

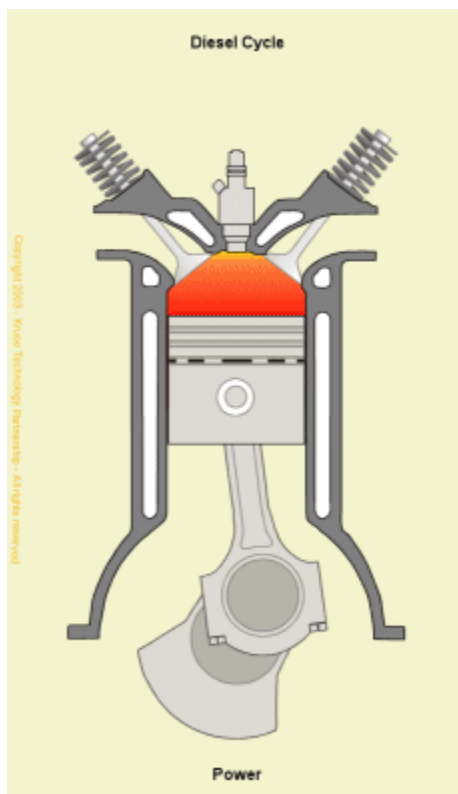
1. Title – Emission characterization on a CAT3410 engine.

2. Objective –

- To import the CAD model of engine in converge Software and check for errors.
- To make sector for both omega piston and w piston, with make engine sector surface.
- To solve the case using suitable solver and convert the result for Paraview software.
- To import output files in Paraview and generate required contours and plots.

3. Introduction –

A heat engine is a device which transforms chemical energy of a fuel into thermal energy and uses it to produce work. Mainly, Heat engine is classified into two categories External combustion engine and internal combustion engine. when the products of combustion of air and fuel transfer heat to a second fluid which is the working fluid of the cycle, then engine is called external combustion engine and when the combustion of air and fuels take place inside the cylinder and are used as the direct motive force then engine is called as internal combustion engine.



Internal combustion engine can be classified further, according to the type of fuel like petrol engine, diesel engine and gas engine. Diesel engine works on diesel cycle which was proposed by Rudolf diesel in 1892. In Diesel engine, First, air is allowed into the cylinder and the piston compresses it—but much more than in a gasoline engine. In a gasoline engine, the fuel-air mixture is compressed to about a tenth of its original volume. But in a diesel engine, the air is compressed by anything from 14 to 25 times. Air will become hotter and injection of fuel results into explosion, which pushes piston, Simply, it generated mechanical energy. Diesel engines are up to twice as efficient as gasoline engines—around 40–45 percent efficient at best.

4. Theory

Simulating internal combustion (IC) engines is challenging due to the complexity of the geometry, spatially and temporally varying conditions, and complex combustion chemistry in the engine. Converge software provides special feature to simulate IC engine. In this study we are going to simulate emission characteristics of CAT 3410 engine.

One of the biggest advancements in piston technology is the use of different piston tops or crowns, the part that enters the combustion chamber and is subjected to combustion. While older piston tops were mostly flat, many now feature bowls on top that have different effects on the combustion process. The piston bowl is primarily used in diesel engine. Diesels don't have an ignition phase, so the piston crown itself may form the combustion chamber. The shape of the piston bowl controls the movement of air and fuel as the piston comes up for the compression stroke and it contributes to expel exhaust gases during exhaust stroke as well. So, piston shape can increase the combustion efficiency. In this study we are going with two different piston configuration one is omega and second is w. We will look how piston shape effects the heat rate, pressure, temperature by plot and we will look some animation as well.

5. Procedure –

IC engine is always going to be tricky due to its complex nature. To generate desired result it is very important to choose right physical model with a perfect solver. In these of simulation it is advisable to grab right initial conditions, boundary conditions, physical model etc. because it will take a lot of time to solve. In this study we simulated emission characteristic of CAT3410 engine, for it the procedure was as followed –

1. First, we imported the model and ran diagnosis tool to find errors. We found no errors.
2. We went with the creation of sector and considered close loop analysis. Piston body divided into sectors to save simulation time.
3. In the case setup we started with crank angles-based IC engine as application type. In crank angle-based menu some parameters were defined as shown in the following image.

✓ Crank angle-based (e.g., IC engine)



Physical Parameters

Cylinder bore:	<input type="text" value="0.13716"/>	m
Stroke (2 * crank radius):	<input type="text" value="0.1651"/>	m
Connecting rod length:	<input type="text" value="0.263"/>	m
Crank offset:	<input type="text" value="0.0"/>	m
Swirl ratio:	<input type="text" value="9.78e-01"/>	
Swirl profile:	<input type="text" value="3.11e+00"/>	
Head position (Z-coordinate):	<input type="text" value="0.0"/>	
Crank speed:	<input type="text" value="1600.0"/>	RPM <input type="checkbox"/> Use file

References

Piston surface ID:	<input type="text" value="Piston"/>
Liner ID:	<input type="text" value="cylinder_wall"/>
Head ID:	<input type="text" value="cylinder_head"/>

☐ Use crevice model

Compression Ratio

OK Validate

4. In gas simulation parameter therm.dat file was imported which contains gas thermodynamic data specifically related to IC engine.

5. From the materials option parcel was enabled. In parcel simulation fuel Diesel2 was selected, which imported all the properties of fuel. Converge employs discrete Lagrangian parcels to simulate a special type of liquid in conjunction with spray modelling. In converge the Parcel simulation dialog box is for configuring properties of Lagrangian liquid parcels (such as for spray simulations).

✓ Parcel simulation

Liquid Name
DIESEL2

DIESEL2
Molecular weight: 178.6 kg/kmole
☐ Constant liquid properties
Non-Newtonian (enabled if it exists in species.in::Non-Newtonian section) **HERSCHEL_BULKLEY_MODEL**

Zero Shear Viscosity (Pa-s): 1.0 Inf Shear Viscosity (Pa-s): 1.0
Power Index: 1.0 Lambda (s): 1.0

Compressibility settings (enabled if 'Liquid flow solver' is compressible)
Reference pressure (Pa): 101325.0 Reference density (kg/m³): 848.0 Bulk modulus (Pa): 1.9e+09

Critical temperature (K): 736.0 ==> 75 rows must be specified below

	Temperature, [K]	Viscosity, [N*s/m^2]	Surface Tension, [N/m]	Heat of Vaporization, [J/kg]	Vapor Pressure, [Pa]	Conductivity, [W/(m*K)]	Density, [kg/m^3]	Specific Heat, [J/(kg*K)]
1	0	0.0047	0.03001	380000	0	0.1215	848	2167.51
2	10	0.0047	0.03001	378700	0	0.1215	848	2167.51
3	20	0.0047	0.03001	377400	0	0.1215	848	2167.51
4	30	0.0047	0.03001	376100	0	0.1215	848	2167.51

Total number of entries: 75

Predefined liquids...
Liquid calculator...

Plot Interpolate Undo Clear all

OK Validate

6. In reaction mechanism windows properties were checked to see the available species, which were imported by therm.dat file.

