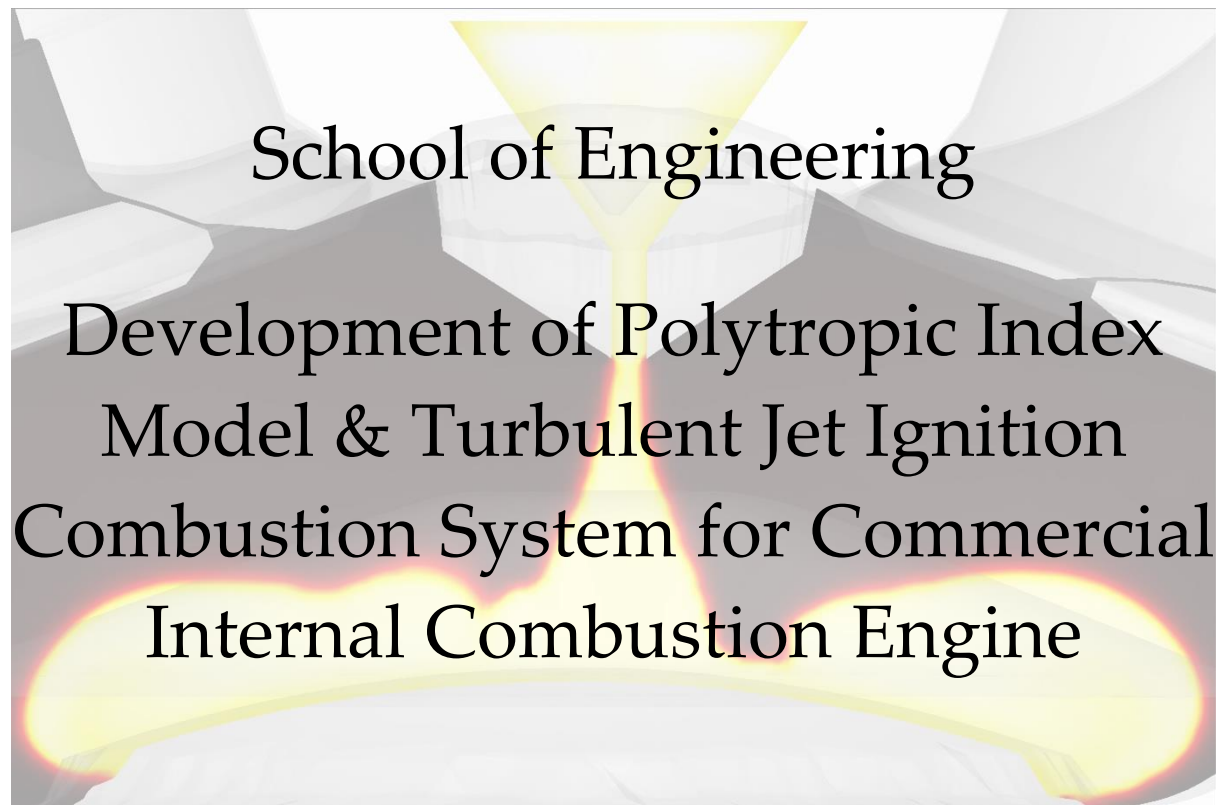




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**Development of Polytropic Index
Model & Turbulent Jet Ignition
Combustion System for Commercial
Internal Combustion Engine**

Major Project M6X00417

BEng: Motorcycle Engineering

MAY, 2020

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I would like to thank my family, Mr. Malcolm McDonald & Mr. Owen Williams from University of Wales Trinity Saint David, as well as Mike Parry from Race Techniques Ltd. for supporting me over the years.

PREFACE

Additional figures such as pictures and videos/ animations, as well as information have been attached in the corresponding Appendix chapters, which portray the additional work that was carried out by the author but wasn't talked about in the main body.

1 TABLE OF CONTENTS

Preface.....	0
2 Nomenclature	4
2.1 Symbols	4
2.2 Subscripts	5
2.3 Notations.....	6
2.4 Abbreviations	6
3 Introduction	9
4 Polytropic Index Model.....	10
4.1 0D Model Introduction.....	10
4.2 Combustion Efficiency	11
4.3 Heat Transfer Model.....	13
4.4 Heat Release Rate.....	23
4.5 2-Zone Combustion Model.....	25
4.6 Ratio of Specific Heats in un-Burnt Zone	27
4.7 Dissociated Ratio of Specific Heats in Burnt Zone	29
4.8 Thermal Equilibrium Error Correction.....	36
4.9 Polytropic Index During Combustion.....	39
4.10 Polytropic Index During Combustion: Conclusion.....	43
5 Measurements & Experiments	44
5.1 Geometrical Acquisition.....	44
5.1.1 Engine Components.....	44
5.1.2 Valve Lift Profiles.....	45
5.2 Flow-Bench Experiment.....	46
5.2.1 Method.....	46

5.2.2	Results.....	47
5.2.3	Flow Turbulence Utilising Pyrotechnics.....	48
5.3	Flow-Bench 3D Model Validation	49
5.3.1	Method.....	49
5.3.2	Validation.....	50
5.4	Spray Experiment.....	51
6	3-Dimensional Engine Modelling	53
6.1	Modelling Original Ford Fox GTDI Engine	53
6.1.1	Case Setup	53
6.1.2	Model Validation.....	56
6.2	Modelling Turbulent Jet Ignition.....	61
6.2.1	Aims and Limitations	61
6.2.2	Determining the Case Specifications & Simulation Results.....	61
6.2.3	Comparison of Case Results	62
6.2.3.1	Pre-Chamber Geometry: A, B & C.....	67
6.2.3.2	Nozzle Diameter: B, D & E	70
6.2.3.3	Nozzle Geometry: B & F.....	71
6.2.3.4	Pre-Chamber Mixture: B & G	72
6.2.3.5	Nozzle Count: G & H.....	74
6.2.4	Final TJI Setup	76
6.2.4.1	Comparison of Final TJI System.....	76
6.2.4.1.1	Cylinder Pressure.....	77
6.2.4.1.2	Mass Fraction Burned & Burn rate	78
6.2.4.1.3	Thermal Efficiency	79
6.2.4.1.4	NOx Production, Temperatures & O2 Levels	80
7	Conclusion	82

