Validation of CFD models of a second-stage combustion system using STAR-CCM+

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Abstract
A computational fluid dynamics (CFD) model of a second-stage combustion system was created in STAR-CCM+ and validated against experimental data in order to validate the software and provide recommendations for best practices for modelling reacting flow in CFD simulations for gas turbine combustor applications. The second-stage combustion system is a reacting jet in a cross flow and is the second half of a two-stage scaled test rig based on a Siemens gas turbine combustion system. The test rig was experimentally characterized with OH chemiluminescence and particle imaging velocimetry (PIV) measurements. The geometry simplifications, turbulence and combustion models, and boundary conditions used in the simulation were varied and their effects compared against experimental OH chemiluminescence PIV measurements of the test rig to determine which models are in best agreement. Recommendations for best practices in modelling based off of the results are provided. The results of this work will aid in the creation of high-fidelity CFD models for design exploration.
# Contents

Abstract ................................................................................................................................................. 1  
Introduction .......................................................................................................................................... 3  
Motivation......................................................................................................................................... 3  
Objectives.......................................................................................................................................... 3  
Test Rig .............................................................................................................................................. 3  
Experimental Setup .............................................................................................................................. 5  
Physical Models ................................................................................................................................ 5  
Computational Domain and Geometry ........................................................................................... 9  
Mesh Generation ............................................................................................................................ 10  
Boundary Conditions ...................................................................................................................... 11  
Summary of Studied Parameter Variations .................................................................................. 16  
  Degree of CAD Geometry Simplification................................................................................... 16  
  Turbulent Schmidt Number ....................................................................................................... 17  
  Turbulence Models..................................................................................................................... 17  
  Chemistry Modelling .................................................................................................................. 18  
Results and Discussion ....................................................................................................................... 18  
Experimental Characterization ...................................................................................................... 18  
CFD Results ...................................................................................................................................... 20  
  Degree of Cad Geometry Simplification ................................................................................... 20  
  Chemistry Modelling: FGM Table Size ...................................................................................... 23  
  Turbulent Schmidt Number ....................................................................................................... 26  
  Turbulence Models..................................................................................................................... 28  
  Chemistry Modelling: Reacting Species Transport .................................................................. 32  
Conclusions and Outlook .................................................................................................................... 35  
  Conclusions ..................................................................................................................................... 35  
  Outlook............................................................................................................................................ 36  
Acknowledgements ............................................................................................................................ 37  
Works Cited ......................................................................................................................................... 38
Introduction

Motivation
Gas turbine combustors are complex reacting systems that are beyond approximation with simple models and assumptions. The development and advancement of such combustors in the pursuit of reducing emissions and maximizing efficiency requires design exploration. While actual experimental characterization of every potential design would provide the most accurate evaluation of its performance, such testing is prohibitively time consuming and expensive. It is therefore beneficial to be able to do design exploration and down-select promising candidates using computational fluid dynamics (CFD) simulations. However, for these simulations to be of value and useful for performance prediction, the CFD software in which the designs are evaluated must be validated against experimental data, and best practices for modelling must be established in order to enable the application of CFD design exploration to general cases.

Staged combustion is a combustion strategy in which fuel is burned in separate combustion stages and has been shown to decrease nitrogen oxide (NOx) emissions [1]. In a two-stage axial combustion system, a portion of the total injected fuel is burned in an upstream combustor. More fuel and air are injected further downstream where they are ignited by the hot exhaust gases of the first stage. By using such a staged system, the residence time of gases at high temperatures may be reduced, therefore reducing the formation of NOx [2]. A common configuration for the second stage of a two-stage combustion system is a jet in cross flow system, in which the second-stage fuel and air are injected as a jet into the vitiated crossflow from the first stage combustor [3].

In this work, the second stage of a two-stage combustion system based on a gas turbine combustor with a jet in crossflow second stage has been simulated in STAR-CCM+ CFD software and the results compared against experimental measurements of the rig in order to validate the software and to determine recommendations for best practices for modelling reacting flows characteristic of combustor turbines.

Objectives
Objectives of this work are to validate STAR-CCM+ as a design tool for turbine systems and to establish best practices for modelling reacting flow problems relevant to turbine combustion system design. This is achieved by comparing the simulation results against experimental measurements of the second half of a scaled two-stage combustion system.

Test Rig
The system to be investigated is a scaled two-stage combustion system. The system consists of two combustion stages representative of those used in Siemens gas turbines. A schematic of the system is shown in Figure 1.
The combustion system was operated with methane (CH₄) as the fuel and standard air as the oxidizer.

The first combustion stage is a partially premixed combustion system with a diffusion pilot flame and circumferential partially premixed main flames. The pilot stage consists of a diffusion flame which is shielded from the main burner flow by a pilot cone. The purpose of this cone is to produce a recirculation zone which stabilizes the pilot flame in order to prevent extinction. The main burners consist of swirlers with fuel injection holes. The fuel is injected into the swirling air flow and becomes partially premixed before being ignited by the pilot flame and flame of the first combustion stage. The fuel flow is split between the pilot and main stages in a ratio of approximately 1:10, and may be varied for engine control. A scaled version of the first-stage combustion system has been experimentally characterized at DLR Stuttgart [4]. A CFD analysis of the system has been performed by Bastian Schmidl in ANSYS Fluent [5]. The second-stage combustion system which was analyzed in this work has been modeled in ANSYS Fluent by Robert Haussmann [6].

The second stage of the two-stage combustion system consists of a partially pre-mixed jet which is injected into the cross flow of the pre-burnt exhaust gases from the first stage combustor. The second-stage jet is injected via a cross stage perpendicular to the main flow channel. The cross stage has an annular flow of air into which fuel is injected through a central injector nozzle, stationed in the center of the jet. The fuel partially mixes with the air in the annulus of the cross stage before entering the main flow channel where it is burned in the exhaust gases of the first stage.

The scaled two-stage combustion rig was constructed and characterized at DLR Stuttgart. Dimensions of the test rig are nondimensionalized by the cross stage inlet diameter. The rig consists of a square channel of height and width 3.7dₒ. The channel is made of quartz to allow optical access for the measurements of OH chemiluminescence and PIV velocity measurements which were used to characterize the system. A figure of the combustion rig is shown in Figure 2.
Figure 2: Combustion rig used for characterization of the system. Flow travels from left to right. On the left, the pilot cone of the first stage combustion system is visible. The second stage injector, located on the bottom wall of the chamber, is not visible in the figure. Figure from [4].

The second-stage combustion system was characterized by measuring the following: OH chemiluminescence, OH planar induced laser fluorescence (PLIF), particle imaging velocimetry (PIV) at three different planes, and NOx and CO emissions via an emissions probe. The setup and details of the measurements are similar to those disused in Lükerath et al. [7]. In this study, only the detailed data of OH chemiluminescence and PIV velocity measurements were available, and thus these were used to validate the results of CFD obtained in STAR-CCM+.

