EFFECT OF RAYLEIGH-TAYLOR INSTABILITY ON FUEL CONSUMPTION RATE: A NUMERICAL INVESTIGATION

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EFFECT OF RAYLEIGH-TAYLOR INSTABILITY ON FUEL CONSUMPTION RATE: A NUMERICAL INVESTIGATION

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ABSTRACT

EFFECT OF RAYLEIGH-TAYLOR INSTABILITY ON FUEL CONSUMPTION RATE:
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An extensive numerical investigation is conducted in order to assess the effect of Rayleigh-Taylor instability on fuel consumption rate (or flame speed). Two geometries are used for this investigation, viz., a high pressure high-g (HPHG) cavity stabilized combustor and a curved duct with a backward facing step. The former geometry is a more practical combustion system that contains liquid fuel injectors with operating conditions that mimic gas turbine cycles, whereas the latter is a canonical combustor used to study turbulent premixed flames. Reynolds averaged Navier-Stokes (RANS) and large eddy simulations (LES) are used. RANS is used for the practical combustor, and both RANS and LES are used for the canonical combustor. The combustion models used are the flamelet generated manifold (FGM) and the two-step species transport for the practical and canonical combustor, respectively.
The HPHG combustor is designed to induce bulk rotational flow in the cavity, inducing centrifugal acceleration. The centrifugal force acts from the high-density reactants towards the low-density products creating a Rayleigh-Taylor instability (RTI). Rayleigh-Taylor instabilities are expected to increase the turbulent flame speed and reduce the size of the combustor by increasing the flame wrinkling and/or corrugation. Simulations at two different levels of centrifugal acceleration, and, consequently, dissimilar Rayleigh-Taylor instability were performed. It was found that the nominal g-loads are overestimating the local g-loads from the simulation because thermal expansion is not taken into account. From these simulations it was not possible to discern the effect of RTI on fuel consumption rate due to the complex physical-chemical process inherent to this combustor such as fuel vaporization, molecular mixing, spray-turbulence interaction, turbulence-chemistry interaction, and partial premixing.

Therefore, gaseous premixed turbulent flames were simulated in a curved duct with a backward facing step. Two radius of curvature were used, viz., an infinite (straight duct) and a finite radius of curvature (curved duct). These combustors were operated at low and high Reynolds number (3,200 and 32,000). The computational results are compared with broadband chemiluminescence and shadowgraph images reported in the literature for similar conditions and geometries. Both RANS and LES results are in general agreement with measurements. Both experiments and simulations show that increasing the Reynolds number in both straight and curved canonical combustor the flame cannot withstand the Karlovitz number effects and the flame is positioned behind the backward-facing step. In addition, the LES results indicate that at high Reynolds
number the flame blows out for the straight channel while it remains stabilized for the curved channel. This result is in agreement with the blowout data reported in the literature. On the other hand, RANS over predict the flame stabilization for the straight channel. Consequently, RANS should not be used in research involving RTI-induced blowout.

In conclusion, RTI interacts with a turbulent premixed flame and its overall effect is to extend the conditions under which turbulent premixed flames can be stabilized. This improved flame stabilization is a direct manifestation that the fuel consumption rate (or flame speed) has been enhanced in order for the flame to withstand higher Karlovitz number effects induced by high Reynolds number. However, the mechanism through which RTI works on the turbulent premixed flame is not clear. A new hypothesis is proposed. The increase in RTI should increase the turbulent length scale as well as increase the Karlovitz number. The corrugated flame would withstand the higher Karlovitz number because RTI temporarily and periodically reverses the turbulent energy cascade by minimizing the potential energy of the stratified flow.
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This work would not have been completed without all the help that I have received along the way. I would like to thank Brent Rankin and Jamie Ervin for being on my committee and for their encouragement and guidance through this process, especially my advisor Scott Stouffer. A special thanks to Alex Briones for assisting me getting my simulations running, for helping through all the computer issues, helping me to draft my thesis, and everything else along the way. I would also like to thank Tim Erdmann, Dave Burrus, and Drew Caswell for your help along the way. I would like to especially thank all of my friends and family for all their love and support, and for letting me vent about my simulations all while pretending to understand what it was I was doing and what I was working on. Finally, I would like to acknowledge the funding of this research by the combustion branch of AFRL through contract number FA8650-15-D-2505.
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**NOMENCLATURE**

\[
\begin{align*}
A_f & = \text{flame surface area [m}^2]\text{]} \\
A_C & = \text{cross sectional combustor area [m}^2]\text{]} \\
a_c & = \text{centrifugal acceleration [Earth’s g]} \\
A_e & = \text{Effective Area} \\
\bar{c} & = \text{Farve mean c-progress variable} \\
C_p & = \text{specific heat capacity [J/kg-K]} \\
\bar{\varphi}_{im} & = \text{mixture-averaged diffusivity of species “i” to the mixture} \\
\bar{\tilde{f}} & = \text{Farve mean mixture fraction} \\
\bar{f}^{1/2} & = \text{Farve mean mixture fraction variance} \\
g & = \text{Earth’s gravitational acceleration, 9.81 m/s}^2 \\
\bar{h}_s & = \text{Farve mean sensible enthalpy [J/kg]} \\
\bar{H} & = \text{Farve mean total enthalpy [J/kg]} \\
k & = \text{turbulent kinetic energy [m}^2/\text{s}^2]\text{]} \\
\bar{k}_{SGS} & = \text{Farve mean turbulent subgrid-scale turbulent kinetic energy [m}^2/\text{s}^2]\text{]} \\
l & = \text{turbulent intensity} \\
Le & = \text{Lewis number} \\
\mathcal{L} & = \text{Markstein length [m]} \\
\dot{m} & = \text{mass flow rate [kg/s]} \\
MW & = \text{molecular weight [kg/kmol]} \\
n & = \text{flame normal vector} \\
N & = \text{refraction index} \\
p & = \text{pressure [Pa]} \\
\bar{p} & = \text{Farve mean pressure [Pa]} \\
Pr_{SGS} & = \text{subgrid-scale Prandtl number} \\
Pr_t & = \text{turbulent Prandtl number} \\
r & = \text{radial coordinate, } r = \sqrt{x^2 + y^2} [\text{m}] \\
Re & = \text{Reynolds number} \\
\bar{R}_i & = \text{mean rate of production of species “i”} \\
S & = \text{strain rate [1/s]} \\
Sc & = \text{Schmidt number} \\
Sc_t & = \text{turbulent Schmidt number} \\
S_f & = \text{local flame speed [m/s]} \\
\dot{S}_H & = \text{total enthalpy source [J/kg-s]} \\
\end{align*}
\]
\( S_L^o = \) unstretched laminar flame speed [m/s]
\( \dot{S}_m = \) mass source [kg/s]
\( S_T = \) turbulent flame speed [m/s]
\( S_{\Phi} = \) generic source term [units depended upon \( \Phi \)]
\( t = \) time [s]
\( T = \) temperature [k]
\( \bar{T} = \) mean temperature [k]
\( u = \) streamwise velocity [m/s]
\( \bar{u} = \) Farve mean streamwise velocity [m/s]
\( u_i = \) velocity in tensor notation [m/s]
\( U_0 = \) inlet velocity [m/s]
\( U_{rms} = \) root-mean square velocity [m/s]
\( v = \) transverse velocity [m/s]
\( \bar{v} = \) Farve mean transverse velocity [m/s]
\( v_{tan} = \) tangential velocity [m/s]
\( w = \) spanwise velocity [m/s]
\( \bar{w} = \) Farve mean spanwise velocity [m/s]
\( x = \) spanwise Cartesian coordinate [m]
\( y = \) transverse Cartesian coordinate [m]
\( \bar{y}_i = \) Farve mean mass fraction of species \( i \)
\( z = \) streamwise/axial Cartesian coordinate [m]

\( \Gamma_{\Phi} = \) generic diffusion coefficient [unit depends upon variable \( \Phi \)]
\( \Delta_f = \) filter length [m]
\( \varepsilon = \) eddy dissipation rate [m2/s3]
\( \eta = \) Kolmogorov length scale
\( \kappa = \) total stretch rate [s-1]
\( \lambda = \) thermal conductivity [W/m-K]
\( \mu = \) viscosity [Pa-s]
\( \mu_{SGS} = \) subgrid-scale viscosity [Pa-s]
\( \mu_t = \) turbulent viscosity [Pa-s]
\( \xi^* = \) fine spatial scale [m]
\( \rho = \) density [kg/m3]
\( \sigma_k = \) turbulent kinetic energy Prandtl number
\( \sigma_{\varepsilon} = \) eddy dissipation rate Prandtl number
\( \sigma_s = \) turbulent Schmidt number for mean mixture
\( \sigma_{\omega} = \) specific dissipation rate Prandtl number
\( \tau_{ij} = \) subgrid-scale stress tensor [Pa/m3]
\( \phi = \) equivalence ratio
\( \Phi = \) generic transport variable [unit depends upon the variable]
\( \omega = \) specific dissipation rate [1/s]
CHAPTER 1

INTRODUCTION

The Introduction is subdivided into Motivation, Background, and Objectives. The latter also discusses the purpose of this investigation.

1.1 Motivation

There is a high demand for the development of gas turbine engines with improved performance, increased durability, and lower emissions. One way to achieve this goal is by increasing the thrust to weight ratio of an engine which can be done by reducing the combustor size which would thereby reduce the engine weight. This objective is being met by exploring new and revisiting old less conventional methods. One such method is to utilize Rayleigh-Taylor (RT) instabilities to shorten the flame by increasing turbulence, which increases the mixing rate, leading to an increased fuel consumption rate. Rayleigh-Taylor instability (RTI) is the phenomenon associated with the interface between two dissimilar density fluids. RT instabilities force the high density unburnt mixture through the lower density burnt mixture, inducing turbulence mixing between the reactants and products. RTI can be driven by either constant body force (e.g., buoyancy-driven RTI) or a varying body force (e.g., centrifugal-force-driven RTI). This body force leads to pressure gradients across the interface, which, in turn, cause perturbations of higher density fluid that displaces towards the lower density fluid,
while the latter moves towards the former. This creates a complex mixing structure, illustrated in Figure 1 [1]. These perturbations of the lower density fluid form into bubbles that then begin to travel through the higher density fluid. Concurrently, pockets of the higher density fluid are forced through the lower density fluid filling the void created by the opposing lower density fluid creating a mushroom-like shape. This process continues until a more complex mixing structure is created and the fluids have completely mixed. There are three main regimes to this process, viz., (1) the initial perturbations (cf. Figure 1 (top)), onset of unstable growth at accelerating rates (cf. Figure 1 (middle)), and enhanced mixing due to longer wavelengths (cf. Figure 1 (bottom)) [1]. From this third stage of the development of RTI there comes a secondary process of the perturbations rolling up underneath the initial perturbation, these roll up features cause localized Kevin-Helmholtz instabilities (KHI) within the existing RTI further increasing the amount of mixing that is occurring. This process of the mixing of two different density fluids and creating RTI/KHI has been often studied and applied to many different fields of research in both numerical and experimental studies as shown in Figure 2 [2] and Figure 3 [1] respectively.
Figure 1. Development of mixing through Rayleigh-Taylor instabilities [1]. In this figure the upper fluid in each figure is the higher density fluid and the lower fluid is the lower density fluid.
Figure 2. Numerical simulation snapshots of the development of Rayleigh-Taylor Instabilities chronologically moving from (a), being the simulated initial perturbation, to (d) being the simulated late stage Rayleigh-Taylor Instabilities. [2] Reprinted from Computers and Mathematics with Applications, 66, Lee, Hyun Geun, Kim, Junseok, Numerical Simulation of the Three-Dimensional Rayleigh-Taylor Instability, 1466-1474,(2013), with permission from Elsevier.
Figure 3. Experimental planar laser-induced fluorescence images displaying the development of Rayleigh-Taylor Instabilities from an early development stage (left) to a late development stage (right) [1].

