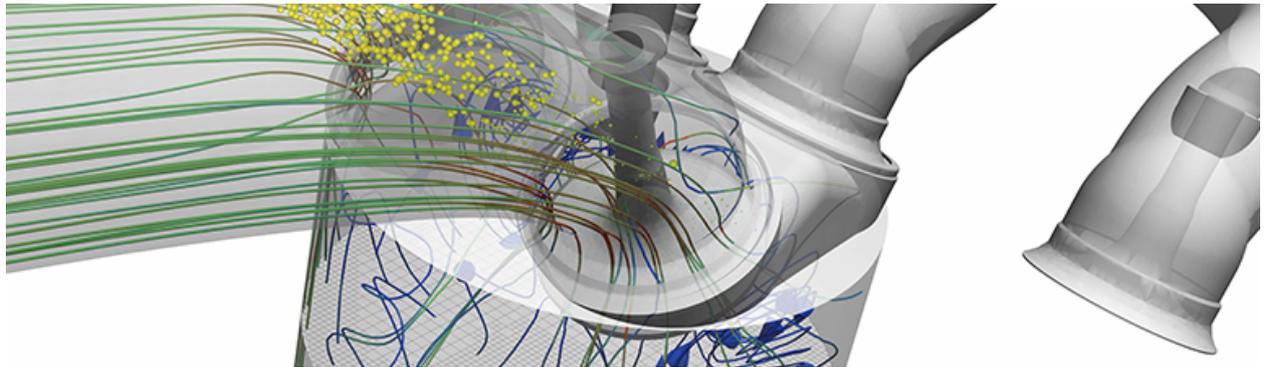




CHALMERS
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Characterization of Fuel Injection and Mixing process in a GDI engine using CFD

Master's thesis in Automotive Engineering - MPAUT

Department of Mechanics and Maritime Sciences
CHALMERS UNIVERSITY OF TECHNOLOGY
Gothenburg, Sweden 2021

MASTER'S THESIS IN AUTOMOTIVE ENGINEERING 2021:08

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Gothenburg, Sweden 2021

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Supervisor and Examiner: Petter Dahlander
Professor at division of Combustion and Propulsion Systems
Mechanics of Maritime Sciences, Chalmers University of Technology

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Department of Mechanics and Maritime Sciences
Division of Combustion and Propulsion systems
Chalmers University of Technology
SE-412 96 Gothenburg
Telephone +46 31 772 1000

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Abstract

In this thesis, computational fluid dynamics(CFD) simulations were carried on a gasoline direct injection (GDI) engine to study the thermal behavior, Piston fuel film mass accumulation, Heat release rate and emissions with different injection timings, piston temperatures and boundary temperatures. Simulating an internal combustion (IC) engine on any CFD platform is challenging because of its complex moving geometries, varying conditions, complex chemistry, and changing fluid structure. Gasoline Direct Injection can help increase engine efficiency and specific power output and reduce exhaust emissions.

Also, simulation of internal combustion engines offers a significant challenge in the field of CFD research. Moving boundaries of the solution domain, caused by valves' motion, piston leads to deformation of the computation grid, which decreases the quality of the results. The GDI surface file was imported onto the Converge work-space to change case setup parameters depending on which fuel was used. Also, changes were made during the simulations to check the resulting behavior with varying parameters.

Once after the initial description of the case setup process, studies of fuel film accumulation on the piston were investigated. The simulations showed that a mixture of Primary Reference Fuels (PRF) provided the best results for piston fuel film accumulation, spray-distribution, in-cylinder temperature, and pressure at particular injection timing and piston temperature. Lastly, standard physical models such as the Extended Coherent Flamelet Model (ECFM) combustion model, Imposed Spark Stretch Ignition model (ISSIM) ignition model, and K-epsilon turbulence model were used for simulations.

Acknowledgements

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I want to give my endless gratitude to my father, mother and sister. Thank you for always being there for me and supporting my decisions. I am forever grateful to all of you.

Dongre Varun, Gothenburg, March 2021.

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1

Introduction

In a competitive world, engine performance improvement has become a challenging and significant issue for automotive manufacturers because of the standard regulations for emissions to fight against global warming. Research is still going on to find out how to increase engine efficiency and reduced emissions, technology and research are going on in the engine design sector to achieve the legalized emission standards. The two standard methods can be utilized to develop and visualize the combustion process; Experimental study with different valve configurations and mathematical modeling (CFD modelling) with many other case setup parameters.

Even though the experimental method provides accurate results, an investment, cost, and time become a significant hurdle in conducting different test experiments. Multi-dimensional computational fluid dynamics (CFD) codes are used for quite a long time to solve the combustion and study the spray pattern with different valve timing and boundary conditions. The CFD simulations take a longer calculation time, thus requires a powerful machine with more cores and high-resolution solver capability. These problems have been solved with improved modern computers, making the system run faster to solve the combustion phenomena, which might be difficult or expensive with experimental studies.

Computational Fluid Dynamics (CFD) is one of Fluid Mechanics' main branches, which deals with problems occurring between fluid-fluid, fluid-gas, or fluid-solid interaction. As a result of solving these problems, CONVERGE CFD came up with a unique CFD software that features autonomous meshing, state-of-the-art physical models, detailed chemistry solvers, and the tool can accommodate complex moving geometry, which makes it very simple for an internal combustion engine simulation. Simulating an Internal Combustion (IC) engine will get more comfortable when incorporated with specific Computational Fluid Dynamics (CFD). As a result, CONVERGE CFD is the best tool to solve problems concerning moving boundaries with varying conditions both spatially and in time. The advanced mesh refinement and Autonomous meshing make CONVERGE spending its resources effectively to solve more significant hurdles and capture relevant flow features, Heat distribution, emissions, and film thickness both in space and time. Its fully detailed chemistry kinetics make it a robust tool for modelling complex chemistry in various systems. In an internal combustion engine, or Gas turbine, or compressors, complexity arises because of its geometry and fluid flow structure. CONVERGE CFD tool includes multi-phase fluid flows, Spray modules, turbulence models, and chemistry to meet these requirements. For simulation purposes, it automatically couples these models, making it user-friendly.

For a shorter run time, a simplified combustion model can be used, and if accuracy is paramount, CONVERGE's detailed combustion model and chemistry solver can be incorporated to study complex chemistry kinetics, Spray modelling, Emissions modelling, Turbulence modelling with stretch spark ignition model.

This master thesis project aims to introduce how effectively CONVERGE CFD tool can be utilized to solve complex CFD problems on internal combustion (IC) engines. The software can be utilized to develop and solve further computational fluid dynamics problems, which the next master thesis group will study at the department.

2

Background work

2.1 Literature survey

CONVERGE CFD was very new at the department of Combustion and Propulsion Systems. Converge CFD's implementation in studying 3D analysis of internal combustion (IC) engines was very challenging because of limited resources and case studies. In order to fill the knowledge gap before running the simulations, several journals were being studied and implemented on paper. The overall aim of this master thesis work was to investigate how Converge CFD could be used completely in studying complex internal combustion (IC) combustion and chemistry. The scope then expanded to simulate the Gasoline Direct Injection (GDI) with different case setups and crank angle degrees (CAD) to visualize both 2D and 3D modules. CONVERGE tools' detailed chemistry, combustion model, and emissions model makes it a powerful tool, and thus, the processing simulation time increased with increasing case setup. Similarly, the Converge CFD platform can be implemented to study different variants of internal combustion engines, Gas turbines, Compressors, Pumps, and after-treatment systems. The results are very accurate as compared to the experimental study.

To start with downloading and installing CONVERGE CFD, you must have administrative access to download the Convergent-Science-Full-Package<version>.msi file from the Convergent Science website. A License.lic file from the convergent science team and Reprise License Manager (RLM) should be installed so that RLM keeps track of the number of licenses running on the host machine for a floating license. Once the full package is downloaded, the Converge will be installed in the Program Files directory. A detailed Converge installation manual to the host machine is added.

2.2 Workflow for a Converge CFD Simulation

The workflow for Converge simulations consists of three main steps:

1. Pre-processing (Preparing surface geometry either by a surface.lic file or a CAD file of a Gasoline Direct Injection engine and configuring the case setup on Converge Studio to vary case setup parameters).
2. Running the Simulation (The simulation should be run from the Command Prompt with several procedures to make the machine running for a longer time).
3. Post-processing (Analyzing the *.out ASCII files in the case directory and Tecplot 360 to view the simulated output either on one or three dimensional plane).

2.3 Example Cases

The process of building a Gasoline-Direct Injection (GDI) engine geometry and simulating it on CONVERGE CFD requires a good level of knowledge with IC engines and CFD. First, the case-setup, simulation, and post-processing of a GDI engine, Tumble GDI ECFM Transient RANS, and Tumble GDI SAGE catalog were used as reference cases to know various specifications and attributes about the cylinder model which was being dealt with.

Table 2.1: Parameters of 6-cylinder engine

Parameters	Unit	Value
Base engine configuration	-	Single cylinder GDI
Valve configuration	-	2 valves
Injection system	-	Gasoline Direct Injection
Stroke (S)	mm	98
Bore (B)	mm	85
Connecting rod length (L)	mm	143.7
Compression ratio	-	10:1
Crank Speed	rpm	3000
Simulation time	CAD	-381.0 to 339.0

2.4 Running Simulation

Before running simulation, the case setup should be exported to a folder and under file inputs.in, the shared memory flag should be set from 1 to 0 (This will activate to run all the *.in files in batches). Navigation to the case directory should be done from the command prompt, and before submitting a job, enter mpivars.bat (This command prepares the batch files for simulation). Once the batch files are prepared, the Intel MPI setup script should be prompted for the last job. For this, enter -mpiexec -n*Number of Processors -converge-intelmpi.exe super (super command should only be used if it's a super-base floating license). The more the number of cores in the machine, the faster the simulation will be. The RAM memory also plays some important role for speeding-up the simulation, higher the RAM and clock speed, faster the simulation will be. The simulation output files will be stored in the same folder that the extracted files will be saved before running the simulation.

2.5 Line Plotting

The line plotting module on CONVERGE studio will be used to visualize the output data generated by CONVERGE solver. The solver writes output data to ASCII file (dynamic.out, thermo.out, etc.), saved in the case directory. The Line plotting then reads the data obtained from CONVERGE solver and allows for the creation of plots of various output data, which can then be saved in numerous formats. These multiple actions in the Line plotting module will not affect the simulation's *.cvg file or any of the output files.

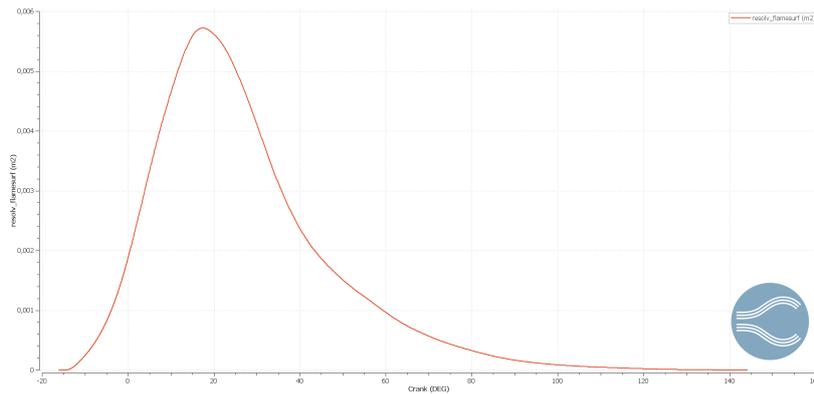


Figure 2.1: Line plotting window

2.6 Post-processing 3D-module

In the post-processing 3D module, you can convert binary format output files generated by CONVERGE during a simulation into a format readable by a three-dimension structure called Tecplot 360. The post-processing 3D module uses the same post convert utility as a command-line-based utility with CONVERGE. Post-processing in CONVERGE studio is an easy way to execute this utility to convert binary output files to your choice's visualization program files. The post-processing 3D module also allows the user to launch Tecplot 360 from CONVERGE studio only. After every simulation, all the post convert files have to be converted to the format that should be readable by Tecplot 360 for 3D visualization.

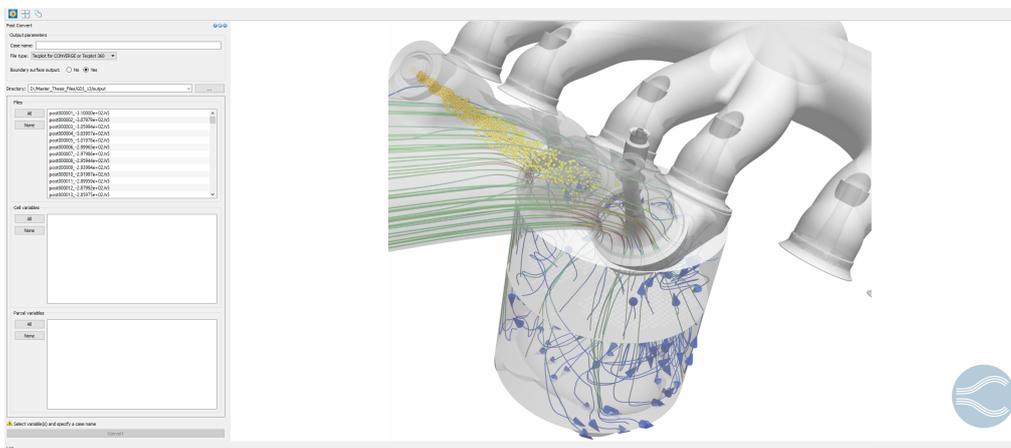


Figure 2.2: Post-Processing Window

2.6.1 Tecplot 360

Tecplot 360 EX is a tool to visualize the post-processed data either in 1D or 3D formats and a significantly faster way of visualizing the Computational Fluid Dynamics results. Tecplot 360 has advanced features to enable the view of the results with different color contours. Its slicing option allows the user to split the model into sections so that detailed results can be viewed from any phase.