8	References	84
9	Appendix.....	87
9.1	Heat Transfer Model.....	87
9.2	2-Zone Combustion Model.....	101
9.3	Ratio of Specific Heats.....	106
9.4	Polytropic Index During Combustion.....	111
9.5	Geometrical Acquisition.....	118

2 NOMENCLATURE

2.1 SYMBOLS

A	area
C	specific heat capacity
E	energy
G	Gibbs free energy
h	convective heat transfer coefficient
h _f	specific enthalpy of formation
k	conductive heat transfer coefficient or reaction rate
K	equilibrium constant
m	mass
M	molecular weight
mol	number of moles
n	polytropic index
P	pressure
p _p	partial pressure
Q	heat
$\dot{Q}$	heat transfer rate
R	gas constant
s	wall thickness
T	temperature
V	volume
x	substance
γ	ratio of specific heats

η	efficiency
λ	air fuel ratio
φ	fuel air ratio

2.2 SUBSCRIPTS

$\sim$	molar
a	air
avg	average
Burnt	burnt zone
c	combustion
co	cooling
f	fuel
F	forward
g	gas
gc	gas convective
gr	gas radiative
i	at current instance
i - 1	one instance before current
l	lost
m	motored or mixture
p	products
R	reverse
r	released
re	reactants

u	universal
un-Burnt	un-burnt zone
w _i	internal wall
w _o	external wall

2.3 NOTATIONS

$\bar{}$	averaged over certain period
d	rate
[]	concentration
Δ	difference

2.4 ABBREVIATIONS

ABDC	after bottom dead centre
AFR	air fuel ratio
AMR	adaptive mesh refinement
ATDC	after top dead centre
BBDC	before bottom dead centre
BDC	bottom dead centre
BTDC	before top dead centre
C.A.	crank angle
CAD	computer aided design
CFD	computational fluid dynamics
D.C.E.	Dissociation Calculation Error
DCCM	dissociation completion correction multiplier

DES	detached eddy simulation
DI	direct injector
EGR or RRI	residual exhaust gas
EOC	end of combustion
EV	exhaust valve
EVC	exhaust valve closing
EVO	exhaust valve opening
GTDI	gasoline turbocharged direct injected
GTTJI	gasoline turbocharged turbulent jet ignited
H	cylinder-head
HC	hydrocarbon
HRR	heat release rate
HTCMC	heat transfer correction multiplier during compression
HTCME	heat transfer correction multiplier during expansion
IC8H18	iso-octane
ICE	internal combustion engine
IT	ignition timing
IV	intake valve
IVC	intake valve closing
IVO	intake valve opening
L	liner
LES	large eddy simulation
LHV	lower heating value
Mch	main chamber
MFB	mass fraction burned

MS	Microsoft
OEM	original equipment manufacturer
P	piston
Pch	pre-chamber
PD	potential difference
RANS	Reynolds averaged Navier stokes equations
RNG	re-normalisation group
rpm	revolutions per minute
SI	spark ignition
SOC	start of combustion
SOI	start of injection
T	total
TDC	top dead centre
TJI	turbulent jet ignition
VBA	visual basic for applications

3 INTRODUCTION

Powertrain industry is under pressure to create engines which produce less emissions, more power and require less fuel, more than ever before due to environmentally driven legislation, as well as the increasing consumer competitiveness of electrification. One of the technologies proven to greatly benefit the ICE efficiency is TJI. As the technology is still novel for the industry, author has decided to investigate TJI systems and develop feasible design which can be relatively easily and cheaply implemented into the Ford Ecoboost 1.0l inline 3, codenamed “Fox”. To do so, author at first developed a novel 0D self-correcting combustion analysis model, which calculated the real polytropic index during combustion and so, allowed for more accurate calculation of HRR. Converge CFD package was used to simulate 3D combustion, in the stock ICE, as well as eight different TJI designs. Final design has been chosen based on combustion performance. Author has carried out extensive literature research as shown by the use of references to ensure valid application of methods and theories throughout the project.

4.2 COMBUSTION EFFICIENCY

Due to the many complicated phenomena which occur inside the combustion chamber, author believes that to achieve confident HRR results, it is crucial to firstly determine the total released heat, which Author has calculated by utilising the analysis of the exhaust gases, as shown in Equation 1, to accurately determine the combustion efficiency as shown in Figure 4-2.

$$\eta_c = 1 - \frac{\sum_i x_i LHV_i}{\frac{m_f}{m_m} * LHV_f}$$

Equation 1: Combustion Efficiency (Heywood, 1988, p. 154)