✓ Reaction mechanism

Available elements:
H C O N

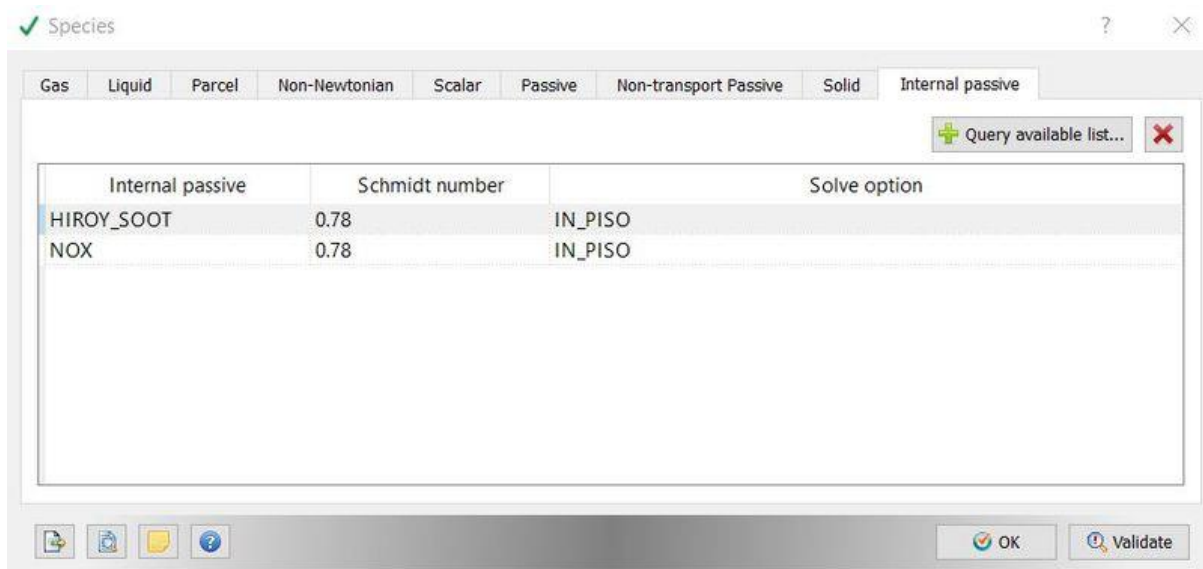
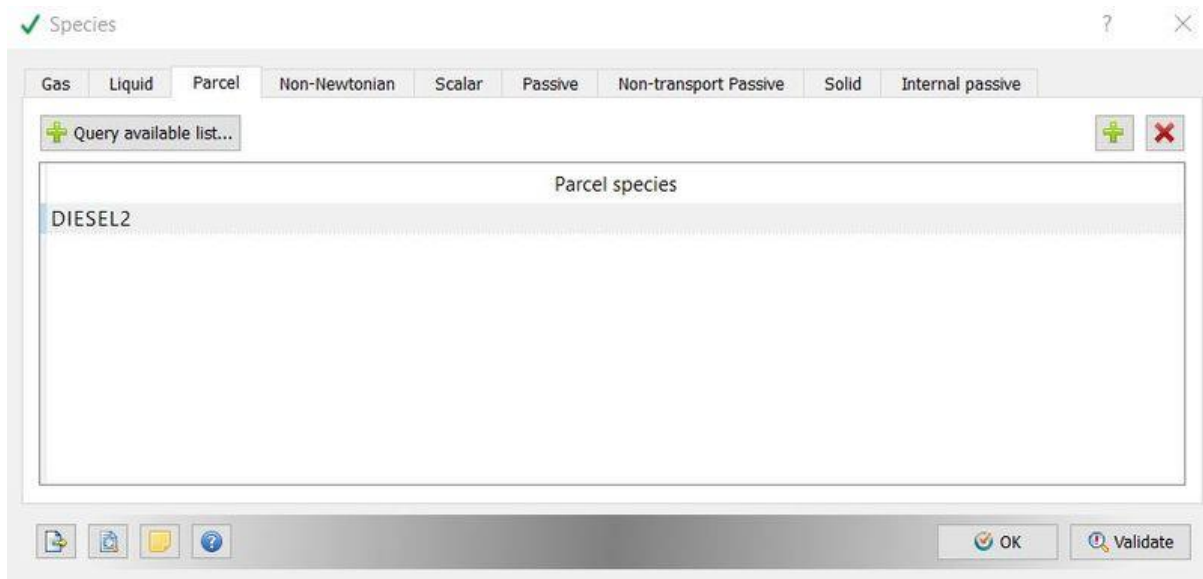
Available species:
C7H16 O2 N2 CO2 H2O CO H2 CH4 C2H2 C2H4 H2O2 HO2
OH H O CH3 CH3O CH2 CH2O CH3O2 CH4O2 HCO C7H15-1
C7H15-2 C7H15O2 C7H14O2H C7H14O2HO2 C7KET12
C6H12 C5H11CHO C5H11CO C5H11 C4H9 C3H7 C3H6 C3H5
C3H4 C2H3 C2H5 C2H6 NO N

Number of available elements: 4
Number of available species: 42
Number of available reactions: 168

Check properties

OK Validate

7. Diesel2 was defined in parcel option of species. SOOT and NOX were defined in internal passives.



8. In run parameter transient was chosen as solver type with hydrodynamic simulation mode to simulate with the effect of liquid and gases. In temporal type crank angle-based engine simulation was chosen, because we wanted to run simulation on crank angles.


✓ Run parameters ? X


Run Mode

☒ New run
☐ Restart append this number to restart output

☒ Generate surface file from current geometry ...

Solver Misc. File names Domain size


Solver: 





Temporal type: 

Simulation mode:

Gas flow solver:

Liquid flow solver:

☐ Fixed flow  (req. fixed_flow.in)

9. In simulation time parameter start and end time were specified in degrees, these were crank angles. Other parameters were defined as in the following image. Solver parameters were left as defaults.

General
Misc.

Start time:

deg

End time:

☐ from GT-SUITE

deg

Time-step selection:

Use variable time-step algorithm

Fixed time-step:

1e-08

s

Initial time-step:

1e-07

s

Minimum time-step:

1e-08

s

☐ Use file

Maximum time-step:

0.0001

s

☐ Use file

Maximum convection CFL limit:

1.0

☐ Use file

Maximum diffusion CFL limit:

2.0

☐ Use file

Maximum Mach CFL limit:

50.0

☐ Use file

Droplet motion time-step control multiple:

1.5

Drop evaporation time-step control multiple:

9999.0

Chemical time-step control multiple:

0.5

Collision grid time-step multiple:

1.0

Moving boundary time-step multiple:

0.5

☐ Use file

Set recommended values

OK
 Validate

10. There were 5 boundaries created in flagging process. Boundary conditions were given as the following images –

Boundary

☐ Has rotational axis

Axis:

Change all boundaries to WALL

ID	Color	Name	Region Name
0	[Green]	Not Assigned	Region Undefined
1	[WAL-F]	Piston	In_cylinder_region
2	[PER-F]	Front_face	In_cylinder_region
3	[PER-F]	Back_face	In_cylinder_region
4	[WAL-F]	cylinder_wall	In_cylinder_region
5	[WAL-F]	cylinder_head	In_cylinder_region

Copy Edit Regions

☐ Sort boundaries by region for export

Boundary Type: WALL

Velocity Boundary Condition

Wall motion type: Translating

Surface movement: MOVING

☐ UDF ☐ User-specified ☒ Piston motion

☐ Motion config: Motion not defined

☐ Output piston motion file 'piston_profile#.out'.

Φ :

Temperature Boundary Condition

☐ UDF ☐ CHT1D

K ☐ Use file

Law of wall roughness parameters

Absolute roughness: m

Roughness constant:

Heat model: Global

Turbulent Kinetic Energy (tke) Boundary Condition

Turbulent Dissipation (eps) Boundary Condition

Wall model:

Near wall treatment: Global

☐ Torque center




OK Validate

✓ Boundary







?