2. Background work

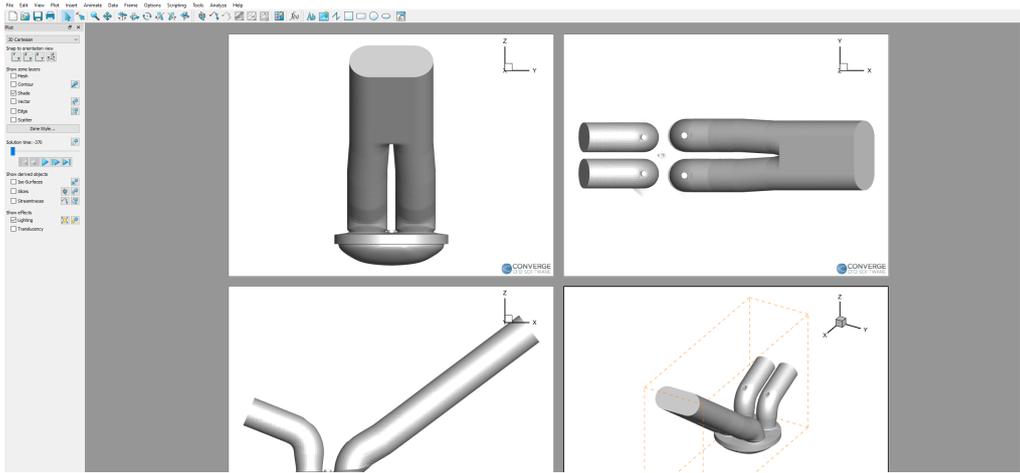


Figure 2.3: Tecplot Window

3

Methods

3.1 Surface Geometry of a GDI engine

Spatial tools integrated into CONVERGE Studio allows the user to import either a surface file, CAD file, or an STL file. The geometry must be represented in a closed triangle to run a Converge simulation. The CAD file, which will be in the form of an STL file, can be imported to Converge studio and can edit geometry to make it a closed loop and then export in the data file format (surface.dat). Once the surface.dat file is prepared, it can be imported to the New blank page on Converge studio for other case setup settings.

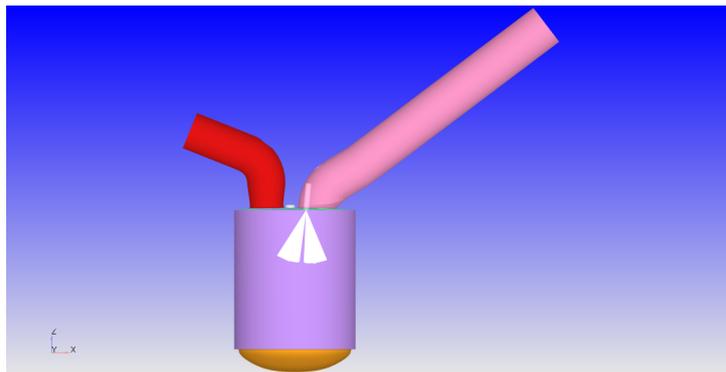


Figure 3.1: Surface file of a GDI engine

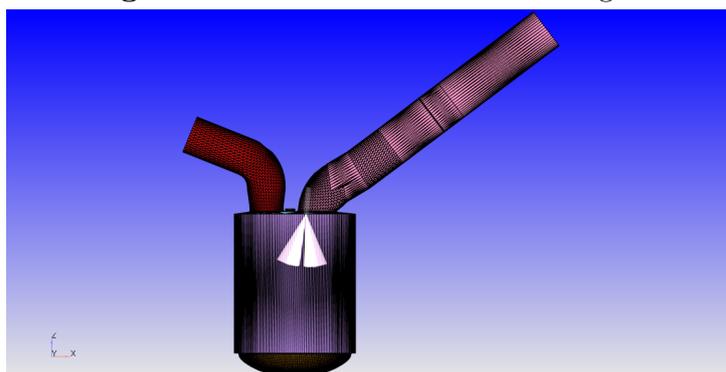


Figure 3.2: Meshed surface file from Converge workspace

3.2 Autonomous Meshing

Converge solver uses Adaptive Mesh Refinement (AMR) to generate triangulated grid to the surface file automatically. With this feature, the grid on the surface file can be automatically refined considering moving or fluctuating boundary conditions depending

on temperature, pressure, velocity, and flame propagation. AMR feature will allow the complicated grid simulation to run without slowing down the simulation time.

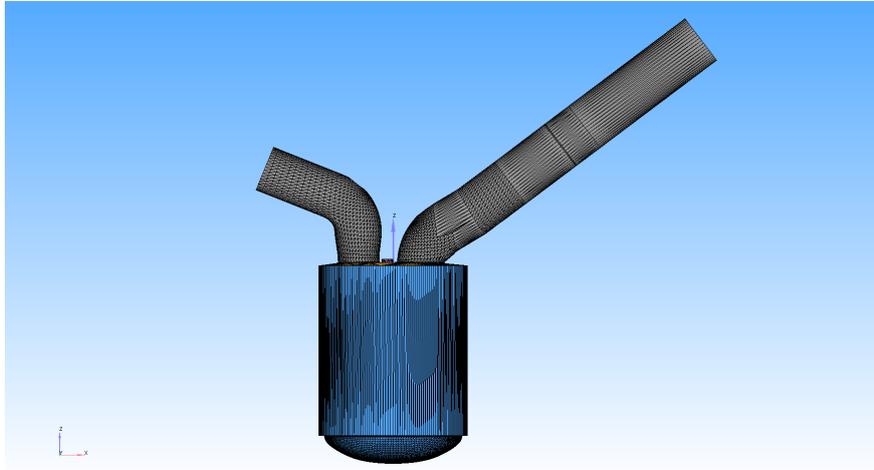


Figure 3.3: Meshed Single Cylinder GDI model

3.3 Import and Exporting Files

In Converge, the input file format is YAML, a plain text data serialization script. The YAML format uses the file's text structure to provide information to the input file parser without excessive use of syntax elements. YAML formatted Converge input files can include repeated sections, optional keywords, one-line lists, and some degree of arbitrary ordering.

Open an import file (*.in or *.dat) dialog box and navigate to the directory that contains one or more input and data files. Converge studio automatically enters the information from the relevant file into the case setup module when you click the import button.

3.4 Application Type

For Internal Combustion Engine Simulation, select crank-based IC engine measuring time in crank angle degrees (CAD). Then specify the engine parameters in the physical parameters section such as Bore, Stroke, connecting rod length, Swirl profile, crank speed, and in the references section, assign the boundaries for piston, liner, and head. The compression ratio will be automatically calculated by CONVERGE studio, which uses engine data like connecting rod length, stroke, and crank offset. It takes the value of chamber volume at the bottom dead center (V_{bdc}) using boundaries at their initial position. The CR calculator temporarily translates the piston boundary by this displacement and calculates the resulting clearance volume (V_c). Then Compression ratio is calculated as,

$$C.R = V_{bdc}/V_c \quad (3.1)$$

Table 3.1: Parameters of 6-cylinder engine

Parameters	Unit	Value
Base engine configuration	-	Single cylinder
Valve configuration	-	4 valves
Injection system	-	Gasoline Direct Injection
Stroke (S)	mm	95
Bore (B)	mm	93
Connecting rod length (L)	mm	143.7
Crank Speed	rpm	2000
Swirl profile	-	3.11
Compression ratio	-	9.5:1

3.5 Materials

CONVERGE Studio will automatically load the relevant thermodynamic data, gas transport data, and chemical reaction mechanism files when the air will be chosen as a predefined mixture. CONVERGE employs discrete Lagrangian parcels to simulate a particular type of predefined liquid or gas in conjunction with spray modelling. The chemistry for these liquids and gases is predefined in its reaction mechanism module. The predefined mixture (Air) should be checked, so the amount air to fuel ratio can be defined at the beginning of the case setup. Gas simulation, parcel simulation, global transport parameters, and species should be checked, where a lot of predefined fuel's chemistry will be used as a combustion element.

Simulations were carried out with three different fuel combinations to check single component and multi-component surrogates behavior against piston film thickness at different injection timings, injection pressure, piston temperature, in-cylinder pressure, and injection duration.

Table 3.2: Fuel parameters

Parameters	Unit	Value
Molecular weight(iso-octane)	kg/Kmole	114.233
Critical temperature	kelvin	543.9
Reference density	kg/m ³	843.0
Molecular weight (n-heptane)	kg/Kmole	100.204
Critical temperature	K	540.26
Reference density	kg/m ³	680.02
Molecular weight (n-hexane)	kg/Kmole	86.177
Critical temperature	K	507.43
Reference density	kg/m ³	654.63
Molecular weight (n-decane)	kg/Kmole	142.285
Critical temperature	K	618.45
Reference density	kg/m ³	727.0

3.6 Regions

The collection of all three boundaries make a region. Converge Studio uses different areas to initialize other variables (temperature, atm. pressure, Turbulent kinetic energy, Turbulent dissipation, and species mass fraction). The user must manually select the grid to one of the created regions before the simulation in other CFD simulation tools. But, Converge automatically creates the grid. During the run time, it looks onto each cell's orientation in the region, and connecting all the areas makes it a closed boundary for simulations to run. The GDI engine system is divided into three major areas, Intake system, Cylinder, and Exhaust system. In the regions dialog box, temperature, pressure, species, turbulence can be assigned for each location. The atmospheric air pressure of 101.325KPa and temperature 288K is considered an ideal condition with 23 % oxygen and 77 % Nitrogen in air, making its mass fraction sum to 1.0. During the combustion process, the cylinder region and the exhaust system are exposed to carbon and NOx emissions. In order to that, the mass fraction that constitutes 1.0 contains 73% Nitrogen, 15% carbon dioxide, 7.87% H₂O, and 2% oxygen. Each boundary in the Converge should be assigned to only one region, and if the geometry shares the portion with two boundaries, then two independent boundaries have to be set up and then assigned to its own region. Figure 3.4 shows the case setup values for the intake system. The values were considered for the ideal case. Figure 3.5 and figure 3.6 shows the case setup values for cylinder region and exhaust system.