The RT instability in a gas turbine combustor would induce turbulence mixing. In turn, this would promote flame front wrinkling and corrugation, increasing the flame surface area. Turbulence fluctuations also increase flame stretching, which reduces the local flame speed. This concept can be mathematically depicted as [3] where $S_T$ is the turbulent flame speed, $S_L^0$ is the unstretched laminar flame speed, $L$ is the Markstein length, $\bar{\kappa}$ is the mean stretch rate, $A_f$ is the flame surface area, and $A_c$ is the cross sectional area of the combustor.

$$\frac{S_T}{S_L^0} = \left(1 - \frac{\bar{\kappa}}{S_L^0}\right)\left(\frac{A_f}{A_c}\right).$$ (1)

1.2 Background

The concept of increasing turbulent flame speeds by increasing RT instabilities was first investigated in experiments conducted by Lewis [5,6,7]. In these experiments, a cylindrical tube, as illustrated in Figure 4(a), was filled with premixed fuel (propane or hydrogen) and air. The cylindrical tube was rotated about its center, and the mixture
was then ignited from one end of the cylinder. Rayleigh-Taylor instabilities are generated due to the centrifugal forces induced from the rotation of the cylinder. Lewis concluded that an increase in centrifugal acceleration, resulting in an increase of mixing due to Rayleigh-Taylor instabilities, results in faster turbulent flame speeds. This effect, however, did not occur until inducing a centrifugal acceleration greater than 500 times Earth’s gravitational acceleration (g-load of 500). For g-loadings greater than 500 Earth g’s, Lewis reported that the propagation velocity increases significantly until a g-loading of approximately 3,500 where flame propagation velocity is reported to decrease dramatically. From the conclusions gathered by Lewis et al. [5,6,7] many more studies and experiments have been conducted to further this understanding and application of gravitational acceleration and Rayleigh-Taylor instabilities on combusting flows.

Lapsa and Dahm [8,9] used the aforementioned curved duct with a backward facing-step to experimentally assess the effect of centrifugal force on turbulent flames as illustrated in Figure 4(b). They utilized several combustors with several radius of curvature varying from a few inches to infinite (hereafter referred to as the straight duct) as illustrated in Figure 4(c). The backward-facing step was placed at either the inner or outer radius of the combustor surface to either suppress or promote RTI, respectively. The backward facing step on the outer wall was utilized to force the higher density flow through the lower density flow using the centrifugal acceleration of the curved duct while the backward facing step on the inward wall causing recirculation on this inner wall and preventing this forced mixing caused by RTI. A premixed propane-air mixture is ignited to stabilize a turbulent flame at the backward facing step. The
experiments were performed at varying inlet velocities to vary the centrifugal acceleration being exerted on the flow and flame. The authors concluded that with large centrifugal acceleration there is significant mixing induced due to RTI. It was also concluded that for positive centrifugal acceleration the RTI is the dominant mechanism for flame propagation and enhanced turbulent flame speed. Moreover, they showed that the flame blew out at much higher inlet velocities when RT instability was induced. The experimental results from Lapsa and Dahm [8,9] agree with the results from Lewis et al. [5,6,7].

Subsequently, Katta et al. [10] and Briones et al. [11] explored the effect of RT instability on turbulent flame propagation through numerical simulations. Katta et al. [10] simulated the Lewis experiments by imposing a constant body force in the momentum equation parallel to the dominant flow direction. The geometry consisted of a two-dimensional tube with an open end. Therefore, Katta et al. [10] simulations were performed at constant pressure and the RT instability was induced by gravitational forces greater or equal to Earth’s gravitational acceleration as illustrated in Figure 4(d). They found that RT instability enhances flame propagation velocity. It is important to recognize that the computational work of Katta et al. [10] was performed at constant pressure and at constant body force on the flow field, whereas the experimental work of Lewis et al. [5,6,7] was conducted at constant volume and radially varying centrifugal force.

Consequently, Briones et al. [11] more closely mimicked the Lewis experiments in a two-dimensional geometry in a constant volume setup and in a non-inertial
reference frame. These numerical simulations were performed with premixed mixtures of propane-air, kerosene-air, and n-octane-air and at g-loadings ranging from 1 to 3000 as illustrated in Figure 4(e). The mixtures were ignited from one end of the rotating tube. It was found that the simulations produced good agreement with the literature [5,6,7]. The authors concluded that (for all fuels) the (absolute) flame propagation velocity increases with increasing RT instability until it reaches a peak and then rapidly decreases. However, the turbulent flame speed does not increase substantially as had been suggested in previous experiments. The flame propagation velocity is the summation of the turbulent flame speed and the local flow velocity \( S_f \) (cf. Eq. (2)), whereas the turbulent flame speed is the relative flame speed with respect to the flow motion. The flame propagation velocity increases due to RT instability and thermal expansion and not because fuel consumption rate (or flame speed) increases.

\[
V_f = S_T + S_f \tag{2}
\]

This work was followed by another study by Briones et al. [4], in which the concept of using centrifugal acceleration was applied to a combustor design known as a High-G Cavity Ultra-Compact Combustor illustrated in Figure 4(f). The UCC-HGC geometry consists of a main core inlet air flow which feeds into a metering plate. The core flow is then directed by a vane and mixes with the flow that feeds in from the circumferential cavity. The flow from the (high-g) circumferential cavity consists of air which enters through 24 cavity driver jets, creating high centrifugal acceleration in the cavity, and mixes with the fuel injected from the cavity fuel pocket. These inlet flows mix at the base of the cavity and continue flowing where the flow mixes with a cooling
flow that enters at the aft base of the cavity before exiting the combustor. Simulations were run on this geometry with varying driver jet angle and varying circumferential-cavity-to-core inlet area ratios as to vary the centrifugal acceleration induced by the cavity driver jets. The simulations demonstrated that while the g-loading appeared to enhance the progress variable source term, which was used to estimate the location of the flame and turbulent flame speed, it is not known if this turbulent flame speed exceeded the turbulent flame speed under suppressed Rayleigh-Taylor instability.
Figure 4. (a) Experimental schematic of Lewis et al. [5,6,7]; (b) experimental schematic of Lapsa and Dahm [8,9] straight duct combustor; (c) experimental schematic of Lapsa and Dahm [8,9] curved duct combustor; (d) numerical simulations of Lewis tube by Katta et al. [10] colored by temperature; (e) numerical simulations of the Lewis tube by Briones et al. [11] colored by temperature; and (f) a 3-D model of the experimental setup of the high-pressure high-g combustor [12]. Figure 2 (b) and (c) Reprinted from Proceedings of the Combustion Institute, 32, Lapsa, Andrew P., Dahm, Werner J.A., Hyperacceleration effects on turbulent combustion in premixed step stabilized flames, 1731-1738, (2009), with permission from Elsevier.
In summary, there is no clear or convincing evidence that RTI enhances fuel consumption rate (or turbulent flame speed). If RTI actually promotes consumption rate the mechanism through which it works is unknown. The investigation on the effect of RTI on fuel consumption rate is nearly scarce in the literature.

1.3 Objectives
The purpose of this investigation is to improve the understanding of the effects of Rayleigh-Taylor instabilities on turbulent flame speed or fuel consumption rate. First, the effect of RTI on fuel consumption rate is investigated utilizing the High-pressure high-g (HPHG) combustor shown in more detail in Figure 5.

![Figure 5. Flow diagram for the HPHG Combustor from the side view (Left) and front view (Right). The blue arrows signify the air driver jet locations and main inlet flows, the green arrows signify the fuel jet locations, and the red arrows signify the cooling jet locations [12].](image)

The HPHG UCC is a more practical device and more challenging apparatus because it involves multiphase heat and mass transfer as well as molecular mixing and partially premixed combustion. The RT instability in this device is induced by swirling the flow in
a circumferential cavity. Fuel is injected from the outer surface of the circumferential cavity (cf. Figure 4e). The fuel evaporates, mixes and reactants with the air. The (low-density) hot products are forced to move radially inward, while the (high-density) air is forced radially outward. This, in turn, promotes mixing between fuel and air and reactants and products. The angle of inclination of the outer driver jets is increased to further augment centrifugal force and, in turn, RT instability.

Second, the effect of RTI on fuel consumption is also investigated in the canonical geometry of Lapsa and Dahm [8,9] (cf. Figure 4b). This geometry poses advantages. Premixed fuel and air flows from the inlet of the duct towards the backward-facing step. The walls of the combustor exert a centripetal force in order for the streamlines to curve. A fluid particle, in the relative reference frame, experiences a centrifugal acceleration in the curvilinear streamlines in order for the particle to balance the centripetal force. The flame is stabilized downstream of the backward facing step. The high density reactants are forced outward, while the low density products are forced inwards by the centrifugal force. The centrifugal force induces RTI. This arrangement enables observation of the effects of RTI on the flame in a more simplified geometry than that of a full combustor. By increasing the inlet flow velocity, the centrifugal force is increased, which, in turn, promotes both turbulence and RTI.

The specific objectives of this investigation are to (1) model the abovementioned combustors, (2) compare the numerical results with available experimental data, (3) to quantify the centrifugal force and fuel consumption rate, (4) to draw general conclusions from this investigation, (5) and to propose future research directions.
CHAPTER 2
PHYSICAL-NUMERICAL MODEL

The governing equations and closure models that are used to customize FLUENT commercial software for both RANS and the LES simulations are illustrated. Also in this section the geometries, meshes, and boundary conditions are discussed.

2.1 Governing Transport Equations
The steady three-dimensional governing equations of continuity momentum, turbulence, total enthalpy, mixture fraction, mixture fraction variance, progress variable are solved using the SIMPLE pressure-based solver of Fluent [13] for the HPHG portion of this investigation. The turbulence is modeled using Reynolds-averaged Navier-Stokes (RANS) with both the Realizable k-ε model and the Standard k-ω model and scalable wall functions to describe the flow near the walls. The governing equations are discretized using the second order scheme for pressure and third-order MUSCL scheme for momentum, turbulent kinetic energy, turbulent dissipation rate, total enthalpy, mean mixture fraction, mixture fraction variance, and progress variable. The gradients and derivatives of the governing equations are obtained using a Least Squares Cell Based Gradient [13]. The Eulerian governing equations can be represented in tensor notation in general conservative form as in:
\[
\frac{\partial (\bar{\rho}\Phi \bar{u}_j)}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \Gamma^\Phi \frac{\partial \Phi}{\partial x_j} \right) + S^\Phi
\]  