Experimental Setup

Physical Models

The physics models used in the CFD simulations are summarized in Table 1.

Table 1: Summary of models used in CFD simulation

<table>
<thead>
<tr>
<th>Solver</th>
<th>Three dimensional</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time</td>
<td>RANS steady state</td>
</tr>
<tr>
<td>Flow</td>
<td>Ideal gas (compressible)</td>
</tr>
<tr>
<td></td>
<td>Multi-component gas</td>
</tr>
<tr>
<td></td>
<td>Segregated fluid enthalpy</td>
</tr>
<tr>
<td></td>
<td>Segregated flow</td>
</tr>
<tr>
<td></td>
<td>Reacting flow</td>
</tr>
<tr>
<td>Turbulence</td>
<td>k-epsilon realizable, k-epsilon standard, k-epsilon elliptic blending, k-omega</td>
</tr>
<tr>
<td>Chemistry</td>
<td>Flamelet generated manifold with kinetic rate source term</td>
</tr>
<tr>
<td></td>
<td>Reacting species transport with complex chemistry</td>
</tr>
</tbody>
</table>
The simulation was run as a Reynolds Averaged Navier Stokes (RANS) steady state simulation with reacting, multi-component gas. Segregated fluid flow and enthalpy solvers were used. Different turbulence models were used and compared to determine which was best suited for modelling the flow field. The models used were k-epsilon realizable, k-epsilon standard, k-epsilon elliptic blending, and k-omega. Other than for the turbulence model study, the k-epsilon realizable turbulence model was used for all simulations.

The combustion chemistry was modeled using a flamelet generated manifold (FGM), and later using species transport with a reduced chemical mechanism. The flamelet model is appropriate for flows in which reactions happen faster than turbulent mixing. This is the case for the flow of the studied combustion system. The FGM models the chemistry by solving the complex chemistry for a simplified 0D constant pressure reactor and parametrizes species concentrations and temperatures as functions of mixture fraction, mixture fraction variance, progress variable, and heat loss ratio. The engineering parameters of interest, such as temperature and species mass fractions, are tabulated with respect to each of these parameters. When queried, the values in the cell are looked up in the table with linear interpolation. Details of the implementation are discussed in the STAR-CCM+ documentation [8], and only a brief summary is given here.

Mixture fraction, $Z$, is defined as the fraction of mass of a mixture originating from the fuel stream, as shown in Eq. (1):

$$Z = \frac{m_{fuel}}{m_{fuel} + m_{oxidizer}}$$  \hspace{1cm} (1)

Thus, there is no source term for mixture fraction and it is transported as a conserved scalar.

In order to take into account the effects of turbulence, the mixture fraction variance is also transported. The parameter accounts for turbulent fluctuations in local mixture fraction values, with areas of higher turbulence leading to an increase in the mixture fraction variance.

The progress variable is a dimensionless parameter which characterizes the completeness of the reaction and is defined such that it is monotonically increasing from unburnt to fully burnt mixture. For the work in this study it is defined as the sum of the mass fractions of CO and CO$_2$. This definition ensures that the progress variable is monotonically increasing for both rich and lean mixtures. The source term for the progress variable transport equation was calculated using the chemical kinetic rate which is looked up from the precomputed FGM table. There are other source terms that may be chosen for the progress variable, including the flame speed closure and coherent flame models. These models calculate the source term of the progress variable transport equation using the laminar flame speed and concentration gradients. These rely on empirical data for flame speed and may be tuned to better match data with the use of a tuning parameter. However, due to the limitations of empirical data and the flexibility of a tuning parameter, these models are not as well suited for predictive simulations as the FGM kinetic source term model.

The heat loss ratio is a measure of the heat loss or addition and is defined as given in Eq. (2).
\[
y = \frac{h_{ad}(Z) - h}{h_{sens}(Z)}
\]  

In which \(h_{ad}(Z)\) is the adiabatic enthalpy at mixture fraction \(Z\), \(h\) is the enthalpy, and \(h_{sens}(Z)\) is the sensible enthalpy of the mixture at mixture fraction \(Z\). The inclusion of this heat loss ratio allows for the FGM to account for heat loss or addition, for example, at the walls of the combustion chamber. It also enables the fuel streams to be at different temperatures than the reference temperatures at which the table is generated.

The FGM model allows for definition of the fuel and oxidizer streams. The fuel stream consisted of 99% methane and 1% nitrogen (mass percent), and the oxidizer stream consisted of 76.7% nitrogen and 23.3% oxygen (mass percent). The FGM table was generated at conditions which were selected such that the table is able to cover the entire range of temperatures which occur in the actual test rig. The temperatures of the fuel and oxidizer for which the FGM are calculated do not need to be equal to their respective inlet temperatures in the combustion rig, as the parameter of heat loss ratio accounts for the temperature difference.

The FGM table was generated in STAR-CCM+ using the GRI 3.0 full chemical kinetic mechanism [9]. This reaction mechanism was selected because it is well-validated for methane combustion, which is what is being investigated in this study.

An adaptive gridding method was used when generating the table. This method spaces tabulated points closely together in areas where the parameters of interest have high gradients (e.g. mixture fractions near stoichiometric condition), and spaces them out where the parameters are linear [8]. This serves to limit the size of the table while reducing interpolation error.

Example plots of the FGM tabulated temperature and OH mole fraction as functions of mixture fraction and progress variable are shown in Figure 3 and Figure 4. These plots demonstrate the effect of the adaptive gridding, showing densely packed points around areas with high nonlinearity and fewer points in areas that are linear. The interpolated points (red circles in Figure 3 and Figure 4) show example interpolated values for points which do not lie within the set of computed points of the table.
Modelling the chemistry with an FGM table has the advantage of reduced computational expense, as the chemistry is parameterized by four variables which are transported. The temperature and species mole fractions are then found via a table lookup.

The combustion chemistry was also modeled by using a chemical kinetic mechanism and transporting reacting species. This method is more computationally expensive, as every reacting species in the chemical kinetic model must be transported.

In order to determine the effects of modelling the chemistry by transporting the reacting species directly while maintaining a reasonable computational time, a reduced chemical kinetic mechanism was used. The mechanism which was chosen is drm22, which is a reduced version of the full GRI mechanism. The drm22 mechanism has 22 species and 104 reactions. The thermodynamic and transport properties for the species were taken from the GRI3.0 mechanism.
**Computational Domain and Geometry**

The focus of this study was the second stage of the two-stage combustion system. This is highlighted schematically in Figure 1. The second-stage combustion system was modeled separately from the first stage system. This was done in order to reduce the number of cells in the simulation in order to reduce computational time requirements and enable rapid evaluation of simulation parameters. It also served to isolate the physics of the second-stage combustion system for more targeted simulation refinement.