✕

☐ Has rotational axis

Axis:  0.0  1.0  0.0





Change all boundaries to WALL

ID	Color	Name	Region Name
0		Not Assigned	Region Undefined
1		Piston	In_cylinder_region
2		Front_face	In_cylinder_region
3		Back_face	In_cylinder_region
4		cylinder_wall	In_cylinder_region
5		cylinder_head	In_cylinder_region

Copy

Edit Regions

☐ Sort boundaries by region for export




   




Boundary Type: PERIODIC

Periodic Type: Stationary

Periodic Shape: Rotational

Angle: 60 degree

Rotation Axis:  0.0  0.0  1.0

Rotation Center:  0  0  0






Matching Boundary: Back_face


OK

Validate

☐ Has rotational axisAxis:  0.0 1.0 0.0

Change all boundaries to WALL

ID	Color	Name	Region Name
0		Not Assigned	Region Undefined
1		Piston	In_cylinder_region
2		Front_face	In_cylinder_region
3		Back_face	In_cylinder_region
4		cylinder_wall	In_cylinder_region
5		cylinder_head	In_cylinder_region

 Copy Edit Regions☐ Sort boundaries by region for export

Boundary Type: PERIODIC ▾

Periodic Type: Matched Boundary


Matching Boundary: Front_face

Break periodic matching dependency







OK



 Validate

☐ Has rotational axis





Axis:  0.0 1.0 0.0

Change all boundaries to WALL

ID	Color	Name	Region Name
0		Not Assigned	Region Undefined
1		Piston	In_cylinder_region
2		Front_face	In_cylinder_region
3		Back_face	In_cylinder_region
4		cylinder_wall	In_cylinder_region
5		cylinder_head	In_cylinder_region

 Copy  Edit Regions

☐ Sort boundaries by region for export

Boundary Type: WALL


Velocity Boundary Condition

Wall motion type: Stationary

Surface movement: FIXED

☐ UDF Law of wall

Temperature Boundary Condition

☐ UDF Law of wall ☐ CHT1D 

433.0 K ☐ Use file

Law of wall roughness parameters

Absolute roughness: 0.0 m

Roughness constant: 0.0

Heat model: Global


Turbulent Kinetic Energy (tke) Boundary Condition

Zero normal gradient (NE)

Turbulent Dissipation (eps) Boundary Condition

Wall model

Near wall treatment: Global

☐ Torque center  0.0 0.0 0.0

OK Validate

✓ Boundary ? X

☐ Has rotational axis

Axis:

Change all boundaries to WALL

ID	Color	Name	Region Name
0		Not Assigned	Region Undefined
1	WAL-F	Piston	In_cylinder_region
2	PER-F	Front_face	In_cylinder_region
3	PER-F	Back_face	In_cylinder_region
4	WAL-F	cylinder_wall	In_cylinder_region
5	WAL-F	cylinder_head	In_cylinder_region

Copy Edit Regions

☐ Sort boundaries by region for export

Boundary Type: WALL

Velocity Boundary Condition

Wall motion type: Stationary

Surface movement: FIXED

☐ UDF Law of wall

Temperature Boundary Condition

☐ UDF Law of wall ☐ CHT1D K ☐ Use file

Law of wall roughness parameters

Absolute roughness: m

Roughness constant:

Heat model: Global

Turbulent Kinetic Energy (tke) Boundary Condition

Zero normal gradient (NE)

Turbulent Dissipation (eps) Boundary Condition

Wall model

Near wall treatment: Global

☐ Torque center

OK Validate

11. One region was defined, which was in cylinder. Since we were analysing emission characteristics of engine, so one region was enough. Species and their mass fraction were defined as follows.

Regions and initialization

Region

Connect all regions

Automatically assign streams

ID	Region Name
0	In_cylinder_region

Copy Add Delete

Assign all boundaries into

Region count: 1

In_cylinder_region

Stream ID: 0 ☐ Solid

Velocity: 0.0 0.0 0.0 m/s

Temperature: K 355.0

Pressure: Pa 197000.0

Turbulence initialization

☒ Value ☐ Viscosity ratio/Length scale

Turbulent Kinetic Energy: 62.0271 m²/s²

Turbulent Dissipation: 17183.4 m²/s³

Species

Species Name	Mass Fraction
Sum = 1.00000	
CO2	0.0014304
H2O	0.0006296
N2	0.76765
O2	0.23029

Normalize

Passive

Passive Name	Value
HIROY_SOOT	0
NOX	0

OK Validate

12. From physical model's menu spray and combustion with emission was enabled.

13. The Spray modelling dialog box is used to configure nozzles, injectors, boundary injections, injection rate-shapes, set various spray-related constants, and choose from several injection and drop models. We started with choosing drop evaporation option with frossling model, it determines how the radius of drop changes with time.

✓ Spray modeling

General Collision/Breakup/Drag Wall Interaction Injectors Combine parcels Misc.

Parcel distribution: Cluster parcels near cone center

Turbulent Dispersion: O'Rourke model

Drop evaporation Film evaporation Penetration Mass diffusivity constants Scaling Porous media

☒ Use evaporation model

General Flash boiling

☒ Frossling model ☐ Chiang model ☐ with boiling model

Evaporation source: 0 - Source specified species

Name of sourced species: C7H16

☒ Temperature discretization

Radius above which 1D heat diffusion will be solved: 1000.0 m

Number of FV cells per spray parcel: 15

Thermal conductivity: Physical

OK Validate

Converge contains the widely used O'Rourke and NTC collision models. These models are designed to estimate the number of droplet collisions and their outcomes in a relatively computationally efficient manner. We went with NTC model, since it is faster and more accurate than O'Rourke model.

✓ Spray modeling

General Collision/Breakup/Drag Wall Interaction Injectors Combine parcels Misc.