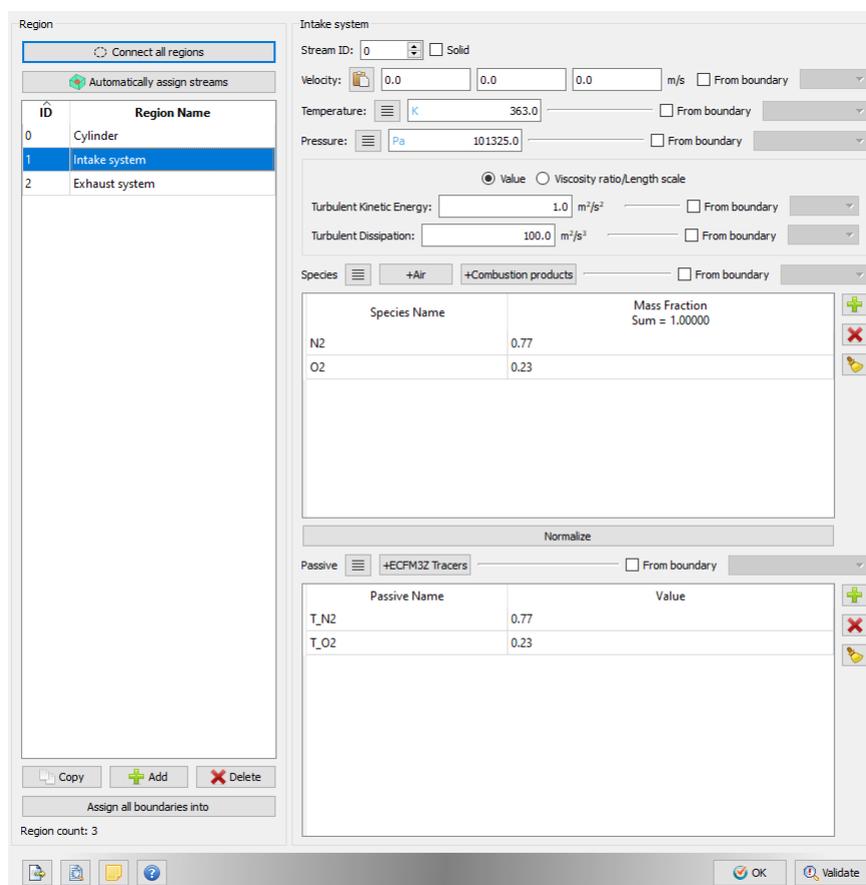


Figure 3.4: Regions - Intake system

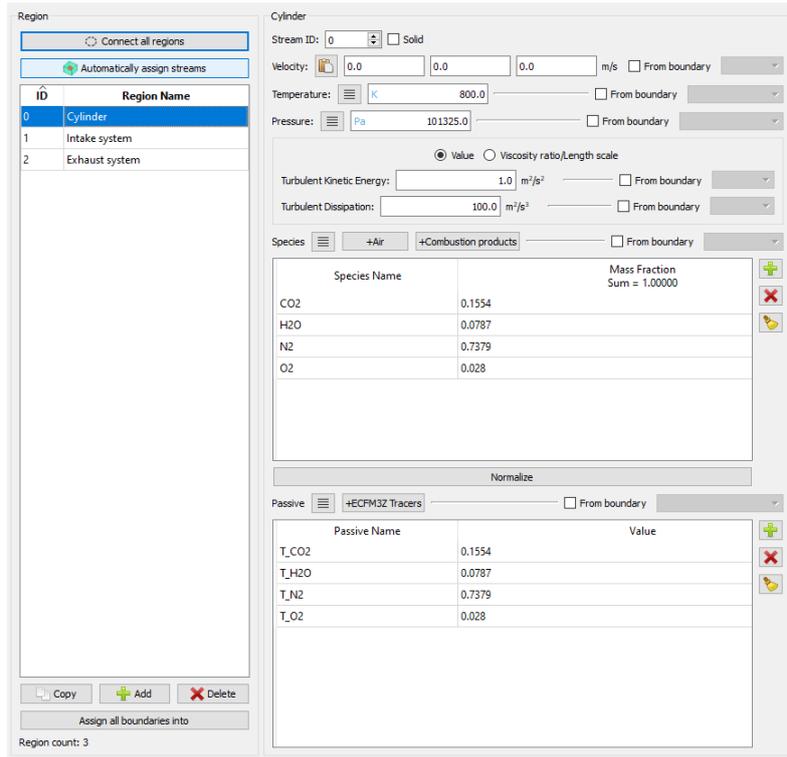


Figure 3.5: Regions - Cylinder

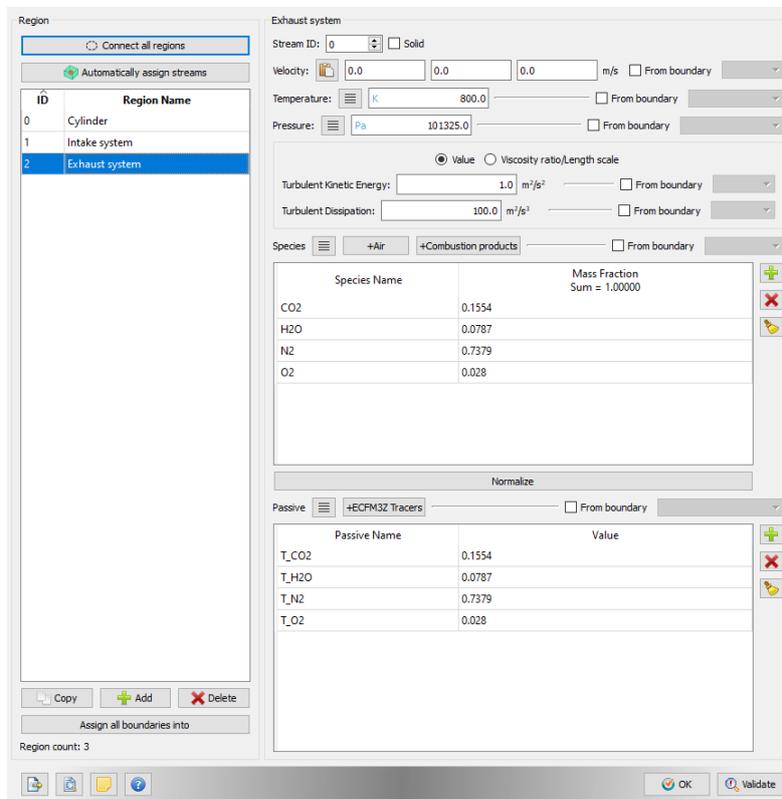


Figure 3.6: Regions - Exhaust system

3.7 Physical Models

3.7.1 Spray modelling

In the spray modelling, the first step is to set up an injector with the selected region's location and orientation. The next step is to configure the spray modelling area to set up a number of nozzles, injectors, species data, and injector temperature. The following are the data specified for each injector model. A constant 300 bar injection pressure was maintained throughout the simulation, which is shown in 3.7. Table 3.3 shows the parameters set for an injector along with the type of injector model used on the model.

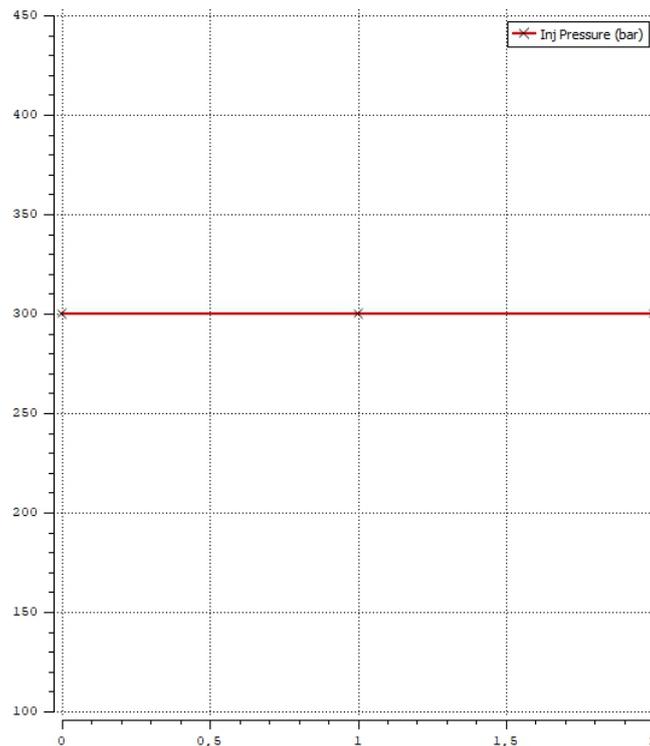


Figure 3.7: Injection Pressure

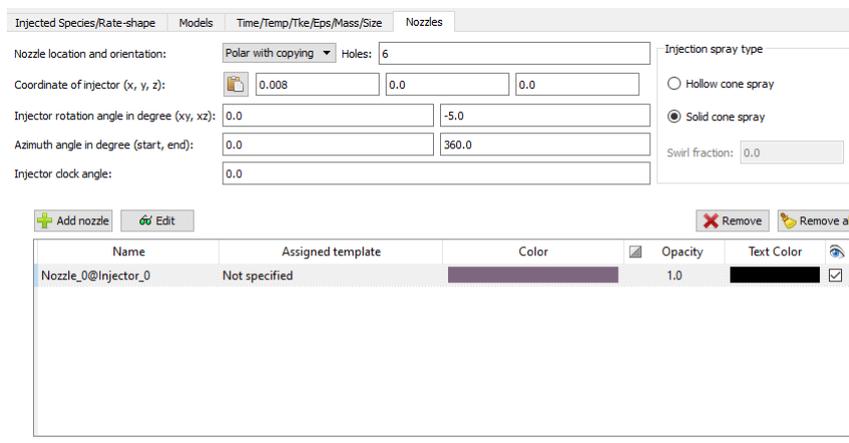


Figure 3.8: Regions - Injector Orientation

Table 3.3: Spray modelling case setup

Parameters	Unit	Value
Injection Temporal type	-	Cyclic
Cyclic period	CAD	720
Start of Injection	CAD	(-310 to -340)
Injected mass	mg	34.7
Fraction of injected mass/nozzle	-	0.05
Number of Nozzles	-	6
Total number of injected parcels/nozzle	-	60000

3.7.2 Combustion modelling

The combustion modelling was developed to simulate and visualize the combustion inside the cylinder with different fuel surrogates or fuel blends. The entire set of simulations were performed on ECFM [Extended Coherent Flamelet Model], which will be used for pre-mixed combustion simulations.

The screenshot displays the configuration interface for the ECFM model. The 'Laminar flamespeed' section is set to 'Gulder model'. The parameters and their values are as follows:

Parameter	Value	Unit
Constant laminar flame thickness:	0.0	m
Reference temperature:	298.0	K
Reference pressure:	101325.0	Pa
Metghalchi fuel:	User-defined	
Metghalchi constant 1:	0.2632	*
Metghalchi constant 2:	-0.8472	*
Metghalchi reference equivalence ratio:	1.13	*
Gulder fuel:	Isooctane	
Gulder constant, ω :	0.4658	*
Gulder constant, η :	-0.326	*
Gulder constant, ξ :	4.48	*
Temperature exponent constant, a_T :	1.56	*
Pressure exponent constant, a_p :	-0.22	*
Temperature exponent slope m_T :	-0.8	
Pressure exponent slope m_p :	0.22	
Dilution species mole fraction:	0.0	

Figure 3.9: Combustion modelling - ECFM model

3.7.3 Spark Ignition modelling

✓ Imposed stretch spark ignition model ? ×

Correction factor for the ignition mass, (>1):

Initial flame surface wrinkling:
(1 is for laminar spherical ignition; >1 is for turbulent ignition)

Spark plugs configuration

	Name	Plug location	Resistance, Ohm	Inductance, Henry	Elec. distance, m	. diameter
1	SpPlug1	-0.00345, 0, -0.00285	20000	20	0.001	0.001

Ignitions configuration

	Spark plug	Start time, deg	Type	Period, deg	Circuit energy, J
1	SpPlug1	-15	CYCLIC	720	0.04

Figure 3.10: Spark Modelling - ISSIM model

3.7.4 Turbulence modelling

Turbulence model: RNG k-ε

Wall Modeling

Von Karman's constant: Law of the wall parameter:

Wall heat transfer model: Base distance to wall on full cell size

Near wall treatment:

RANS Constants

C_μ $C_{\epsilon 3}$

Reciprocal μ Prandtl Reciprocal ϵ Prandtl

$C_{\epsilon 1}$ β

$C_{\epsilon 2}$ η_0

Buoyancy effects

v²-f/ ζ -f model constants

C_1 C_2 C_3 C_4

C_μ Reciprocal ζ Prandtl C_2'

Spray dissipation constant Drop turbulent dispersion constant

Figure 3.11: Turbulence Modelling - RANS model

3.8 Post-variable selection

The results which should be visualized on Tecplot 360 or Line-plotting module should be checked here before running the simulation. Film thickness, in-cylinder temperature,

and pressure, Film mass, spray characteristics, Fuel mixing at each boundary, Lambda, Flame speed will be selected in the post-variable selection case set up before running the simulations.

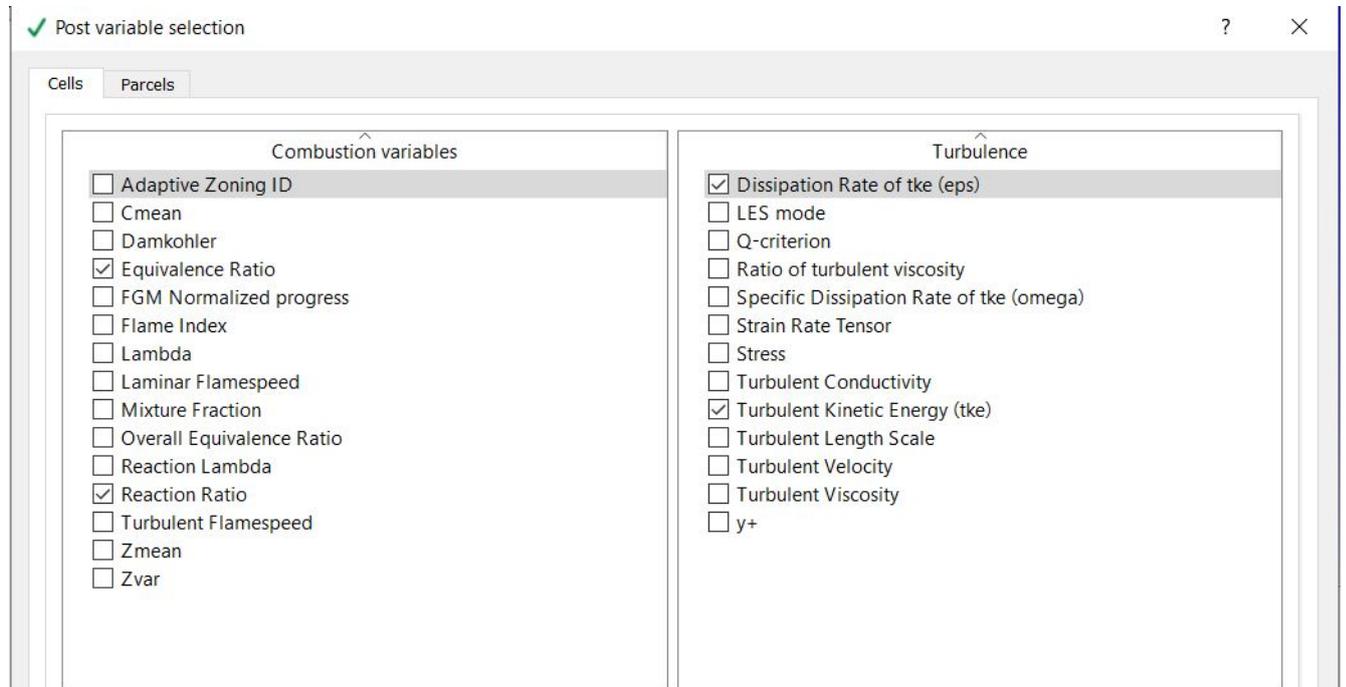


Figure 3.12: Post variable selection window

4

Results

Three-Dimensional(3D) combustion simulations using Computational Fluid Dynamics (CFD) with integrated fuel and combustion chemistry on Converge CFD was used in the simulation of Gasoline Direct Injection (GDI) engines. The real fuel is a blend of a lot of hydrocarbons that exceeds the present computational capabilities. To simplify the computational resources and a feasible approach, several simplifications are done, keeping engine development as the main purpose. This is done to simulate surrogate fuels to simulate and visualize the real engine performance during the entire 4-strokes. Iso-octane and n-heptane are the simplified surrogate fuels used for IC engine simulations, which are also called primary reference fuels (PRF). Converge CFD has its inbuilt fuel chemistry, making the tool user-friendly by minimizing the real-time to build the mechanism. Along with its Spray modelling, Combustion modelling, Emissions modelling, and Turbulence modelling, Converge CFD stands at the top among CFD simulation software, as its already been implemented with the case setup.