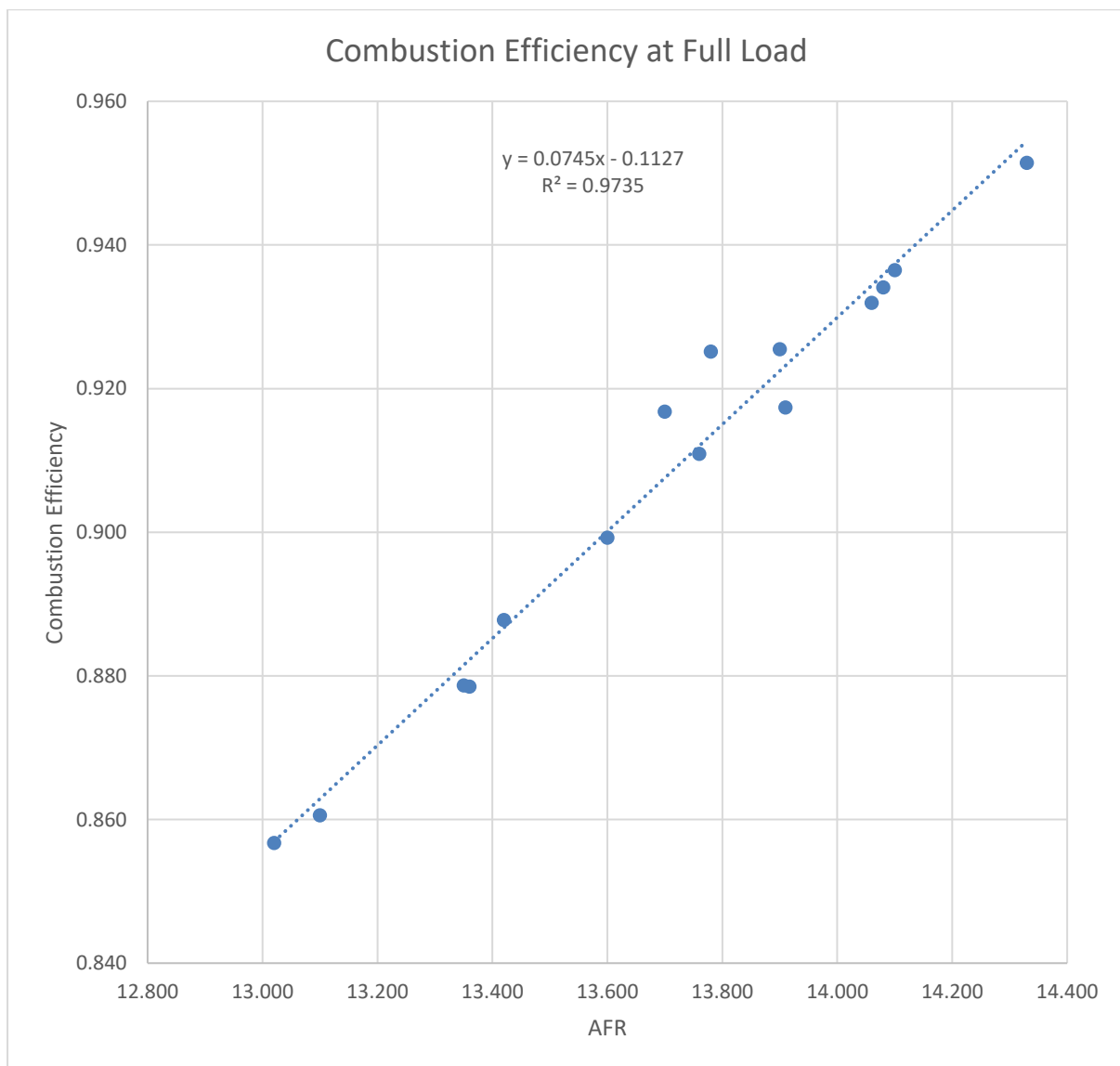


Figure 4-2: Combustion Efficiency @ Full Load

Figure 4-2 shows a clear positive linear correlation with a R^2 value of 0.97, between combustion efficiency and “in-cylinder” AFR. This is primarily due to the chemistry of combustion: as concentration of O_2 increases, it is more likely for the hydrocarbon molecules to collide and react with the O_2 molecules, thus causing more complete combustion. Although other parameters such in-cylinder turbulence, local mixture qualities etc. affect combustion efficiency as well but with much smaller effect. It, estimation of “in-cylinder” AFR by Ford, as well as the gas analyser measurement tolerance, are the primal reasons why perfectly linear correlation hasn’t been established. Additionally, due to lack of data on the H_2 quality in the exhaust gasses, author wasn’t able to account for all combustables, which is why author believes the calculated combustion efficiencies to be overestimated. Despite this, author still had the most confidence in this method because of the input’s un-affiliation with rest of the model and very good correlation with the results shown in Figure 4-3.