Collision model: NTC collision

Collision outcomes: Post collision outcomes

☐ Use a collision mesh

Level for collision: 2

Drop drag model: Dynamic drop drag

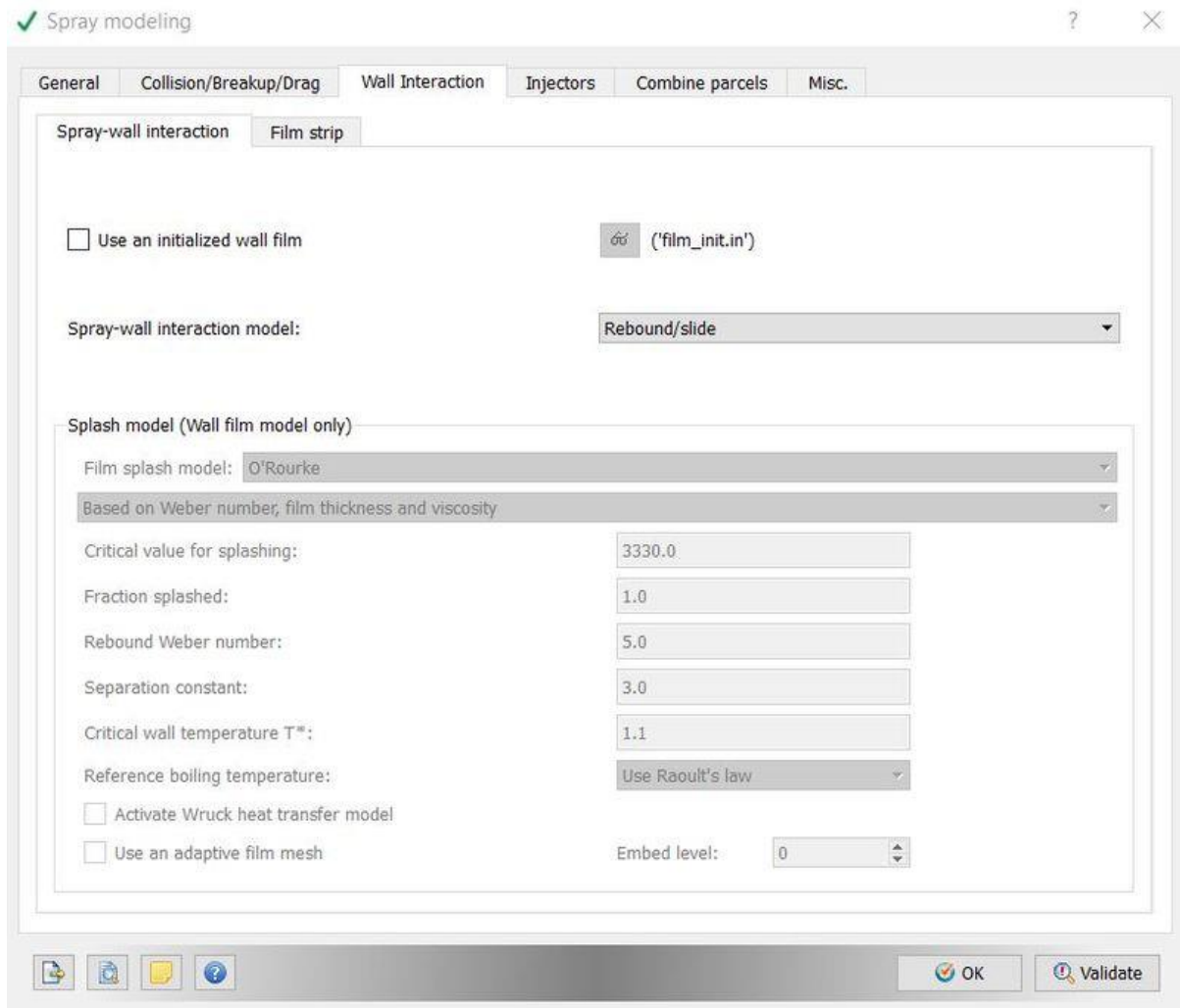
TAB/Dynamic drag var 1: 0.08333

TAB/Dynamic drag var 2: 10.0

TAB/Dynamic drag var 3: 8.0

OK Validate

In wall interaction dialog box when define how liquid interacts with the walls and its parameter. wall film model is used for the modelling the interaction of liquid drops with solid surface and it comes with wall splashing option also. To determine the splash O'Rourke model is used and spray wall interaction wall film model was used.



Converge offers two categories of liquid injection mechanisms: injectors and nozzles. An injector is a group of nozzles that have some of the same characteristics. Each injector can have any number of nozzles, each with its own hole size, cone angle, position, and orientation. We went with one nozzle with Kelvin-Helmholtz and Rayleigh-Taylor model. These models were responsible for prediction of liquid atomization and drop breakup. Time of injection, temperature, species and nozzle parameters were given as shown in following image.

General
Collision/Breakup/Drag
Wall Interaction
Injectors
Combine parcels
Misc.

+ Injector
Edit
Tools...
Remove
Remove all

Name	Assigned template	Model	Nozzles	
Injector_0	Not assigned	KH+RT	1	<input checked="" type="checkbox"/>

+ Template
Edit
Remove
Remove all

Template	Description	Common fields	Linked inj.
----------	-------------	---------------	-------------

OK
Validate

Injected Species/Rate-shape Models Time/Temp/Tke/Eps/Mass/Size Nozzles

Injected parcel species and mass fraction



	Parcel species	Mass fraction
1	DIESEL2	1.0

Normalize

Clear All

Injection rate-shape

☒ Profile

☐ Constant

☐ VOF-Spray coupling

☐ ELSA

☒ Injection using VOF data file

Max mass per parcel, kg:

Threshold:



Open 'Spray modeling' panel

Apply

OK

Injected Species/Rate-shape	Models	Time/Temp/Tke/Eps/Mass/Size	Nozzles
<div><div><div><input checked="" type="checkbox"/> Kelvin-Helmholtz model (KH) <input checked="" type="checkbox"/> Create child parcels Fraction of injected mass/parcel: <input type="text" value="0.05"/> Shed mass constant: <input type="text" value="1.0"/> Model size constant: <input type="text" value="0.61"/> Model velocity constant: <input type="text" value="0.188"/> Model breakup time constant: <input type="text" value="7.0"/> <input type="checkbox"/> KH-ACT model Config... <input type="checkbox"/> Turn off drop enlargement</div><div><input type="checkbox"/> Linearized Instability Sheet Atomization (LISA) Model breakup length constant: <input type="text" value="12.0"/> Model breakup size constant: <input type="text" value="0.5"/> No distribution with LISA Injection pressure: <input type="text" value="101300.0"/> Pa TAB secondary breakup: No distribution with TAB</div></div><div><div><input checked="" type="checkbox"/> Rayleigh-Taylor model (RT) RT model without breakup length Model breakup time constant: <input type="text" value="1.0"/> Model size constant: <input type="text" value="0.1"/> Model breakup length constant: <input type="text" value="99999.0"/> No distribution with RT</div><div><input type="checkbox"/> Taylor Analogy Breakup (TAB) No distribution with TAB <div>Additional params are available under Spray/Collision/Breakup/Drag ⚙</div></div></div><div><input checked="" type="checkbox"/> Discharge coefficient model Use correlation for Cv Discharge coefficient value: <input type="text" value="0.7"/> <input type="checkbox"/> Use file Velocity coefficient value: <input type="text" value="1.0"/> <input type="checkbox"/> Use file</div></div> <div>⚙ Set recommendations for...</div>			
<div>⚙ Open 'Spray modeling' panel 🗨 Apply ✅ OK</div>			



Injected Species/Rate-shape

Models

Time/Temp/Tke/Eps/Mass/Size

Nozzles

Nozzle location and orientation:

Polar

Holes: 2

Coordinate of injector (x, y, z):

0.0

0.0

-0.0032208

Injector rotation angle in degree (xy, xz):

0.0

0.0

Azimuth angle in degree (start, end):

0.0

360.0

Injector clock angle:

0.0

Injection spray type

☐ Hollow cone spray

☒ Solid cone spray

Swirl fraction: 0.0

+ Add nozzle

✎ Edit

✖ Remove

🗑 Remove all

Name	Assigned template	Color	Opacity	Text Color	
Nozzle_0@Injector_0	Not specified		1.0		<input checked="" type="checkbox"/>

+ Add template

✎ Edit

✖ Remove

🗑 Remove all

Template	Description	Common fields	Linked nozzles
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?

