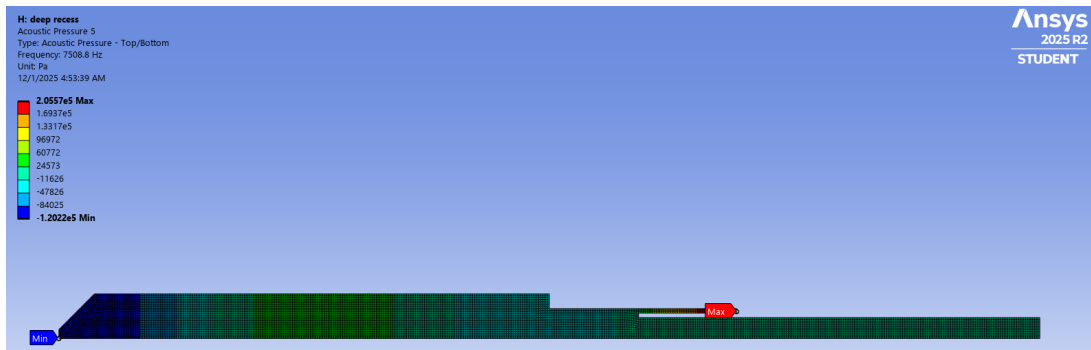


(c) Flush

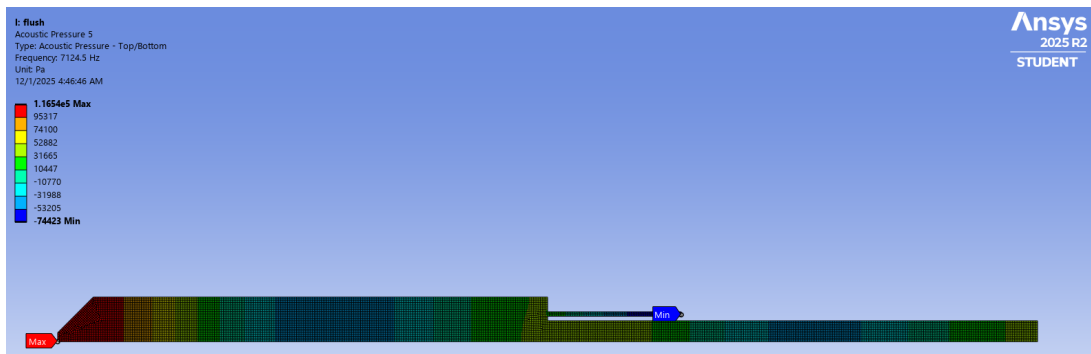
Figure 4.12: Comparison of acoustic mode 4 contours across injector recess configurations.



(a) 6 mm Recessed

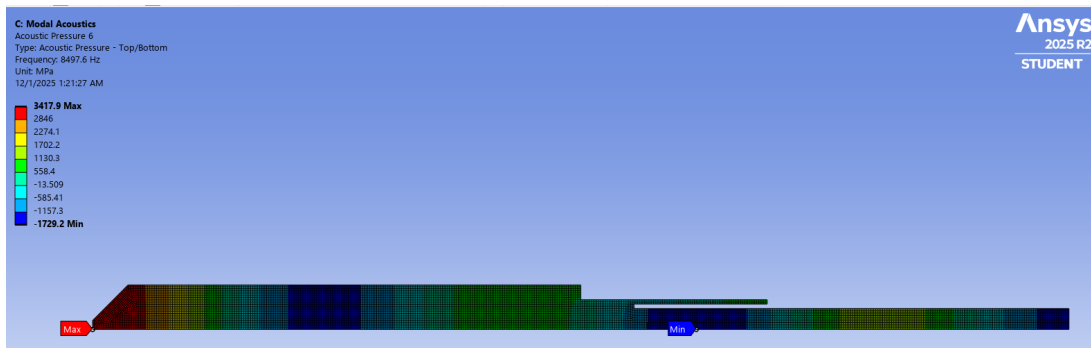


(b) Deep Recessed

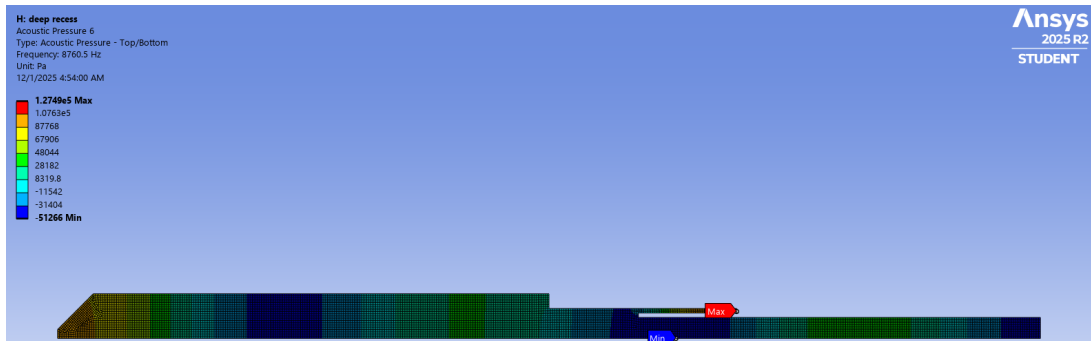


(c) Flush

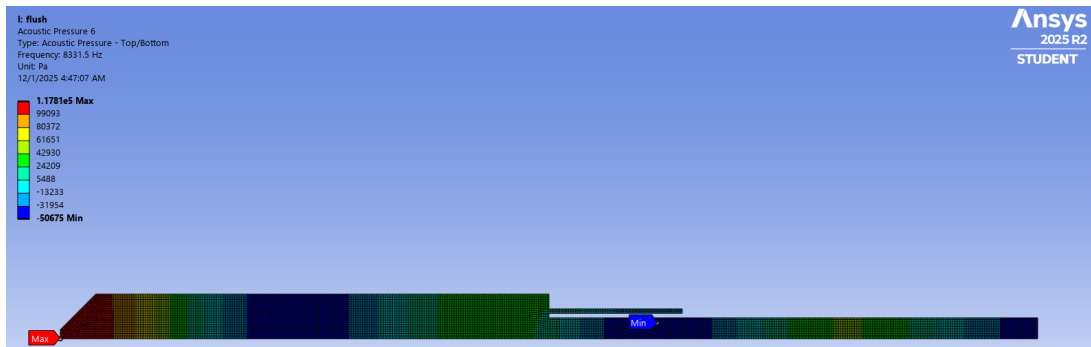
Figure 4.13: Comparison of acoustic mode 5 contours across injector recess configurations.



(a) 6 mm Recessed



(b) Deep Recessed



(c) Flush

Figure 4.14: Comparison of acoustic mode 6 contours across injector recess configurations.

TABLE III. Comparison of dominant frequencies and pressure oscillation amplitudes for the experiment, theoretical analysis, and numerical simulation.

Comparison	1W (Hz)	2W (Hz)	3W (Hz)	Chamber pressure (MPa)	$p'_{p-p}(\%)$
Experiment	2995	6004	8995	0.96	76.5
Simulation	3326	6653	9979	1.01	82.2
Theory	3250	6500	9750	1.09	...