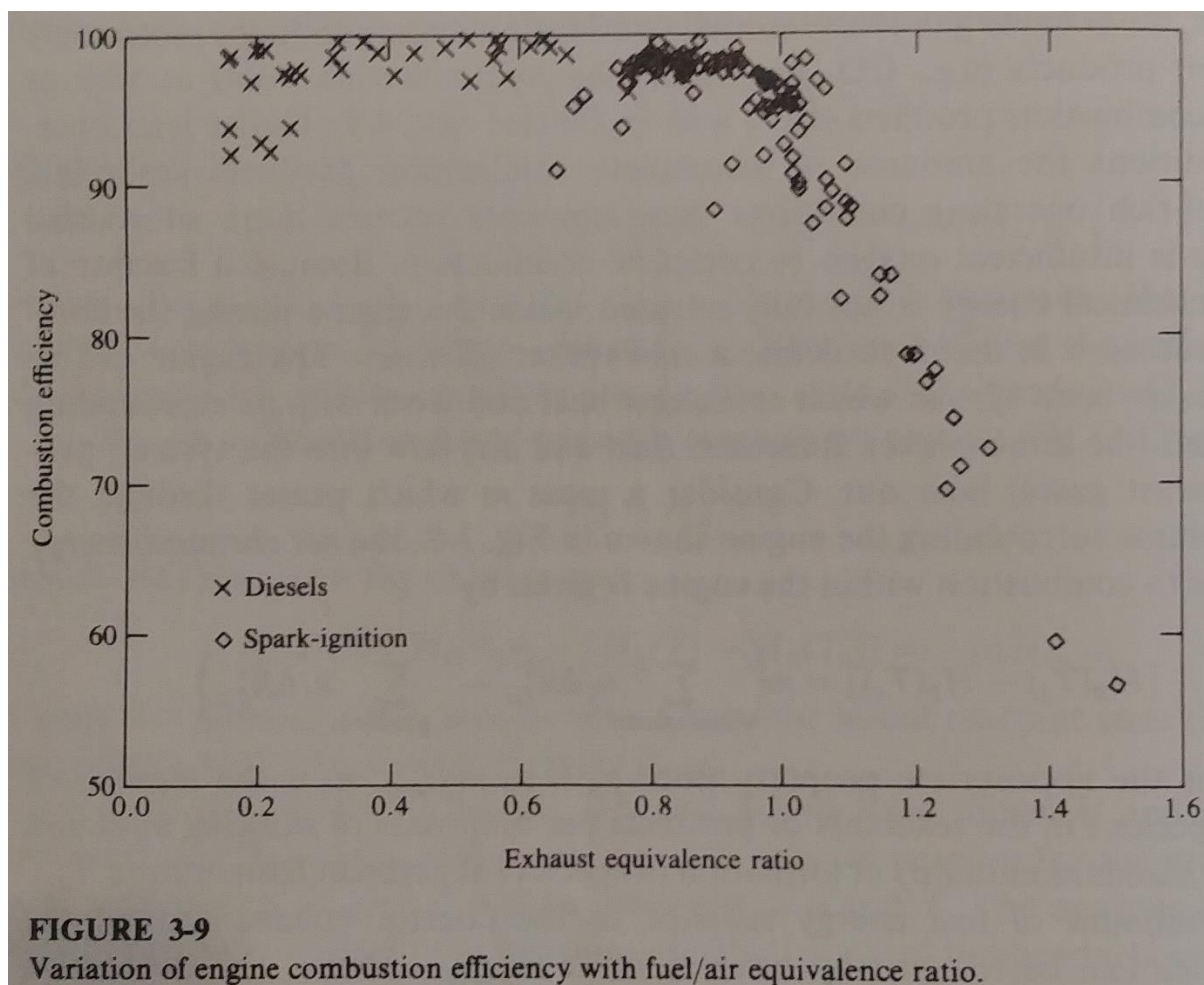


Figure 4-3: Expected Combustion Efficiency as Function of Equivalence Ratio for Spark-ignited and Diesel ICES (Heywood, 1988, p. 82)

4.3 HEAT TRANSFER MODEL

Due to absence of heat transfer data such as wall temperatures, author had to develop a sub-model which would calculate the total heat transfer rate on degree by degree basis.

Author has achieved this by assuming quasi-static process and consequently created the following equations:

$$\dot{Q} = \frac{KA(T_g - T_{co})}{s + \frac{K}{h_g}}$$

Equation 2: General Heat Transfer

$$T_{wi} = T_g - \frac{\dot{Q}}{h_g A}$$

Equation 3: General Interior Wall Temperature

$$\dot{Q} = \frac{h_g(T_g - T_{co})}{1 + h_g(\frac{S_p}{K_p} - \frac{S_w}{K_w})}$$

Equation 4: Heat Transfer Considering Plated Component

$$\dot{Q} = T_g - \frac{\dot{Q}}{h_g A} - \frac{\dot{Q} S_p}{AK_p}$$

Equation 5: Interior Wall Temperature Considering Plating

$$\dot{Q} = K(\frac{A_1(T_g - T_{co1})}{S_1 + \frac{k}{h_g}} + \frac{A_2(T_g - T_{co2})}{S_2 + \frac{K}{h_g}})$$

Equation 6: Heat Transfer Considering Compound Regime

After implementing all 3 ways of heat transfer, it became apparent that the effective differences between each way is minimal and the implementation of more advanced heat transfer techniques only introduces more uncertainty. Thus, author has decided to only use the ‘general’ method in this project.

To estimate convective heat transfer coefficient, author has chosen the ‘classical’ Woschni correlation, as shown in Equation 7. This is because according to the carried-out research, this correlation is the most reliable and applicable, since it yields to the most accurate results compared to other correlations such as Eichelberg or Annand.

$$h_{gc} = 0.01297829376B^{-0.2}P^{0.8}T^{-0.53} \left(C_1S_p + C_2 \frac{V_dT_{ref}}{P_{ref}V_{ref}} * (P - P_m) \right)^{0.8}$$

Where:

$C_1 = 2.28$, $C_2 = 0.0$ on Compression & $C_1 = 2.28$, $C_2 = 3.24 \cdot 10^{-3}$ on Expansion.