In Equation (3), \( \rho \) denotes density, \( \bar{u}_j \) denotes the velocity components (\( \bar{u}, \bar{v}, \) and \( \bar{w} \)), and \( x_j \) denotes the directional components (\( x, y, \) and \( z \)). The general form of the equation can be used to represent any number of equations depending of the variable used for \( \Phi \), the diffusive transport coefficient \( \Gamma^\Phi \) and the source term \( S^\Phi \). The governing equations for the HPHG portion of this investigation are shown in Table 1.
<table>
<thead>
<tr>
<th>Equations</th>
<th>$\Phi$</th>
<th>$\Gamma^\Phi$</th>
<th>$\Sigma^\Phi$</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Continuity</strong></td>
<td>1</td>
<td>0</td>
<td>$\frac{m_{b}}{V_{cell}} + \frac{m_{p,0} - m_{p,0}m_{p,0}}{m_{p,0}V_{cell}} \hat{m}_{p,0}$</td>
</tr>
<tr>
<td><strong>Favre Mean Momentum</strong></td>
<td>$\bar{u}_i$</td>
<td>$\mu + \mu_t$</td>
<td>$- \frac{\partial \rho}{\partial x_i} + \frac{\partial}{\partial x_j} (\mu + \mu_t) \left( \frac{\partial \bar{u}<em>j}{\partial x_i} - \frac{2}{3} \frac{\partial \mu_t}{\partial x_k} \delta</em>{ij} \right) - \frac{2}{3} \rho k \delta_{ij}$</td>
</tr>
<tr>
<td><strong>Turbulent Kinetic Energy</strong></td>
<td>$k$</td>
<td>$\mu + \frac{\mu_t}{\sigma_k}$</td>
<td>$\mu_t S^2 - \rho \varepsilon$</td>
</tr>
<tr>
<td><strong>Eddy Dissipation Rate</strong></td>
<td>$\varepsilon$</td>
<td>$\mu + \frac{\mu_t}{\sigma_\varepsilon}$</td>
<td>$\rho \cdot C_1 S \varepsilon - 1.9 \rho \frac{\varepsilon^2}{k + \sqrt{\mu_t \varepsilon/\rho}}$</td>
</tr>
<tr>
<td><strong>Specific Dissipation Rate</strong></td>
<td>$\omega$</td>
<td>$\mu + \frac{\mu_t}{\sigma_\omega}$</td>
<td>$\frac{\omega}{k} \mu_t S^2 0.00648 \rho \left[ 1 - \left( \frac{0.09 \left( \frac{0.267 + \left( \frac{\rho k}{\mu} \delta_{k/\omega} \right)^4}{1 + \left( \frac{\rho k}{\mu} \delta_{k/\omega} \right)^4} \right)}{0.072} \right) F(M_\omega) \left( \frac{0.267 + \left( \frac{\rho k}{\mu} \delta_{k/\omega} \right)^4}{1 + \left( \frac{\rho k}{\mu} \delta_{k/\omega} \right)^4} \right) \omega^2 \right]$</td>
</tr>
<tr>
<td><strong>Favre Mean Total Enthalpy</strong></td>
<td>$\bar{H}$</td>
<td>$\mu + \frac{\mu_t}{\rho_{p_t}}$</td>
<td>$\frac{m_{b}}{V_{cell}} \int_{T_{ref}}^{T_{p, out}} c_{p_a} d\bar{T} + \frac{m_{p,0}}{m_{p,0}V_{cell}} \left( m_{p, out} - m_{p, in} \right) h_f - \frac{m_{p, out}}{m_{p,0}V_{cell}} \int_{T_{ref}}^{T_{p, out}} c_{p_p} d\bar{T} + m_{p, in} \int_{T_{ref}}^{T_{p, in}} c_{p_p} d\bar{T}$</td>
</tr>
<tr>
<td><strong>Mixture Fraction</strong></td>
<td>$\bar{f}$</td>
<td>$\frac{k}{c_{p}} + \frac{\mu_t}{\rho_{c_t}}$</td>
<td>$\frac{m_{p, out} - m_{p, in}}{m_{p,0}V_{cell}} \hat{m}_{p,0}$</td>
</tr>
<tr>
<td><strong>Mixture Fraction Variance</strong></td>
<td>$\bar{f}'^2$</td>
<td>$\frac{k}{c_{p}} + \frac{\mu_t}{\rho_{c_t}}$</td>
<td>$C_g \mu_t \left( \frac{\partial \bar{f}'}{\partial x_j} \right)^2 - C_d \rho \frac{\varepsilon}{k} \bar{f}'^2$</td>
</tr>
<tr>
<td><strong>Progress Variable</strong></td>
<td>$\bar{Y}_c$</td>
<td>$\frac{k}{c_{p}} + \frac{\mu_t}{S c_t}$</td>
<td>$\rho Y_c \bar{S}_c$</td>
</tr>
</tbody>
</table>
In Table 1 $\dot{m}$ is the mass flow rate, $\mu_t$ is the turbulent viscosity, $\overline{p}$ is the Farve mean pressure, $k$ is the turbulent kinetic energy, $\sigma_k$ is the turbulent kinetic energy Prandtl number, $S$ is the strain rate, $\varepsilon$ is the eddy dissipation rate, $\sigma_\varepsilon$ is the eddy dissipation rate Prandtl number, $\omega$ is the specific dissipation rate, $\sigma_\omega$ is the specific dissipation rate Prandtl number, $\gamma$ is the heat capacity ratio, $R$ is the ideal gas constant, $T$ is the temperature, $\overline{H}$ is the Farve mean total enthalpy, $Pr_t$ is the turbulent Prandtl number, $C_p$ is the specific heat capacity, $\sigma_t$ is the turbulent Schmidt number for mean mixture, $\overline{f}$ is the Farve mean mixture fraction, $\overline{f^2}$ is the Farve mean mixture fraction variance and, $Sc$ is the turbulent Schmidt number. Regarding the specific dissipation rate, $F(M_T)$ is defined in (4) below.

$$
F(M_t) = \begin{cases} 
0 & \frac{2\kappa}{\sqrt{\gamma RT}} \leq 0.25 \\
\frac{2\kappa}{\sqrt{\gamma RT}} - 0.0625 & \frac{2\kappa}{\sqrt{\gamma RT}} > 0.25 
\end{cases}
$$

(4)

For both the mixture fraction and the progress variable (c), their second moments (i.e. variance) is required by the Beta probability density function (PDFs). The un-normalized progress variable $\overline{\gamma_c}$ and its variance $\overline{\gamma_c^n}$ can be obtained using the algebraic consideration presented in (5).

$$
\tilde{c} = \frac{\overline{\gamma_c}}{Y_{eq}}, \tilde{c^2} = \left(\frac{\overline{\gamma_c}}{Y_{eq}}\right)^2 = \frac{0.1 l_t^2}{Sc_t} \left(\nabla \overline{\gamma_c}\right)^2
$$

(5)
The unsteady three-dimensional governing equations of continuity momentum, turbulence, total enthalpy, and species transport are solved using the PISO pressure-based solver of Fluent for the canonical duct portion of this investigation. The turbulence is modeled using Reynolds Averaged Naiver Stokes (RANS) and Large Eddy Simulation (LES) with the kinetic energy transport subgrid-scale model. The governing equations are discretized using the second order scheme for pressure, bounded central differencing for momentum and species transport, and third-order MUSCL scheme for the subgrid kinetic energy and the energy with a bounded second order implicit transient formulation. The gradients and derivatives of the governing equations are obtained using a Least Squares Cell Based Gradient [13]. The Eulerian governing equations can be represented in tensor notation in general conservative form as in (6).

\[
\frac{\partial (\rho \Phi)}{\partial t} + \frac{\partial (\rho \Phi \bar{u}_j)}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \Gamma^\Phi \frac{\partial \Phi}{\partial x_j} \right) + S^\Phi \tag{6}
\]

In (6), \( t \) denotes time, \( \rho \) denotes density, \( \bar{u}_j \) denotes the Favre-filtered velocity components (\( \bar{u}, \bar{v}, \) and \( \bar{w} \)), and \( x_j \) denotes the directional components (\( x, y, \) and \( z \)). The general form of the equation can be used to represent any number of equations depending of the variable used for \( \Phi \), the diffusive transport coefficient \( \Gamma^\Phi \) and the source term \( S^\Phi \). The governing equations for the curved duct portion of this investigation are shown in Table 2.
Table 2. Governing equations for dynamic subgrid turbulent kinetic energy LES model.

<table>
<thead>
<tr>
<th>Equation</th>
<th>$\Phi$</th>
<th>$\Gamma^\Phi$</th>
<th>$\mathcal{S}^\Phi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Filtered Continuity</td>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Filtered Momentum</td>
<td>$\ddot{u}_i$</td>
<td>$\mu + \mu_r$</td>
<td></td>
</tr>
<tr>
<td>&amp;</td>
<td>&amp;</td>
<td>$- \frac{\partial \bar{\rho}}{\partial x_j} + \frac{\partial \bar{\rho}}{\partial x_j} \left( \frac{\partial \bar{u}_{i}}{\partial x_j} \right) - \frac{\partial}{\partial x_j} \left( \bar{\rho} \bar{u}_i \bar{u}_j - \bar{\rho} \bar{u}_i \bar{u}_j \right)$</td>
<td></td>
</tr>
<tr>
<td>Filtered Enthalpy</td>
<td>$\ddot{\tilde{h}}_s$</td>
<td>$\frac{\lambda + \frac{C_p \mu_{t}}{P_{t}}}{\sigma_k} \frac{\partial \bar{\rho}}{\partial t} + \bar{u}<em>j \frac{\partial \bar{\rho}}{\partial x_j} + \frac{\partial}{\partial t} \left( \frac{\lambda + \frac{C_p \mu</em>{t}}{P_{t}}}{\sigma_k} \right) \sum \left( \frac{\rho \tau_{ij}}{\Delta_f} \right) - 1 \frac{\partial \bar{\rho}}{\partial x_j} \left( \rho \bar{h}_s \bar{u}_j - \rho \bar{\tilde{h}}_s \bar{u}_j \right)$</td>
<td></td>
</tr>
<tr>
<td>Dynamic Subgrid-Scale Kinetic Energy</td>
<td>$\bar{k}_{SGS}$</td>
<td>$\frac{\mu_{t}}{\sigma_k}$</td>
<td>$- \tau_{ij} \frac{\partial \bar{\tilde{u}}<em>i}{\partial x_j} - C</em>{e} \rho \frac{k_{SGS}^{2/3}}{\Delta_f}$</td>
</tr>
<tr>
<td>Species Transport</td>
<td>$\ddot{\bar{y}}_i$</td>
<td>$\rho_{lm} \bar{y}<em>i - \frac{\mu</em>{t}}{5C_{e}}$</td>
<td>$- \frac{\partial}{\partial x_j} \left( \bar{\rho} \bar{y}_i \bar{u}_j - \bar{\rho} \bar{y}_i \bar{u}_j \right) + \bar{R}_i$</td>
</tr>
</tbody>
</table>

In Table 2 $\ddot{h}_s$ is the Farve mean sensible enthalpy, $\lambda$ is the thermal conductivity, $Le$ is the Lewis number, $\bar{R}_i$ is the mean rate of production of species “$i$”, $\bar{k}_{SGS}$ is the Farve mean turbulent subgrid-scale turbulent kinetic energy, $\tau_{ij}$ is the subgrid-scale stress tensor, $\Delta_f$ is the filter length, $\ddot{\bar{y}}_i$ is the Farve mean mass fraction of species “$i$”, and $\rho_{lm}$ is the mixture-averaged diffusivity of species “$i$” to the mixture.

### 2.2 HPHG-UCC Simulation Closure Models

#### 2.2.1 Realizable k-ε Model

$$C_1 = \max \left( 0.43, \frac{S \cdot \frac{k}{\varepsilon}}{5 + S \cdot \frac{k}{\varepsilon}} \right)$$
C₁ is a constant in the eddy dissipation equation used for the Realizable k-ε model where S is the strain rate magnitude for the eddy dissipation rate.

### 2.2.2 Subgrid Momentum Flux Closure

The subgrid momentum flux closure is modeled following Kim and Menon [14].

\[
\frac{\partial}{\partial x_j} \left( \rho \overline{u_i u_j} - \rho \tilde{u}_i \tilde{u}_j \right) = \frac{2}{3} \rho K_{SGS} \delta_{ij} - C_k \rho K_{SGS}^{1/2} \Delta_t \tilde{s}_{ij} \tag{8}
\]

In (8), \(K_{SGS}\) is the subgrid-scale kinetic energy which is equal to \(\frac{1}{2} \left( \overline{u_k^2} - \overline{\tilde{u}_k^2} \right)\), \(C_k\) is determined dynamically [15], and \(\Delta_t\) is the filter length.