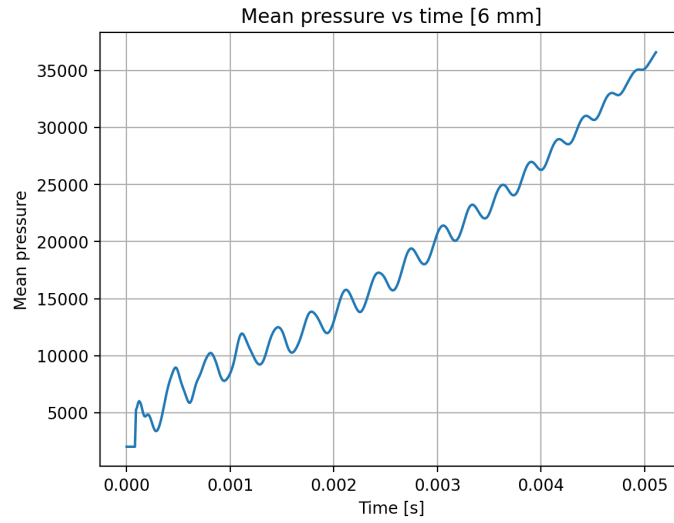
Figure 4.15: Referenced data from Guo et al.[16]

4.3 Time Series Data

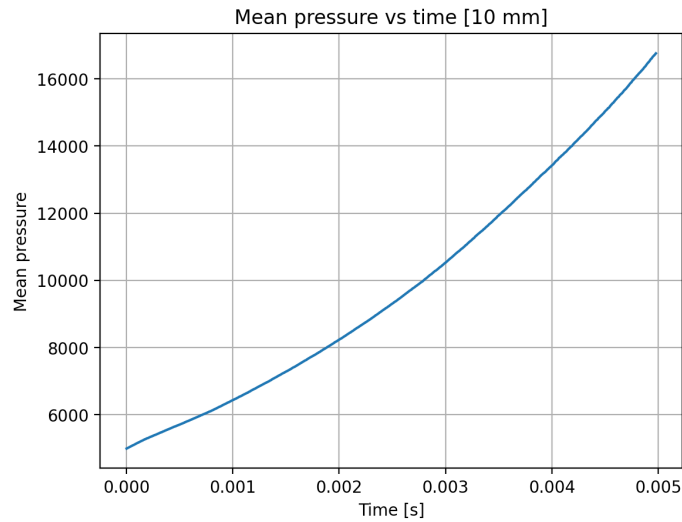
The zero time was selected to be as soon as the turbulence model was selected to be SBES, thus briefly before spark ignition. Figs. 4.16a — 4.17a calculate the mean pressure as a function of time along the centerline. The centerline is an arbitrary line that runs between the injector posts positioned at the most recessed point running for 20 mm into the combustion chamber. It was selected to collect data in the region of initial fuel and oxidizer mixing. Figs. 4.18a — 4.19a calculate the instantaneous pressure fluctuation as a function of time along the centerline. Figs. 4.20a — 4.21a calculate the mean heat release as a function of time along the centerline. Figs. 4.22a — 4.23a calculate the instantaneous heat release as a function of time along the centerline. Figs. 4.24a — 4.25a calculate the cumulative Rayleigh integral as a function of time along the centerline. Figs. 4.26a — 4.27a calculate the Rayleigh criterion as a function of time along the centerline. Figs. 4.28a — 4.29a calculate the mean temperature as a function of time along the centerline. Table 4.2 shows the $\mathcal{R}$ values, where $\mathcal{R} > 0$ is unstable, $\mathcal{R} < 0$ is stable and $\mathcal{R} = 0$ is neutrally stable.

Table 4.2: Rayleigh criterion values

Geometry	Value
Case 01 Flush	-0.0104
Case 02 6 mm Recessed	-0.0213
Case 03 Deep Recessed	1.437e-21

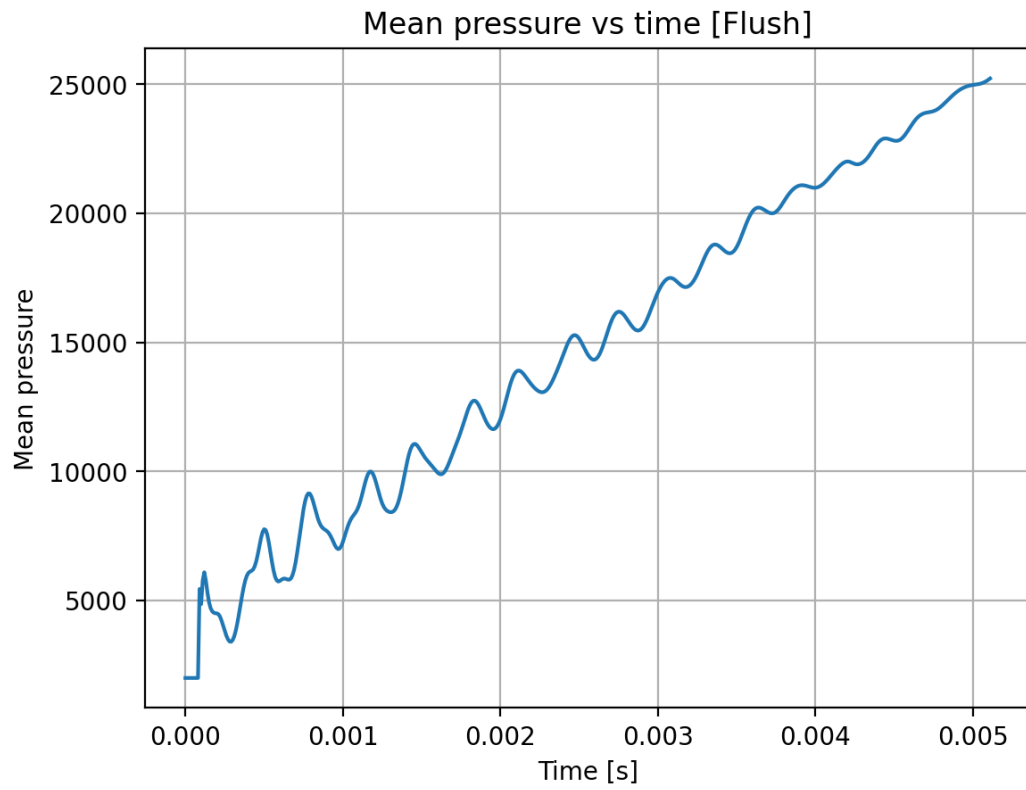


(a) Case 06 mm recessed



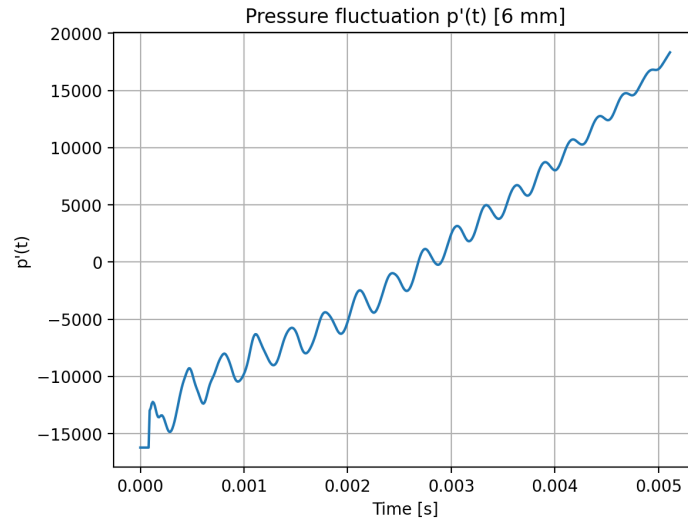
(b) Case 10 mm recessed

Figure 4.16: Mean pressure versus time for the recessed injector configurations.