The geometry of the simulation domain is shown in Figure 5. The model was created in the native CAD system of STAR-CCM+ in order to allow for parametrization and control over the geometry and meshing. The coordinate system used in the simulation is centered with the Z axis collinear with the axis of the cross stage injector. The positive X axis along the direction of flow, and the Y axis is in the lateral direction, as shown in the figure.

![Figure 5: Geometry of simulation domain for the second-stage combustion system.](image)

The system may be broadly divided into two components: The main channel and the cross stage.

The main channel consists of a square cross section with chamfers on the corners. The far upstream end of the chamber, referred to here as the headend, is the inlet in which the pre-burnt combustion products of the first stage combustor are introduced. At the far downstream end, the channel has a converging nozzle with a circular exit profile. The nozzle is used in order to control the pressure and flow rate in the system.

The central axis of the cross stage is located laterally centered in the main channel downstream of the headend inlet. The cross stage air inlet has an inner diameter of $d_j$. The cross stage inlet to the main channel is not level with its bottom face, but rather protrudes approximately $0.23d_j$ into the main channel, as seen in Figure 5. The overall length of the cross stage is approximately $4d_j$. 


At the bottom of the cross stage air inlet are 60 air inlet holes, arranged in five rows of twelve circumferential holes. Preheated air enters the cross stage through these holes from a settling chamber surrounding the bottom part of the cross stage.

Centered within the cross stage is the fuel injector. The injector is a jet-in-crossflow nozzle. It has 16 circumferential holes. The tip of the injector is conical in shape. The holes are located \(1.6d_j\) from the entrance to the main channel. Fuel exits the nozzle and mixes with the annular flow of air in the cross stage as it enters the main channel, where it burns in the vitiated cross flow.

**Mesh Generation**

The mesh on which the CFD equations are solved was generated in STAR-CCM+. The mesh consisted of approximately 3 million polyhedral cells. Polyhedral cells were selected over tetrahedral and hexahedral cells due to their many-faces which are orthogonal to almost any flow direction. This makes polyhedral cells well-suited for modelling highly swirling flows such as the one in the second-stage combustion system.

A cross section of the mesh is shown in Figure 6.

![Cross section of the mesh at the y=0 midplane.](image)

**Figure 6**: Cross section of the mesh at the y=0 midplane. The areas around the jet exit and slightly downstream are refined with volumetric controls in order to capture the reacting zone and areas of high gradients. Approximate cell sizes are shown overlaid on the mesh. Details are shown in the zoomed subfigures.

The mesh was refined in key areas in order to capture the reaction zone and resolve large gradients. These areas of refinement are located close to the outlet, as shown in Figure 6.

Prism layers were used on the walls of the system in order to model the boundary layers of the flow. As a conjugate heat transfer analysis was not used and the primary goal of the prism layers was to obtain the velocity profile close to the wall, high \(y+\) wall treatment and wall function approach were used. This resulted in having two to three prism layers for most parts of the system.

A mesh size independence study was not carried out. However, the results of the simulation were in good agreement with the experimental measurements of the test rig, and all
comparisons of any particular parameter change (aside from geometrical changes, which are by nature linked to the mesh) are performed on the same mesh to remove its influence on the results. For investigating the influence of different geometries, the mesh parameters were kept constant which resulted in similar meshes for key areas such as the top half of the cross stage and the entirety of the combustion channel.

**Boundary Conditions**

The boundary conditions used in the model are summarized in Table 2. The corresponding location of each of the boundaries is summarized in Figure 7. Values are nondimensionalized to reference values, which are not provided for reasons of confidentiality.

Table 2: Summary of boundary conditions. The region numbers in the table correspond to the numbers in Figure 7.

<table>
<thead>
<tr>
<th>Region</th>
<th>Type</th>
<th>Parameter</th>
</tr>
</thead>
</table>
| 1            | Headend inlet             | \( \dot{m} = 226.3 \dot{m}_{ref}, T = 2.25 T_{ref} \)  
\( Z = Z_{ref}, c = 1.0 \)  
Or  
Field functions from LES |
| 2            | X-stage air inlet         | \( \dot{m} = 29.9 \dot{m}_{ref}, T = 0.886 T_{ref} \)  
\( Z = 0.0, c = 0.0 \) |
| 3            | X-stage fuel inlet        | \( \dot{m} = \dot{m}_{ref}, T = 0.454 T_{ref} \)  
\( Z = 1.0, c = 0.0 \) |
| 4            | Outlet                    | 0.895 \( P_{ref} \)                            |
| All Walls    | Wall                      | No slip,                                        
adiabatic or fixed \( T = 1.38 T_{ref} \) |

\( \dot{m} = \text{mass flow rate, } T = \text{temperature, } Z = \text{mixture fraction, } c = \text{reaction progress variable} \)
Figure 7: Summary of boundary conditions. The labels in the figure correspond to the numbers in Table 2.

The headend inlet (boundary 1) and the walls were modeled with different assumptions at different stages in the characterization to determine the effects of each set of assumptions.

All boundaries that were not inlets or outlets were modeled as non-slip walls. The walls were first modeled as adiabatic, but this was found to lead to high wall temperatures in the combustion channel. The combustion channel of the test rig was made of quartz to allow for optical access for the diagnostics. Assuming adiabatic walls yielded wall temperatures greater than the recommended highest operating temperature for quartz for all of the channel walls, as shown in Figure 8.
In order to more realistically model the conditions of the experiment, the combustion channel walls were modeled as non-slip walls with a fixed temperature within the quartz operating temperature range. The walls of the cross stage were modeled as non-slip adiabatic walls. No heat conduction through the injector was modeled, although in reality it is expected that the injected fuel is preheated by the hot co-flow air via conduction through the injector itself.

The outlet of the system was modeled as a constant pressure outlet at a pressure of $0.895 P_{\text{ref}}$. This yielded a pressure of approximately $P_{\text{ref}}$ in the combustion chamber, matching experimental conditions. In the steady state solution, there was no reversed flow on the outlet face for any of the combinations of conditions tested.

The cross stage air and fuel inlets were modeled as mass flow inlets. The air inlet was modeled as a mass flow inlet of unreacted pure air (progress variable and mixture fraction both equal to 0.30) at a mass flow rate of $239.9 \dot{m}_{\text{ref}}$, and a temperature of $0.886 T_{\text{ref}}$. The mass flow was divided evenly among the 60 air inlet holes.