Equation 7: Woschni’s ‘classical’ convective heat transfer correlation (ZDENĚK ŽÁK, 2016)

To accurately model heat transfer, the radiation from gas is accounted for. Due to the complexity of determining the net emissivity (emissivity – absorptivity) of the burnt and unburnt mixtures, author has decided to use Annand’s radiative term of the convective heat transfer correlation, as shown in Equation 8, since it has proven to be the only reliable method of implementing radiation known to author. The implementation of radiation has proven to be equal to about 5% and under of the total peak heat transfer, agreeing with notion of relatively low radiative heat transfer in spark ignited engines (Heywood, 1988, p. 684).

$$h_{gr} = c\sigma \frac{T_g^4 - T_{wi}^4}{T_g - T_{wi}}$$

Where:

$c = 0.075$ for petrol & $c = 0.576$ for diesel

Equation 8: Annand’s radiative term of convection heat transfer coefficient equation (ZDENĚK ŽÁK, 2016)

Due to the radiative term being expressed as convective heat transfer coefficient equivalent, the net convective heat transfer coefficient is described in Equation 9.

$$h_g = h_{gc} + h_{gr}$$

Equation 9: Net Convective Heat Transfer Coefficient

To estimate the conductive heat transfer coefficient, author has used tabulated data (Turns, 2006) from which equation of the line was determined, as shown in Figure 4-4.

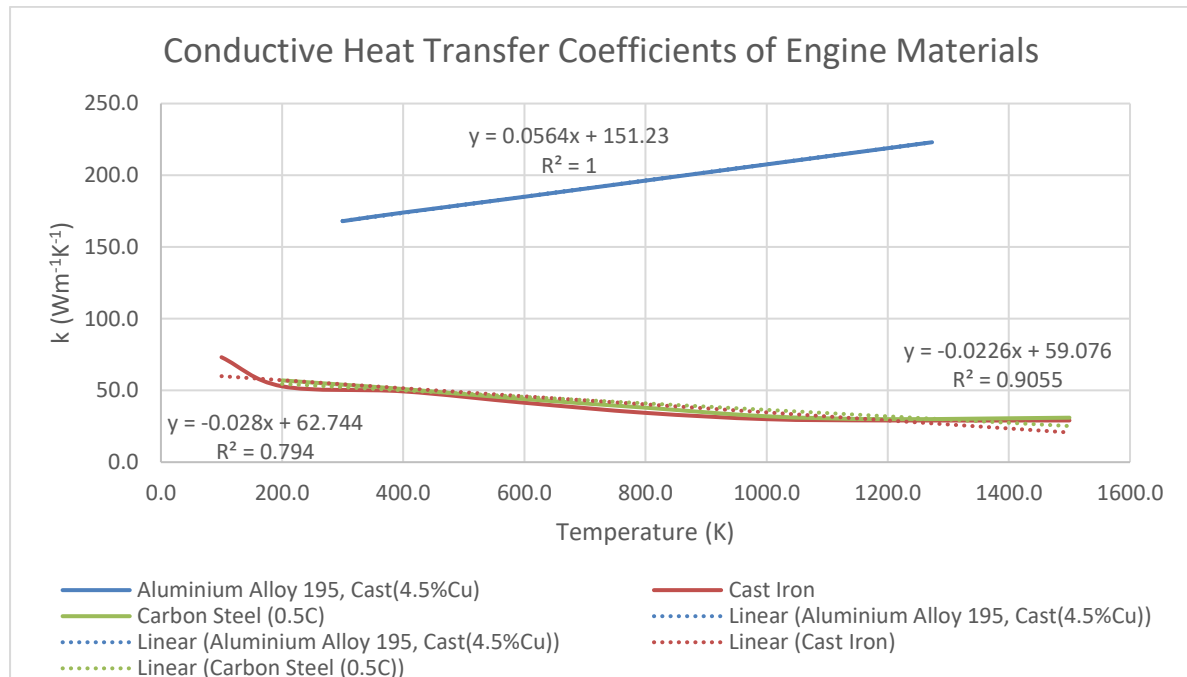


Figure 4-4: Conductive Heat Transfer Coefficients of Engine Materials

The temperature used to predict the instantaneous conductive heat transfer coefficient was the average of the instantaneous T_{wi} & T_{co} .

Due to the quasi-static nature of the model, author had to implement phasing so that all of the T_{wi} values are always 1° behind the calculation front. Author believes this to cause a very minor error in the overall accuracy of the sub-model. Consequently, a T_{wi} initialization value must be assumed, which is adjusted so that it is equal to the 1st calculated T_{wi} value. Author believes this method to be valid since there is no practical difference between the values. Figure 4-5 shows how the initialization value is found.

```
Sub Conduction_Ratio()
'
' Conduction_Ratio Macro Written by Kacper Kaczmarczyk
'
'
Dim i 'Declare row variable
Dim n 'Declare column variable

For n = 1 To 5 'go through all columns
    For i = 1 To 7 'go through all rows
        Cells(16 + n, 50 + i).GoalSeek Goal:=1, ChangingCell:=Cells(10 + n, 50 + i) 'find value so that the target is equal to 1
    Next i 'next row
Next n 'next column

End Sub
```

Figure 4-5: VBA code of the Conduction Ratio Macro

Table 4-1 shows the component areas used in modelling of the heat transfer in Ford Fox engine. All values have been collected from the 3D CAD model, as shown in Figure 4-6, which is talked about in the Geometrical Acquisition chapter.