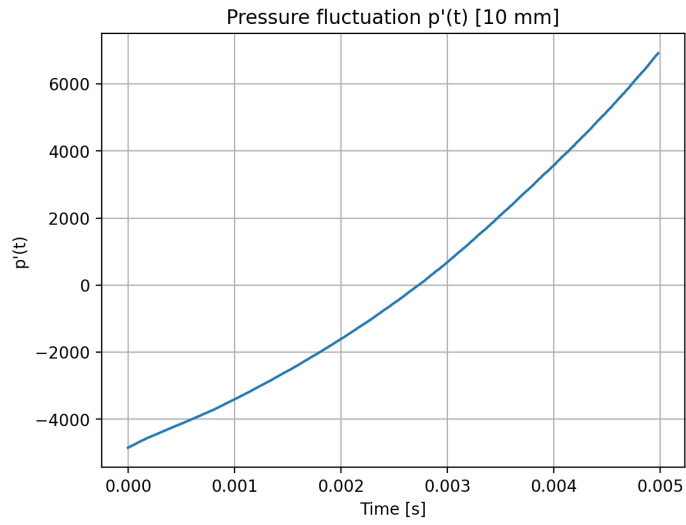


(a) Case flush

Figure 4.17: Mean pressure versus time for the flush injector configuration.

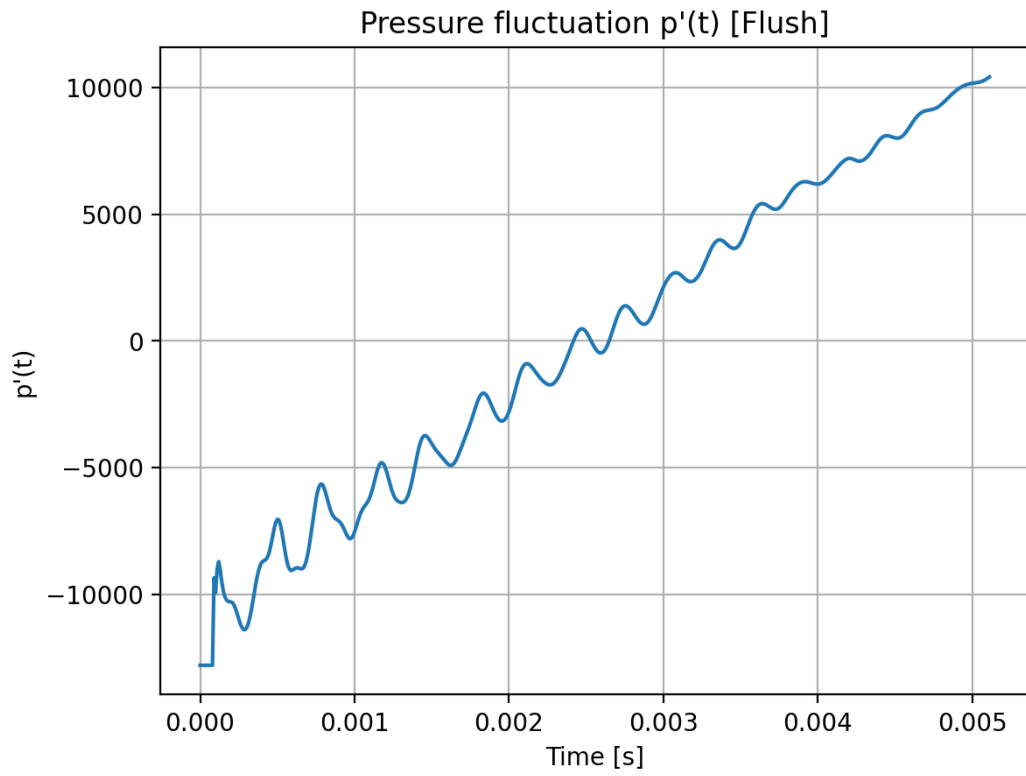


(a) Case 06 mm recessed



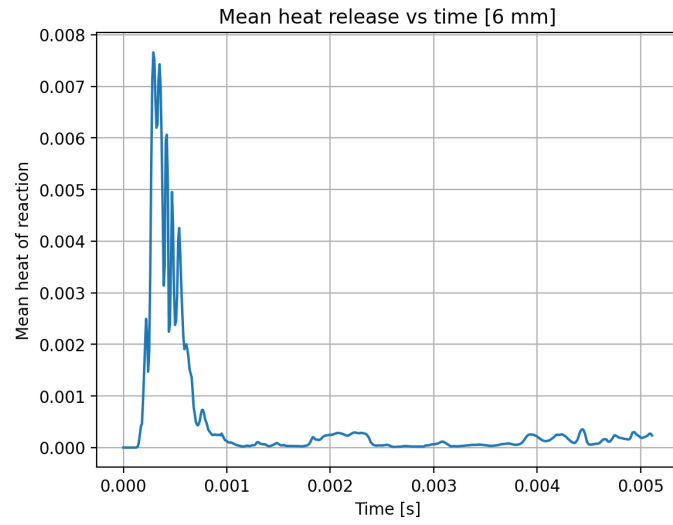
(b) Case 10 mm recessed

Figure 4.18: Pressure fluctuation p' versus time for the recessed injector configurations.

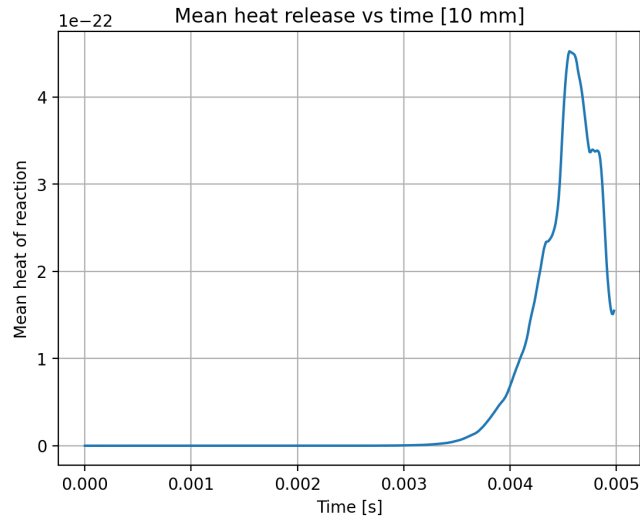


(a) Case flush

Figure 4.19: Pressure fluctuation p' versus time for the flush injector configuration.