The fuel inlet was modeled as a mass flow inlet of pure, unreacted fuel (progress variable equal to 0.0 and mixture fraction equal to 1.0) at a mass flow rate of $\dot{m}_{\text{ref}}$ and a temperature of 363 K. For the case of complex chemistry modelling, the inlets were modeled as mass flow inlets with species mass fraction profiles equal to their respective streams in the FGM.

The headend inlet was first modeled as a mass flow inlet with uniform conditions approximately equal to those at the exit of the first-stage combustion system, in order to obtain approximate results. Later the headend inlet was modeled as a velocity inlet with mapped spatial profiles obtained from a previously run LES simulation of the first combustion stage in order to simulate the experimental conditions more closely.

The conditions used when modelling the headend inlet as a mass flow inlet boundary were bulk parameters close to those of the first stage combustor exit. The mass flow rate was set to $226.3 \dot{m}_{\text{ref}}$. The inlet mixture fraction was set to $Z = Z_{\text{rel}}$, the temperature to $2.25 T_{\text{ref}}$, and the
progress variable to 1.0. These conditions are representative of those at the exit of the first stage combustion system.

After initial simulations were conducted using the estimated bulk flow conditions with a mass flow inlet boundary condition, spatial profiles of the inlet conditions of the headend were obtained from a simulation performed of the first-stage combustion system by itself. This simulation was performed in ANSYS Fluent as an LES with time-averaged profiles of key parameters saved.

The field functions for the time-averaged parameters were extracted at a plane at the headend in the computational domain of the two-stage combustion system model. Temporal averaged spatial distributions were available for the static temperature, pressure, density, mixture fraction, velocity components in the x, y, and z directions, and RMS velocity fluctuations of the velocities in the x, y, and z directions. Some field functions of interest, including progress variable, turbulence intensity, and mixture fraction variance, were not saved as time-averaged parameters in the original simulation and were therefore not able to be extracted directly. These parameters were therefore estimated using the relevant available time-averaged and instantaneous profiles.

The time-averaged profiles for temperature, mixture fraction, and the x, y, and z velocity components are shown in Figure 9. The model of the second-stage combustions system was set up such that its coordinate system was oriented in the same way as that of the LES simulation of the first-stage combustion system. The extracted profiles could therefore be directly mapped to the headend inlet.

Figure 9: Sample extracted time-averaged profiles from the LES simulation of the first-stage combustion system at a location equal to that of the headend inlet. The profiles are the mean (time-averaged) values of (a) temperature, (b) mixture fraction, (c) x velocity, (d) y velocity, and (e) z velocity.
For the reaction progress variable, the time-averaged spatial profile was not available, and the only profile which could be extracted was the instantaneous profile at the last time step of the simulation. This is shown in Figure 10.

Figure 10: Instantaneous reaction progress variable spatial profile at the headend inlet plane location for the last time step.

As can be seen in Figure 10, the reaction progress variable is nearly completely equal to 1.0 throughout the entire plane, except for some turbulent patches of unreacted mixture near the edges. Since the majority of the profile is completely reacted, especially towards the core of the domain, the headend inlet was assumed to have a uniform reaction progress variable of 1.0. This is the same as was used in the mass flow boundary condition earlier.

Mixture fraction variance was another parameter which was unavailable as a time-averaged value. An attempt was made to calculate the mixture fraction variance from the mean mixture fraction profile and the instantaneous mixture fraction profile at the final time step, but it yielded an unrealistically high value. This is not an unexpected result, as the variance is a value calculated over many time steps, and cannot be accurately estimated with only a single value and the mean.

The mass flow averaged mixture fraction variance at the exit of the second-stage combustion system from the simulations run using the mass flow boundary condition for headend inlet were on the order of $10^{-5}$ to $10^{-6}$. This was after the only partially-premixed jet of fuel and air was introduced and combusted in the cross flow. Since the second-stage combustion system has, by design, poorer mixing than the first stage combustion system, it was assumed that the mixture fraction variance of the first combustion stage was close to zero by the time the fuel and air had combusted and travelled down the channel. The headend inlet was thus assumed to have a mixture fraction variance of zero.

Turbulent kinetic energy and dissipation rates were also not available as time-averaged parameters as desired. Turbulence intensity was thus estimated from the mean velocity field and RMS velocity fluctuations as described by Eq. (3) [8].
Turbulence intensity was thus calculated for each point and a spatial distribution obtained. Values obtained were reasonable, ranged from about 7% to a max of 20%. Turbulence was specified by turbulence intensity and length scale. For the turbulent length scale, a constant value of 7% of the sidewall length dimension of the headend inlet.

**Summary of Studied Parameter Variations**

Multiple parameters were varied in order to determine the extent of their influence on the solution. These include the degree of CAD geometry simplification, the value of the turbulent Schmidt number, turbulence models, and chemistry modelling.

**Degree of CAD Geometry Simplification**

The influence of the extent of geometry simplification on the model was studied by varying the level of detail used in modelling the air inlet to the cross stage.

The actual inlet geometry is as shown in Figure 11. Air flows in through the tube on the left and is metered by flow metering plates before entering the settling chamber, from which it passes through the 60 perforated holes and enters the cross stage.

![Figure 11: Inlet geometry for cross stage air supply. Labeled components are (1) air inlet channel, (2) flow metering plates, and (3) settling chamber.](image)

Three different levels of detail were used to model the air inlet geometry. The levels of detail were to model the full inlet geometry, model discrete inlet holes, and modelling the inlet as a single annular band with the same surface area as the combined surface area of the holes. The geometry is shown in Figure 12.
The full inlet geometry was modeled, including the air inlet channel, flow metering plates, settling chamber, and cross stage inlet holes. This configuration is shown in Figure 12 (a). This full level of detail allows for the flow to develop as it would in the real system.

The inlet geometry was then simplified by modeling only the cross stage and discrete inlet holes, as shown in Figure 12 (b). This intermediate level of detail allowed for the effects of the holes on the flow inside of the cross stage to be accounted for, but assumed an even distribution of air flow through each of the holes.

The geometry was further simplified by modeling all 60 of the inlet holes as a single air inlet band, as shown in Figure 12 (c). The area of this band was equal to that the sum of the areas of all of the injector holes.

For all cases, the mass flow of air into the cross stage was equal, and is specified in the summary of boundary conditions.

**Turbulent Schmidt Number**

Another parameter which was varied was the turbulent Schmidt number, which is the ratio between the turbulent transports of momentum and mass. A lower turbulent Schmidt number leads to better mixing, as the mass transport is relatively higher. It is suggested in the documentation of STAR-CCM+ to use a turbulent Schmidt number of 0.7, although using a value of 0.4 has also been suggested. This parameter was therefore tested at each of the two values in order to determine which better modeled the second-stage combustion system.