### 2.2.3 Subgrid Enthalpy Flux Closure

\[
\frac{\partial}{\partial x_j} \left( \rho h_{sg} \overline{u_j} - \rho \overline{h_i} \tilde{u}_j \right) = - \mu_{SGS} C_p Pr_{SGS} \frac{\partial T}{\partial x_j} \tag{9}
\]

In (9), \(\mu_{SGS}\) is the subgrid viscosity, \(Pr_{SGS}\) is the subgrid Prandtl number which is set to 0.85, and \(C_p\) is the specific heat capacity.

### 2.2.4 Progress Variable Closure Model

\[
\tilde{S}_{FR} = \int_0^1 \int_0^1 S_{FR}(f, c) \beta(f) \beta(c) df dc \tag{10}
\]

In (10), \(S_{FR}\) is the summation of the net reaction rates of CO and CO₂ (i.e., \(S_{FR} = \frac{\dot{\omega}_{CO}}{\rho_{CO}} + \frac{\dot{\omega}_{CO₂}}{\rho_{CO₂}}\)).

### 2.2.5 Chemical Kinetics Model

Flamelets were calculated by solving laminar n-dodecane/air counter flow non-premixed flame equations using the JetSurF 2.0 mechanism [16].
2.3 Canonical Duct Simulation Closure Models

2.3.1 Rans Turbulence Closure Model

The Realizable k-ε turbulence closure model with the low-Reynolds number wall formulation [25] is used in the RANS simulations. The turbulent viscosity, $\mu_t$, is computed from

$$\mu_t = C_\mu \rho \frac{k^2}{\varepsilon}.$$  \hfill (11)

The model constant, $C_\mu$, is dynamically computed from

$$C_\mu = \frac{1}{4.04 + \sqrt{6 \cos \phi} \frac{S_{ij} S_{ij} + \delta_{ij} \delta_{ij}}{\varepsilon \sqrt{S_{ij} S_{ij}}}}.$$  \hfill (12)

2.3.2 LES Subgrid-Scale Closure Model

In the large eddy simulations, the subgrid-scale kinetic energy ($k_{SGS}$) is equal to $\frac{1}{2} (\bar{u}_k^2 - \bar{u}_k^2)$, and the subgrid scale eddy viscosity, $\mu_t$, is computed as

$$\mu_t = C_k \rho k_{SGS}^{1/2} \Delta f.$$  \hfill (13)

The subgrid-scale momentum flux closure is modeled following Kim and Menon [14],

$$\bar{\rho} \bar{u}_i \bar{u}_j - \bar{\rho} \bar{u}_i \bar{u}_j = 2 \rho k_{SGS} \delta_{ij} - 
\quad C_K \rho k_{SGS}^{1/2} \Delta f \delta_{ij}.$$  \hfill (14)

The subgrid-scale enthalpy flux is given by

$$\bar{\rho} \bar{h}_z \bar{u}_j - \bar{\rho} \bar{h}_i \bar{u}_j = - \frac{\mu_t C_p}{\Pr_{SGS}} \frac{\partial \bar{T}}{\partial x_j}.$$  \hfill (15)

The subgrid-scale species flux is given by
\[
\rho \bar{y}_i \bar{u}_j - \bar{\rho} \bar{y}_i \bar{u}_j = -\frac{\mu_t}{1.0} \frac{\partial \bar{y}_i}{\partial x_j}
\]  

(16)

The subgrid Prandtl number (Pr$_{SGS}$) is prescribed to be 0.85. The model constants, $C_\varepsilon$ and $C_k$, are computed dynamically [13]. The filter-size length, $\Delta_f$, is computed as cubic root of the cell volume.

### 2.3.3 Chemical Kinetics Model

The following two-step global reaction mechanism for propane-air [25] combustion is used in the simulations:

\[
C_3H_8 + 3.5(O_2 + 3.76N_2) \rightarrow 3CO + 4H_2O + 18.8N_2
\]

\[
k_1 = 5.62 \times 10^9 \exp \left( \frac{1.256 \times 10^8}{8345T} \right) [C_3H_8]^{0.1}[O_2]^{1.65}
\]

\[
CO + 0.5O_2 \leftrightarrow CO_2
\]

\[
k_{2f} = 2.239 \times 10^{12} \exp \left( \frac{1.7 \times 10^8}{8345T} \right) [CO][O_2]^{0.25}[H_2O]^{0.5}
\]

\[
k_{2b} = 5.0 \times 10^8 \exp \left( \frac{1.7 \times 10^8}{8345T} \right) [CO_2]
\]

### 2.3.4 Turbulence-Chemistry Interaction

Reactions only occur in small turbulent structures (i.e., fine scales) [17]. The spatial scale (17), time scale (18), and source term for enthalpy (19) and species conservation equations (cf. Table 1) are given as:

\[
\xi^* = 2.1377 \left( \frac{\nu \varepsilon}{k^2} \right)^{1/4}
\]

(17)
\[ \tau^* = 0.4082 \left( \frac{\nu}{\eta} \right)^{1/2}. \]  

(18)

\[ \bar{R}_i = \frac{\rho(\xi^*)^2}{\tau^* [1 - (\xi^*)^3]} (\bar{y}_i^* - \bar{y}_i). \]  

(19)

2.4 Geometries, Boundary Conditions and Mesh

2.4.1 HPHG Geometry and Configurations

Figure 6 illustrates the geometry of the HPHG model and describes the boundary conditions. The HPHG-UCC geometry consists of a main core inlet air flow which feeds into a metering plate. This metering plate consists of 36 equally spaced windows in order to constrict the airflow to a constant combined air flow from the core flow and driver jet flow [4]. This allows the varying of centrifugal forces induced on the cavity from the driver jets. The core flow is then directed by a vane and mixes with the flow that feeds in from the high-g circumferential cavity. The flow from the circumferential cavity consists of air which enters through 24 cavity driver jets, creating high-g conditions in the cavity that mixes with the fuel injected from the cavity fuel pocket (i.e., cavity-in cavity feature). These inlet flows mix at the base of the cavity and continue flowing where the flow mixes with additional cooling flow that enters through the aft circumferential outer wall downstream the circumferential cavity before exiting the combustor. To reduce computational cost and time, a 60° sector was simulated with periodic boundaries.
Lewis [5,6,7] concluded that centrifugal-force fields, when applied at levels high enough, greater than 500 g, become a dominant factor on the combustion, and can significantly increase the fuel consumption rate due to increased buoyant-like effects. It is based on these findings that the prospect of the high-pressure high-g combustor was pursued in order to attempt to take advantage of the increased fuel consumption rate associated with Lewis’s findings. This would allow the length of combustor section of a gas turbine engine to be reduced by shortening the flame length, allowing engines to be smaller and lighter. In an attempt to optimize the combustion efficiency of this HPHG combustor the angle of the driver jets, the diameter of the driver jets, and the blockage area of the main inlet flow metering plate were all varied. This was done in order to maintain a constant global equivalence ratio as well as keeping the total air flow rate constant by increasing the airflow rate from the driver jets and decreasing the air flow rate through the main inlet or vice versa. This causes a change in the circumferential
cavity equivalence ratio and the circumferential cavity g-loading such that increasing g-loading causes a lower cavity equivalence ratio allowing the examination of the effects when the circumferential cavity was subjected to a number of different gravitational loads.

For post experimental comparison with simulations the HPHG low cavity loading and mid cavity loading configurations were selected because they represent two different cavity loadings while maintaining a constant driver jet angle of 32.5°. These configurations showed the most significant drop-off in performance going from a lower cavity loading to the higher cavity loading. The low cavity loading HPHG configuration has a 0.187” diameter driver jet hole diameter, and a main inlet metering plate with 50% physical area blockage. The mid cavity loading HPHG configuration has a 0.276” diameter driver jet hole diameter, and a main inlet metering plate with 60% physical area blockage.

2.4.1.1 HPHG Mesh

For the simulations of both the low cavity loading and mid cavity loading configurations of the HPHG geometry a cutcell mesh with a minimum size of 0.5 mm and a maximum size of 1.5 mm, giving an average Courant-Frederich-Levy (CFL) number of 0.9, was used for creating meshes in the ANSYS Meshing program with 3.3 and 3.1 million cells, respectively. Both meshes were created using the same settings in an attempt to match the mesh as much as possible with the two different geometries resulting in meshes that are mostly similar but with slightly different numbers of cells and element type. Figure 7 illustrates the mesh used for the low cavity loading HPHG
configuration and shows the feature locations of the mesh. Figure 7 (a) illustrates an isometric view of the entire mesh. Figure 7 (b) and Figure 7 (c) show the inflation layers as well as the scaling of the cutcell. Figure 7 (d) illustrates the mesh features on the top of the cavity and in the vicinity of the driver jets. Figure 7 (e) presents the mesh feature at the back of the high-g cavity, where the cooling jets are located. The meshes consist of hexahedral dominant elements with inflation on each wall consisting of ten layers giving an overall average orthogonal quality of 0.96. The boundary mesh is not meant to work with resolved transport equations up to the cells adjacent to the wall because this would increase mesh size, which in turn increases computational time. Instead, the cell adjacent to the wall within the boundary layer is large enough so that it can be used with scalable wall functions [13].
Figure 7. (a) Isometric mesh view of high-pressure high-g. (b) Side view of HPHG inlet and metering plate. (c) Side View of HPHG outlet. (d) Top view of HPHG cavity. (e) Isovew of HPHG cooling jets.

2.4.1.2 HPHG Boundary Conditions

The operating conditions for the simulations of the HPHG low cavity loading and mid cavity loading configurations were determined based on the testing conditions provided from the separate experimental testing prior to the simulations [18]. This experimental testing was conducted using a full combustor; the simulations, however,
were run using one sixth of the geometry with periodic boundaries. Operating conditions and flow splits used in the simulations were obtained from the corresponding experiments and are shown in Table 3 and Table 4, respectively.
**Table 3.** Inlet and operating conditions for high-pressure high-g low cavity loading and mid cavity loading configurations.

<table>
<thead>
<tr>
<th></th>
<th>HPHG Low Cavity Loading</th>
<th>HPHG Mid Cavity Loading</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Main Inlet</strong></td>
<td>$\dot{m}=0.1015 \frac{kg}{s}$, $T=467$ K, $I=5%$, $\bar{f}=0$, $f'^2=0$, $c=0$</td>
<td>$\dot{m}=0.0801 \frac{kg}{s}$, $T=467$ K, $I=5%$, $\bar{f}=0$, $f'^2=0$, $c=0$</td>
</tr>
<tr>
<td><strong>Cooling Inlet</strong></td>
<td>$\dot{m}=0.005775 \frac{kg}{s}$, $T=467$ K, $I=5%$, $\bar{f}=0$, $f'^2=0$, $c=0$</td>
<td>$\dot{m}=0.005733 \frac{kg}{s}$, $T=467$ K, $I=5%$, $\bar{f}=0$, $f'^2=0$, $c=0$</td>
</tr>
<tr>
<td><strong>Fuel Inlet</strong></td>
<td>$\dot{m}=9.41 \frac{kg}{hr}$, $T=303$ K, $I=5%$, $\bar{f}=0$, $f'^2=0$, $c=0$</td>
<td>$\dot{m}=8.54 \frac{kg}{hr}$, $T=300$ K, $I=5%$, $\bar{f}=0$, $f'^2=0$, $c=0$</td>
</tr>
<tr>
<td><strong>Outlet</strong></td>
<td>$P=-35.2$ kPa</td>
<td>$P=-35.2$ kPa</td>
</tr>
<tr>
<td><strong>Global</strong></td>
<td>$\dot{m}=0.175 \frac{kg}{s}$, $P=688$ kPa</td>
<td>$\dot{m}=0.163 \frac{kg}{s}$, $P=688$ kPa</td>
</tr>
<tr>
<td><strong>Discrete Phase</strong></td>
<td>$\dot{m}_p=0.01568 \frac{kg}{s}$ (per injector), $</td>
<td>\vec{v}_p</td>
</tr>
</tbody>
</table>

In Table 3 $I$ is the turbulent intensity.
Table 4. High-Pressure High-G experimentally measured boundary flow splits [18].