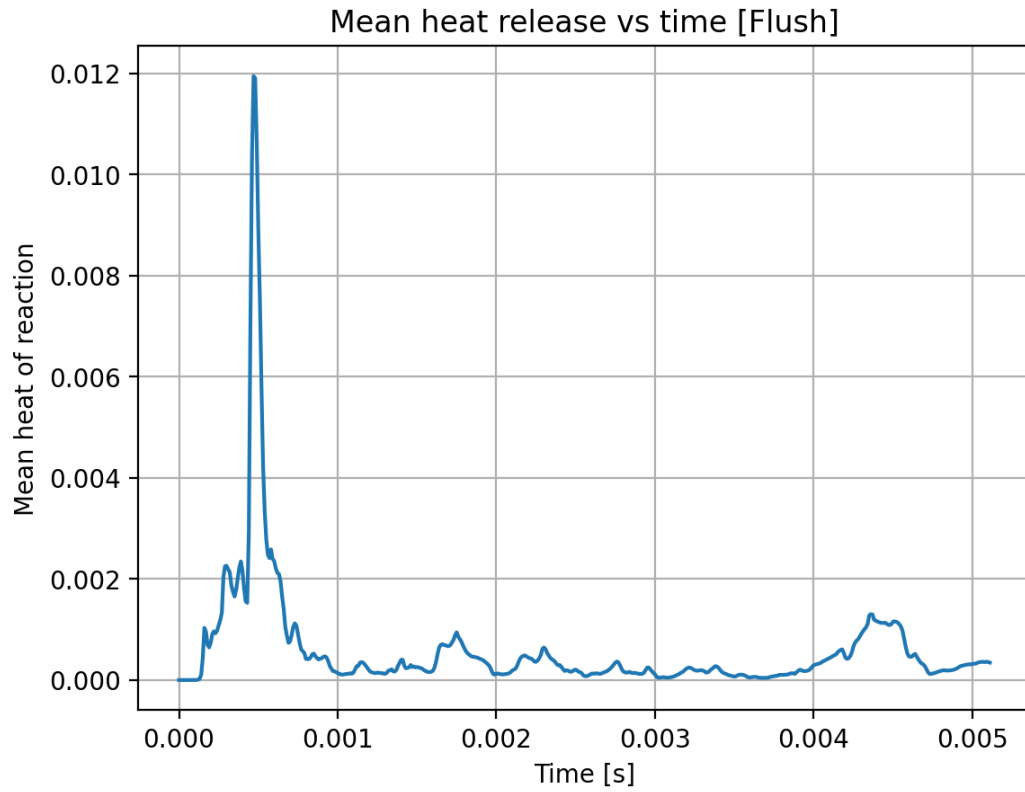


(a) Case 06 mm recessed



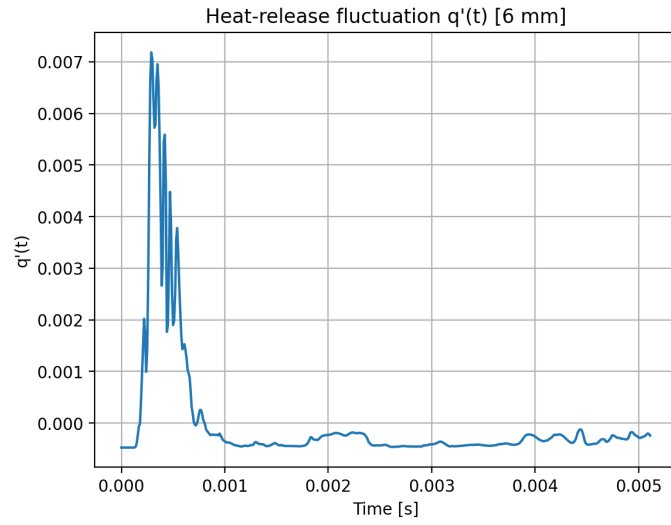
(b) Case 10 mm recessed

Figure 4.20: Mean heat-release rate q versus time for the recessed injector configurations.

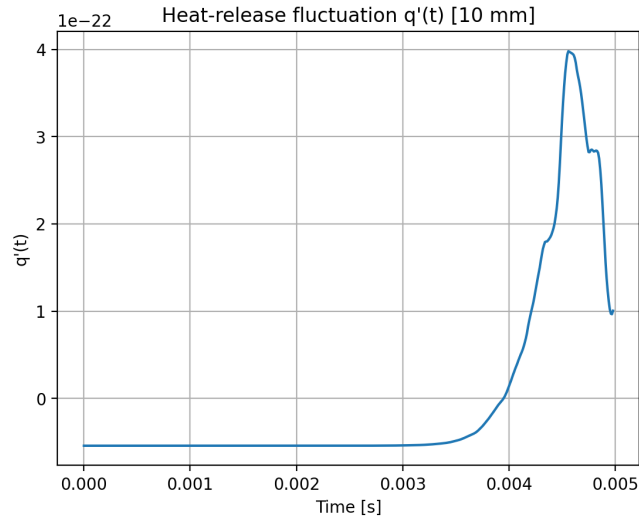


(a) Case flush

Figure 4.21: Mean heat-release rate q versus time for the flush injector configuration.

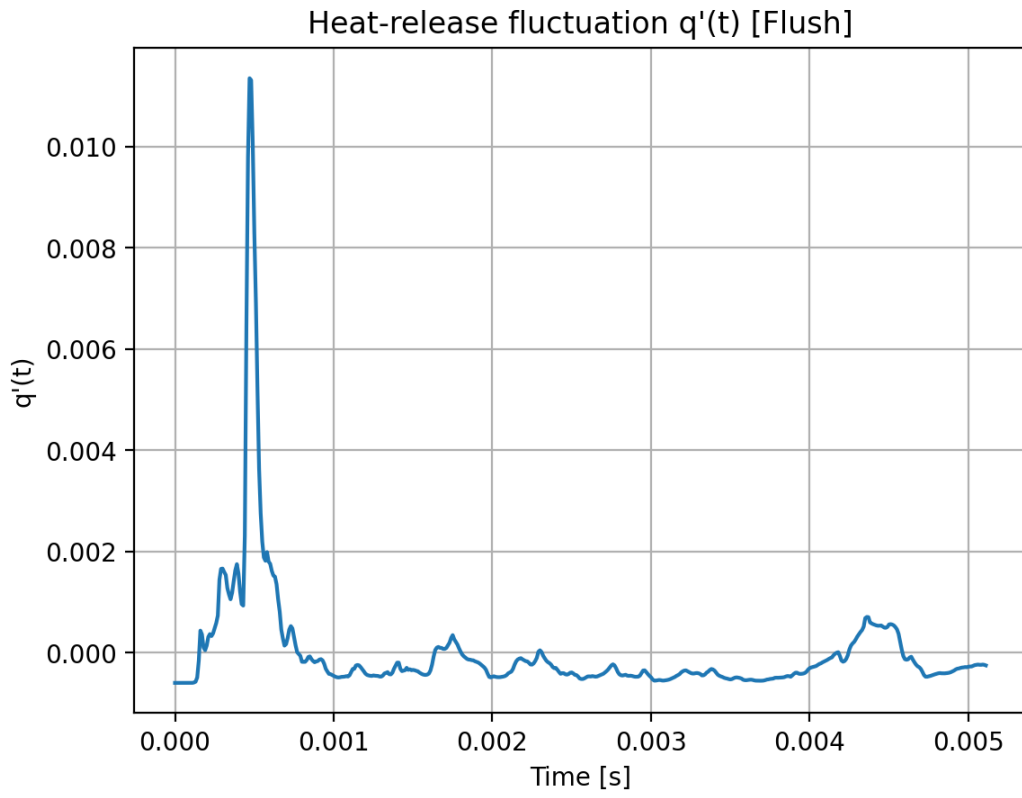


(a) Case 06 mm recessed



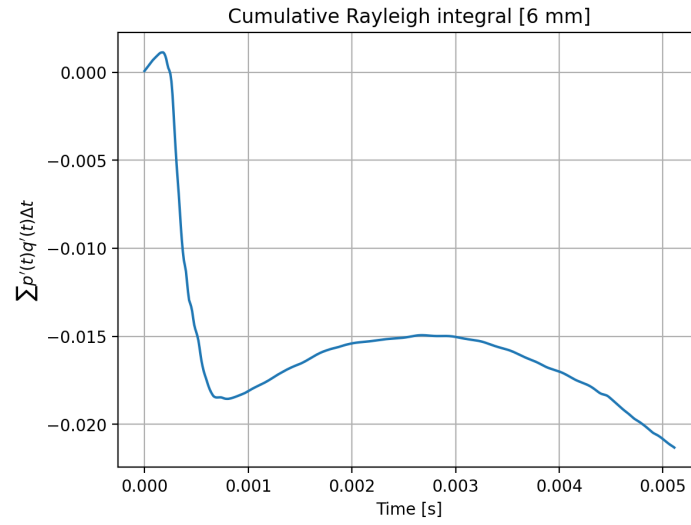
(b) Case 10 mm recessed

Figure 4.22: Heat-release fluctuation q' versus time for the recessed injector configurations.

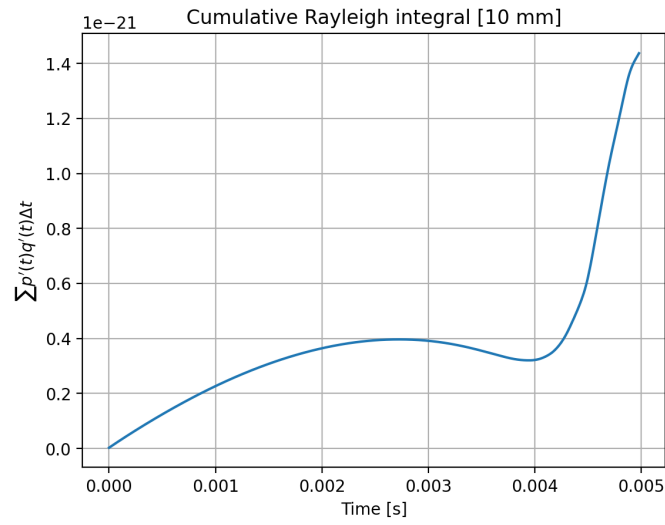


(a) Case flush

Figure 4.23: Heat-release fluctuation q' versus time for the flush injector configuration.