The wetting of the combustion chamber walls with liquid fuel is the dominant particulate emissions source in the GDI engines. So, to visualize the emissions and piston mass, a model with different case setup was simulated during the thesis work. The main parameters influencing the spray-wall interactions were discussed in the following section of the CFD calculations of a single-cylinder GDI engine. The surface temperature represents another essential parameter influencing the spray-wall business inside the cylinder. The fuel composition could also be an essential factor in determining spray-wall thickness, But also the piston wall temperature plays a vital role in the spray-wall fuel accumulation.

The simulations were performed only for single-component fuel [Iso-octane] with different injection timings, piston temperatures, and case setup variables. But in the later stages, with the reference of few journal papers, two-component and three-component fuels were simulated with various case setup parameters to study the piston fuel film accumulation both in liquid and gaseous form.

4.1 Single component fuel

4.1.1 SOI = -310 CAD and room temperature piston 300k

2,2,4-Trimethylpentane or iso-octane was used as the primary reference fuel (PRF) because of the simplified combustion kinetics integrated on Converge CFD. Several simulations were tested to set some of the case setup parameters that provided the best output result. The case setup was prepared for SOI = -310 CAD at piston temperature 300k (room temperature) to study the in-cylinder temperature, pressure, piston mass accumulation and heat release rate.

Figure 4.3 shows the amount of fuel accumulation on the piston's surface. Since the piston is at room temperature, which is very cold for the sprayed fuel to get vaporized, there will be a lot of spray mass accumulated. Before the start of combustion, i.e., at -16 CAD, 11.1mg of 34.7mg was still accumulated on the piston's surface. This leads to a reduction in the fuel efficiency and the life of the piston and increases the emissions. Figure 4.4 also shows a significantly lower heat release during the combustion, contributing to the increase of emissions. This crank angle timing and it is easily noticed that the mixture formation remains very lean even at the end of 720 degrees. There will be higher NOx emissions as the mixture remains lean, requiring an efficient catalytic converter system. The results below are showed at low load of 2000rpm.

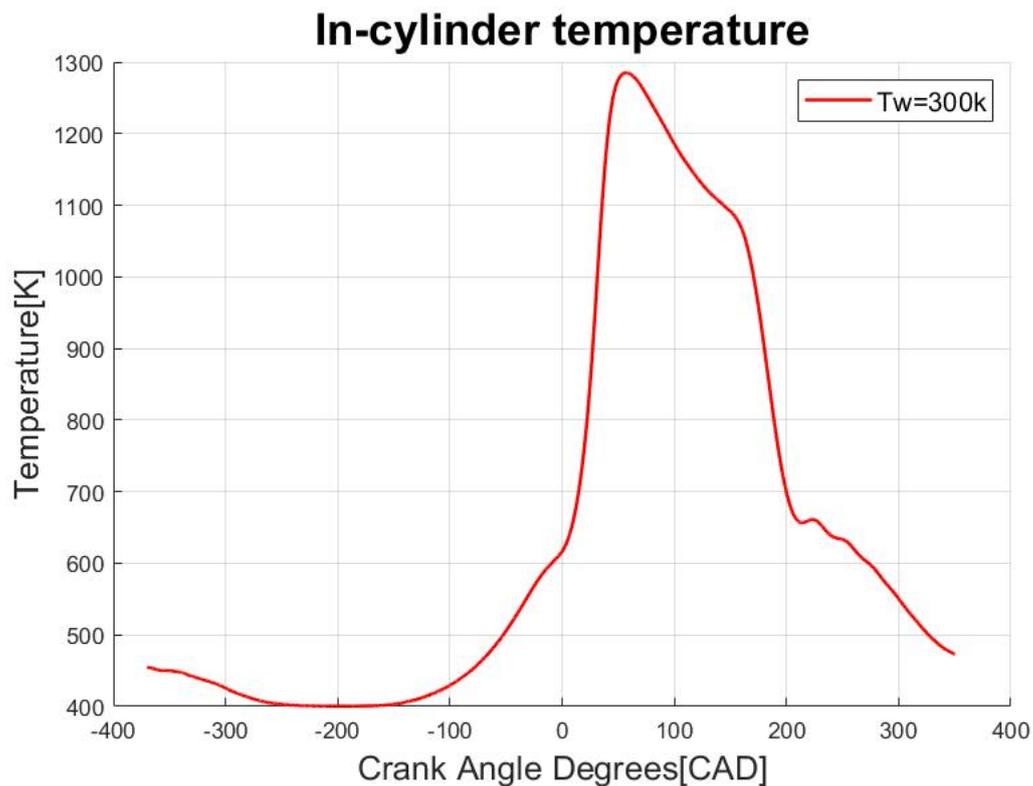


Figure 4.1: In-cylinder temperature

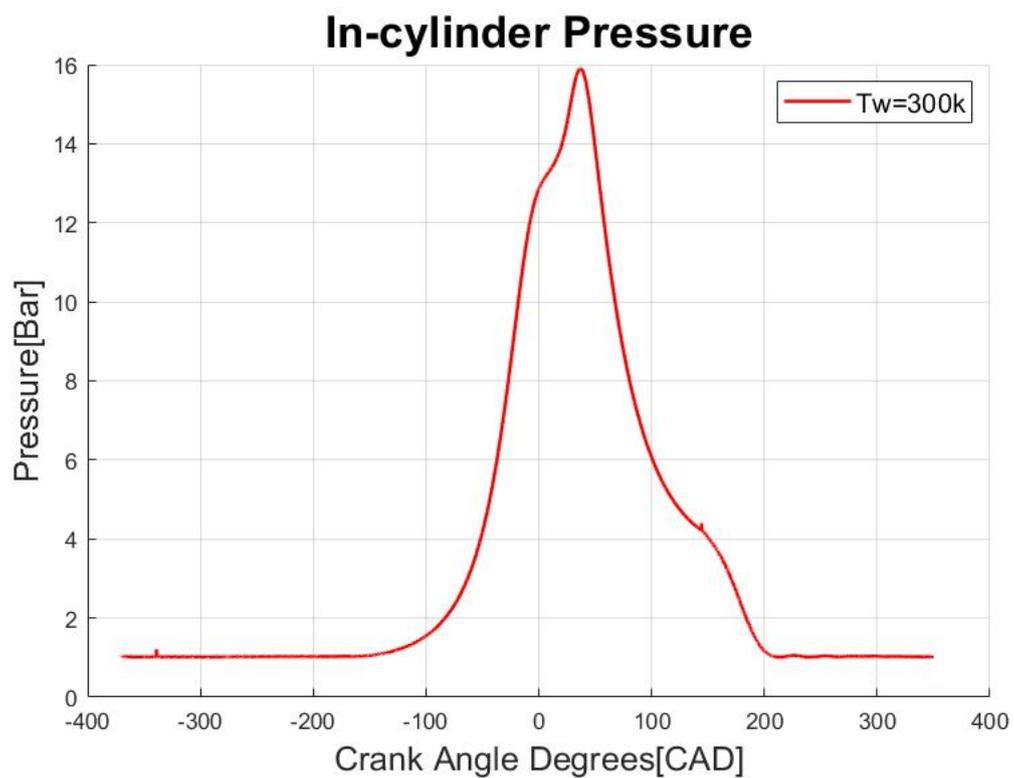


Figure 4.2: In-cylinder pressure

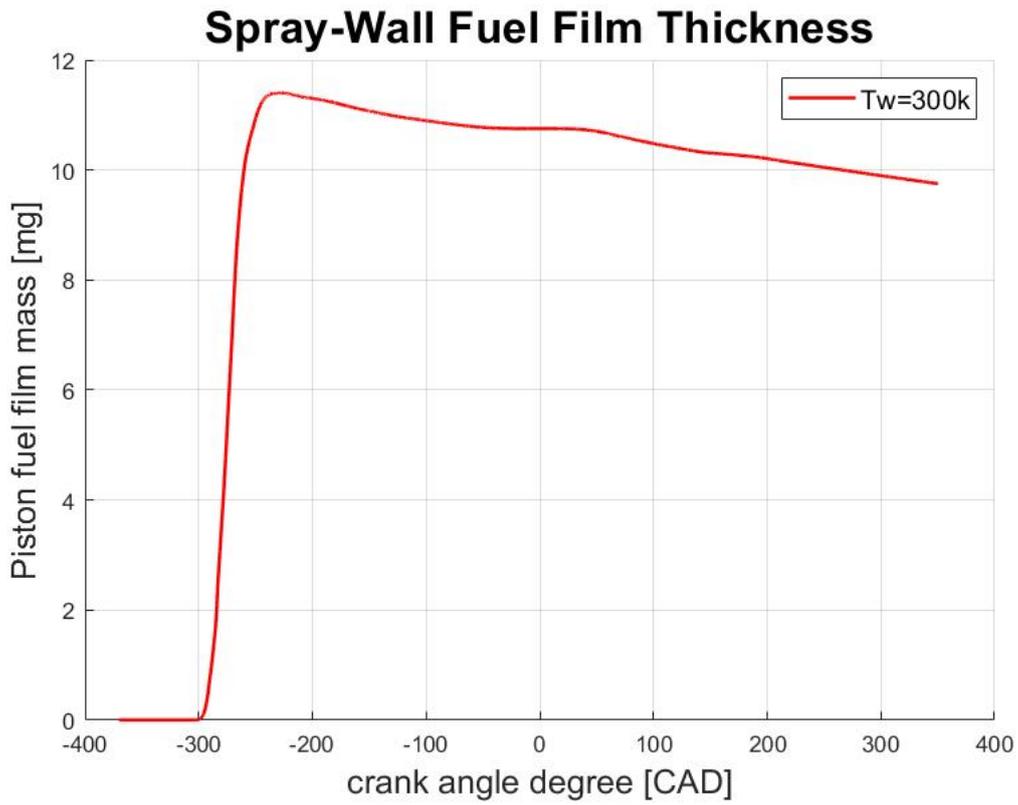


Figure 4.3: Piston Fuel film mass accumulation

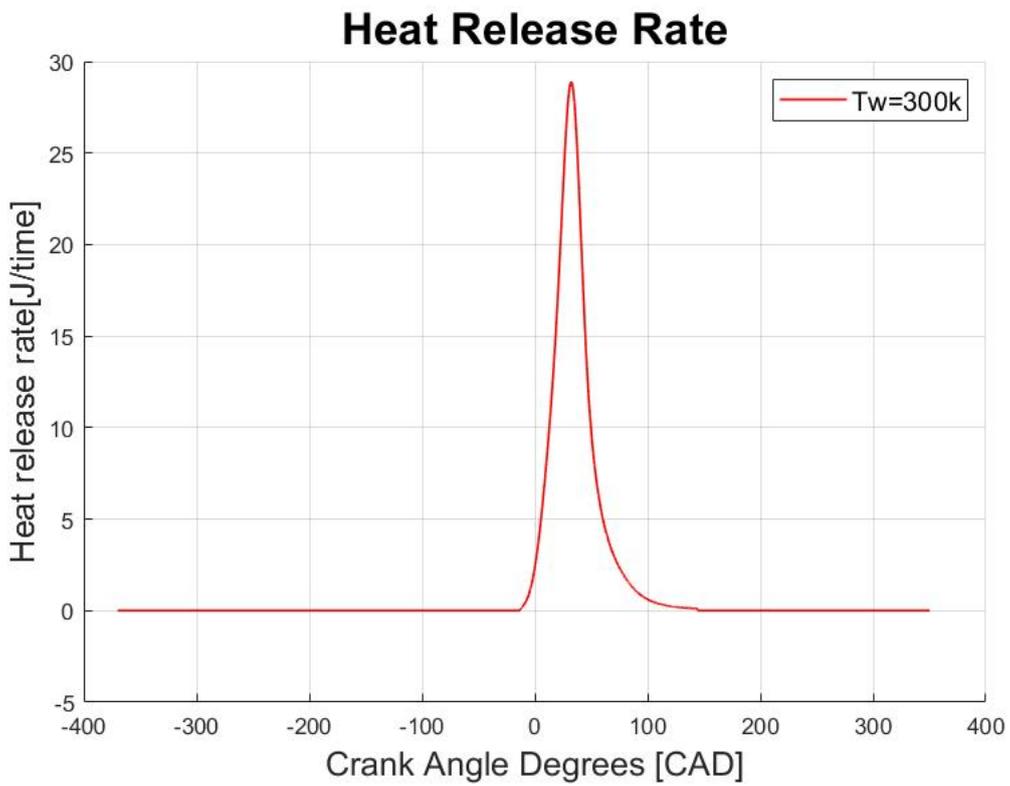


Figure 4.4: Heat Release Rate

4.1.2 SOI = -310 CAD and Piston temperatures 380k, 420k and 450k

To find the best timing and piston temperatures, simulations were performed at injection timing SOI = -310 CAD and piston temperatures $T_w = 380\text{k}$, 420k , and 450k to determine the variations in the performance of the engine with given case setup parameters. According to the standards, these piston temperatures are the best operating points for the piston to provide the best efficiency and limited emissions. Referring to the above plots, SOI=-310 CAD was the best injection timing, giving minor emissions and piston fuel-film mass accumulation. The piston temperatures of 380k , 420k , and 450k and other case setup parameters are shown below.