The turbulent Prandtl number is the ratio of turbulent eddy diffusivities of momentum and heat transfer. This parameter was set equal to 0.9 for locations within $3.8 \times 10^{-4} \frac{d}{d_j}$ of a wall and equal to the value of the turbulent Schmidt number (0.7 or 0.4, depending on the simulation) in the flow.

**Turbulence Models**

The choice of turbulence model was varied to determine which is best suited for modelling the studied test rig. The models which were used were realizable k-epsilon, standard k-epsilon, k-
epsilon lag (elliptic blending), and k-omega. The default settings were used for each of the models. Details of these models and their implementation in STAR-CCM+ may be found in the software documentation [8].

Chemistry Modelling

For the majority of the cases that were run in this study, chemistry was modeled using an FGM which was generated from the GRI3.0 chemical kinetic mechanism. The number of grid points in the FGM table was varied in order to determine the effect of table resolution on the resultant chemistry.

Chemistry was also later modeled using complex chemistry and reacting species transport. For this, the chemistry was modeled using the drm22 [10], which is a reduced chemical kinetic mechanism based upon the GRI 1.2. This mechanism has 22 reacting species, compared to the 53 species of GRI3.0. The drm22 mechanism was selected to address the tradeoff between accuracy and computational expense. The complex chemistry was simulated both with and without chemistry acceleration in order to determine the effect of acceleration on the solution and the computational time.

Results and Discussion

Experimental Characterization

The results of the CFD simulations were compared to experimental results of the test rig from DLR Stuttgart by OH chemiluminescence and PIV measurements.

An image of the experimental OH chemiluminescence data is shown in Figure 13.

![Figure 13: Sample OH chemiluminescence image. The second-stage combustion system is visible in the right-most panel.](image)

The OH chemiluminescence image is line of sight integrated along the width of the combustion channel. In order to model this and compare the CFD results more accurately, a volume rendering of the OH mole fraction was used with an opacity gradient color scale. This was viewed in parallel projection from the side, resulting in a line of sight integrated image.

The image of OH chemiluminescence is line of sight integrated. To model this, a volume rendering of OH mole fraction with a gradient scale was used. This results in areas with higher line-of-sight integrated values of OH having a darker color. Viewed from the side, the OH volume rendering is line of sight integrated in the same way as the OH chemiluminescence
measurement, giving the most realistic comparison. An example of the OH volume rendering, viewed from an angle and from the side, is shown in Figure 14. There was always a small amount of OH present throughout the entire combustion channel due to slight interpolation error, so the minimum mole fraction of OH shown was increased past this threshold, with lower values omitted.

Figure 14: Example of volume rendering of OH with opacity gradient scale. The darker regions have a higher value for line-of-sight integrated OH. (a) Angle view and (b) parallel projection side view of line of sight integrated OH mole fraction.

Velocities were measured via PIV at two planes in the rig, one at the centerline of the channel and one at the edge of the cross-stage injector jet. Two dimensional velocity distributions were obtained in the X-Z coordinate plane. A sample velocity image is shown in Figure 15.

Figure 15: Sample PIV velocity image taken at the off-center plane. Vectors show the flow direction while the color indicates velocity magnitude.

Results from the CFD simulation were compared to the measured velocities along vertical lines located in the mid and off-center plane. The sampling locations in the CFD simulation and their corresponding locations in the test rig are shown in Figure 16.
These probe lines were selected at the entrance plane of the cross stage and at locations 1, 2, and 4 times the cross stage jet inlet diameter downstream. These locations were selected to capture the recirculation zone and free-stream flow. Results are presented as a nondimensionalized velocity versus a nondimensionalized vertical distance at each of the eight probe lines.

**CFD Results**

The following sections detail the results obtained from the CFD simulations and how each of the varied parameters impact the agreement between the simulation and experimental data.

**Degree of Cad Geometry Simplification**

The degree to which the inlet geometry was simplified had an effect on the velocity fields in the cross stage, ultimately affecting mixing and flame profile. The geometry simplification study was performed with the reduced size FGM table.

Cross-sectional views of the cross-stage velocity profiles along the y=0 midplane of the domain are shown in Figure 17.
Figure 17: Cross-sectional views of the velocity profiles in the cross-stage for the system with (a) the full inlet geometry, (b) discrete air inlet holes, and (c) a single air inlet band. The color scale indicates the velocity magnitude. Values above the maximum velocity are clipped and appear as white in the figure.

A slight difference is observed between modelling the full inlet geometry and discrete air inlet holes. Modelling the full inlet geometry captures the velocity imbalance between the left and right hand sides of the fuel injector. However, as can be seen by comparing Figure 17 (a) and (b), the difference between the velocity profiles is small. The single inlet band simplification of Figure 17 (c), on the other hand, leads to a significantly higher velocity near the walls of the injector, differing greatly from the predictions of the single full or discrete air inlet geometries.

The mixture fraction profile along the $y=0$ midplane of the injector and main combustion channel are shown in Figure 18.

Figure 18: Normalized mixture fraction profiles for (a) the full inlet geometry, (b) the discrete air hole inlet geometry, and (c) the single band simplification geometry. Bulk flow travels from left to right in the figure.
As seen in Figure 18 (a), and (b), the extent of the mixture fraction extent downstream of the cross stage is similar for the full inlet geometry model and for the discrete air inlet holes simplification. This is due to the similar velocity profiles within the cross stage. However, the extent of mixing that occurs within the cross stage is predicted to be higher for the discrete air inlet hole model than for the full inlet model. This may be explained by lower turbulence produced by the even velocity distribution within the discrete air inlet hole model compared to the full inlet model. An increase of turbulence within the cross stage would act to promote mixing, leading to a more even mixture fraction distribution. The single inlet band model shows more mixing occurring within the cross stage, due to the higher velocity of the air along the injector. However, it does not predict the mixture fraction extending as far downstream as the full inlet geometry and discrete air inlet holes geometries.

The OH chemiluminescence was compared with the line of sight integrated OH mole fractions as shown in Figure 19.

![Figure 19: Comparison of OH chemiluminescence to line-of-sight integrated OH mole fraction for (a) the full inlet geometry, (b) the discrete air inlet hole geometry, and (c) the single inlet band geometry simplification. Orange lines are guides for referencing position, showing the cross stage inlet and the approximate extent of OH chemiluminescence.](image)

The full inlet geometry and discrete air inlet holes geometries behaved similarly, and showed reasonable agreement with the experimental measurement. The single inlet band simplification did not match the results from the other geometry models or experimental data well, predicting a flame that is attached at the trailing edge of the cross stage inlet and not extending as far downstream as the experimental measurements. The attached flame predicted by the single inlet band is of a completely different behavior than the lifted flame and is due to the over predicted mixing caused by the high inlet velocity in the cross stage with the single inlet band.