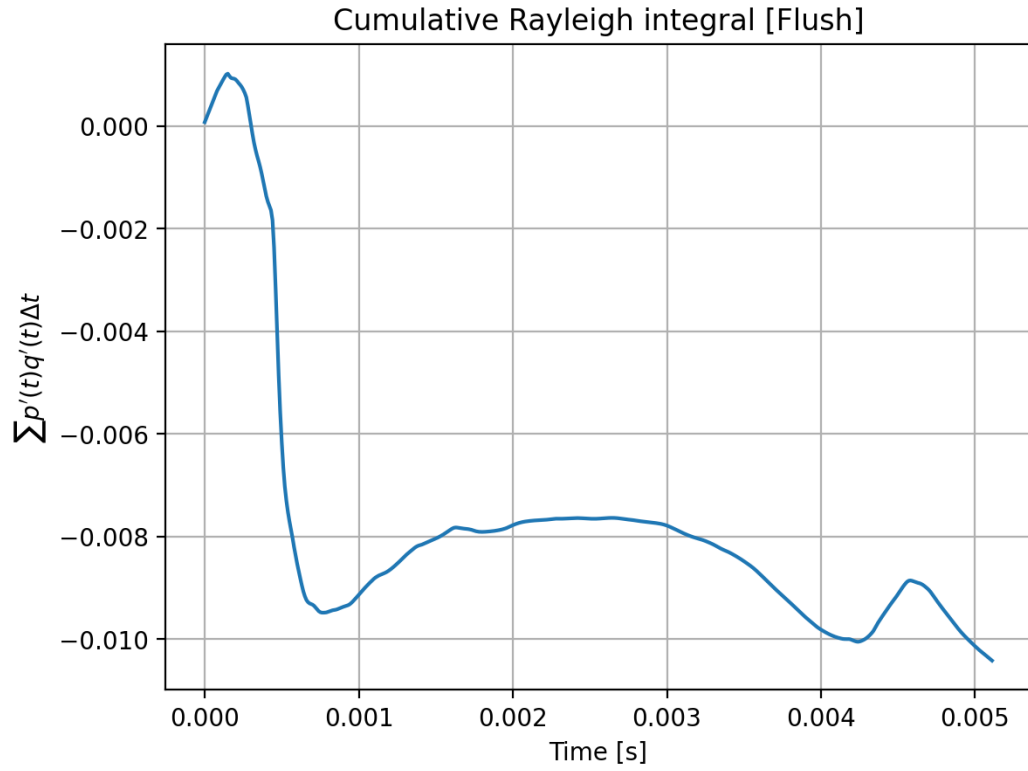


(a) Case 06 mm recessed



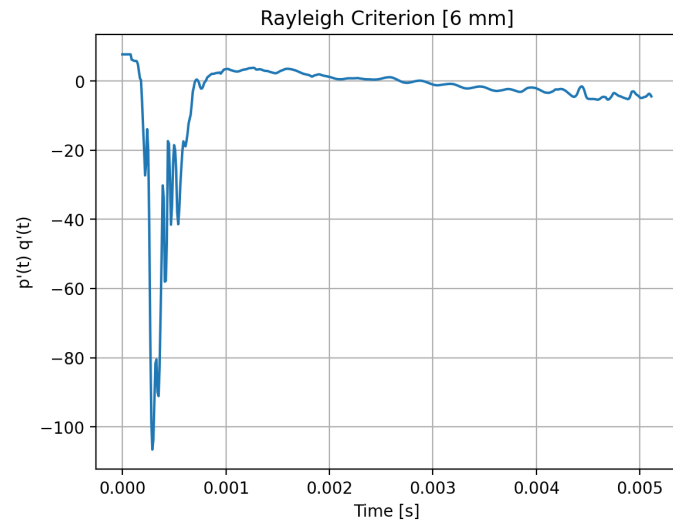
(b) Case 10 mm recessed

Figure 4.24: Cumulative Rayleigh index versus time for the recessed injector configurations.

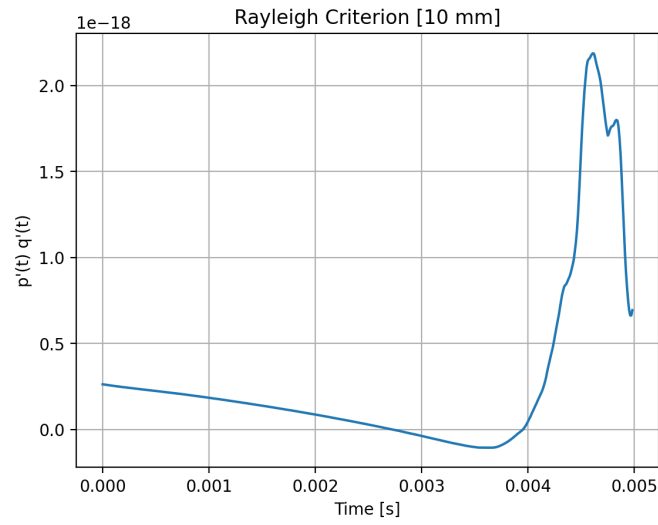


(a) Case flush

Figure 4.25: Cumulative Rayleigh index versus time for the flush injector configuration.