<table>
<thead>
<tr>
<th></th>
<th>HPHG Low Cavity Loading</th>
<th>HPHG Mid Cavity Loading</th>
</tr>
</thead>
<tbody>
<tr>
<td>Main Inlet</td>
<td>57.99%</td>
<td>49.20%</td>
</tr>
<tr>
<td>Cav. Fwd. Wall Cooling</td>
<td>4.27%</td>
<td>4.01%</td>
</tr>
<tr>
<td>Cav. Top Wall Cooling</td>
<td>7.49%</td>
<td>6.90%</td>
</tr>
<tr>
<td>Cav. Driver Jets</td>
<td>9.00%</td>
<td>17.74%</td>
</tr>
<tr>
<td>Cav. Aft Wall Cooling</td>
<td>4.99%</td>
<td>4.90%</td>
</tr>
<tr>
<td>Corner Cooling</td>
<td>3.30%</td>
<td>3.52%</td>
</tr>
<tr>
<td>Aft Liner Effusion Cooling</td>
<td>12.96%</td>
<td>13.73%</td>
</tr>
<tr>
<td></td>
<td>100%</td>
<td>100%</td>
</tr>
</tbody>
</table>

For the low cavity loading and mid cavity loading HPHG simulations the boundary conditions used for the main inlet, the driver jet inlet, and the cavity corner cooling inlet were all mass flow inlets as to better match the simulated flow splits against the experimental flow splits. The exit for the HPHG low cavity loading and mid cavity loading simulations was a pressure outlet in order to attempt to match the measured pressure drop. The conditions for the cavity forward, top, and aft wall cooling were prescribed from an effusion cooling model scheme that was applied. This effusion cooling model introduced volumetric mass and enthalpy source adjacent to the walls were the effusion cooling holes exist in the actual hardware. However, this model neglects both volumetric momentum sources adjacent to these patches as well as discrete distribution of effusion cooling jets.
Using these conditions and the equations described in (3) and Table 1 simulations were run in order to validate the model against data obtained in testing the simulated configurations as well as to apply the investigation of the effects of Rayleigh-Taylor instability on the turbulent flame speed to a real world applicable combustion system. Based on the results that will be presented in the Results and Discussion section it was determined that in the HPHG it is nearly impossible to decouple the multi-combustion flame regimes to the heterogeneous and anisotropic turbulence. In order to better assess the effect of RTI on fuel consumption rate a canonical pre-vaporized, premixed system is utilized to remove the complex two-phase flow with heat and mass exchange as well as molecular mixing that leads to partially premixed combustion.

2.4.2 Curved-duct with Backward Facing Step Geometry and Configurations

There are two geometries used in this investigation that mimic the experimental arrangements studied by Lapsa and Dahm [8,9]. Both geometries contain a backward facing step. One geometry is a straight channel with a converging inner wall downstream of the backward-facing step. This is the baseline geometry, and it is referred as the straight channel in this study. The second geometry is a curved channel with a backward-facing step on the outer radius. The curved channel geometry is used to investigate the effects of Rayleigh-Taylor instabilities, and it is referred as the curved duct in this study. Figure 8 and Figure 9 depict the computational domain and mesh for the straight and the curved duct, respectively.
Figure 8. Straight channel mesh displaying the region of interest.

Figure 9. Curved duct mesh displaying the three sections and the inlet boundary mesh. The cross section at the inlet boundary is also shown.

2.4.2.1 Curved Backward Facing Step Mesh
The curved duct contains three sections, viz., upstream, middle and downstream.

There is particular interest in the middle section, which is where centrifugal forces
induce Rayleigh-Taylor instability within the flame. For this reason, a fine mesh with a spatial resolution of 0.2 mm is used in this section. The Kolmogorov length scale is estimated to be 0.03 mm for the operating conditions studied in this work using (20).

\[
\eta = \left( \frac{\mu}{\rho \varepsilon} \right)^{\frac{1}{4}} \tag{20}
\]

The laminar flame thickness is estimated to be 1.3 mm for propane-air at standard temperature and pressure conditions and an equivalence ratio of 1.1. The mesh is stretched geometrically in the axial direction such that the spatial resolution is 0.5 mm near the inlet and exit of the curved duct. The boundary layer contains 20 cells perpendicular to the wall that increase in size towards the core cells, as shown by the cross section at the inlet boundary. The mesh is fully structured containing nearly 16 million hexahedral cells.

2.4.2.2 Curved Backward Facing Step Boundary Conditions

For the inlet boundary, the inlet velocity \( U_0 \) is either 4 m/s or 40 m/s, giving Reynold’s numbers of 3,200 and 32,000 respectively, the temperature is 300 K, the turbulence intensity is 5 % and the viscosity ratio is 10 (for the RANS cases). For the LES, the inlet velocity is fluctuating through a perturbation method [19]. The subgrid turbulence kinetic energy is 2%. The outlet boundary condition is prescribed to be atmospheric pressure. Isothermal (300K) boundary conditions were used for the walls to mimic the experiments. The experiments [8,9] utilized aluminum, which is highly thermally conductive for transferring heat from the combustor.
CHAPTER 3

RESULTS AND DISCUSSIONS

These sections are sub-divided in two main sections corresponding to the results pertaining to the high-pressure high-g combustor and the canonical curved backward facing step. These two main sections are further sub-divided into specific discussions.

3.1 Practical Research on a High-Pressure High-G Combustor

In this section the results from the HPHG low and mid cavity loading simulations are examined in a number of different ways. In Figure 10 and Figure 11 the streamlines are presented from forward looking aft and the side views, respectively. From Figure 10 it is observed that the HPHG low loading case has fewer streamlines that persist throughout the cavity compared to the mid-level loading case. This would imply that the HPHG mid-level loading case would have a higher flow in the cavity as well as a higher g-loading as expected meaning that as the cavity loading increases the g-loading also increases. From Figure 11 it is seen that the mixing of the streamlines increases from the HPHG low loading case to the HPHG mid loading case as can be seen toward the exit of the combustor in Figure 11.
Figure 10. Forward looking aft view of flow streamlines from mainstream plenum (red), driver jet plenum (blue), and cooling jets (green) for the low (left) and mid loading (right) HPHG.

Figure 11. Side view of flow streamlines from mainstream plenum (red), driver jet plenum (blue), and cooling jets (green) for the low (left) and mid loading (right) HPHG.

In order to see where and how this dimensionless centrifugal acceleration is affecting the fuel consumption rate throughout the cavity the flow in a number of planes were examined in order to view the variation between the two cases moving axially and radially through the cavity in Figure 12 and Figure 13, respectively. Using the fuel consumption rates from Figure 12 and Figure 13 the percentage of the combustion that occurs in the cavity was calculated and is displayed in Table 5. From Figure 12 it can be seen that in both the low and mid loading cases, the axial profiles of dimensionless acceleration and fuel consumption rate peak at nearly the same location ~77% the
circumferential cavity width which is in contrast with the findings with this geometry where Briones et al. [4] observed that these same peaks are symmetric across the driver jets. This difference in peak location is likely attributed to the flow in the cavity. As seen from the streamlines in Figure 11, the flow in the cavity moves mostly aftward in the cavity and, consequently, more mixing takes place near the cavity aft wall explaining this discrepancy seen between these simulations and the findings of Briones et al. [4]. Figure 13 illustrates that in both the low and mid loading cases, the centrifugal acceleration peaks at approximately 20% the total radial distance while the fuel consumption rate for both configurations exhibits two peaks at ~57% and ~92% the total radial length. The centrifugal acceleration peak from Figure 13 is likely attributed to that the centrifugal acceleration is calculated using (21) causing the cells with lower radius to have a higher centrifugal acceleration.

Table 5 examines the overall fuel consumption rates taking place in the cavity. From Table 5 it is seen that for the low loading HPHG case 71% of the combustion happens in the cavity and for the mid loading HPHG case 83% of the combustion happens in the cavity.
Figure 12. Radially- and azimuthally-average axial profiles of centrifugal acceleration and fuel consumption rate for the low (left) and mid loading (right) HPHG combustor.

Figure 13. Axially- and azimuthally-average radial profiles of centrifugal acceleration and fuel consumption rate for the low (left) and mid loading (right) HPHG.

Table 5. Fuel Consumption Rate Percentage Distribution.

<table>
<thead>
<tr>
<th></th>
<th>HPHG Low Loading</th>
<th>HPHG Mid Loading</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cavity Fuel Consumption Rate [kg/s]</td>
<td>0.01037</td>
<td>0.01082</td>
</tr>
<tr>
<td>Total Fuel Consumption Rate [kg/s]</td>
<td>0.01409</td>
<td>0.01367</td>
</tr>
<tr>
<td>Cavity Fuel Consumption Rate [%]</td>
<td>73.60</td>
<td>79.13</td>
</tr>
</tbody>
</table>
A number of different contours, such as equivalence ratio, reaction progress, temperature, and centrifugal acceleration, have been taken of both cases at the center plane and at the periodic boundary of the simulation in order to qualitatively analyze and compare the low- and mid-loading HPHG-UCC. It can be seen from Figure 14 that the equivalence ratio is highest close to the fuel injector and is also quite high through the middle of the circumferential cavity and becomes relatively uniform throughout the expansion zone to the exit. There is more heat release in the circumferential cavity than there is in the main passage. This indicates that the flame is located mostly within the circumferential cavity. However, there is still heat release in the main passage which could be detrimental for the inlet guide vane (IGV). Special cooling techniques would have to be developed for the IGV. There are no clear distinctions between the low and middle loading cases from this figure. In Figure 15 it can be seen that the reaction progress shows a very similar pattern to that of the equivalence ratio in Figure 14 with peaks in the circumferential cavity and evening out toward the exit. This leads to the same conclusion that the flame is most likely located in the peak sections within circumferential cavity seen in Figure 12. From Figure 16 it can be observed that the pockets of higher temperature are located in the centrifugal cavity which as with Figure 14 and Figure 15 would indicate that the flame front is located at these pockets and the flame is mostly within the cavity. From these contours it is evident that the pattern factor of the middle cavity loading is better than that of the low cavity loading case. The temperature distribution near the trailing edge of the IGV is more uniform for the image.
on the right than from the image on the left. Figure 17 illustrates a contour of the dimensionless centrifugal acceleration in the high-g cavity section of the combustor. There are multiple ways to compute the dimensionless g-loads. Here, the dimensionless centrifugal acceleration is calculated using (21) where \( V_{\text{tan}} \) is the tangential velocity at each point of the cavity, \( g \) is the gravitational constant, and \( r \) is radius of each cell. The figure below clearly shows that low cavity loading leads to lower g-loading as indicated by the contours. Note that the low cavity loading case reaches g-loading up to 2000 g’s, whereas the middle cavity loading case reaches g-loading up to 4000 g’s. The g-loading is higher near the corner cooling region for both cases which is likely due to the high speed of the flow and the viscosity as the flow turns out of the cavity into the main passage. From Figure 17 it is observed that both the low cavity loading and the mid cavity loading configurations have similar patterns showing of dimensionless centrifugal acceleration with them being relatively uniform with a pocket of high dimensionless centrifugal acceleration as the lower aft portion of the centrifugal cavity with the mid cavity loading having significantly higher dimensionless centrifugal acceleration, as expected.
Figure 14. Contours of equivalence ratio for high-pressure high-g combustor at low cavity loading (left) and mid cavity loading (right) configurations.