As can be seen from figure ??, the in-cylinder temperature is very much better than compared to piston temperature 300k . At piston temperature 380k , the temperature reaches 1620k , which is again lower compared to the other two because of the low piston temperature required for complete combustion to happen. But in the case of 450k P.T., the in-cylinder temperature reaches 1770k , which is very good for a GDI to perform complete combustion. Figure 4.5 shows the pressure variations at different piston temperatures. For P.T. 380k and 420k , the pressure fluctuates between 28 to 31 bar. Still, in P.T. 450k , the pressure shoots to 50 bar, which is because of the difference in fuel chemistry integrated with Converge CFD. This uneven chemistry leads to variations in a lot of thermal and physical parameters inside the cylinder. But referring to piston fuel-film mass accumulation on figure 4.6, for P.T. 380k , during the mixing process, the fuel mass shoots to 6.7 mg, but it reaches 1.2mg before the start of combustion, which is very efficient. But for P.T. 420k and 450k , the sprayed fuel will vaporize immediately after the mixing process is done because of the higher P.T. and air temperature. No mass will be accumulated on the piston before the start of combustion. Even the heat release rate [fig 4.7] for 380k and 420k is quite moderate, but for higher temperature, it shoots up to 84 J/time because of the differences in the fuel chemistry of Iso-octane.

The CO₂ emissions vary from 105mg to 115mg as shown in fig 4.8, which is under the E.U. standards for emissions. But, CO emissions [fig ??] relatively vary with the difference in P.T., which is very inconsistent for a GDI engine's best output. For P.T. 380k , 10.4mg of C.O. emissions will be produced during the combustion peak, which escapes during the exhaust stroke. But, for P.T. 420k and 450k , C.O. emissions are pretty nominal, where a proper exhaust after-treatment system can be utilized to reduce it still.

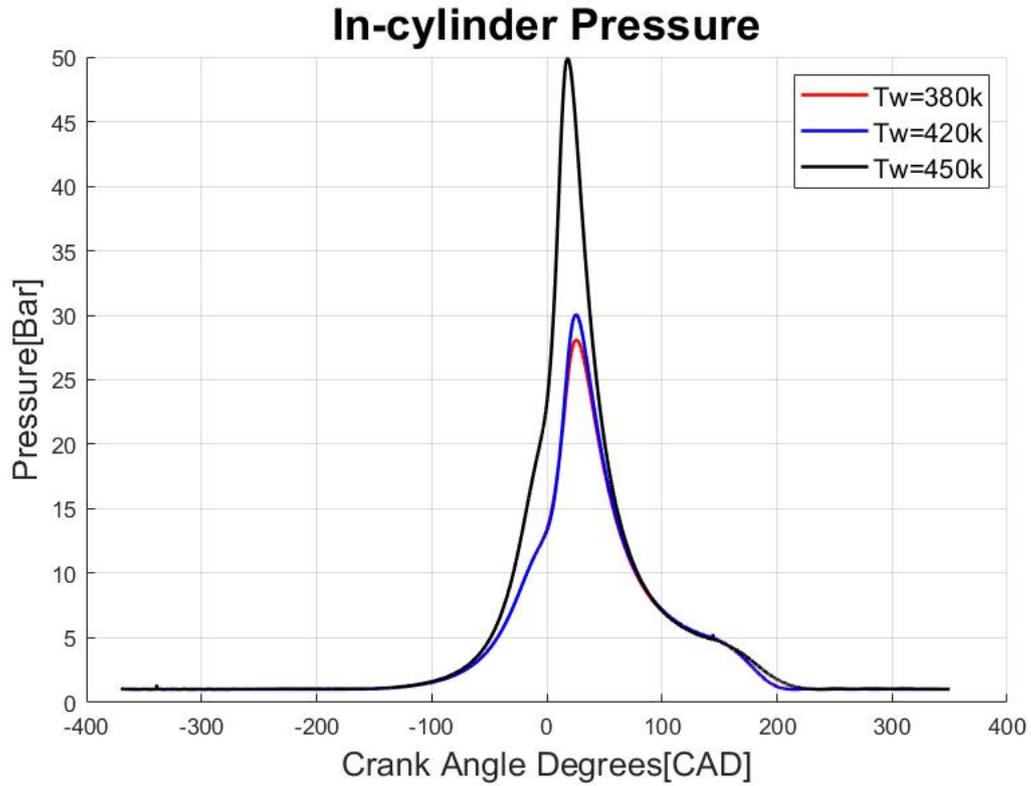


Figure 4.5: In-cylinder pressure

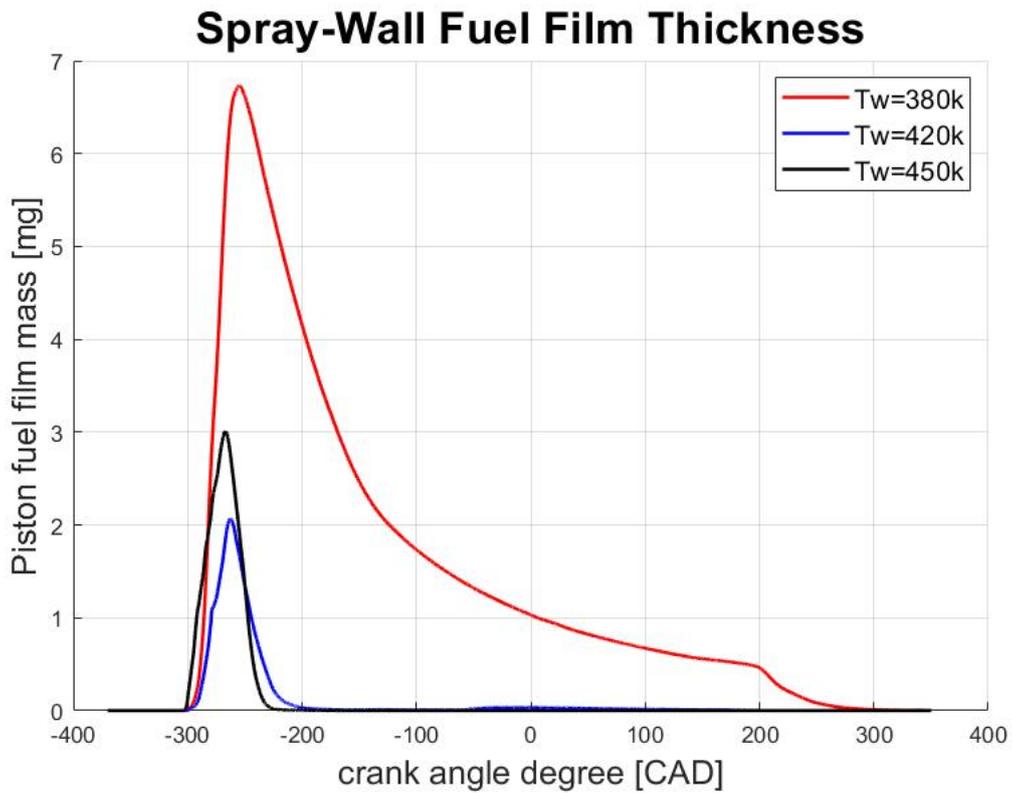


Figure 4.6: Piston mass accumulation

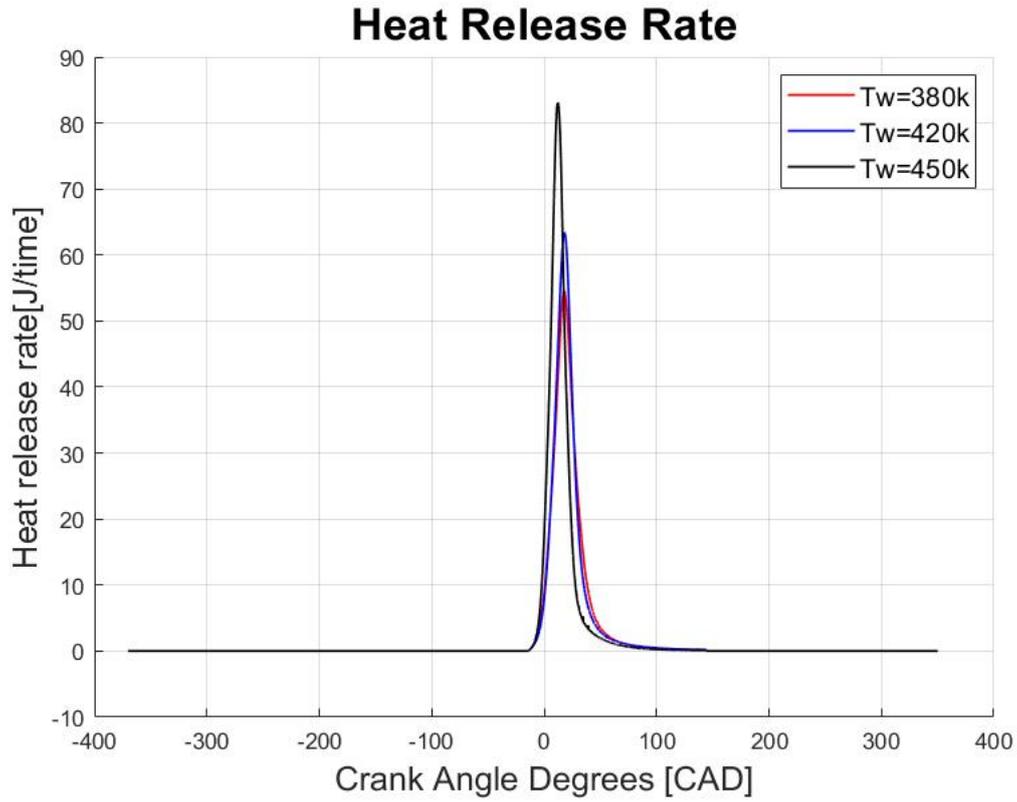
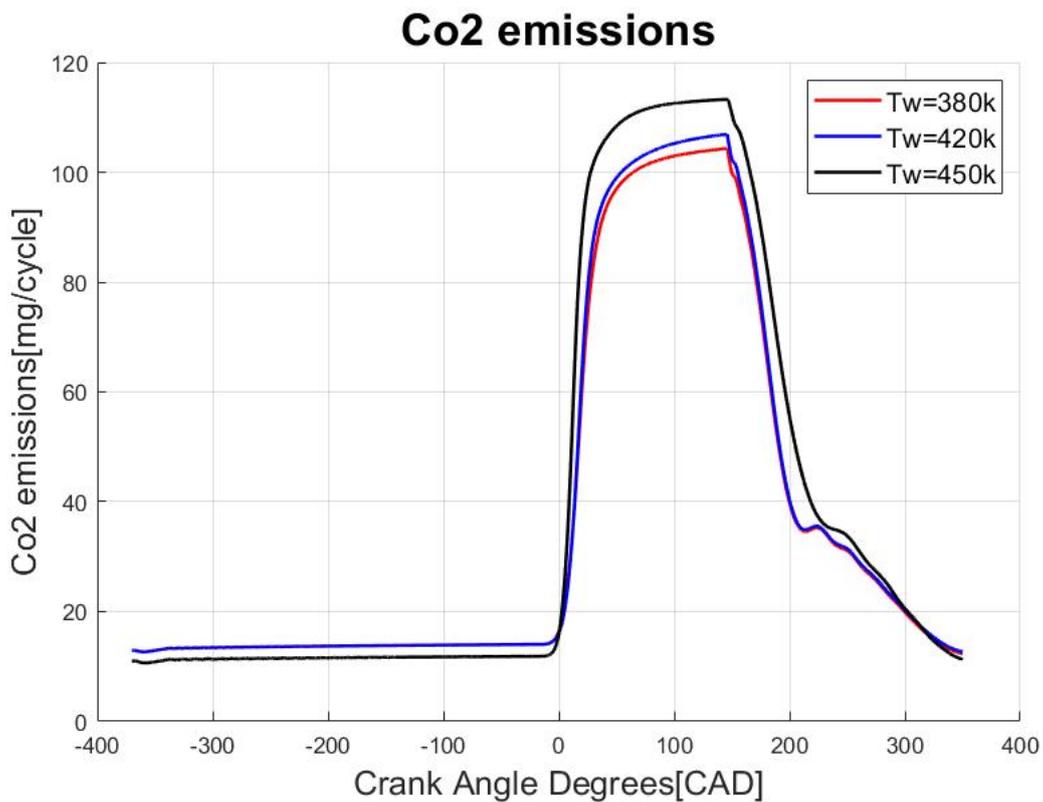


Figure 4.7: Heat release rate

Figure 4.8: CO₂ emissions

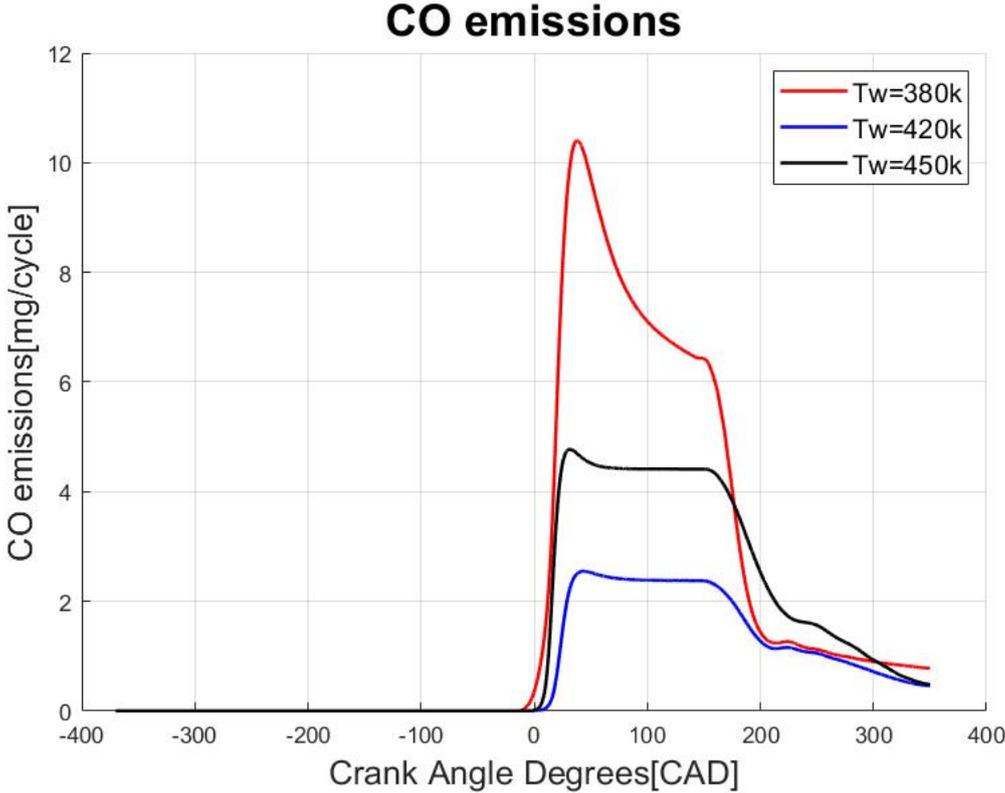


Figure 4.9: CO emissions

4.2 Two component Fuel

The two-component fuel includes 80% iso-octane and 20% n-heptane. These are Primary Reference Fuels, which are popular gasoline surrogates used in the study of the combustion process in an I.C. engine.