Table 4-1: Heat Transfer Model, Component Areas

Component	A (m ²)
Comb. Chamber	0.00400100
Intake Valve Head	0.00065229
Exhaust Valve Head	0.00047599
Piston Crown	0.00529560

Table 4-2: Heat Transfer Model, Component Thicknesses

Component	Thickness (mm)
Liner Thickness (mm)	6.86
Head (mm)	5.00
Intake Valve Head (mm)	4.00
Exhaust Valve Head (mm)	4.00
Piston (mm)	8.00
Deck Height (mm)	1.00

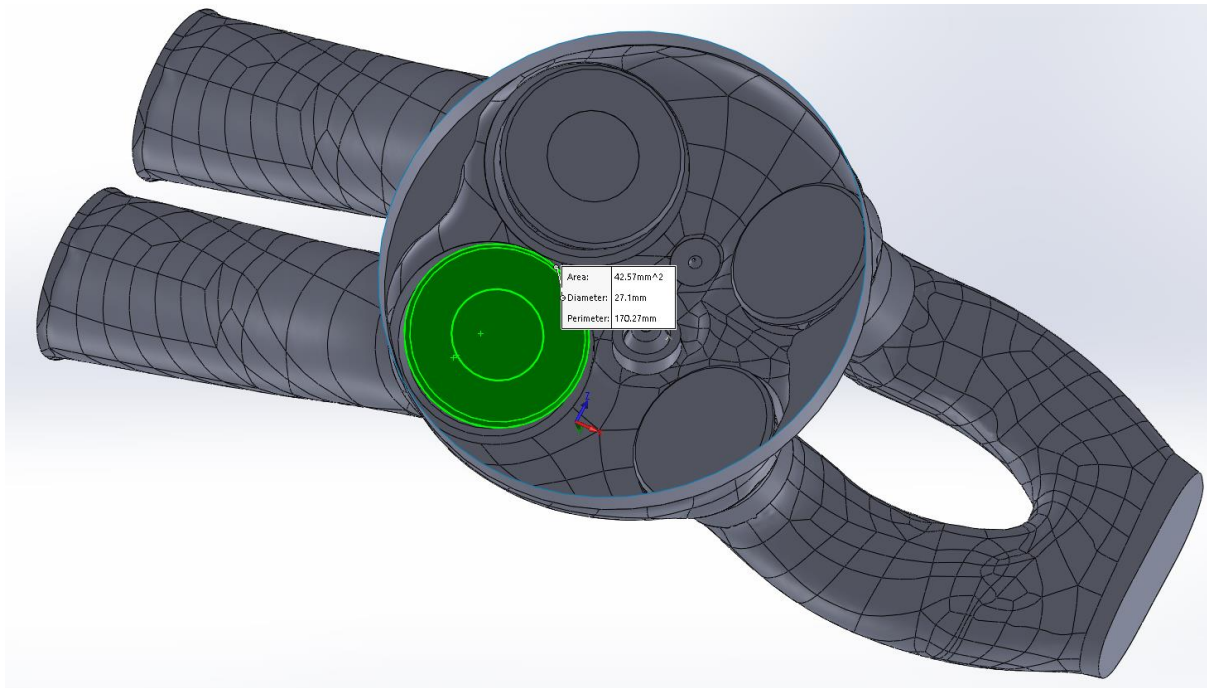


Figure 4-6: Intake Valve Area Measurement

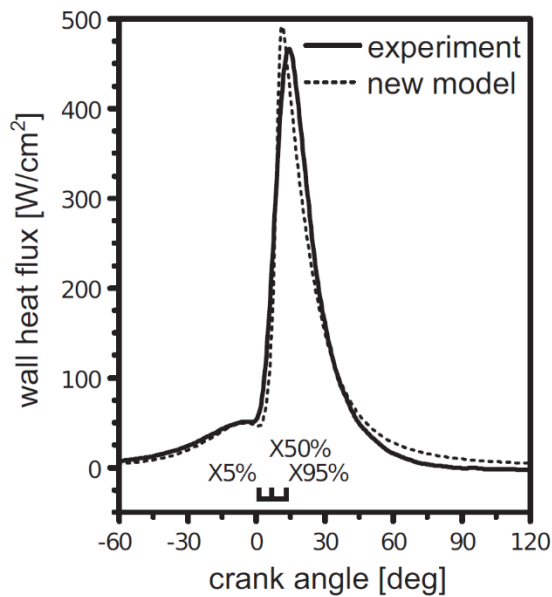


Figure 4-8: Measured Wall Heat Flux @ 2,000rpm and $\lambda=1.0$, in Hydrogen Engine (Johannes Michl, 2015)

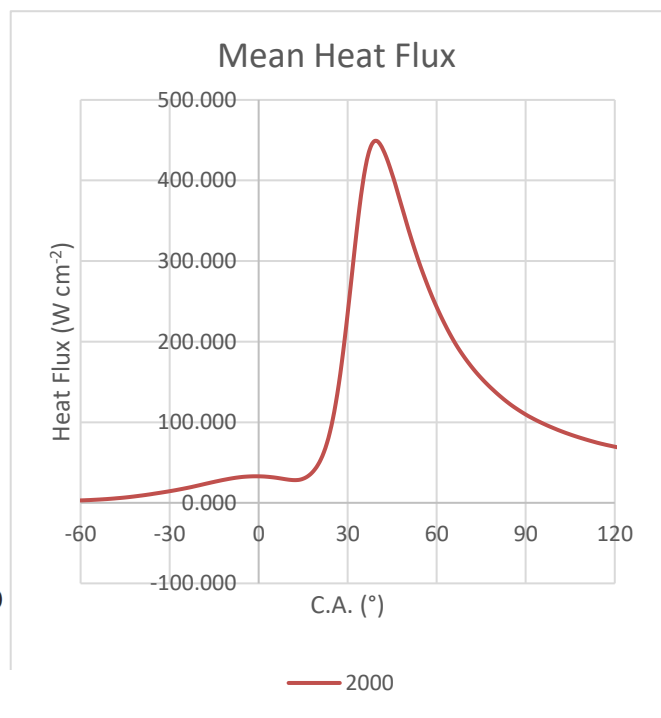


Figure 4-7: Mean Heat Flux from Heat Transfer Model @ 2,000rpm

Figure 4-7 shows that the calculated heat flux is very similar to the one showed in Figure 4-8, which was measured on a physical research engine. The differences are most likely due to differences in the engines, such as fuel type, total released heat, EGR% etc. However, it was clear to author that bull-park values have been achieved, which is the best that author believes

to be possible without any heat transfer data. The absolute values themselves are not as crucial since heat transfer correction multiplier is applied to all heat transfer values.