Figure 15. Contours of normalized reaction progress for high-pressure high-g low cavity loading (left) and mid cavity loading (right) configurations.
Figure 16. Contours of temperature for high-pressure high-g low cavity loading (left) and mid cavity loading (right) configurations.

Figure 17. Contours of dimensionless centrifugal acceleration for high-pressure high-g low cavity loading (left) and mid cavity loading (right) circumferential cavity configurations.
Comparisons are taken between the simulated HPHG cases in order to ensure that the simulations accurately represent the experimental results provided as shown in Table 6 and Table 7. From Table 6 and Table 7 it can be seen that the flow splits from the experiment and both the low cavity loading and mid cavity loading simulations agree with the experiments. From Table 6 and Table 7 it can similarly be seen that exit temperatures, exit equivalence ratios, static and total pressures at the experimental probe plane, and cavity static pressures all agree relatively well with each other. These values were taken as average across a plane that was created at the same axial location as the experimental probes. The slight discrepancy between the experimental and simulation temperatures is likely due to the small increase in the equivalence ratio from the experimental to the simulated case.
Table 6. Comparison of simulated and experimentally obtained flow splits [18].

<table>
<thead>
<tr>
<th></th>
<th>Exp [%]</th>
<th>Sim [%]</th>
<th></th>
<th>Exp [%]</th>
<th>Sim [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Low Cavity Loading HPHG</strong></td>
<td></td>
<td></td>
<td><strong>Mid Cavity Loading HPHG</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Main Inlet</td>
<td>57.99</td>
<td>58.24</td>
<td>Main Inlet</td>
<td>49.20</td>
<td>49.30</td>
</tr>
<tr>
<td>Cav Fwd Wall</td>
<td></td>
<td></td>
<td>Cav Fwd Wall</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cooling</td>
<td>4.27</td>
<td>4.28</td>
<td>Cooling</td>
<td>4.01</td>
<td>3.65</td>
</tr>
<tr>
<td>Cav Top Wall</td>
<td></td>
<td></td>
<td>Cav Top Wall</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cooling</td>
<td>7.49</td>
<td>7.51</td>
<td>Cooling</td>
<td>6.90</td>
<td>6.90</td>
</tr>
<tr>
<td>Cav Driver Jets</td>
<td>9.00</td>
<td>9.05</td>
<td>Cav Driver Jets</td>
<td>17.74</td>
<td>17.79</td>
</tr>
<tr>
<td>Cav Aft Wall</td>
<td></td>
<td></td>
<td>Cav Aft Wall</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cooling</td>
<td>4.99</td>
<td>4.96</td>
<td>Cooling</td>
<td>4.90</td>
<td>4.90</td>
</tr>
<tr>
<td>Cav Corner Cooling</td>
<td>3.30</td>
<td>3.31</td>
<td>Cav Corner Cooling</td>
<td>3.52</td>
<td>3.53</td>
</tr>
<tr>
<td>Aft Liner Effusion</td>
<td></td>
<td></td>
<td>Aft Liner Effusion</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cooling</td>
<td>12.96</td>
<td>12.99</td>
<td>Cooling</td>
<td>13.73</td>
<td>13.73</td>
</tr>
<tr>
<td></td>
<td>100</td>
<td>100</td>
<td></td>
<td>100</td>
<td>100</td>
</tr>
</tbody>
</table>
Table 7. Comparison of simulated and experimentally obtained values at the combustor exit.

<table>
<thead>
<tr>
<th></th>
<th>Low Cavity Loading HPHG</th>
<th>Mid Cavity Loading HPHG</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Exp.</td>
<td>Sim.</td>
</tr>
<tr>
<td>Temperature [K]</td>
<td>1028</td>
<td>1051</td>
</tr>
<tr>
<td>Equivalence Ratio</td>
<td>0.2183</td>
<td>0.2199</td>
</tr>
<tr>
<td>Average Probe Plane Static Pressure [kPa]</td>
<td>651.35</td>
<td>640.39</td>
</tr>
<tr>
<td>Average Probe Plane Total Pressure [kPa]</td>
<td>648.24</td>
<td>659.07</td>
</tr>
<tr>
<td>Average Cavity Static Pressure [kPa]</td>
<td>685.34</td>
<td>666.03</td>
</tr>
</tbody>
</table>

In order to make the best possible comparison of the g-loading from the experiments to the simulations a number of different ways to calculate or measure the g-loading were considered and are displayed in Table 8.
Table 8. Comparison of simulated and experimentally obtained values at the combustor exit.

<table>
<thead>
<tr>
<th></th>
<th>Low Cavity Loading HPHG</th>
<th>Mid Cavity Loading HPHG</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density [kg/m³]</td>
<td>5.142</td>
<td>5.110</td>
</tr>
<tr>
<td>Effective Area (Aₑ) [mm²]</td>
<td>283.87</td>
<td>310.97</td>
</tr>
<tr>
<td>Mass Flow [kg/s]</td>
<td>0.0943</td>
<td>0.0948</td>
</tr>
<tr>
<td>Tangential Velocity (V₉ₐₜ) [m/s]</td>
<td>54.51</td>
<td>50.27</td>
</tr>
<tr>
<td>Driver Jet-Based g-Loading</td>
<td>3017</td>
<td>2566</td>
</tr>
<tr>
<td>Volume Average g-Loading</td>
<td>-</td>
<td>611</td>
</tr>
<tr>
<td>Experimental Bulk g-Loading</td>
<td>295</td>
<td>-</td>
</tr>
</tbody>
</table>

\[ V_{tan} = \frac{m}{\rho A_e} \]  

(22)

In Table 8 the driver jet-based g-loading is the calculated g-loading based on the tangential velocity from the driver jets where the tangential velocity is calculated using (22). The cavity volume averaged g-loading is the volume average of (21) of the cavity from the simulated cases. The experimental bulk g-loading is based on the bulk flow into the experimental rig which could not be mimicked in the simulation due to the effusion cooling model air flow contributing to the flow as a source rather than through flowing into the combustor. This experimental bulk g-loading was calculated by using (22) with a mass flow obtained from a single pressure tap inside the circumferential cavity. Of these ways to calculate the g-loading the only direct comparison that was able to be made...
was the jet-based g-loading. This jet-based g-loading was experimentally calculated using (22) where the density is of the unburned gas and the effective area is the area of the cavity driver jets. From this jet-based g-loading it can be seen that the simulations tend to under predict the measured values used to calculate the jet-based g-loading from experiments. This discrepancy is, however, consistent between the cases and is attributed to the thermal expansion which is not accounted for in the experimental calculation of the jet-based g-loading which is only based of the nominal values as well as that the experimental calculations being made using initial density values instead of local values throughout the combustor as in the simulated combustor. However, it can also be seen that, while the inlet centrifugal acceleration is in the range of several thousands, the effective volume averaged g-loading that is affecting the flow is more on the order of several hundred.

In summary, it is believed that there is an overall positive effect caused by inducing centrifugal acceleration in this HPHG combustor. It can be seen that there is a coinciding increase in centrifugal acceleration and fuel consumption rate which was expected. This, however, could be caused by a number of different flow effects, in order to try to see the effects more specific to RTI the results of the curved backward facing step study.

3.2 Canonical Research on a Curved Backward Facing Step

The computational results are compared with measurements of time-averaged broadband chemiluminescence and instantaneous shadowgraph images reported by Lapsa and Dahm [8,9]. Figure 18 and Figure 19 present, respectively, the broadband chemiluminescence and shadowgraph comparison for the straight channel. The
Experimental chemiluminescence is a path-integrated light emitted by many species. These species are “excited” at high temperature and not just where heat release rate occurs. The volume rendered temperature was chosen to represent this broadband chemiluminescence. The volume rendering displays multiple parallel planes (with respect to the line of sight) while varying the transparency [20]. The opacity is maximum when temperature is the highest and it is minimum when temperature is the coldest. The experimental results show that the flame is lifted away from the backward-facing step when the inlet velocity is 4 m/s. The flame is angled by approximately 20° to 30° with respect to the bottom wall, and the flame spans the entire channel from bottom to top. Increasing the inlet velocity to 40 m/s results in the flame being positioned closer to the backward-facing step, and the angle between the attachment location and an imaginary surface parallel to the inner (bottom) wall is nearly 0°. The RANS results show similar qualitative trends when compared to the experiments. However, the RANS results indicate that both flames are attached to the backward-facing step. It is plausible that the experimental broadband chemiluminescence images do not capture the weak signal near the backward-facing step, or the simple combustion model does not accurately predict the turbulent flame speed.
Figure 18. Measurements [8,9] (left), RANS computations (center), and LES computations (right) of the chemiluminescence images for the straight channel at $U_0 = 4$ m/s (top) and $U_0 = 40$ m/s (bottom). Experimental figures on left reprinted from Proceedings of the Combustion Institute, 32, Lapsa, Andrew P., Dahm, Werner J.A., Hyperacceleration effects on turbulent combustion in premixed step stabilized flames, 1731-1738, (2009), with permission from Elsevier.

Figure 19 illustrates the comparison between the measured instantaneous [8,9] and computed time-averaged shadowgraph images created using (25). A shadowgraph is an image of the shadows caused by non-uniformity in a gaseous or liquid flow field such as by temperature or density differences which is represented by the second derivative of the index of refraction ($N$). Equation (23) represents a shadowgraph (i.e., the dimensionless change of intensity) and Equation (24) is the linearly varying refraction index for gases.

\[
\frac{\Delta I}{I_o} = D \int \left( \frac{\partial^2 N}{\partial x^2} + \frac{\partial^2 N}{\partial y^2} \right) (\ln N)dz. \tag{23}
\]

\[
N = k \rho + 1. \tag{24}
\]

Here, the Gladstone-Dale coefficient, $k$, is 0.23g/cm$^3$ for air standard conditions. After differentiating (23) with respect to $z$ and combining this result with (24), the shadowgraph equation is obtained as shown in Equation 25.
\[
\frac{d(\Delta I/I_0)}{dz} = Dk \left( \frac{\rho}{P} \nabla^2 P - \frac{\rho}{T} \nabla^2 T - \sum_i \frac{\rho_i}{MW_i} \nabla^2 Y_i \right) \ln(kp + 1), \text{ where} \\
\n\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}.
\]

This equation, which was used to create the simulated shadowgraphs, demonstrates that changes in intensity (for an ideal gas) are due to second-order gradients in pressure, temperature and species mass fractions (in the direction parallel to the image). A laminar-to-turbulent transitional flow regime is observed when the inlet velocity is 4 m/s. Heterogeneous and non-isotropic turbulence is observed when the inlet velocity is 40 m/s. Similar to the broadband chemiluminescence images, the 4 m/s flow shows that the shear layer interacts with the upper wall at further upstream locations when compared with the 40 m/s flow. The RANS results qualitatively capture this trend.

**Figure 19.** Measurements [8,9] (left), RANS computations (center), and LES computations (right) of the shadowgraph images for the straight channel at \(U_0 = 4\) m/s (top) and \(U_0 = 40\) m/s (bottom). Experimental figures on left reprinted from *Proceedings of the Combustion Institute, 32*, Lapsa, Andrew P., Dahm, Werner J.A., Hyperacceleration effects on turbulent combustion in premixed step stabilized flames, 1731-1738, (2009), with permission from Elsevier.
Both the measured and predicted chemiluminescence and the shadowgraph images suggest that the flame is not located at the region of large density curvature. For the straight channel discussed above, the pressure drop (due to viscous dissipation) precedes changes in both the temperature and species distributions. Thus, the shadowgraph images show larger changes upstream relative to those observed in the chemiluminescence images. This occurs for both the experimental and computational results.