Figure 4.10, shows the variations in the in-cylinder temperature for a two-component fuel blend iso-octane and n-heptane. Many simulations were performed to fix the case setup parameters with different injection timings, piston temperatures, and fuel surrogates concentrations. During the combustion peak, for all three piston temperatures, the in-cylinder temperatures were quite similar which varied between 1620k to 1650k. This is because of the Primary Reference Fuels' stability, which will be used for most of the Computational Fluid Dynamics simulations. Figure 4.11, shows the distribution of in-cylinder pressure during the entire 720 CAD. The maximum pressure reached is 31 bar for P.T. 450k, which is because of the high piston temperature, which quickly vaporizes the fuel.

Figure 4.12 shows the gaseous spray distribution of the fuel molecule inside the cylinder. Because of the lower boiling points and higher air temperature, pressure, and fuel quantity, n-heptane gets quickly vaporized before the iso-octane gets vaporized. The piston fuel film mass accumulation for P.T. 380k before combustion is like 0.3mg, and for P.T. 420k and 450k, the sprayed fuel gets quickly vaporized because of the higher piston and air temperature. But compared to single-component fuel, the heat release rate [4.14] for two-component fuel is stable for all three temperatures. Figure 4.15 is relatively low compared to single-component fuel. The carbon molecules and the previous combustion cycle, a small amount of CO₂, will be present until the beginning of combustion at -16 CAD. Once the combustion starts, the CO₂ percentage rises to a peak of 105mg/cycle to 108mg/cycle for three different piston temperatures. But, the amount of CO₂ emissions is consistent for all the three-piston temperatures. But, CO emissions [??] drastically rises for lesser P.T. of 380k, which reaches 12.1mg/cycle, and for higher P.T.'s of 420k and 450k, the process only emits around 2.2mg of C.O. per cycle.