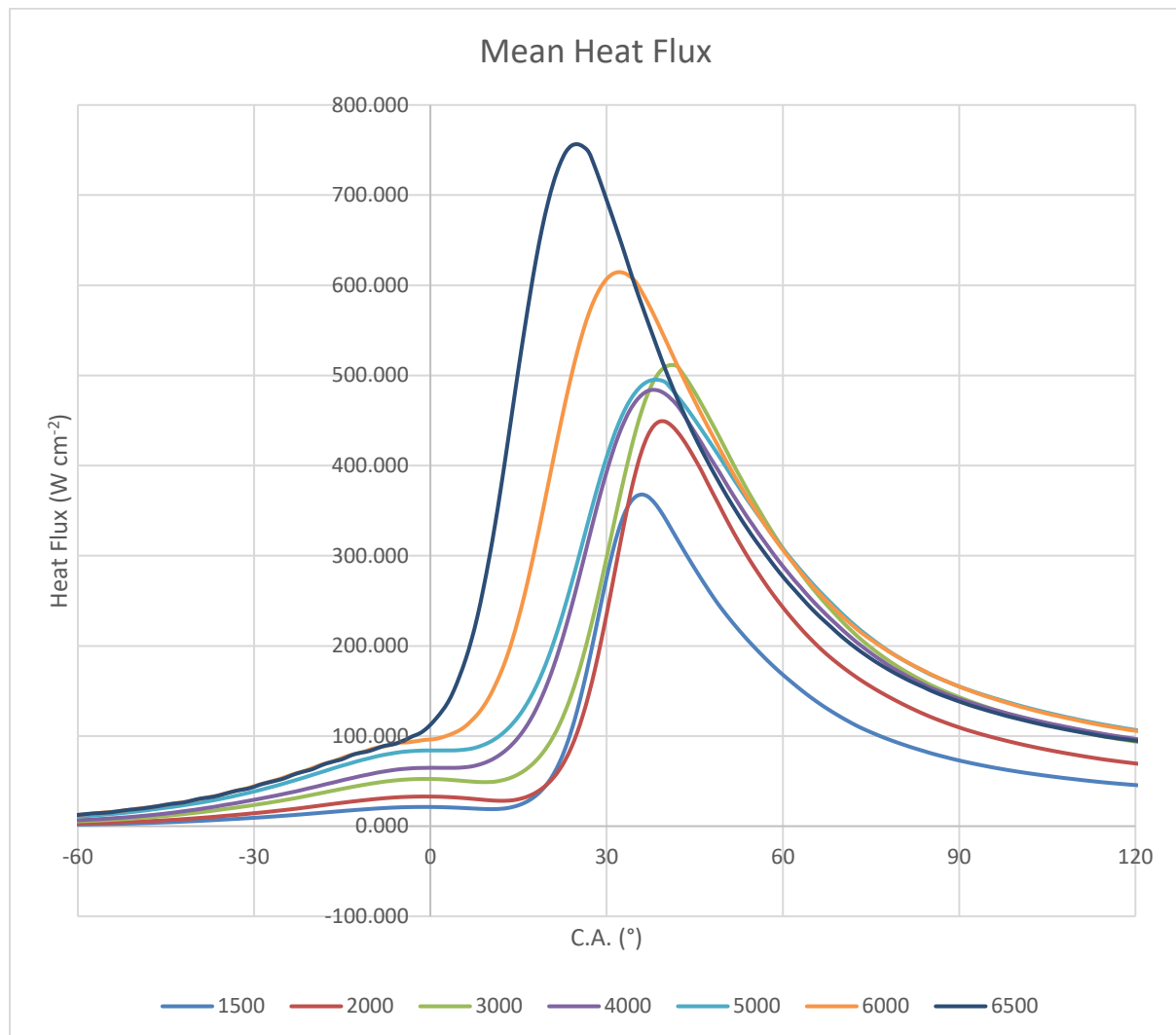


Figure 4-9: Mean Heat Flux @ all RPMs

Figure 4-9 shows that mean heat flux increases with rpm. Author has expected this since combustion time decreases with rpm, causing more heat per second to be transferred to the surroundings. Furthermore, there is also a good relation between SOC and mean heat flux peak. This can be explained since the peak cylinder temperature point is highly dependent on SOC. Despite author's best efforts to find reliable and applicable heat transfer data of other ICEs, author was unable to do so, creating a lack of model verification at higher rpms. However, the model is based on very well developed and known thermodynamic principles, the coefficients are calculated via very well-known ICE specific correlations and the model has been verified at low rpm, giving author great confidence in the validity of the model, considering the lack of data.