⚙ Open 'Spray modeling' panel

📄 Apply

✓ OK

Injected Species/Rate-shape Models Time/Temp/Tke/Eps/Mass/Size Nozzles

Injected parcel species and mass fraction



	Parcel species	Mass fraction
1	DIESEL2	1.0

Normalize

Clear All

Injection rate-shape

☒ Profile

☐ Constant

☐ VOF-Spray coupling

☐ ELSA

☒ Injection using VOF data file

Max mass per parcel, kg:

Threshold:



Open 'Spray modeling' panel

Apply

OK

Injected Species/Rate-shape	Models	Time/Temp/Tke/Eps/Mass/Size	Nozzles
<div><div><input checked="" type="checkbox"/> Kelvin-Helmholtz model (KH) <input checked="" type="checkbox"/> Create child parcels Fraction of injected mass/parcel: <input type="text" value="0.05"/> Shed mass constant: <input type="text" value="1.0"/> Model size constant: <input type="text" value="0.61"/> Model velocity constant: <input type="text" value="0.188"/> Model breakup time constant: <input type="text" value="7.0"/> <input type="checkbox"/> KH-ACT model Config... <input type="checkbox"/> Turn off drop enlargement</div><div><input type="checkbox"/> Linearized Instability Sheet Atomization (LISA) Model breakup length constant: <input type="text" value="12.0"/> Model breakup size constant: <input type="text" value="0.5"/> No distribution with LISA Injection pressure: <input type="text" value="101300.0"/> Pa TAB secondary breakup: No distribution with TAB</div></div>			
<div><div><input checked="" type="checkbox"/> Rayleigh-Taylor model (RT) RT model without breakup length Model breakup time constant: <input type="text" value="1.0"/> Model size constant: <input type="text" value="0.1"/> Model breakup length constant: <input type="text" value="99999.0"/> No distribution with RT</div><div><input type="checkbox"/> Taylor Analogy Breakup (TAB) No distribution with TAB <div>Additional params are available under Spray/Collision/Breakup/Drag ⚙</div></div><div><input checked="" type="checkbox"/> Discharge coefficient model Use correlation for Cv Discharge coefficient value: <input type="text" value="0.7"/> <input type="checkbox"/> Use file Velocity coefficient value: <input type="text" value="1.0"/> <input type="checkbox"/> Use file</div></div>			
<div>⚙ Set recommendations for...</div>			
<div>⚙ Open 'Spray modeling' panel Apply OK</div>			

✓ [Injector_0] configuration

?

✕

Injected Species/Rate-shapeModelsTime/Temp/Tke/Eps/Mass/SizeNozzles

MainTemperature/Tke/Eps

Injection temporal type:

CYCLIC

▼

Cyclic period:

720.0

deg

Start of injection:

-9.0

deg

☐ Use file

Injection duration:

21.0

deg

☐ Use file

Total injected mass:

2.70167e-05

kg

☐ Use file

Total number of injected parcels (per nozzle):

50000

Injection drop distribution:

☒ Predefined☐ User-defined

Blob (specified nozzle diameter)

▼

Rosin-Rammler parameter:

3.5

?

⚙️ Open 'Spray modeling' panel

📄 Apply

👌 OK

✓ [Injector_0] configuration

Injected Species/Rate-shape Models Time/Temp/Tke/Eps/Mass/Size **Nozzles**

Nozzle location and orientation: Polar Holes: 2

Coordinate of injector (x, y, z): 0.0 0.0 -0.0032208

Injector rotation angle in degree (xy, xz): 0.0 0.0

Azimuth angle in degree (start, end): 0.0 360.0

Injector clock angle: 0.0

Injection spray type

☐ Hollow cone spray

☒ Solid cone spray

Swirl fraction: 0.0

+ Add nozzle Edit Remove Remove all

Name	Assigned template	Color	Opacity	Text Color	
Nozzle_0@Injector_0	Not specified		1.0		<input checked="" type="checkbox"/>

+ Add template Edit Remove Remove all

Template	Description	Common fields	Linked nozzles

Open 'Spray modeling' panel Apply OK

14. Combustion model is responsible for the chemical reactions and kinetics during combustion. We chose SAGE model, which solves for chemical reaction mechanism and its related parameters. In general setting, the time of combustion were defined in form of crank angles means combustion will take place between crank angle -10 to 135degrees.

General

Models (SAGE)

Fuel species name: C7H16

Timing/Activation

Output

Temporal type:

SEQUENTIAL

Cyclic period:

0.0

deg

Start time:

-10.0

deg

End time:

135.0

deg

Regions:

Not region-dependent

Combustion temperature cutoff:

600.0

K

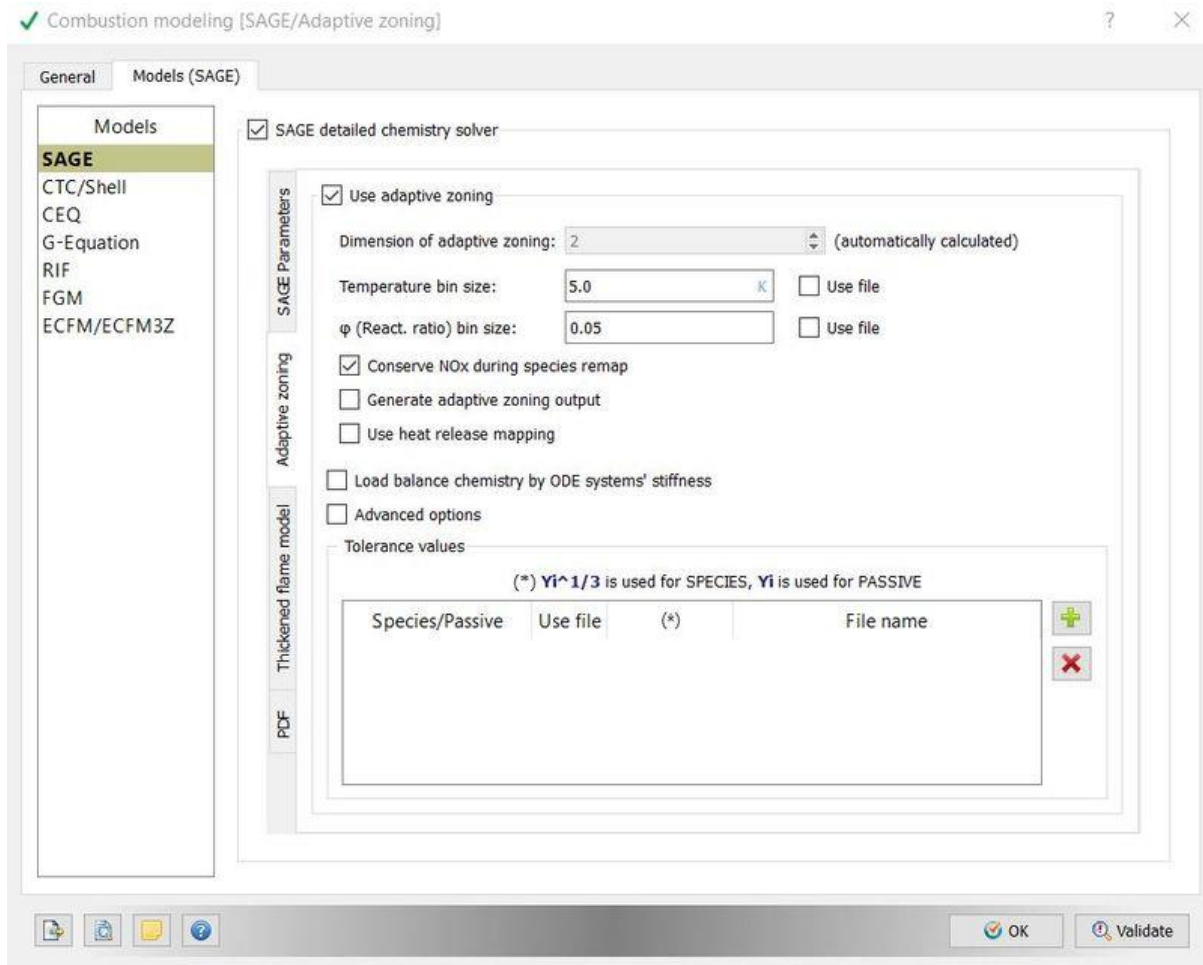
Minimum HC species mole fraction:

1e-08

☒ Emissions model

OK

Validate




15. Converge provides many models to simulate NO_x and SOOT production. Species of interest such as CO, CO₂, and unburned hydrocarbons are always calculated or interpolated in CONVERGE, provided they are included in the reaction mechanism file and are a part of the combustion model used by the simulation.