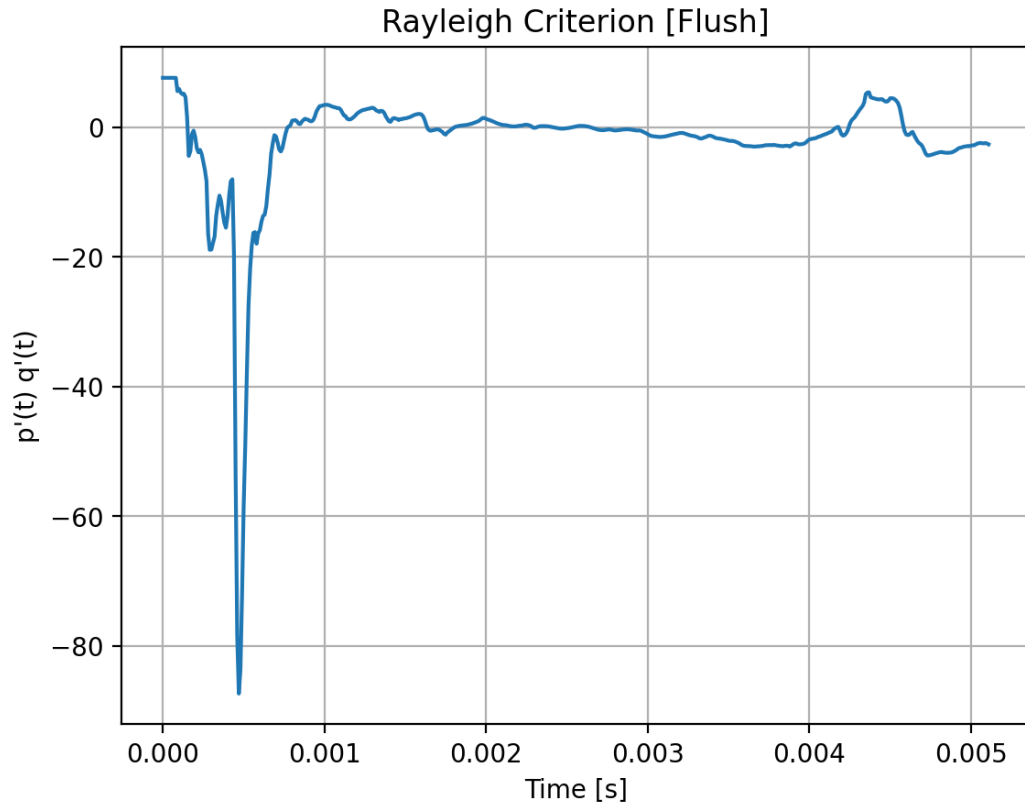


(a) Case 06 mm recessed



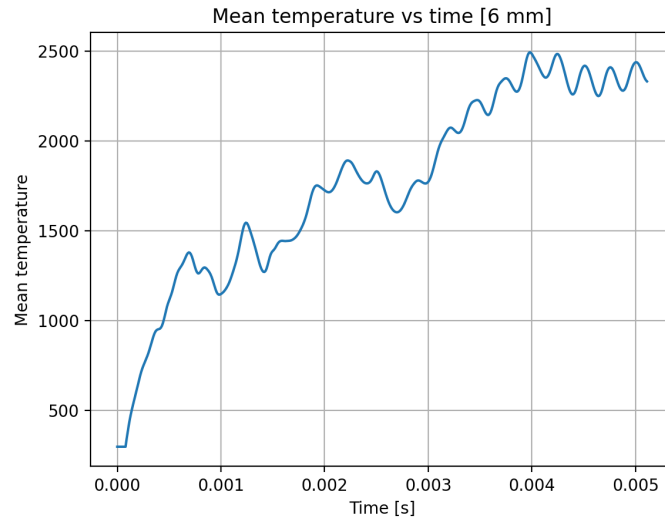
(b) Case 10 mm recessed

Figure 4.26: Rayleigh index integrand versus time for the recessed injector configurations.

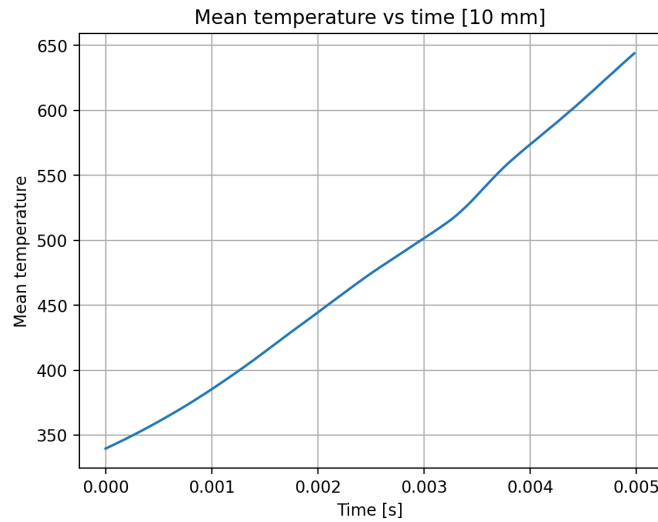


(a) Case flush

Figure 4.27: Rayleigh index integrand versus time for the flush injector configuration.

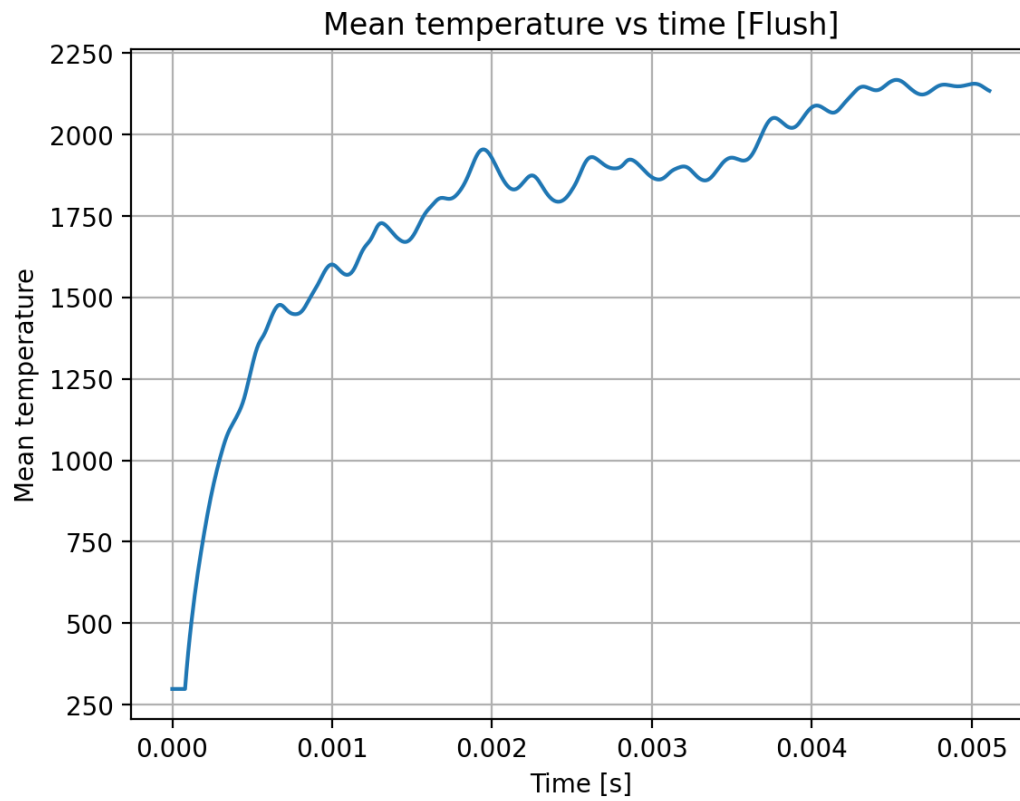


(a) Case 06 mm recessed



(b) Case 10 mm recessed

Figure 4.28: Mean temperature versus time for the recessed injector configurations.



(a) Case flush

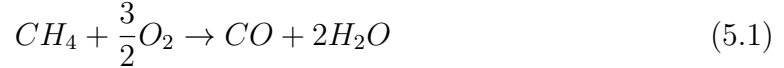
Figure 4.29: Mean temperature versus time for the flush injector configuration.

Chapter 5

Discussion

There are three distinct cases studied: Flush recess, 6 mm recess and 10 mm recess also referred to as deep recess. The three cases were selected on the basis of creating a continuum across which the system changes could be compared against. All cases were ran using the same set of initial conditions with the exception of the number of time steps. The difference in time steps varied with how long it would take the injected flow to reach the recess. In regards to the deep recessed case, a miscalculation occurred in which the spark ignited preemptively before the fuel and oxidizer could properly mix, thus this case's data is compared skeptically. The contours shown are a reflection of the systems state at the final timestep. Animations of the flow were created, but cannot be shared via this medium. By analyzing Figs. 4.1a, 4.22a—4.23a and Figs. 4.20a—4.21a alongside each other a greater understanding of the system can be achieved. In the baseline 6 mm case, the contour map portrays the heat of the reaction occurring close to the exterior wall of the combustion chamber. No data exists for locations beyond the defined centerline; however, the quantitative data indicates a significant instantaneous heat release coinciding with the spark then regressing into negative rate of heat release likely due to dissipative effects. The mean heat release tells a similar story, there is a significant jump in line with the spark ignition followed by a low mean heat release indicating sustained reactions. The deep recessed case portrays a heat of reaction close to the axis of rotation likely indicative of poor mixing due to a mistimed spark ignition. The mean heat release of the deep recessed failed to run for a sufficient amount of time post ignition to obtain a satisfactory signal-to-noise ratio regarding the heat release from the reactants, but still indicates a notable increase at ignition. The instantaneous heat release of the deep recess case follows suit with the mean heat release. The contour of the heat of the reaction for the flush case emulates the baseline case in terms of downstream