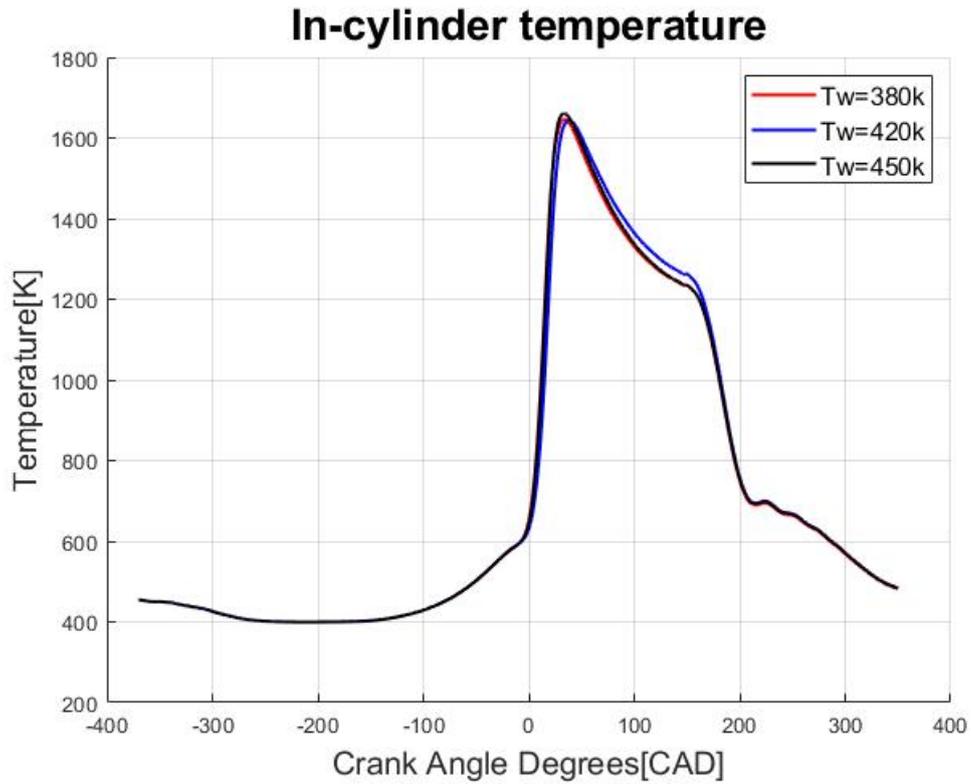


Figure 4.10: In-cylinder temperature

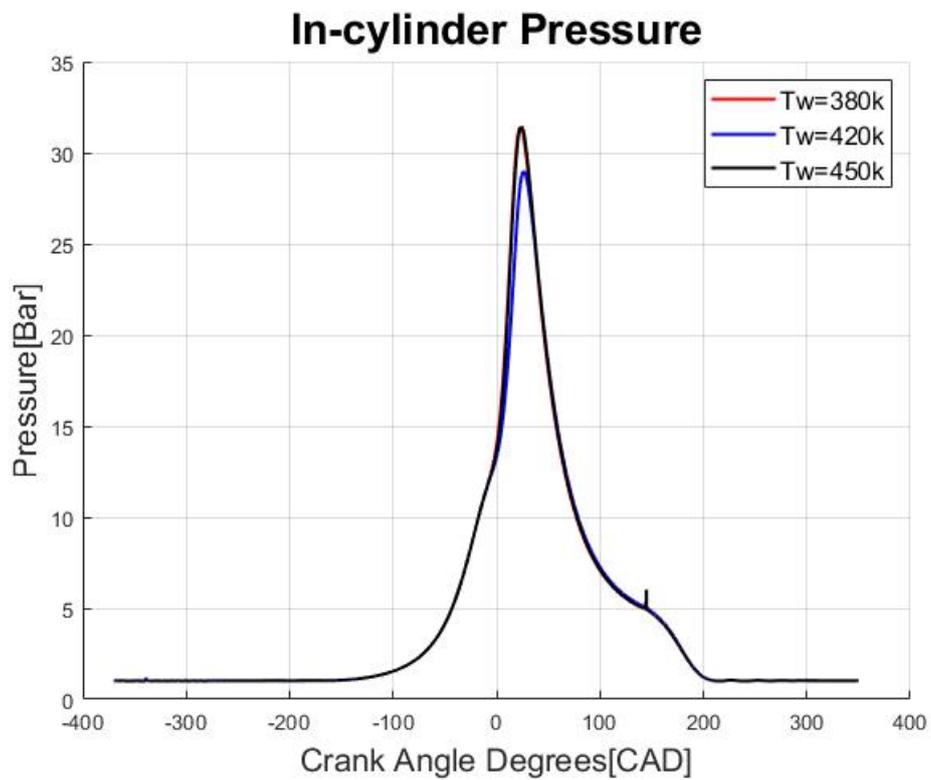


Figure 4.11: In-cylinder pressure

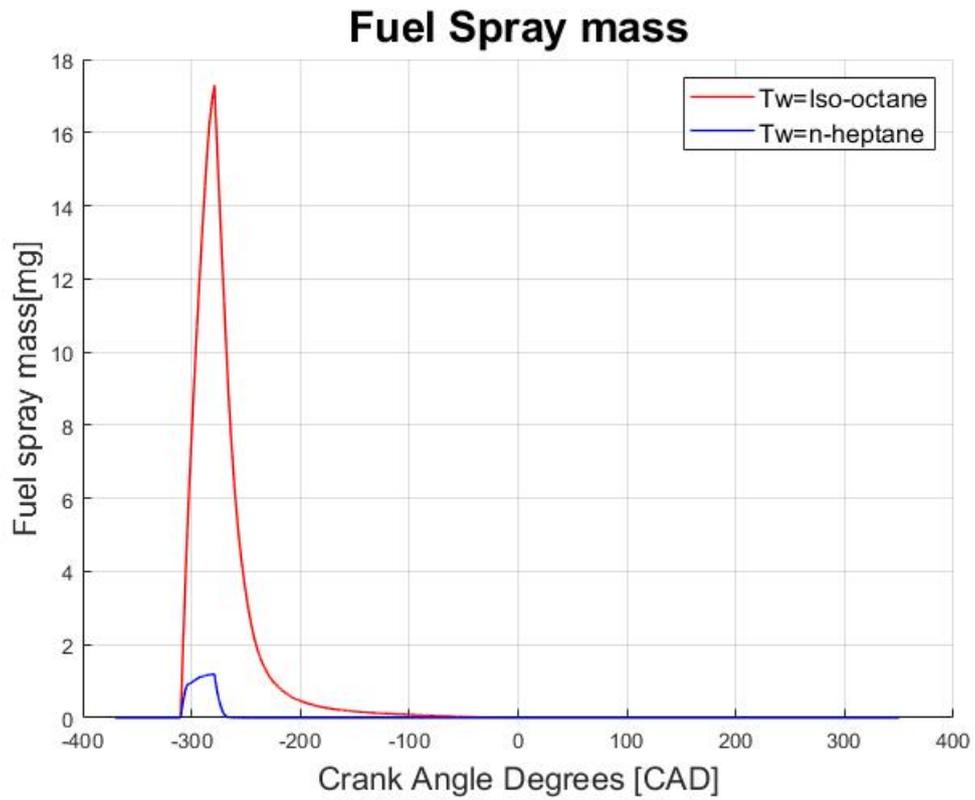


Figure 4.12: Fuel spray distribution

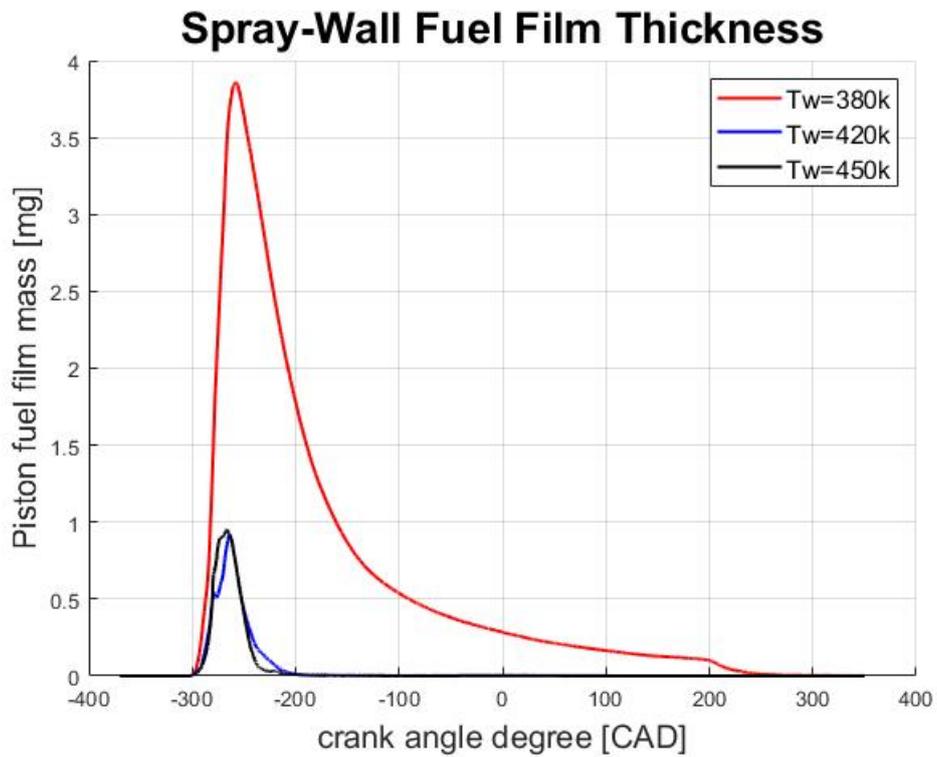


Figure 4.13: Piston fuel film mass accumulation

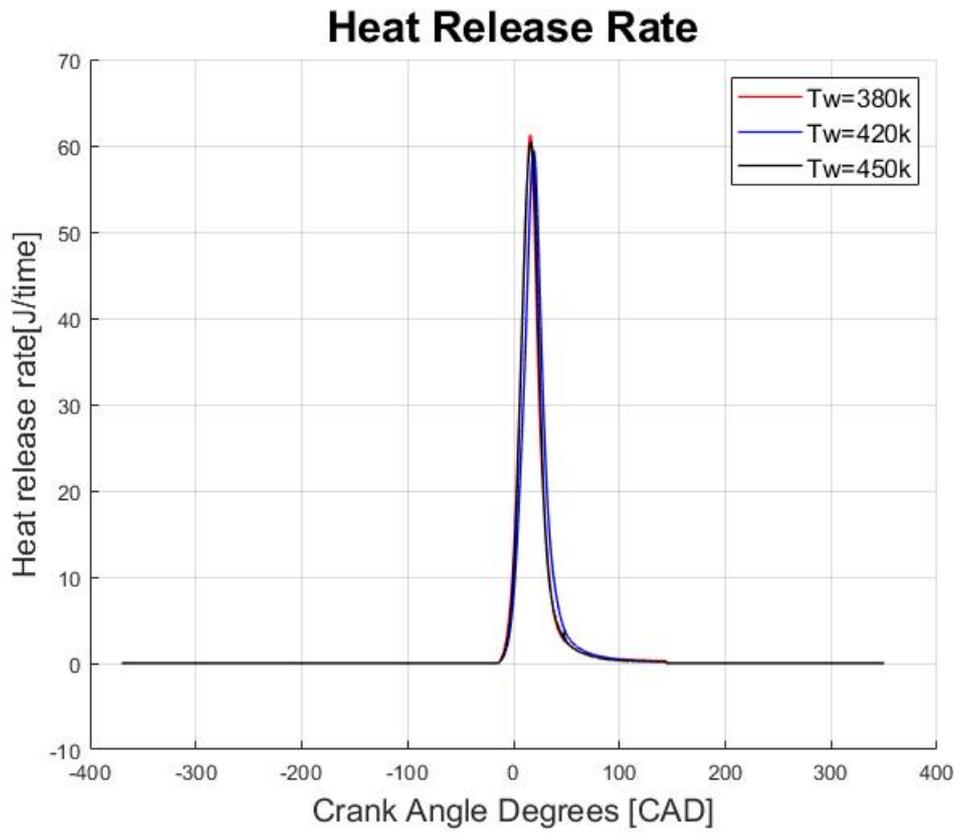


Figure 4.14: Heat release rate

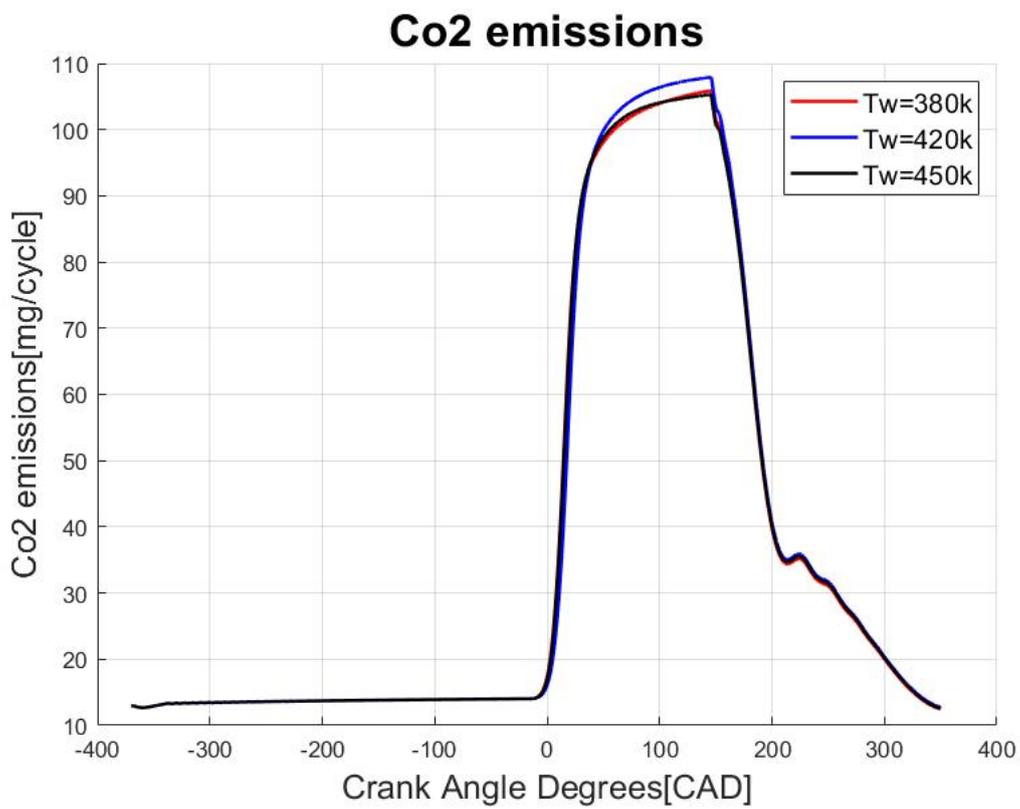


Figure 4.15: CO2 emissions

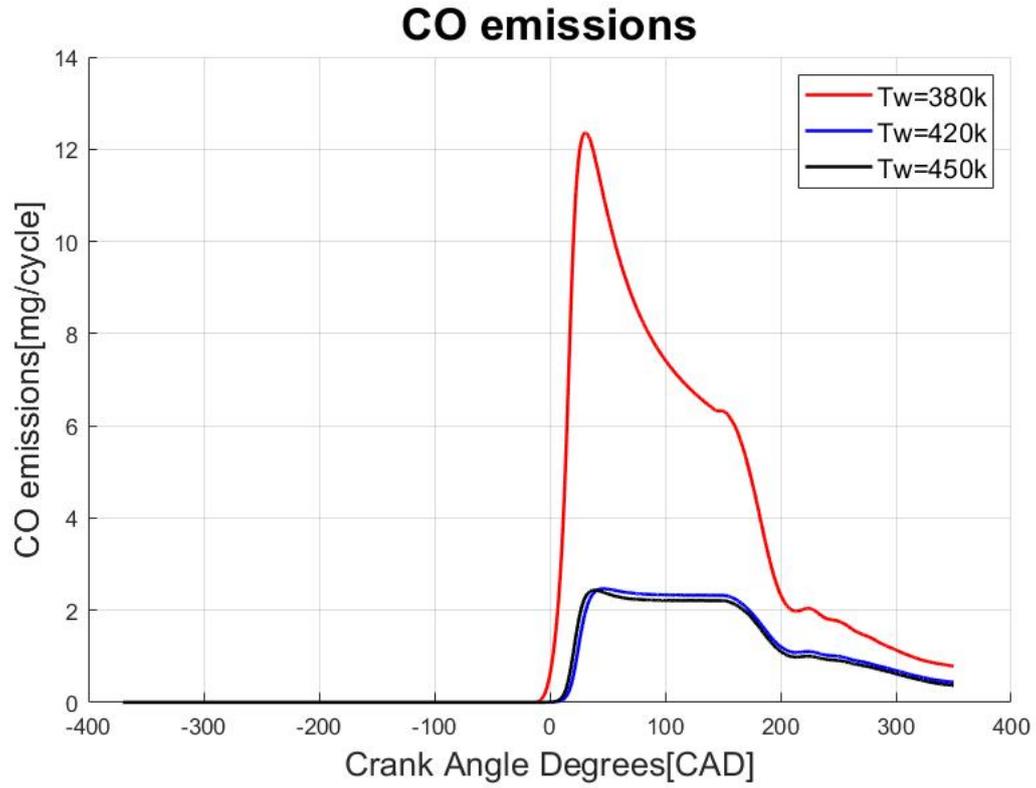


Figure 4.16: CO emissions

4.3 Three component fuel

The three-component surrogate fuel consists of 45% iso-octane, 35% n-hexane, and 20% n-decane. This fuel combination is refereed from the SAE journal paper [6], which says this combination of fuel blend is efficient because of its mixture composition and fuel chemistry. The sprayed fuel's vaporization mixes properly with the air, which results in a lesser piston fuel film accumulation at all three different piston temperatures.

Figure 4.17 shows the temperature variations for a three component fuel surrogate. The peak combustion temperature reaches to 1650k, which is very good for a GDI engine to provide best results. Since the air temperature is quite high, the fuel homogenization happens properly which results in complete combustion of the sprayed molecules. Also, there is a variations with the pressure [4.18]compared to the previous one component and two component fuel. The pressure rises to 33.8 bar, which leads to complete combustion of the mixed molecules with temperature 1650k. Figure 4.19 shows the detailed representation of fuel spray distribution with different variants of fuel. Because of the high air temperature, the fuel with higher boiling point vaporizes immediately after the injection and the fuel with lower boiling point spreads until the start of combustion. This results in some sprayed molecule accumulation on the piston as shown in figure 4.20. For 380k P.T, 1.5mg of fuel is being accumulated on the piston and for 420k, only 0.3mg of fuel is accumulated on the piston. But, because of the higher piston temperature, all the sprayed molecules gets vaporized immediately for 450k P.T. Figure 4.21 shows the Co₂ formation during the combustion and it varies between 105mg to 112mg, which is higher than that of two component fuel. Even for CO emissions, figure 4.22 shows CO emissions and for 380k P.T, the CO emissions shoots to 7.2mg/cycle because of the insufficient P.T. But for 420k and 450k P.T, the Co emissions will be 3.1mg/cycle, which is again a little bit higher than that of three component fuel.