✓ Emissions modeling ? ✕

NOx models Hiroyasu-NSC soot model Phenomenological soot models Detailed soot models

☒ Thermal NOx model (Extended Zeldovich)

☐ Thermal NOx rate flag (passive_nox_rate.dat) 

O/OH models for the thermal NOx (Extended Zeldovich)

☒ Equilibrium assumption (default)

☐ Partial equilibrium assumption



☐ No assumption (requires O and OH in mech.dat)





☐ Prompt NOx model flag

Equivalence ratio

Mass scaling factor converting NO to NOx

☐ Specify custom soot precursors

OK Validate

There are two NOx models one is thermal NOx and other one is prompt NOx. Prompt NOx model predicts formation of NO at low temperature fuel rich conditions and it is suitable for gas turbines. So, we chose thermal NOx model.

✓ Emissions modeling

NOx models Hiroyasu-NSC soot model Phenomenological soot models Detailed soot models

☒ Use Hiroyasu-NSC soot model

Soot pre-exponential formation rate factor: 350.0 (s*bar^{0.5})⁻¹

Soot activation energy in the formation rate: 12500.0 cal/gmol

Soot particle diameter: 2.5e-06 cm

Soot oxidation rate factor: 1.0

Soot density: 2.0 g/cm³

Formation species

☒ Use total hydrocarbons for formation species

☐ Use C2H2 for formation

☐ Specify custom soot precursors

OK Validate

The soot models in converge describe the complex soot formation and oxidation process using several global steps, including soot inception, surface growth, coagulation, and oxidation. Phenomenological and detailed soot model are computationally expensive. So we went with empirical model.

16. We chose k-epsilon turbulent model and base grid was chosen as 0.004m, since we would enable fixed embedding and AMR the global grid size won't be a big problem.

✓ Base grid

?


✕


☐ Automatic relofting


Base grid size

dx, dy, dz:

Grid Preview













Suggestion from target cell count

Cell count estimation

 OK  Validate

17. Adaptive mesh refinement option was enabled to get finer mesh. This option is very important because you cannot deploy same sized mesh on whole model. Velocity and temperature were two criteria which chosen for AMR. In velocity criteria sub grid criteria was 2m/s means above it, cell will be become finer by a factor of 2^n , here n is embedded level, in our case it is 2 and mesh will get finer by 4 times. Similarly, when sub grid temperature goes beyond 5K mesh will get finer by a factor of 4.

Cycle steady: 100

☐ Use file

Minimum cells: 1

☐ Use file

Embed frequency: 1

☐ Use file

*(for 'Steady-state solver' only)

Maximum cells: 2000000

☐ Use file

Release frequency: 25

☐ Use file

AMR Groups

Boundary

Release

Proximity

AMR Group 2

AMR Group 2

Available Regions

Active Regions

In_cylinder_region

<=

=>

Edit Regions

☒ Velocity ☒ Temperature ☐ Pressure ☐ Density ☐ Species ☐ Passive ☐ Void fraction

Embed type: Sub-grid scale (SGS)

Timing control type: PERMANENT

Max embedding level: 2

Start: deg

Sub-grid criterion: 2.0 m/s

End: deg

Embed criterion[0]:

Cycle period: 720.0 deg

Embed criterion[1]:

Use AMR when parcel count exceeds: 50

Add

Delete



OK

Validate

✓ Adaptive Mesh Refinement

Cycle steady: 100 ☐ Use file Minimum cells: 1 ☐ Use file Embed frequency: 1 ☐ Use file
 "(for 'Steady-state solver' only) Maximum cells: 2000000 ☐ Use file Release frequency: 25 ☐ Use file

AMR Groups Boundary Release Proximity

AMR Group 2

Available Regions

Active Regions
In_cylinder_region

≤ ≥

Edit Regions

☒ Velocity ☒ Temperature ☐ Pressure ☐ Density ☐ Species ☐ Passive ☐ Void fraction

Embed type: Sub-grid scale (SGS) Timing control type: SEQUENTIAL

Max embedding level: 2 Start: -12.0 deg

Sub-grid criterion: 5.0 K End: 180.0 deg

Embed criterion[0]: Cycle period: 720.0 deg

Embed criterion[1]:

+ Add - Delete

OK Validate

18. Fixed embedding option was enabled from grid control menu. Fixed embedding makes finer mesh of the basis of time or on the basis of crack angles. It is different from AMR because AMR option was dependent on the particular cell property. Fixed embedded was applied around nozzle, piston and around the boundary of cylinder. The parameter can be seen by following images.

☒ Show all
 ☐ Hide all

Fixed embedding

- ☒ Embedding 1 NOZ
- ☒ Embedding 2 BND
- ☒ Embedding 3 BND

Entity type: NOZZLE

Mode: SEQUENTIAL

Period (cyc. mode): 0.0 deg

Scale: 2

Start time: -12.0 deg

End time: 15.0 deg

Injector ID: Injector_0

Nozzle ID: Nozzle_0@Injector_0

Radius 1: 0.001 m

Radius 2: 0.003 m

Length: 0.01 m

☒ Render volume

☐ Comment out embedding when exporting

+ Add
 ✕ Delete
 📄 Copy

OK
Validate

☒ Show all
 ☐ Hide all

Fixed embedding

<input checked="" type="checkbox"/> Embedding 1	NOZ
<input checked="" type="checkbox"/> Embedding 2	BND
<input checked="" type="checkbox"/> Embedding 3	BND

Entity type: BOUNDARY

Boundary ID: Piston

Mode: SEQUENTIAL

Period (cyc. mode): 0.0 deg

Scale: 1

Embed Layers: 1

Start time: -20.0 deg

End time: 180.0 deg

☒ Render volume

☐ Comment out embedding when exporting

+

 Add

✕

 Delete

Copy

OK

Validate

Fixed embedding

☒ Show all ☐ Hide all

Entity type: BOUNDARY

Boundary ID: cylinder_head

Mode: SEQUENTIAL

Period (cyc. mode): 0.0 deg

Scale: 1

Embed Layers: 1

Start time: -20.0 deg

End time: 180.0 deg

☒ Render volume

☐ Comment out embedding when exporting

Fixed embedding

- ☒ Embedding 1 NOZ
- ☒ Embedding 2 BND
- ☒ Embedding 3 BND

☒ Add ☒ Delete ☒ Copy

☒ OK ☒ Validate

19. Time interval for writing 3D output data files was set to 2second for writing text output it was 0.1 second, other parameters of output files was left as default.