propagation. The mean heat release and instantaneous heat release have a significant spike 1.5x that of the baseline case. This can be attributed to the ignition occurring in the combustion chamber instead of a recess cavity that would limit the amount of reactants present. Looking towards the mass fraction contours of the reactants Figs. 4.2— 4.6 the mixing can be qualitatively analyzed. Starting with the baseline 6 mm case the methane has propagated well throughout the combustion chamber and has sufficiently mixed for sustained combustion. The oxidizer is an almost perfect inverse of the fuel, which is expected. The imperfect invertibility of the contour is attributed to the products of the reaction. Whilst the mixing sustains combustion, the fuel and oxidizer could be reacting more efficiently should the mass flow rates be increased properly. When comparing the flush case to the baseline, there is a lesser turbulent flow leading to poorer mixing. The lack of turbulence is likely due to the reduction in eddies formed in the recess cavity and initial mixing region. The deep recessed case portrays severely suboptimal mixing and a regressed oxidizer. The oxidizer was pushed back by a preemptive ignition source severely impeding reacting flows. Looking at the product mass fractions Figs. 4.3— 4.5 the baseline case 6 mm, shows thorough mixing and flow agitation. CO_2 is the sole product that does not show a significant presence in the recessed region of the geometry. This delay in CO_2 is a result of operating procedure of the methane-2-step chemistry mechanism in Ansys Fluent.



Reaction 2, Eq. 5.2 can only occur after Eq. 5.1 occurs, thus the delay in the mass fraction rate of CO_2 . The flushed case behaves in a similar manner to the baseline case with a reduction in turbulent flow. However, the deep recessed case is near zero and constrained to the recess zone. Moving onto the static pressure analysis of Figs. 4.7 & 4.16a— 4.19a, starting from the baseline, the measured pressure is 37.3 kPa almost everywhere in the geometry with the exception of the outlet. The corresponding mean pressure and instantaneous pressure increase linearly with minor amplitude oscillations slowly dampening as time increases. The slight variance in pressures are a results of the startup combustion periodically mixing and reacting. The two other cases also follow this same phenomena with a slight exception to the 10 mm case. The 10 mm case shows a smooth pressure increase contrary to the jagged nature of the flush and 6 mm case. The smooth nature of this curve can be attributed to an increased mass in the system at a steady rate pre-combustion.

Figs. 4.8 & Figs. 4.28a— 4.29a give insight into how temperature changes spatially and temporally from the contours and graphs respectively. All cases show a hot region of 5000 K at the centerline, this is caused by the ignition spark. The ignition spark is located in this area and heats the immediate and surrounding area. If the temperature reaches 5000 K then the solver caps the temperature and maintains it steady at 5000 K until the heat is dissipated. This introduces some errors into the simulation, but is done to minimize the thermal gradients. The motivation behind throttling the thermal gradients is reducing compute time; the compute time is reduced via this method because when there are steep numerical gradients smaller time steps are required to solve and prevent a numerical explosion. Despite this thermal limitation, the reacting flow still maintains conformity to real life physics sufficiently so to analyze combustion. The spark in the deep recessed case however, occurred too early in regards to the flow. This failed to allow the heat to be properly dissipated by the moving flow. When analyzing the mean temperature as a function of time, the baseline and flush case show remarkable similarities. One of those similarities is the steep temperature gradient followed by a plateau at approximately 2300 K. The deep recessed case sees a temperature increase, but not a climb to 2300 K like the other contours. With regard to the eigenmodes of the geometries, Table 4.1 shows no strong correlation between the mesh fidelity nor the recess length affecting the eigenmodes of the system as seen in Figs. 4.9— 4.14. Comparing the simulated modal data to both theory and [16] there is an alignment with the modes 3, 4 and 6 to the paper, although to different modes. There is an indication of acoustic coupling between modes 3 and 4. These modes' frequencies are close enough where should the proper set of conditions occur, there could be destructive acoustic waves that form. There is the added danger of combustion instabilities resonating at this frequency; it can be seen from Table 4.2 the deep recessed case shows some slight indication towards combustion instability. Whilst the baseline and flush case do not indicate combustion instability due to $\mathcal{R} < 0$ they are only slightly stable by this metric. It is important to note that the method used to calculate $\mathcal{R}$ was based on pressure and heat release values that existed along a 20 mm centerline, thus this is solely an indication of 1-D stability in this section of the geometry. While local stability may exist, further investigation may reveal strong global combustion instabilities. Looking at Figs. 4.24a— 4.27a the 6 mm and flush case tend towards stability in the cumulative Rayleigh integrand while the 10 mm becomes unstable. Contrary to expectation, both the 6 mm and flush case see a strong jump toward stability during ignition while the converse occurs for the 10 mm case. Further investigation is required to truly determine the stability of the respective systems.

Chapter 6

Future Work

6.1 Further Refinement

6.1.1 Model Accuracy & Refinement

When creating the model, there were great efforts to mimic conditions from [16]; however, due to computational constraints some substitutions were included. The paper geometry is an eleven injector 3-D model. There were limitations on the size of the mesh that strongly motivated a reduction to a 2-D single injector geometry. It is understood, this significant change can introduce difficulties when comparing results. Additionally, the mass flow rates were modified as the steep velocity and turbulence gradients created would call for a much smaller time step to be used. Using a proper time step for the intended mass flow rate would prohibitively increase the computational time. The timestep used were a magnitude greater than what was initially desired, however, due to computational constraints the slight reduction in accuracy was deemed acceptable for the conditions. As the results stand, only the eigenmodes for the geometry are referenced to [16]. Future work would include the RSME of various parameters for direct comparison with figures from [16]. The data collected was along a 20 mm line. This minor subset of the geometry generated over 50 GB of numerical data and animations. Storage space prevented the expansion of the area of data collection. Future work should incorporate real time calculation to prevent storage limitations or expand storage capabilities for robust data collection and processing. An expansion to the number of recess lengths would also benefit the study. Additionally, there is great potential to expand the work to include the variance of the L^* parameter and measure changing $\mathcal{R}$ as a result.

6.2 Neural Networks

6.2.1 Theory

The emergence of neural networks began in the 1940's with a formal neuron model proposed by McCulloch and Pitts[54]. A few years later Donald Hebb proposed the Hebb synapse[55] and Rosenblatt the perceptron[56]. This perceptron node is a linear classifier and in contemporary use is the activation function such as ReLu, Sigmoid, Tanh etc[57]. The node is an element that contains various pieces of information such as: weight, bias and activation function. The neuron by itself is will only capture linear behavior; however, coupled with several others they are capable of capturing highly non-linear behavior [58]. At a high level, the architecture of a neural network contains an input layer, one or more hidden layers and an output layer. The input layer is responsible for specifying the expected shape of the input data. If necessary a flattening layer could be inserted to modify the shape of the input data. The dense layers of the network are where the training will occur. Sometimes when the data lacks sufficient diversity, the model overfits. Overfitting is a phenomena in which the dataset trained and validated on fail to generalize to general patterns due to learning the patterns of the noise in the data [59]. The dense layers are the layers in between the input and output layers. These layers are responsible for the "learning". The learning will vary based on network architecture and data. Distinct architectures are more suitable for their respective uses. For example, convolutional neural networks (CNNs) have improved accuracy at image detection whereas Long Short Term Memory networks (LSTM) are better at language processing. The current state of the art in Natural Language Processing (NLP) are Transformers [60].

6.2.2 Data requirements

When considering the data requirements for a neural network, one must first understand the domain of the problem and consider the architecture of the NN. The domain this neural network is computational fluid dynamics (CFD). As such, it should be expected to require a complex architecture to predict anything noteworthy. As stated in the previous section complex behavior will require highly non-linear multidimensional functions to predict. This requirement requires a deep neural network as a shallow network would be insufficient in its predictive capacities. The specialized neural network referred to in the previous section are examples of deep neural networks.