![Figure 20](image)

**Figure 20.** Measurements [8,9] (left), RANS computations (middle), and LES computations (right) of the chemiluminescence images for the curved duct at $U_o = 4$ m/s (top) and $U_o = 40$ m/s (bottom). The dotted magenta line indicates the shift in flame attachment from $U_o = 4$ m/s to $U_o = 40$ m/s. *Experimental figures on left reprinted from Proceedings of the Combustion Institute, 32, Lapsa, Andrew P., Dahm, Werner J.A., Hyperacceleration effects on turbulent combustion in premixed step stabilized flames, 1731-1738, (2009), with permission from Elsevier.*

Figure 20 and Figure 21 present the measured and computed chemiluminescence and shadowgraph images for the curved duct. The measured chemiluminescence images indicate that the flame is lifted when the inlet velocity is 4 m/s and attached to the backward-facing step when the inlet velocity is 40 m/s. The flame is more angled with respect to the lower wall for the lower velocity case. The RANS and LES results
qualitatively capture this behavior, but the LES results more closely emulate the measurements. However, there are large quantitative discrepancies between the measurements and computations. Both the RANS and LES results suggest that the flame attaches to the backward-facing step for both inlet flow velocities. The magenta arrows are showing the impingement points of the flow to the inner wall. It can be seen that there is relatively good agreement from the 4 m/s case LES simulation to the experimental case. However, the other cases do not show as good agreement. The LES shadowgraphs show better agreement with the measurements.

Figure 21. Measurements [8,9] (left), RANS computations (middle), and LES computations (right) of the shadowgraph images for the curved duct at $U_o = 4$ m/s (top) and $U_o = 40$ m/s (bottom). *Reprinted from Proceedings of the Combustion Institute, 32, Lapsa, Andrew P., Dahm, Werner J.A., Hyperacceleration effects on turbulent combustion in premixed step stabilized flames, 1731-1738, (2009), with permission from Elsevier.*

A primary purpose of this work is to examine the effects of centrifugal force results on the flame which is positioned near the middle portion of the curved duct where the mesh is fine (cf., Figure 9 and Figure 23). Consequently, Figure 22 illustrates the
The dimensionless centrifugal acceleration at the center plane for the middle section of the curved duct, which is obtained as Equation 26.

\[ a_c = \frac{V_t \tan^2 \gamma r}{g r} \]  

(26)

The results for the LES are time averaged. Generally, higher centrifugal accelerations are observed towards the inner radius because centrifugal acceleration is inversely proportional to radius. The RANS and LES results demonstrate that by increasing the inlet flow velocity the centrifugal acceleration increases from approximately 110 g to 1600 g near the leading edge of the backward-facing step. The RANS and LES results indicate that when the inlet velocity is 40 m/s and the flame is behind the backward-facing step, the entire flow field is exposed to centrifugal accelerations. The RANS and LES results presented in Figure 22 are qualitatively and quantitatively similar, and the RANS simulations would have been sufficient to compute the centrifugal acceleration flow field. Figure 22 demonstrates that increasing the inlet velocity increases the centrifugal acceleration in the flow field. However, the turbulent flames are only influenced by the centrifugal force at the flame front since the fuel consumption rate is being directly related to the turbulent flame speed for the purposes of this study.
Figure 22. Dimensionless centrifugal acceleration for the RANS (top) and LES (bottom) results for the curved duct at $U_o = 4$ m/s (left) and $U_o = 40$ m/s (right).

Figure 23. Heat release rate distributions at the center plane from the RANS computations for the straight channel (top) and curved duct (bottom) at $U_o = 4$ m/s (left) and $U_o = 40$ m/s (right).
The location of the flame front can be identified in the heat release distributions. Figure 23 shows the heat release rate from the RANS computations for the straight channel and curved duct. For the straight channel and curved duct at 4 m/s, the flame front extends from the corner of the backward-facing step towards the exit of the combustor. Notice the heat release rate thickens downstream for the $U_0 = 4$ m/s case. This is not a physical result but it is due to mesh stretching (cf. Figure 9). On the contrary, for the 40 m/s the flame front cannot withstand the high stretch rates in the shear layer; consequently, the reaction zone is located primarily in the recirculation zone downstream of the backward-facing step.

**Figure 24.** Instantaneous heat release rate distributions at the centerplane from the LES computations for the curved duct at $U_0 = 4$ m/s (left) and $U_0 = 40$ m/s (right).
Figure 24 presents typical instantaneous heat release rate distributions for the LES simulations of the curved duct. The heat release computed by the LES shows that the flame is more wrinkled and corrugated in comparison with that predicted by RANS. Through conservation of mass \( U = S_T = \overline{\Delta} \cdot A_f / A_c \), where \( A_c \) is the geometrical area, the larger the wrinkling and corrugation the larger the flame area \( (A_f) \) and the lower the area-averaged flame speed \( (\overline{\Delta}) \). Consequently, the LES calculated flames are stabilized at locations further upstream in comparison with RANS calculated flames. This is particularly true for the flame with \( U_0 = 4 \text{ m/s} \). There are some similarities between the RANS and LES results as well. Qualitatively, the RANS and LES results indicate that at \( U_0 = 4 \text{ m/s} \), the flame is interacting with the main flow and the flame spans the channel at an angle. At \( U_0 = 40 \text{ m/s} \), the flame cannot withstand the stretching induced by the high-velocity core flow and the flame is positioned behind the backward-facing step. The heat release contours shown in Figure 24 are expected to be under-predicted based on work done by Mantel et al. [21] regarding high stretch and two-step chemistry interactions. This interaction will require additional research in future work regarding Rayleigh-Taylor instabilities using two-step chemistry.

Figure 25-30 show the LES instantaneous snapshots of temperature distributions for the 4 m/s straight channel case and both the 4 m/s and 40 m/s curved duct cases. Figure 25, Figure 27 and Figure 29 illustrate the centerplane temperature distributions whereas Figure 26, Figure 28, and Figure 30 show, respectively, transverse temperature distributions. Irrespective of the geometry or inlet velocity the transverse temperature contours reveal that for all cases the flow is highly three-dimensional.
4m/s straight channel case clearly indicates that throughout the simulation the characteristic turbulence scales are of consistent size (cf. Figure 25). On the other hand, the curved duct at 4 m/s evidently demonstrates that there is a large disturbance that was not seen in the straight channel (cf. Figure 25, Figure 27). This large scale disturbance is circled in the figure. The large scale is convected downstream and by the turbulence cascade mechanism the large scale breaks into smaller scales that is finally dissipated downstream the channel. Hence, the RTI only appears periodically during the simulation. At 40 m/s the strain rates force the flame to nearly blowout and the flame can only be stabilized at the recirculation zone behind the backward-facing step for the curved duct configuration (cf. Figure 29). There still appears to be a large scale disturbance as indicated by the black circle. The corresponding flame for the straight channel blew out when the inlet velocity was 40 m/s. This suggests that RTI appears to be extending the flame stability. This is in agreement with the experimental results of Lapsa and Dahm [8] as shown in Figure 31 in which the flame blew out at ~38 m/s for the same equivalence ratio. The energy cascade in turbulence theory postulates that energy is transferred from the large scales into small scales and the latter into even smaller scales until kinetic energy dissipates into internal energy. RTI attempts to reverse this effect by temporarily transferring energy from the small scales to the larger scales (cf. Figure 27). Another plausible explanation is that the large scales associated with RTI induce lower effective stretch rates and greater flame wrinkling, which combined promotes fuel consumption rate. These two hypotheses are not contradictory with respect to the other.
Figure 25. Instantaneous centerplane temperature distributions of the 4 m/s LES straight channel case. The magenta line indicates the transverse plane for the subsequent figure. The sampled snapshots (a), (b), (c), and (d) are in sequential order.

Figure 26. Instantaneous transverse temperature distributions of the 4m/s LES straight duct case as discussed in the context of Figure 25. The location of these transverse planes are, respectively, indicated in the preceding figure by the magenta lines. The sampled snapshots (a), (b), (c), and (d) are in sequential order.
Figure 27. Instantaneous centerplane temperature distributions of the 4 m/s LES curved duct case. A large scale RTI disturbance is indicated by black circles (left) and the convected disturbance dissipates at later time (right). The magenta line indicates the transverse plane for the subsequent figure. The sampled snapshots (a), (b), (c), and (d) are in sequential order.
Figure 28. Instantaneous transverse temperature distributions of the 4 m/s LES curved duct case discussed in the context of Figure 27. The location of these transverse planes are, respectively, indicated in the preceding figure by the magenta lines. The sampled snapshots (a), (b), (c), and (d) are in sequential order.
Figure 29. Instantaneous centerplane temperature distributions of the 40 m/s LES curved duct case. A large scale RTI disturbance is indicated by black circles (left) and this disturbance subsides at later flow time (right). The sampled snapshots (a), (b), (c), and (d) are in sequential order.
Figure 30. Instantaneous transverse temperature distributions of the 40 m/s LES curved duct case discussed in the context of Figure 29. The location of these transverse planes are, respectively, indicated in the preceding figure by the magenta lines. The sampled snapshots (a), (b), (c), and (d) are in sequential order.
Figure 31. Blowout curves with comparison of accelerations of +1 g, less than +1 g, and greater than +1 g where the blue triangles represent the points on this lot where the simulations in this study fall [8]. Reprinted from Proceedings of the Combustion Institute, 32, Lapsa, Andrew P., Dahm, Werner J.A., Hyperacceleration effects on turbulent combustion in premixed step stabilized flames, 1731-1738, (2009), with permission from Elsevier.

If RTI is truly reversing the energy cascade from the small scales towards the large scales in order to delay kinetic energy dissipation, then Borghi diagrams could provide some insight. Borghi diagrams are a form of diagram that are used to categorize combustion by its regime based on combustion characteristic such as the turbulence and flame thickness. One would expect a lateral shift from the small scales towards the larger scales. These diagrams are shown in Figure 32 for all RANS and LES simulations of the canonical curved duct. The laminar flame speed ($U_L$) and the flame thickness ($\delta$)
were computed using [22]. The turbulent length scale for the RANS and LES were estimated using (27) [13] and (28) [23], respectively.

\[ l_t = 0.37 \frac{\sqrt{k^3}}{\varepsilon} \]

\[ l_t = 0.37 \frac{\sqrt{2} U_{rms}^2}{2 \mu S^2} \]

The results plotted in Figure 32 were filtered with the progress variable for values between 0.45 and 0.55. Both RANS and LES results clearly indicate that the curved duct tends to laminarize the flow as indicated by the green dots extending towards the laminar region. Interestingly, the straight channel forces the flame towards the more turbulent region (i.e., greater turbulent length scale). The location of all the flames are nearly parallel to the Klimov-Williams limit (Ka =1). The RANS results are less scattered than their LES counterparts and this might be due to the fact that RANS is isotropic, whereas LES is not constraint by this condition. Unfortunately, the Borghi diagrams do not shed light into why the 40 m/s flame does not blowout when exposed to RTI (in the curved duct) whereas it blows out when RTI is not present (in the straight duct). The Realizable k-\( \varepsilon \) is only valid for fully turbulent flow, but with an inlet velocity of 4m/s the Reynolds number, 3,200, is transitional.