✓ Output files ? X

Output generation Species output Writing time intervals Custom time unit

Time interval for writing 3D output data files: 2.0 deg ☐ Use file

Time interval for writing text output: 0.1 deg ☐ Use file

Time interval for writing restarting output: 5.0 deg ☐ Use file

Maximum wall-clock time between writing restart files: 1.0 hours

Write restart file based on: Simulation time (s/crank angle/cycle)

Time interval for writing heat transfer data: 10.0 deg ☐ Use file

Maximum number of restart files saved: 5

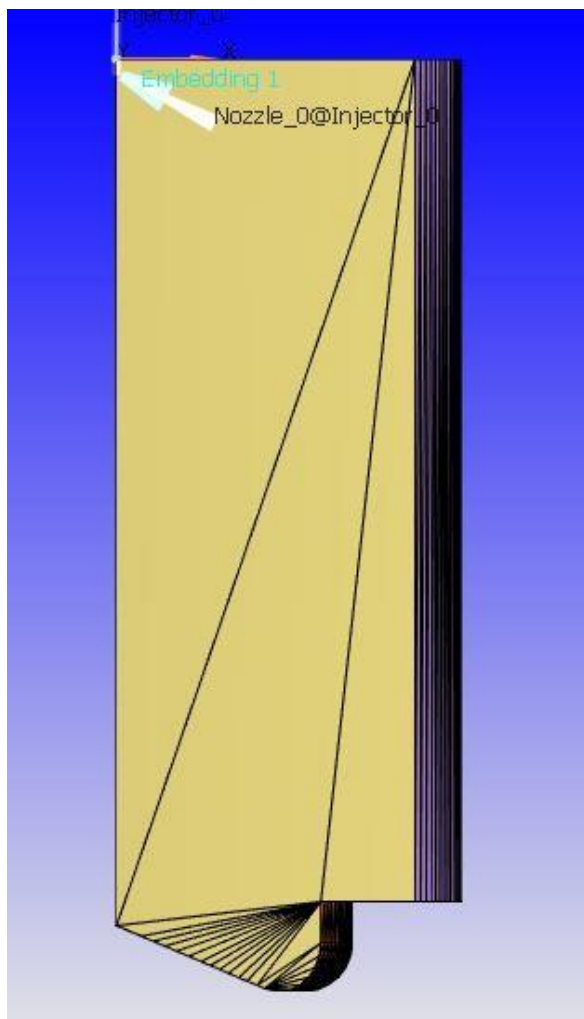
☐ Generate map files

OK Validate

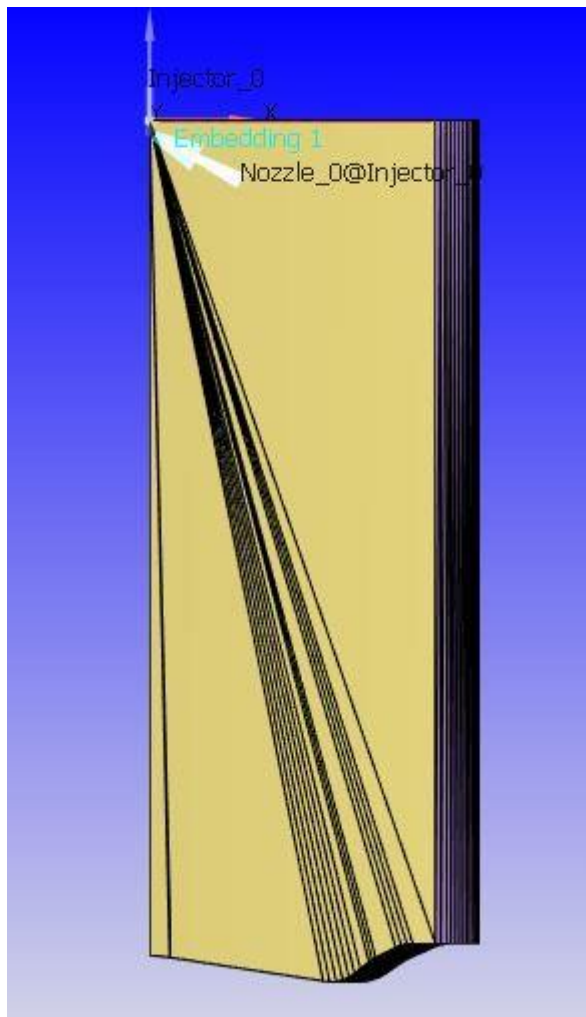
6. Results –

Geometry -

Omega piston -

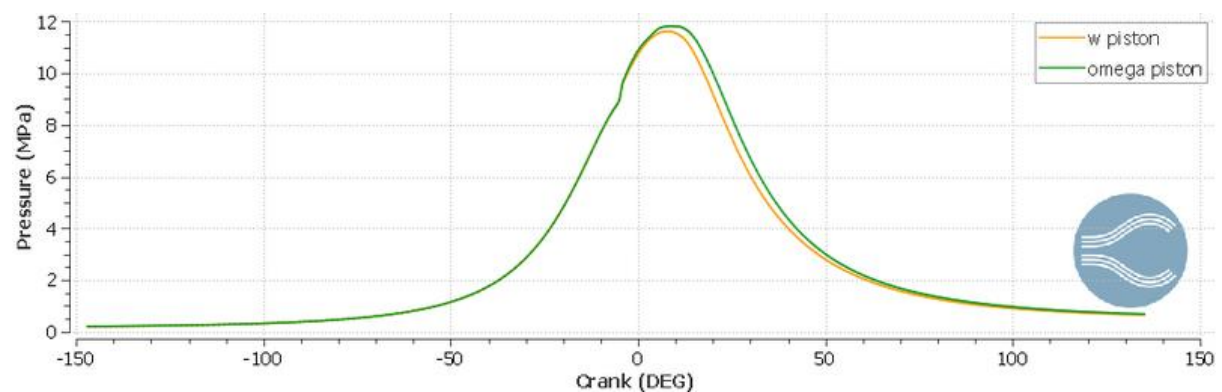


w piston -

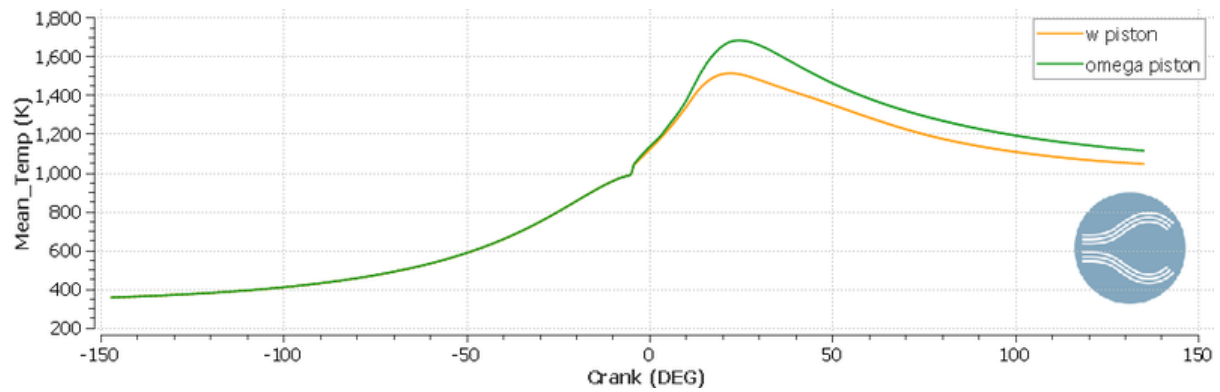


Useful plots and animations were generated to compare the piston profiles. Its very difficult to choose one of the them, because they have their own advantages. Animations were created to see spray wall interaction and piston movement.