Modelling the full inlet geometry is expected to produce the most realistic results, as it makes the fewest assumptions about the flow field within the cross stage. However, modelling the air
inlet to the cross stage as discrete holes showed similar performance to the full inlet geometry, and because it is simpler and reduces the mesh size, is the preferred model for the geometry. Modelling the air inlet as a single band of equal area to the sum of the discrete air inlet hole areas did not yield results similar to that of the full inlet geometry with respect to velocity, mixture fraction, or OH profiles. Because of this, it is not recommended to simplify the geometry to this extent. Overall, some level of geometry simplification in models is acceptable without causing major inaccuracies in the results, but caution should be exercised that the simplification does not remove flow features which would affect parameters important to combustion, such as the level of mixing.

Chemistry Modelling: FGM Table Size

The FGM table size was tested with a coarser and finer grid spacing in order to determine its effect on the solution. A summary of the FGM table parameters for the coarse (small) and fine (large) tables is given in Table 3.

For both table sizes, the FGM table was generated in STAR-CCM+ using adaptive gridding, which is described in the documentation [8]. Due to this, the maximum number of allowed points per table dimension is not equal to that which is returned by the code.

Table 3: Summary of FGM table dimensions for the original, coarse table and the updated, refined table. The max number of points is maximum number of points allowed for the given dimension in the table, and the final number of points is the final number of points in that dimension that the table generation returned after the adaptive gridding procedure.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Coarse (small) FGM</th>
<th>Fine (large) FGM</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Max npts</td>
<td>Final npts</td>
</tr>
<tr>
<td>Heat Loss Ratio</td>
<td>21</td>
<td>11</td>
</tr>
<tr>
<td>Mixture Fraction</td>
<td>61</td>
<td>36</td>
</tr>
<tr>
<td>M.F. Variance</td>
<td>31</td>
<td>19</td>
</tr>
<tr>
<td>Progress Variable</td>
<td>101</td>
<td>73</td>
</tr>
<tr>
<td>Species for post processing</td>
<td>CH₄, CO, CO₂, H₂O, N₂, O₂, OH</td>
<td>CH₄, CO, CO₂, H₂O, N, N₂, O, O₂, OH, NO</td>
</tr>
</tbody>
</table>

Plots of the temperature as a function of mixture fraction for the fully reacted adiabatic case from each of the two tables are provided in Figure 20. While the larger FGM table is more refined, both tables are in good agreement for the temperature. As a result, there was only a minor difference in the temperature distribution obtained in the solutions using the two different tables, as shown in Figure 21.
Figure 20: Plots of temperature points from the coarse (blue stars) and refined (red circles) FGM table as a function of mixture fraction for a completely reacted, adiabatic case.

Figure 21: Temperature profiles at the y = 0 midplane for the (a) coarse and (b) refined FGM tables. The walls are treated as adiabatic for this comparison, so no temperature gradient is visible near the walls.

Plots of the OH mole fraction as a function of mixture fraction for the two tables are shown in Figure 22. The OH profile was not well resolved in the small table. Using the larger table, the OH
profile was better resolved, with a higher number of points concentrated around areas of high nonlinearity, such as mixture fractions of 0.05 and 0.1, as shown in Figure 22.

Figure 22: Plots of OH mole fraction points from the coarse (blue stars) and refined (red circles) FGM table as a function of mixture fraction for a completely reacted, adiabatic case.

The poor resolution of OH in the small FGM table led to interpolation errors resulting in artifacts in the observed OH mole fraction distribution, as shown in Figure 23. The small FGM table suggests that there is excessive OH entering from the headend inlet and that OH extends further downstream of the cross stage than it should, according to experimental measurements. Increasing the resolution of the FGM table eliminates these artifacts and yields a solution in better agreement with the OH chemiluminescence measurement.

Figure 23: Line of sight integrated OH mole fraction for the (a) coarse and (b) refined FGM tables. Refining the table and adding more resolution to the OH profile removed an artifact suggesting an increased OH concentration at the headend inlet, highlighted with orange boxes.

Overall, the FGM table was found to have an impact on the solution if the parameters of interest are not well resolved. Only small differences were observed between the temperature
distributions of the solutions, due to that the temperature profile was reasonably well resolved in both the small and large tables. However, since the OH profile was not well resolved in the small FGM table, increasing the table resolution led to a large difference in the observed OH distribution in the solution. For the remaining studies, an even more refined FGM table was used, with dimensions of 19 points for heat loss ratio, 128 points for mixture fraction, 28 points for mixture fraction variance, and 168 points for progress variable.

In order to obtain the best chemistry resolution with the smallest possible table, it is recommended to use adaptive gridding and select the species of interest as species for post-processing in order to obtain table refinement in areas of high nonlinearity. One limitation of using the FGM for modelling chemistry is that in the current version of STAR-CCM+, the table must be copied in memory once for every CUP that the solution is run on. This may lead to large memory requirements.

**Turbulent Schmidt Number**

The turbulent Schmidt number was set to 0.4 and 0.7 and the effect observed on the solution.

The midplane nondimensionalized mixture fraction at the y = 0 midplane is shown in Figure 24 for both cases.

Figure 24: Nondimensionalized mixture fraction at the midplane for (a) $Sc_t = 0.4$ and (b) $Sc_t = 0.7$. Mixture fraction is nondimensionalized to the combustion channel freestream value. The vertical black bar is a visual reference to demonstrate the difference in extent of high mixture fraction region downstream of the cross stage.

As expected, using the higher turbulent Schmidt number led to the region of higher mixture fraction extending further downstream of the cross stage inlet.

The velocity profiles at the probe lines are shown in Figure 25.
Figure 25: (Top) Locations of probe lines, overlaid on the $y=0$ midplane showing the nondimensionalized $x$ velocity contour. (Bottom) Comparison of the nondimensionalized $x$ velocity profiles ($x$-axis) obtained from the CFD simulations and PIV measurement plotted against the nondimensionalized combustion channel height ($y$-axis). Red circles are the PIV mean velocities, while green dots indicate the +/- RMS fluctuations in the measurement. The solid blue line is the velocity profile using $Sc_t = 0.7$, while the solid orange line is the profile using $Sc_t = 0.4$.

There is good agreement between the PIV measurements and CFD output results for both turbulent Schmidt numbers. The turbulent Schmidt number did not have a significant influence on the observed velocity profile for the two values studied.

The comparison of CFD results to OH chemiluminescence data is shown in Figure 26.
Using a value of 0.7 for the turbulent Schmidt number caused the extent of OH downstream of the cross stage injector to be over predicted and. The results obtained with a turbulent Schmidt number of 0.4 show good agreement with the experimental OH chemiluminescence data.

Since both values for turbulent Schmidt number yield nearly identical velocity profiles which agree well with the PIV measurements, the better agreement with OH chemiluminescence data obtained with a turbulent Schmidt number of 0.4 suggest that it is the better value to use for modelling the flow of the second-stage combustion system.