Although the Borghi diagrams do not really support the hypotheses that RTI delays the turbulent energy cascade they do not oppose it. It is plausible that at low Reynolds number the turbulent flame is located on the left side of the Borghi diagram. This flame is probably closer to the Klimov-Williams limit than when it is exposed at
higher Reynolds number. Augmenting the Reynolds number exposes the flame sheet to higher Karlovitz number and the flame front spreads laterally on the Borghi diagram, but parallel to the Klimov-Williams limit. Simultaneously, the flame front is also exposed to larger turbulence length scales \( l_t \). Hence, the flame front would have been shifted towards the right. This is not observed in this investigation because no intermediate Reynolds number simulation was conducted, for example, at 20 m/s. Further increase of Reynolds number towards blowout diminishes RTI and, consequently, the induced larger scales \( l_t \). Thereby, the flame front shifts back towards the left in the Borghi diagram.
Figure 32. Borghi diagrams for the RANS (left) and LES (right) canonical cases for the 4 m/s (top), 40 m/s (bottom), straight duct (red), and curved duct (green).

The other hypothesis is that RTI exposes the flame front to lower stretch rates while increasing flame corrugation. Table 9 presents the flame-front area-averaged centrifugal acceleration ($\bar{a}_c$), rms velocity ($\bar{U}_{rms}$), total stretch ($\bar{\kappa}_T$), hydrodynamic stretch ($\bar{\kappa}_H$), curvature-induced stretch ($\bar{\kappa}_C$), and local flame speed ($\bar{S}_f$). The latter
quantities are locally computed as shown below for later area-averaging at the flame front.

\[ n = \frac{-\nabla Y_{H_2O}}{\left| \nabla Y_{H_2O} \cdot \nabla Y_{H_2O} \right|} \quad (29) \]

\[ S_f = \left| n \cdot V_{flow} \right| \]

\[ \kappa_T = \nabla \cdot \bar{V} - nn : \nabla \bar{V} + \tilde{S}_f \cdot \nabla \nabla \]

The flame front is assumed to be the iso-surface represented by \( Y_{H_2O} = 0.075 \), which is used in the computing of area-averaged Favre data. These iso-surface has been previously used by Ko and Chung [24] and Briones et al. [25]. The fluctuations \( (U_{rms}) \) at the flame front are \(~15\) - \(~19\) % times the inlet velocity \( (U_0) \) for the RANS, including the straight channel and curved duct. For the straight channel, \( \kappa_T \) remains constant with increasing \( U_0 \) because \( \kappa_H \) and \( \kappa_C \) increase with opposite signs. The flame speed \( (\tilde{S}_f) \) and flame area \( (A_f) \) increase and decrease, respectively, due to conservation of mass \( (U = S_T = \tilde{S}_f \cdot A_f / A_C) \). The flame area \( (A_f) \) increases due to the increase in \( \bar{U}_{rms} \). Hence, \( S_f \) decreases as a response to corrugation (cf. Figure 32).

For the curved duct, the RANS results show that the flame front is exposed to centrifugal accelerations of 38g and 94g for \( U_0 = 4 \) m/s and \( U_0 = 40 \) m/s, respectively. This increases \( \kappa_T \) from \( 57 \) s\(^{-1}\) to \( 140 \) s\(^{-1}\) due to both \( \kappa_H \) and \( \kappa_C \). The increase in fluctuations (0.75 m/s vs. 7.6 m/s) appears to be a response of the system due to the increase in Reynolds number since \( \bar{U}_{rms} / U_0 \) is similar to that of the straight channel. In other words, \( \bar{a}_c \) is not responsible for the increase in \( \bar{U}_{rms} \). In the curved duct the fluctuations have a more pronounced effect on \( A_f \), which reduces \( A_f \) by nearly half.
(15.2 vs. 8.6 cm²) when increasing $U_0$ from 4 m/s to 40 m/s. Consequently, the response of the flame is more pronounced and $S_f$ is three-folded (0.11 vs. 0.34 m/s). This increase in burning is caused by the decrease in $A_f$, but $\bar{a}_c$ might also play a direct role in contributing to enhancing $\bar{S}_f$. The flame speed is able to overcome the rise of $\bar{k}_T$, which is the only mechanism that could reduce $\bar{S}_f$.

The LES results for the curved duct are qualitatively similar to the RANS results. The LES results show that $\bar{a}_c$, $\bar{k}_T$ and $\bar{S}_f$ increase similarly to RANS results, while $A_f$ decreases. Fortunately, under low inlet velocity ($U_0 = 4$ m/s) the absolute fluctuation is very large comparable with the larger velocity case ($U_0 = 40$ m/s). This is a remarkable evidence that RTI is actually present for the low Reynolds number condition. A fluctuation of $U_{rms} = 10$ m/s for an inlet velocity of $U_0 = 4$ m/s is a clear quantitative evidence that RTI is actually converting potential energy (due to flow stratification) into kinetic energy further explained in Figure 33.
Figure 33. Flow diagram displaying explanation of conversion of potential energy to kinetic energy throughout the domain with the curved duct (left) and the straight duct (right).

It can be seen that (cf. Figure 33 left) when the centrifugal acceleration is larger this force induces more potential energy to the flow at the inlet which is then converted to kinetic energy through the region of interest of the curved duct. This effect does not occur when the centrifugal acceleration is zero (cf. Figure 33 right) as in the straight duct. This result with that large scale disturbance present in Figure 28 unmistakably illustrate RTI acting on the reacting flow. Suppose the simple schematic of RTI in Figure 1 in which the inlet velocity is zero, but the potential energy is large due to dissimilar fluids and force vector pointing from the heavier towards the lighter gas. Experiments have shown that this configuration would lead to large $U_{mean}$ and $U_{rms}$ [26]. These velocities are going to be associated to the Atwood number, shown in Equation 30 where $\delta_1$ and $\delta_2$ are the densities of the fluids being compared, among other
parameters. The RTI may not act alone, but could also be inducing Kelvin-Helmholtz instability as have shown in previous numerical investigations [27].

\[ At = \frac{\delta_1 - \delta_2}{\delta_1 + \delta_2} \quad (30) \]

Table 9. Area averaged at the flame surface results in terms of centrifugal acceleration \( (a_c) \), rms velocity \( (U_{rms}) \), total \( (\kappa_T) \), hydrodynamic \( (\kappa_H) \) and curvature-induced stretch \( (\kappa_C) \), flame speed \( (S_f) \) and flame area \( (A_f) \).

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CHAPTER 4

CONCLUSIONS

An extensive numerical investigation is conducted in order to assess the effect of Rayleigh-Taylor instability on fuel consumption rate (or flame speed). Two geometries are used for this investigation, viz., a high pressure high-g (HPHG) cavity stabilized combustor and a curved duct with a backward facing step. The former geometry is a more practical combustion system that contains liquid fuel injectors with operating conditions that mimic gas turbine cycles, whereas the latter is a canonical combustor used to study turbulent premixed flames. Reynolds averaged Navier-Stokes and large eddy simulations are used. RANS is used for the practical combustor and both RANS and LES are used for the canonical combustor. The combustion models used for this research are the flamelet generated manifold (FGM) and the two-step species transport for the practical and canonical combustor, respectively. The numerical results are compared against available experimental results available in literature in terms of emissions-based single point temperature measurements for the practical combustor and broadband chemiluminescence, shadowgraphs and blowout data [8,9] for the canonical combustor. Important conclusions are as follows:
1. The HPHG combustor is designed to induce bulk rotational flow in the cavity, inducing centrifugal acceleration. The centrifugal force acts from the high-density reactants towards the low-density products creating Rayleigh-Taylor instabilities (RTI). These instabilities are expected to increase the turbulent flame speed and reduce the size of the combustor by increasing flame wrinkling and/or corrugation. Simulations at two different levels of centrifugal acceleration, and, consequently, dissimilar Rayleigh-Taylor instability (RTI) were performed. It was found that the nominal g-loads are overestimating the local g-loads from the simulation because thermal expansion is not taken into account. The axial centrifugal acceleration within the cavity peaks at the location of increased fuel consumption rate. However, the radial centrifugal acceleration occurs across the range of lowest fuel consumption rate. From this it was determined that an increase in centrifugal acceleration may cause an increase in fuel consumption rate at large radius, but lower fuel consumption rate occurs at small radius. From these simulations it was not possible to discern the true effect of RTI on fuel consumption rate due to the complex physical-chemical process inherent to this combustor such as fuel vaporization, molecular mixing, spray-turbulence interaction, turbulence-chemistry interaction, partial premixing, etc.

2. Therefore, pre-vaporized premixed turbulent flames were simulated in a curved duct with a backward facing step. Two radius of curvature were used, viz., an infinite (straight duct) and a finite radius of curvature (curved duct). These combustors were operated at low and high Reynolds number (3,200 and 32,000). The computational
results are compared with broadband chemiluminescence and shadowgraph images reported in the literature for similar conditions and geometries. Both RANS and LES results are in general agreement with these measurements. The LES results are qualitatively similar to the RANS results in particular when the latter is compared against time-averaged results of the former. The centrifugal acceleration field from the RANS results is nearly identical to the time-averaged LES results. The LES results better match both the experimental broadband chemiluminescence and the shadowgraphs. This is because the LES lead to flames that are more wrinkled and corrugated positioning the flames further upstream.

3. Both experimental and numerical results demonstrate that the large changes in density, manifested in shadowgraphs, occurs upstream of the flame location. The density is a function of pressure, temperature and species composition. The gradual pressure drop occurs monotonically from the inlet towards the outlet. The temperature and species changes occur only at the flame front location. However, heat loss to the walls makes temperature gradients evident at the walls. Consequently, shadowgraphs reveal density variations due to pressure variation further upstream before they reveal density variations due to temperature and species composition.

4. Both experiments and simulations show that increasing the Reynolds number in both straight and curved canonical combustor the flame cannot withstand the high Karlovitz number effects and the flame is positioned behind the backward-facing step. In addition, the LES results indicate that at high Reynolds number the flame
blows out for the straight channel while it remains lit for the curved duct. This result is in agreement with the blowout data reported in the literature. On the other hand, RANS over predicts the flame stability of the straight channel. Consequently, RANS should not be used in research involving RTI-induced blowout. RTI is unmistakably present at the low Reynolds number in the curved combustor as evidence by the large scale turbulence disturbance observed from the simulations, which exhibits very large fluctuations in comparison with the global Reynolds number. This suggests that RTI is converting potential energy into kinetic energy.

5. Increasing Reynolds number increases turbulent flame speed while reducing flame area in order to maintain mass continuity. RTI periodically interacts with a turbulent premixed flame and its overall effect is to extend the flame stability. This enlarged flame stability is a direct manifestation that the fuel consumption rate (or flame speed) has been further enhanced in order for the flame to withstand higher Karlovitz number effects induced by high Reynolds number. However, the mechanism through which RTI works on the turbulent premixed flame is not clear. A new hypothesis is proposed. The increase in RTI should increase the turbulent length scale as well as increase the Karlovitz number. The corrugated flame would withstand the higher Karlovitz number because RTI temporarily and periodically reverses the turbulent energy cascade by minimizing the potential energy of the stratified flow.
CHAPTER 5

FUTURE WORK

It is determined that a number of more steps are needed to be taken in order to further the understanding of the effect of Rayleigh-Taylor instabilities of a combusting flow. First, detailed chemistry sensitive to stretch effects needs to replace the global chemistry in order to give more accurate representation of the physics occurring in these cases. Second, simulations for various curved duct with different radius should be used to show the effects of increasing and decreasing the centrifugal forces from the studied cases. Hence, curved channel combustors with backward facing steps with smaller radii would hypothetically induce larger Rayleigh-Taylor instabilities. In this manner, the Reynolds number effects on the flame can be decoupled from the simulations. Third, if inducing Rayleigh-Taylor instabilities truly enhances the fuel consumption rate, then, blowout simulations should be run in order to show this effect. Finally, to run cases at intermediate inlet velocities between 4 m/s and 40 m/s in order to observe the effects that these intermediate cases show.
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