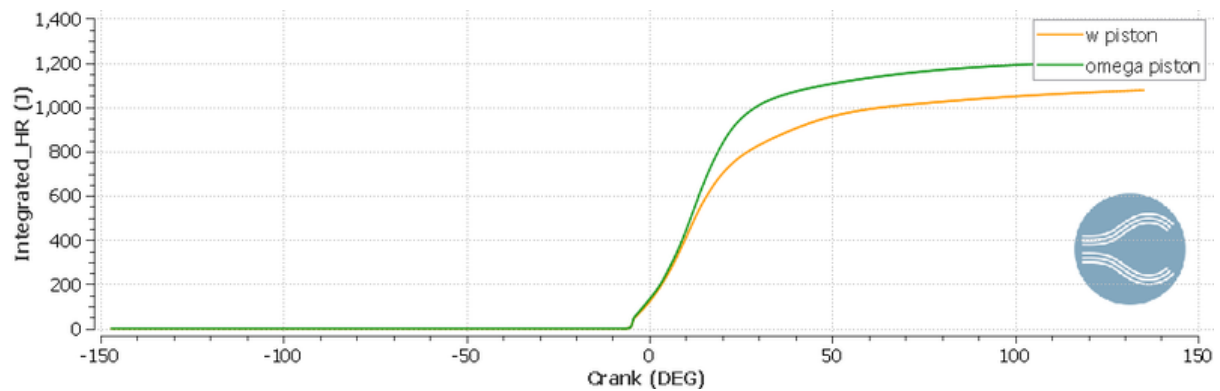
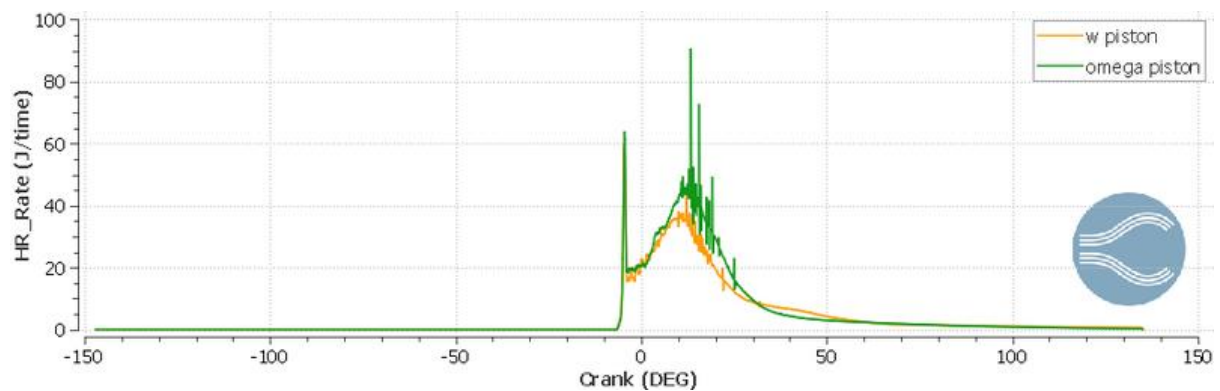
1. We if look at the pressure plot, we can see we are getting higher pressure by omega piston, but we cannot declare it best only on this criteria.



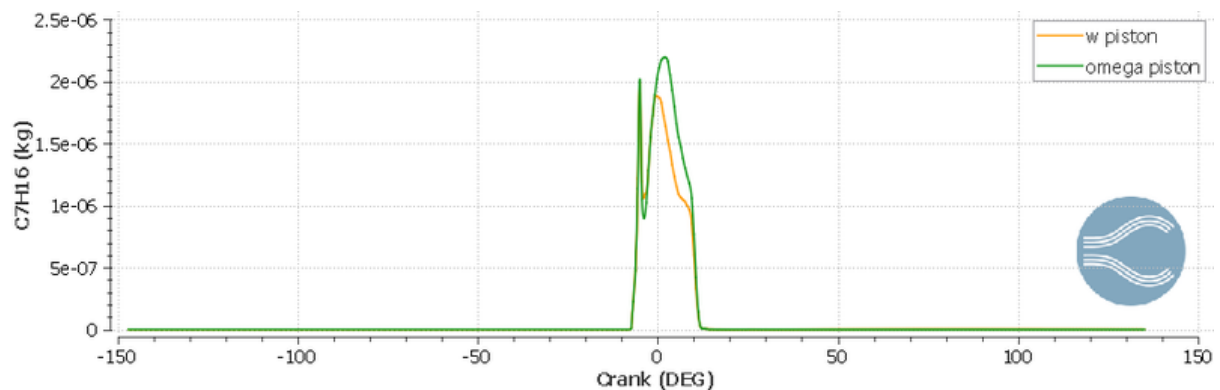
2. Now, look at the mean temperature plot. For w piston mean temperature is low, we can assume there might be some fuel which is unburn, but we have to see further criteria to validate it. Low temperature gives us lower amount of NOx as well.



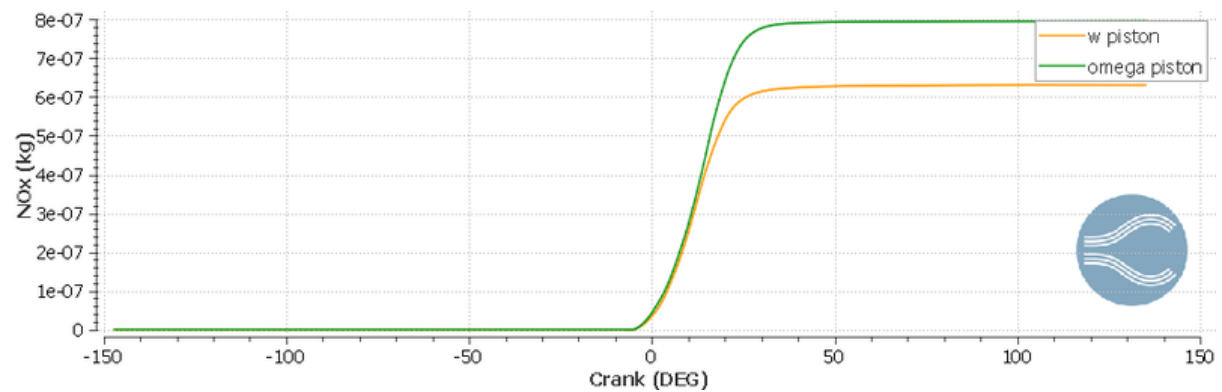
3. Now come to heat rate and integrated heat rate plots. Omega piston has higher heat release rate, that why it has higher temperature compared to omega piston. Integrated heat release rate is accumulation of heat released during whole cycle. IHR is higher for omega piston.



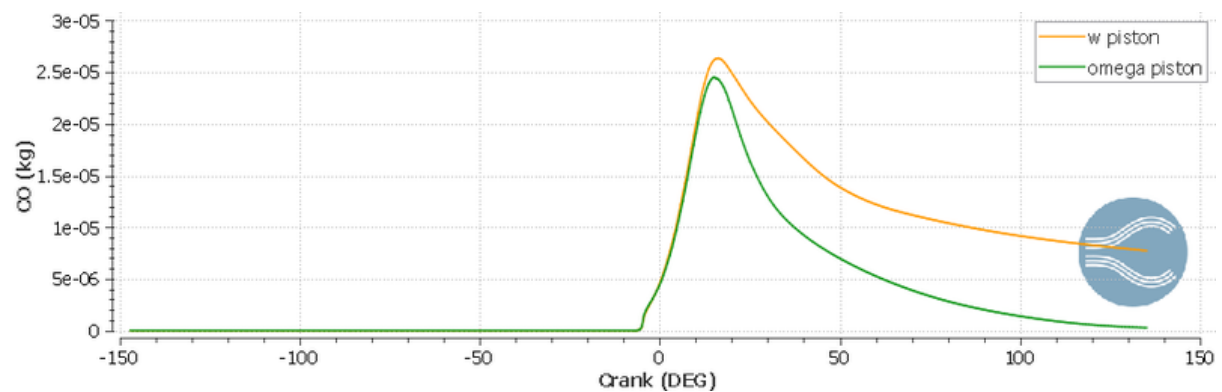
4. If we look the following plot, we can say omega piston has higher gases fuel, which is being burned lately, it can be verified from IHR plot also.



5. With omega piston there is lower NOx and it can be selected, if it someone targets lower NOx.



6. Open w piston has larger amount of carbon mono oxide, so we can say there is a lot of unburn fuel.



7. Omega piston produces lower soot, again, someone can choose it, if he is targeting lower Soot.