**Turbulence Models**

The turbulence model used in the simulation was varied between realizable k-epsilon, standard k-epsilon, k-epsilon lag (elliptic blending), and SST k-omega. A high wall y+ treatment was maintained for all models.

The models were qualitatively compared by their midplane temperature and turbulent kinetic energy profiles. The midplane temperature distribution for each of the turbulence models is shown in Figure 27, and the midplane turbulent kinetic energy distribution in Figure 28.
Figure 27: Temperature profiles at the $y = 0$ midplane for the (a) k-epsilon realizable, (b) k-epsilon lag elliptic blending, (c) k-epsilon standard, and (d) SST k-omega models. All plots are on a common color scale, with temperatures above $2.25T_{ref}$ clipped and appearing as white.

Figure 28: Normalized turbulent kinetic energy profiles at the $y = 0$ midplane for the (a) k-epsilon realizable, (b) k-epsilon lag elliptic blending, (c) k-epsilon standard, and (d) SST k-omega models. All plots are on a common color scale, with values above 1 appearing as white.

The main effects of changing the turbulence model on the midplane temperature distribution were the change in maximum temperature and the extent of the high-temperature region down the main combustion channel. This is due to the difference in mixture fraction profiles for the different models, which is a result of the different levels of turbulent mixing from each.

As shown in Figure 28, the k-epsilon realizable model has the highest kinetic energy at the tip of the jet, while the k-epsilon standard and lag models have lower turbulent kinetic energy at this region. The k-omega model has the lowest turbulent kinetic energy in this region of all of the models studied. The lower turbulent energy leads to reduced turbulent mixing.
This effect is shown in Figure 29, which shows the nondimensionalized mixture fraction of the midplane for the realizable k-epsilon and SST k-omega models. These two models were selected for comparison because they show the highest difference in turbulent kinetic energy around the jet.

Figure 29: Nondimensionalized mixture fraction profiles at the $y=0$ midplane for (a) the k-epsilon realizable and (b) the SST k-omega turbulence models.

The poorer mixing of the models with lower turbulent kinetic energy result richer regions that extending further downstream, leading to the higher temperatures for these models.

The velocity profiles for each of these models were compared against the experimental PIV results and are shown in Figure 30. The k-epsilon family of models all resulted in similar velocity profiles which were in good agreement with the experimental measurements. The velocity profile obtained using the SST k-omega turbulence model did not agree well with experimental measurements, particularly at the position $2d$, downstream of the cross stage. The size and magnitude of the recirculation zone is over predicted by the k-omega turbulence model, with velocities falling outside of the bounds of RMS fluctuations measured in the experiments.
Figure 30: Comparison of the nondimensionalized x velocity profiles (x-axis) obtained from the CFD simulations and PIV measurement plotted against the nondimensionalized combustion channel height (y-axis). Red circles are the PIV mean velocities, while green dots indicate the +/- RMS fluctuations in the measurement. The solid lines are results for the (blue) k-epsilon realizable, (red) k-epsilon standard, (orange) k-epsilon lag elliptic blending, and (purple) SST k-omega models.

The k-epsilon family of models also performed better in predicting the OH profiles, as shown in Figure 31. The k-epsilon realizable turbulence model best matched experimental results, followed by k-epsilon standard, lag elliptic blending, and finally k-omega.

Figure 31: Comparison of CFD OH mole fraction to OH chemiluminescence measurements. The line of sight integrated OH mole fraction is shown for (a) k-epsilon realizable, (b) k-epsilon standard, (c) k-epsilon lag elliptic blending, and (d) SST k-omega models, with regions in which the static temperature $T$ is greater than $2.33 \, T_{\text{ref}}$ highlighted in pink.

The predicted OH profile for each model is consistent with its respective temperature profile, as shown in Figure 27, with turbulence models with lower turbulent kinetic energy yielding a longer flame.
Due to its good agreement with experimental measurements of both velocity and OH chemiluminescence, the k-epsilon realizable turbulence model was determined to be the best suited for modelling the second-stage combustion system.

**Chemistry Modelling: Reacting Species Transport**

The system was also modeled using reacting species transport and complex chemistry instead of an FGM. The chemical kinetic mechanism that was used was the drm22, which is a reduced mechanism based off of the GRI1.2 containing 22 reacting species and 104 reactions. The drm22 was selected as a tradeoff between accuracy in chemistry and computational expense. The thermodynamic and transport data were taken from the GRI3.0 mechanism.

The solution was initialized using a converged solution with an FGM containing all of the species present in the drm22 mechanism. The boundary conditions were updated from progress variable and mixture fraction to mass fractions of each of the species, in order to be consistent with the species transport requirements. Using the initial fields of the FGM initialized solution sped up the convergence for the reacting species transport solution.

![Figure 32: Temperature distribution at the y = 0 midplane.](image)

The temperature distribution at the midplane of the computational domain is shown in Figure 32. The temperature profile shows a qualitatively as expected, showing a peak temperature at the tip of the cross stage jet. The maximum temperature predicted was somewhat higher than that predicted by the FGM simulation.
A comparison of the simulated OH profile with OH chemiluminescence measurement is shown in Figure 33. The lifted flame is well predicted with the location and shape of the OH region in good agreement with the measurement. Furthermore, the region of OH with a temperature greater than 2.33 \( T_{\text{ref}} \) is almost equal in size and shape to the entire high OH region.

The comparison of the simulated and measured velocity profiles is shown in Figure 34. The simulated velocity profiles were found to be in good agreement with the measurements. The location of the recirculation zone is predicted to be slightly too low in the main combustion channel, but the magnitude of velocities is well predicted. These results are similar to those predicted with the FGM model.
Figure 34: Comparison of the nondimensionalized x velocity profiles (x-axis) obtained from the CFD simulations and PIV measurement plotted against the nondimensionalized combustion channel height (y-axis). Red circles are the PIV mean velocities, while green dots indicate the +/- RMS fluctuations in the measurement. The solid blue line is the CFD result from the reacting species transport complex chemistry simulation.

Figure 35: Comparison of time per solver iteration for the FGM and reacting species transport chemistry models on 48 cores of a computational grid. The increase in computational time was approximately a factor of 10.

The increase in computational time for running the reacting species transport with complex chemistry over FGM was approximately an order of magnitude, as shown in Figure 35. The simulations may be sped up if a chemistry acceleration technique such as clustering is used.