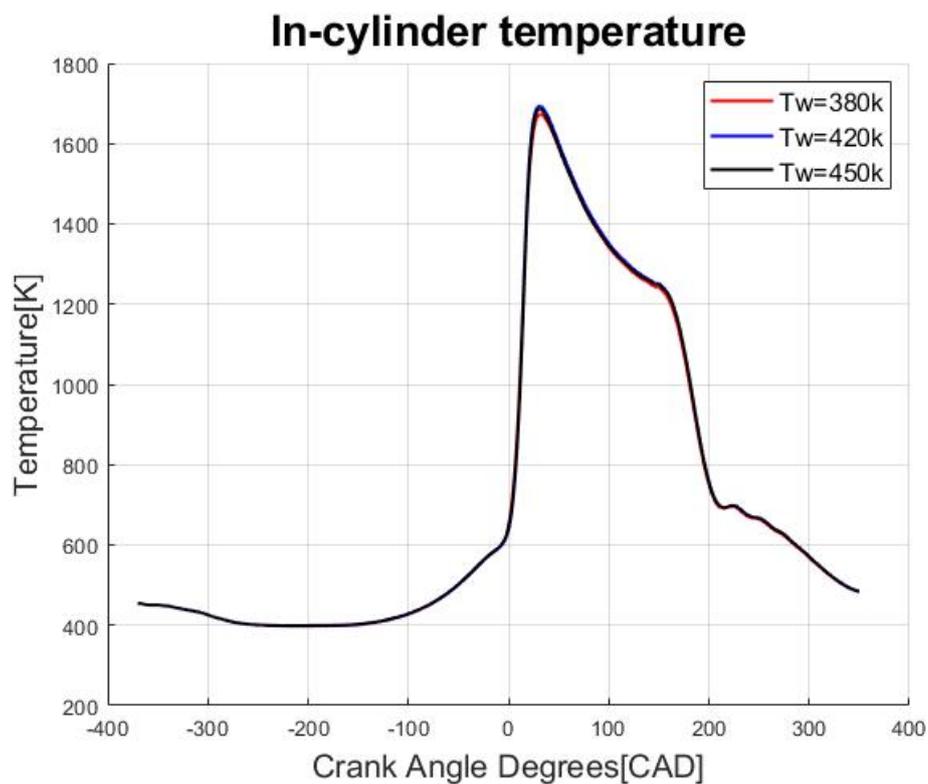


Figure 4.17: In-cylinder temperature for 3-component fuel

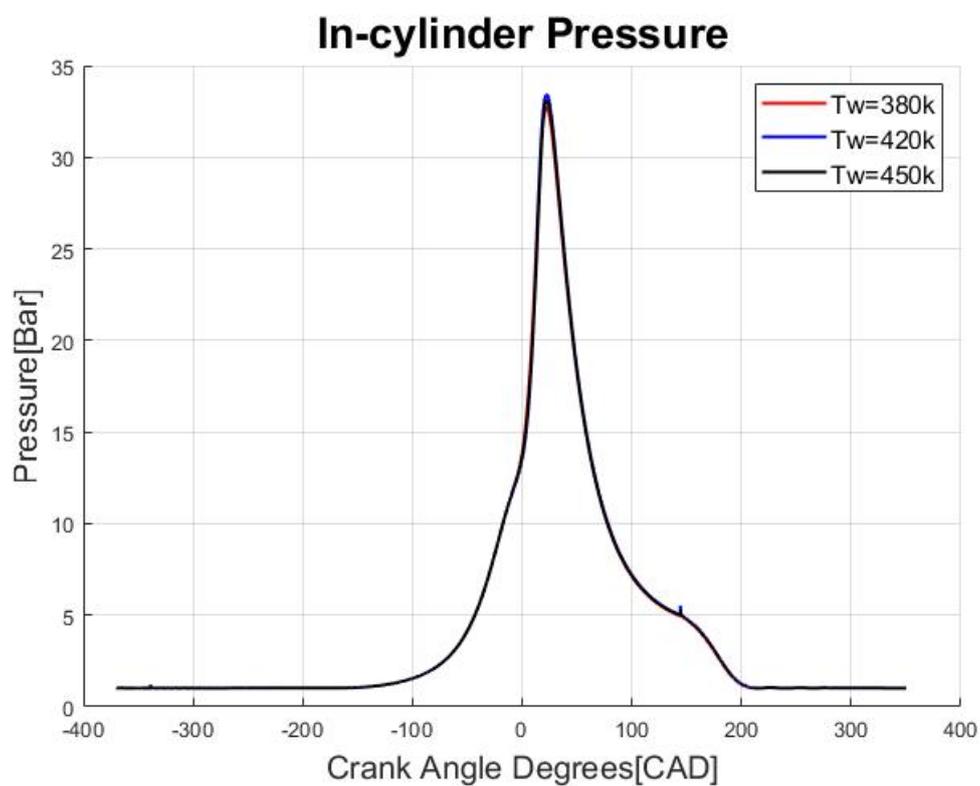


Figure 4.18: In-cylinder pressure 3-component fuel

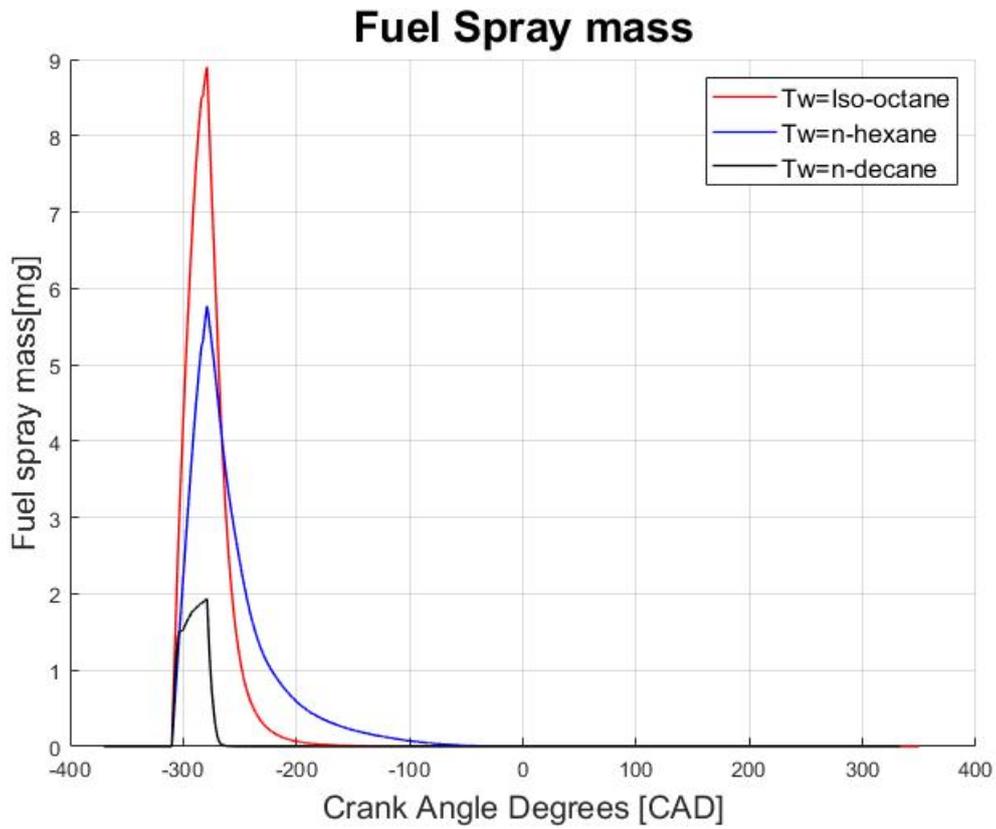


Figure 4.19: Fuel spray distribution for 3-component fuel

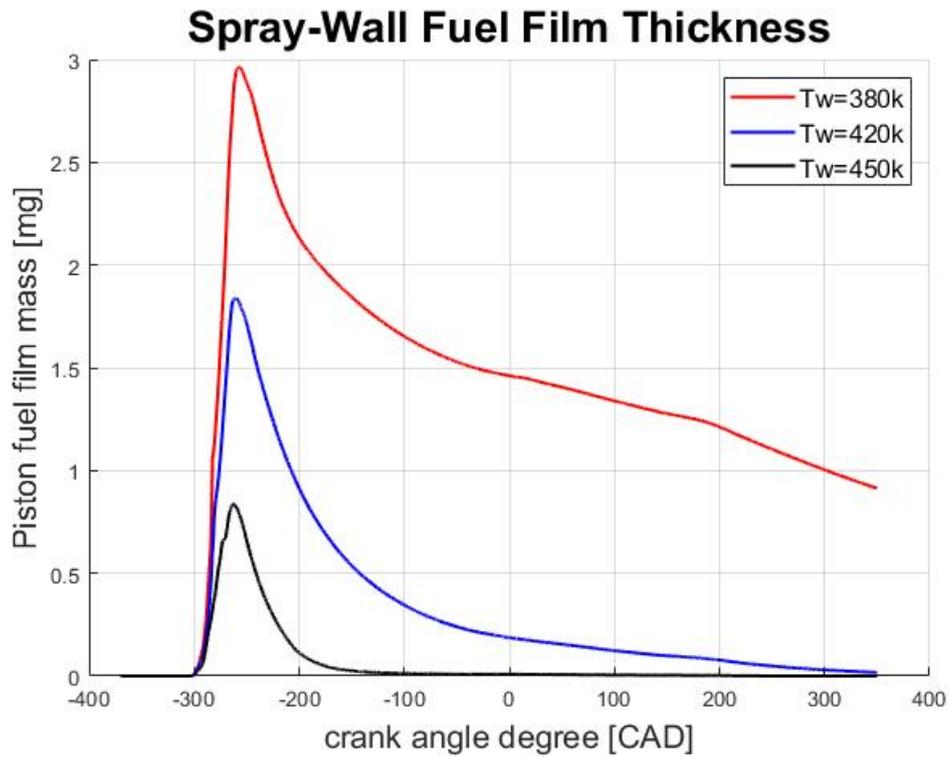


Figure 4.20: Piston fuel film mass accumulation for 3-component fuel

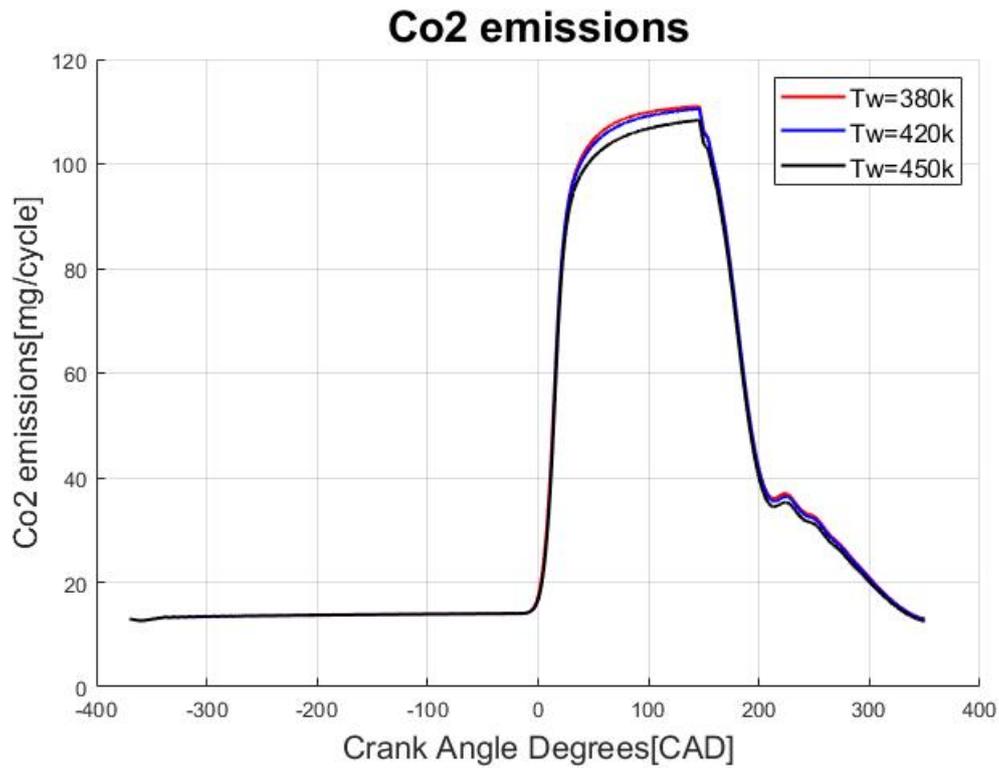


Figure 4.21: CO₂ emissions for 3-component fuel

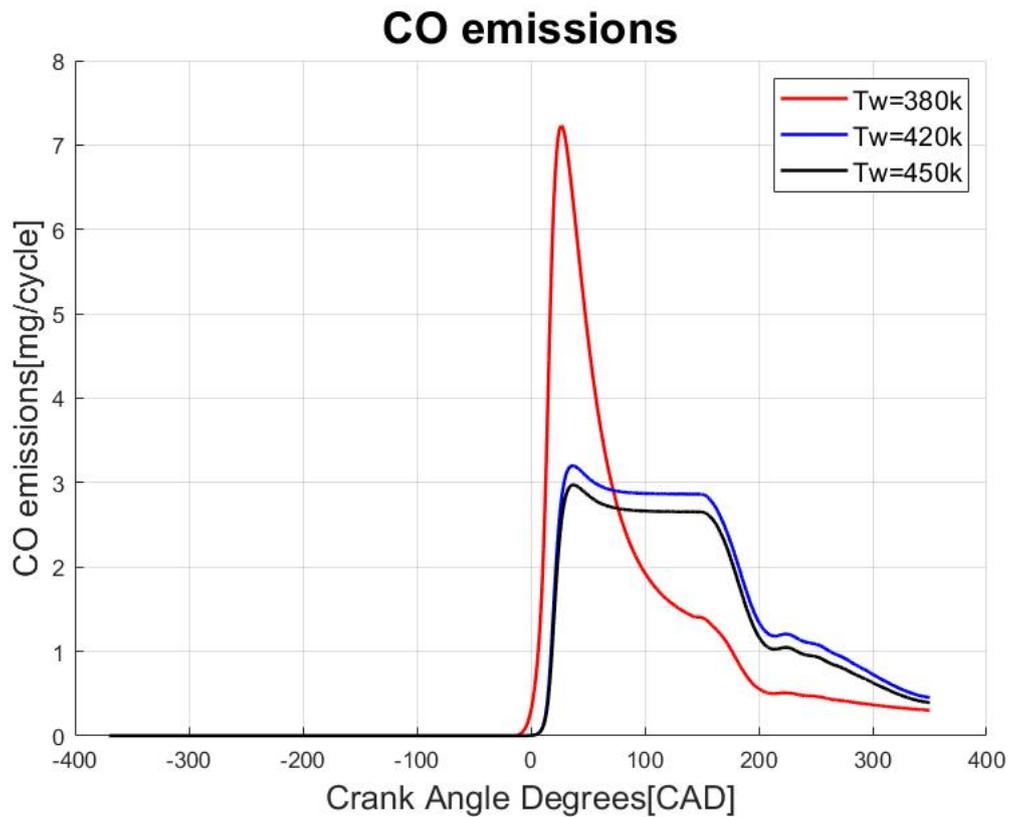


Figure 4.22: CO emissions for 3-component fuel

5

Conclusion

The overall scope of this master thesis was to introduce the effectiveness of how CONVERGE CFD simulations can be utilized to solve problems of mass accumulation on the piston of a internal combustion (IC) engine. The advanced insight into its coupled simulation characteristics, physical model, Combustion models, emissions model, and turbulence model makes CONVERGE CFD a unique simulation tool to carry further computation fluid dynamics (CFD) related work. Even though the CFD simulations take longer computational time, Converge's autonomous meshing and its integrated fuel chemistry reduces a lot of time and effort in preparing it. The results are also satisfying in all contexts, which relates and remains according to industry standards from the case setup the user prepares.

From the simulation results, we can see that the piston temperature plays a very important role in the fuel mass accumulation on the piston. Colder the piston temperature, higher will be the mass accumulation before the start of ignition. Because of the fuel chemistry variations integrated with Converge, the results are quite different for some piston temperatures. For single component fuel (iso-octane) the fuel accumulation showed a lot of inequalities because of the variations in its fuel chemistry. A mixture of two surrogate fuel provided the best result considering piston mass accumulation. There was a limited accumulation of fuel on the piston with all three temperatures. For three component mixture, because of the higher air temperature and boiling point, the fuel gets quickly evaporated, thus leaving a small fuel accumulation on the piston. Considering all the simulations results, two-component fuel gives the best results with case setup and fuel mass distribution parameter.

6

Future Work

Since the entire simulations were tested only for injection pressure of 300bar, future work can be done on varying injection pressure with 600bar, 1000bar, and 1500 bar to visualize the variations in the mixing process and film accumulation on the piston. Instead of sending the mixed fuel from the same injection, the split injection can be adopted to see how the spray distribution occurs with different boiling points. For Gasoline Direct Injection with a basic case setup, the simulation time was quite high because of the machine's lower processors. So, to minimize the simulation time, a Matlab code or change in case setup can be tested. A new CAD model or the surface file can be prepared as per the requirement and standard industry specifications so that still more detailed results can be obtained.

CONVERGE users who also have GT-SUITE licenses can use its detailed chemistry solver, multi-phase flow modelling, and advanced embedding features to calibrate and visualize GT-Suite + CONVERGE advanced coupled simulations. Engine cylinder, After-treatment, and fluid flow structure coupling can be done as extended work. Further work can be carried out with the Hydrogen fuel to study NOx and Flame burning.

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A

Appendix 1

A literature survey was done in the beginning to know more about the concepts of Computation Fluid Dynamics and Converge CFD. A example case was refereed in the beginning to study the case setup and new model was developed in the later stages. The results were also shows for three different blends of fuels.