6.3 Use in CFD

Machine learning has taken root across several fields and subfield, it has been strongly aided by the increasing drive of data output. The increase of data, also referred to as big data, is derived from an ever increase suite of sensors and higher fidelity sweeps. CFD is constantly in pursuit of higher fidelity simulations running, high powered RANS and LES setups with an increasing amount of injector elements is producing copious amounts of data. ML is uniquely positioned to insert itself into this field in various manners. Post processing is a valuable way to digest data and better understand a system. With regards to combustion instability, these ML algorithms are capable of reproducing highly non-linear behavior and has the potential to expedite simulations or augment them in other forms. This is not without its challenges, ML requires big data and depending on the tool, that data may need to be labeled. Supervised learning algorithms require that the data that is fed should be properly labeled to be appropriately classified. Unsupervised learning, on the other hand, does not require that. Unsupervised learning has the capacity to learn underlying patterns that conventional algorithms may be incapable of converging on. A caveat is that these algorithms must be closely monitored for unwanted behaviors such as overfitting.

Chapter 7

Conclusion

This study in injector driven combustion instability serves as an introduction to the topic. Further refinement and expansion is required to meet robust standards. Despite the required and desired future work, the exploration of the application of SBES to mapping combustion instabilities provides insight and the groundwork for derivative studies. The geometry used was purposely simple to provide accessibility for reproducibility given software constraints and has the added benefit of turning the focus to understanding the underlying physics and chemistry. Reacting flows are complicated dynamical systems that require careful consideration of the underlying chemistry mechanisms. These mechanism can be simplified, but if they are simplified the underlying assumptions must be well understood. The assumptions will dictate the accuracy of the simulation. Understanding which assumptions are acceptable for the desired phenomena requires careful curation and thought. The 2 step methane mechanism used in the simulation provided sufficient chemical reactions to observe heat release form the chemistry, but retained the limitations of a real world mechanism. Other assumptions and simplifications such as how to treat the gas results in distinct behavior. Reductions in model fidelity can be desirable so long as they are selected for and not a result of negligence. The physics of the problem lies in the boundary conditions and turbulence model. How the boundary conditions were defined were strongly based on [16]. Some modifications were made using the physical understanding of the model and physics along with some hand calculations. Understanding non-dimensional parameters such as Reynolds number and Lewis number is imperative to correct problem setup. Even with proper initial conditions there are solver specific considerations to weigh that may not be known until after the initial runs of the simulation. The turbulence model used is essential to the problem definition. Certain turbulence models may be unable to resolve the

phenomena desired or require a higher mesh fidelity than the model currently uses. Mesh creation is another significant aspect that will change the results of the simulation. There are several considerations with mesh creation such as unstructured vs structured meshes and mesh fidelity. When the setup is complete the simulation must use the appropriate time steps to resolve the desired problem and reach residual convergence. Proper CFD is hardly a task for a lackadaisical problem setup. With regards to combustion instability, CFD is insufficient to holistically encapsulate the problem. At minimum it should be coupled with FEA to determine acoustic modes of the geometry. Thermo-acoustic coupling cannot be determined without knowledge of the eigenmodes of the geometry nor without knowledge of the chemistry and physics of the combustion. The data collected from the simulations ran are sufficient to determine whether there are localized combustion instabilities along the defined 1-D centerline, but further efforts are required to determine global combustion instability and to determine where stability exists. The work done serves as a well defined starting point for future exploration into injector driven high frequency combustion instabilities.

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Appendix A

Component to Vector form Navier-Stokes Equations

Let $\mathbf{u} = (u, v, w)$

X-momentum

Step 1

$$\frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho u^2)}{\partial x} + \frac{\partial(\rho uv)}{\partial y} + \frac{\partial(\rho uw)}{\partial z} = -\frac{\partial p}{\partial x} + \frac{1}{\text{Re}_r} \left(\frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{xy}}{\partial y} + \frac{\partial \tau_{xz}}{\partial z} \right) \quad (\text{A.1})$$

Step 2

$$\left(\frac{\partial(\rho \mathbf{u})}{\partial t} \right)_x = \frac{\partial(\rho u)}{\partial t}, \quad (\text{A.2})$$

$$(\nabla \cdot (\rho \mathbf{u} \mathbf{u}))_x = \frac{\partial(\rho u^2)}{\partial x} + \frac{\partial(\rho uv)}{\partial y} + \frac{\partial(\rho uw)}{\partial z}, \quad (\text{A.3})$$

$$(-\nabla p)_x = -\frac{\partial p}{\partial x}, \quad (\text{A.4})$$

$$(\nabla \cdot \boldsymbol{\tau})_x = \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{xy}}{\partial y} + \frac{\partial \tau_{xz}}{\partial z}. \quad (\text{A.5})$$

Step 3

$$\left[\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) \right]_x = \left[-\nabla p + \frac{1}{\text{Re}_r} \nabla \cdot \boldsymbol{\tau} \right]_x \quad (\text{A.6})$$

Y-momentum

Step 1

$$\frac{\partial(\rho v)}{\partial t} + \frac{\partial(\rho uv)}{\partial x} + \frac{\partial(\rho v^2)}{\partial y} + \frac{\partial(\rho vw)}{\partial z} = -\frac{\partial p}{\partial y} + \frac{1}{\text{Re}_r} \left(\frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{yz}}{\partial z} \right) \quad (\text{A.7})$$

Step 2

$$\left(\frac{\partial(\rho \mathbf{u})}{\partial t} \right)_y = \frac{\partial(\rho v)}{\partial t}, \quad (\text{A.8})$$

$$(\nabla \cdot (\rho \mathbf{u} \mathbf{u}))_y = \frac{\partial(\rho uv)}{\partial x} + \frac{\partial(\rho v^2)}{\partial y} + \frac{\partial(\rho vw)}{\partial z}, \quad (\text{A.9})$$

$$(-\nabla p)_y = -\frac{\partial p}{\partial y}, \quad (\text{A.10})$$

$$(\nabla \cdot \boldsymbol{\tau})_y = \frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{yz}}{\partial z} \quad (\text{A.11})$$

Step 3

$$\left[\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) \right]_y = \left[-\nabla p + \frac{1}{\text{Re}_r} \nabla \cdot \boldsymbol{\tau} \right]_y \quad (\text{A.12})$$

Z-momentum

Step 1

$$\frac{\partial(\rho w)}{\partial t} + \frac{\partial(\rho uw)}{\partial x} + \frac{\partial(\rho vw)}{\partial y} + \frac{\partial(\rho w^2)}{\partial z} = -\frac{\partial p}{\partial z} + \frac{1}{\text{Re}_r} \left(\frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z} \right) \quad (\text{A.13})$$

Step 2

$$\left(\frac{\partial(\rho \mathbf{u})}{\partial t} \right)_z = \frac{\partial(\rho w)}{\partial t}, \quad (\text{A.14})$$

$$(\nabla \cdot (\rho \mathbf{u} \mathbf{u}))_z = \frac{\partial(\rho uw)}{\partial x} + \frac{\partial(\rho vw)}{\partial y} + \frac{\partial(\rho w^2)}{\partial z}, \quad (\text{A.15})$$

$$(-\nabla p)_z = -\frac{\partial p}{\partial z}, \quad (\text{A.16})$$

$$(\nabla \cdot \boldsymbol{\tau})_z = \frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z} \quad (\text{A.17})$$

Step 3

$$\left[\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) \right]_z = \left[-\nabla p + \frac{1}{\text{Re}_r} \nabla \cdot \boldsymbol{\tau} \right]_z \quad (\text{A.18})$$

Vector Form

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \frac{1}{\text{Re}_r} \nabla \cdot \boldsymbol{\tau}$$