In conclusion, results from complex chemistry were found to be in good agreement with the experimental measurements. The velocity profiles matched those of the experiment well, and the OH concentration profile matched the OH chemiluminescence data well. The complex chemistry was able to predict the lifted flame well, performing better than the FGM.
Overall, results from complex chemistry matched those obtained using a fine FGM table well. Although the FGM does not predict the flame liftoff as well as the reacting species transport chemistry, the location of the bulk of the OH chemiluminescence is in good agreement between the two models, as seen comparing Figure 26 (a) and Figure 33. The velocity profiles predicted by each of the models both also match experimental data well.

Based upon these findings, the use of complex chemistry may be valuable for validating a FGM table against for a new geometry, and then using the validated FGM table to perform design exploration at a reduced computational cost.

Conclusions and Outlook

Conclusions

The second stage of a two-stage combustion system was modeled in STAR-CCM+ and model parameters including the level of geometry simplification, chemistry modeling, turbulent Schmidt number, and turbulence models were varied and their effect on the solution observed. Results from the simulations were compared to experimental OH chemiluminescence and PIV data of the rig in order to determine which combination of parameters was best suited to model the system. Based upon these results, recommendations for each parameter were developed.

The CFD simulations were found to produce results in good agreement with the experimental measurements for both velocity profile and OH distribution for the jet-in-crossflow fuel injector that was studied. Based upon the good agreement of the simulation results with experimental data, the solver may be used as a tool for design exploration of different cross stage injector geometries.

Some level of geometry simplification may not significantly impact the obtained solution. However, care must be taken to preserve important features that would affect the flow. For example, in the studied system, simplifying the inlet holes to a band strongly affected the velocity profile within the cross stage, consequently affecting the mixing and resulting flame.

For modeling the combustion chemistry using an FGM, the manifold should be generated from a full mechanism in order to enable it to capture the most chemistry possible. It is also recommended to use adaptive table generation to concentrate points in non-linear areas in order to reduce interpolation error. This has been shown to reduce artifacts that may change the conclusions drawn from a simulation. It is important to check the FGM table resolution of parameters of interest, particularly those which are being compared to measurements, in order to ensure that they are well resolved and interpolation error is minimized. Overall, the table size should be selected to be large enough to have good resolution but small enough to meet memory limitations of the hardware, as the current implementation requires the table to be copied once per CPU used to run the simulation.

The turbulent Schmidt number was not found to have a significant impact on the velocity profile of the solution, but did impact the degree of turbulent mixing and the resulting flame location. Using a value of 0.4 for the turbulent Schmidt number yielded better agreement.
between the simulation result and the measured OH chemiluminescence profile for the k-epsilon realizable turbulence model than a value of 0.7.

The k-epsilon realizable, k-epsilon standard, k-epsilon lag elliptic blending, and k-omega turbulence models were compared. The velocity profiles of the k-epsilon family of models were in good agreement with one another and with the experimental velocity measurements. The k-omega model over predicted the magnitude of the recirculation zone and did not show good agreement with the experimentally observed velocity profiles. The magnitude of turbulent kinetic energy predicted by each model affected the mixing profiles within the system, leading to a variation in flame position and length among the models. The k-epsilon realizable model had the highest turbulent kinetic energy, leading to the best mixing and a flame located the most upstream of all of the models. This best matched the experimental OH chemiluminescence profile, and was therefore determined to be the recommended model for the system. As an added benefit, the k-epsilon family of models showed stable convergence, while the k-omega SST model had an oscillatory solution. The stability of the k-epsilon models make them well suited for automated design exploration in optimization sweeps.

Reacting species transport with complex chemistry was used to model the system. A reduced mechanism (drm22) was selected as a tradeoff between increase in computational expense and accuracy in the solution. Computational expense was observed to increase by approximately an order of magnitude over the FGM solution for the complex chemistry without the use of any chemistry acceleration. The reacting species transport was better able to predict the lifted flame which was experimentally observed than the FGM model. Due to the significant increase in computational expense, complex chemistry may not be well suited for design exploration. It may, however, be useful to obtain a high fidelity solution for a base-case of a new design for which there is not any experimental data available. An FGM may then be tuned to produce a solution closely matching that of the complex chemistry simulation, and subsequently used for design exploration.

**Outlook**

Recommendations for future work and analyses are provided in this section.

A major source of uncertainty in the modelling done in this study is in the headend inlet conditions at the entrance of the main combustion channel. While efforts were taken to replicate the inlet conditions as accurately as possible by using conditions obtained from an LES solution of the first combustion stage, the best accuracy would be obtained by modelling and simulating the entire test rig. Modelling the full rig would lead to more confidence in the results of the second stage, and provide insight into the models best suited for a combination of complex and simple geometries, such as those from the first and second combustion stages. It would also be valuable to further investigate the effect of changing the boundary conditions of the walls and considering conjugate heat transfer. In the current simulation, the walls of the injector and cross stage were modeled as adiabatic, while the channel walls were modeled with a fixed temperature. In reality, the system which was modeled had heat transfer which was neglected or oversimplified in the analysis. For example, the hot inlet air of the cross stage will
preheat the fuel to some extent as it travels up the injector in the cross stage. It would be valuable to obtain more realistic boundary conditions for the walls and consider conjugate heat transfer in the cross stage to determine how much these assumptions impact the solution and whether they need to be taken into account during design exploration, or if the effect is negligible.

Another valuable aspect to investigate is how well emissions concentrations are modeled in the software. Emissions were not studied in the present work due to uncertainty in the headend inlet conditions. However, emissions limits are important design constraints that drive design changes, so validating the extent to which the CFD can predict the trends and absolute values of emissions such as CO and NOx is important to understand.

Performing a large eddy simulation (LES) would also be useful in better understanding the flow field and validating the turbulence models. Using LES to resolve more of the turbulence in the system may lead to better understanding of which model to use and why. Also, this may be used to check pressure fluctuations against measurements and validate STAR-CCM+ for use in design evaluation with respect to thermoacoustics, which is not possible with the steady state RANS simulations which were performed in this study.

Finally, it would be valuable to validate the complex chemistry model using full GRI3.0 mechanism and investigate the impact of clustering chemistry acceleration. The effect of chemistry acceleration on the solution and computational expense was not investigated in this study. Understanding the extent to which it distorts the non-accelerated solution and the reduction in computational time it enables is important for determining how complex chemistry simulations should be used for future simulations. In the current work, a reduced mechanism was selected for the complex chemistry as a tradeoff between accuracy and computational expense. Understanding the extent to which the results differ between using a reduced mechanism such as the drm22 and using a full mechanism such as the GRI3.0 will guide the way that complex chemistry simulations are implemented in future design evaluations.

Acknowledgements

I would like to thank Siemens Energy and Southwest Research Institute for providing and supporting this internship opportunity through the UTSR program. I would also like to thank Rich Valdes and Cliff Johnson for their guidance and mentorship, as well as Megan Karalus and Omid Madani for their support and training in STAR-CCM+. 
Works Cited