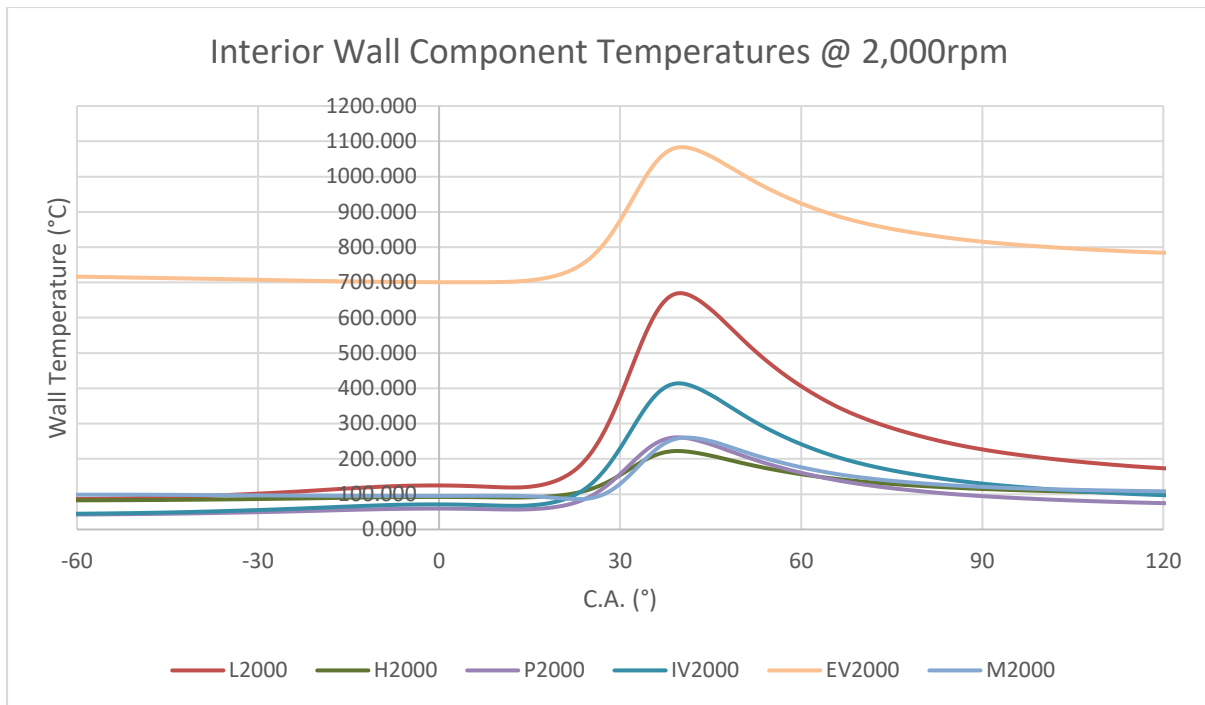


Figure 4-10: Interior Wall Temperatures @ 2,000rpm

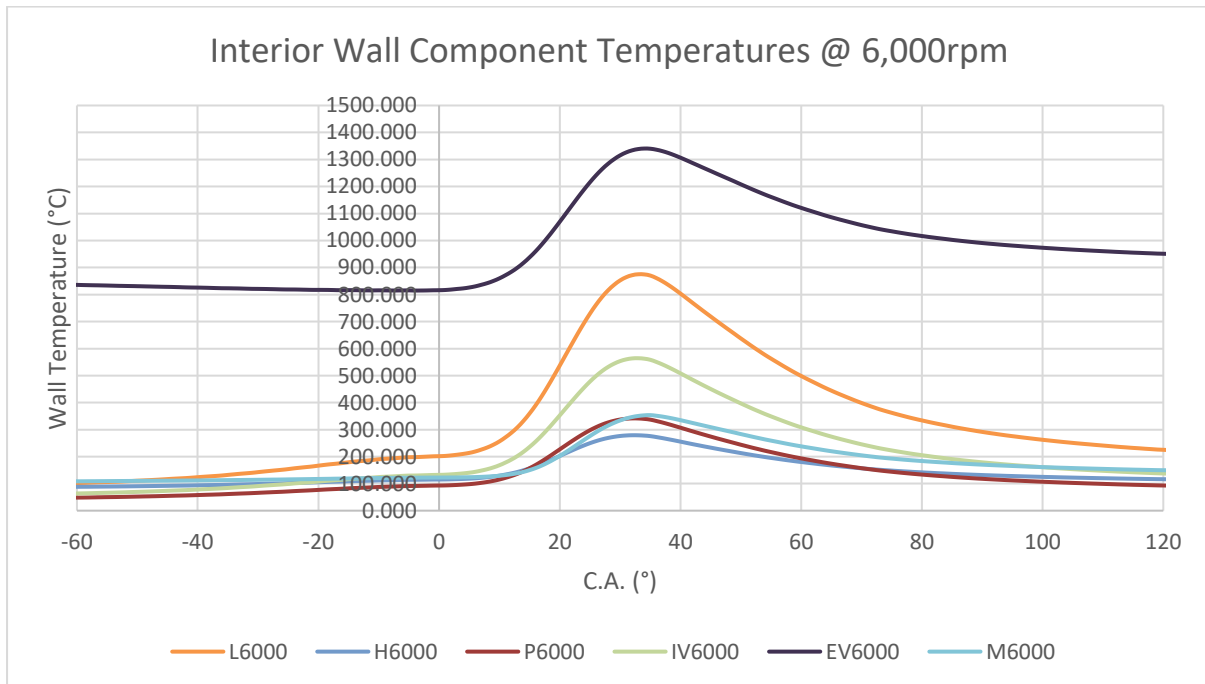


Figure 4-11: Interior Wall Temperatures @ 6,000rpm

As shown in Figure 4-10 & Figure 4-11, the instantaneous interior wall temperatures of all components follow the trend shown in Figure 4-9, as expected. The peak instantaneous temperatures are higher than expected. However, the high temperatures occur only for a fraction of a time. Interestingly, the piston wall temperatures follow the mean temperatures very well throughout the rpm range.

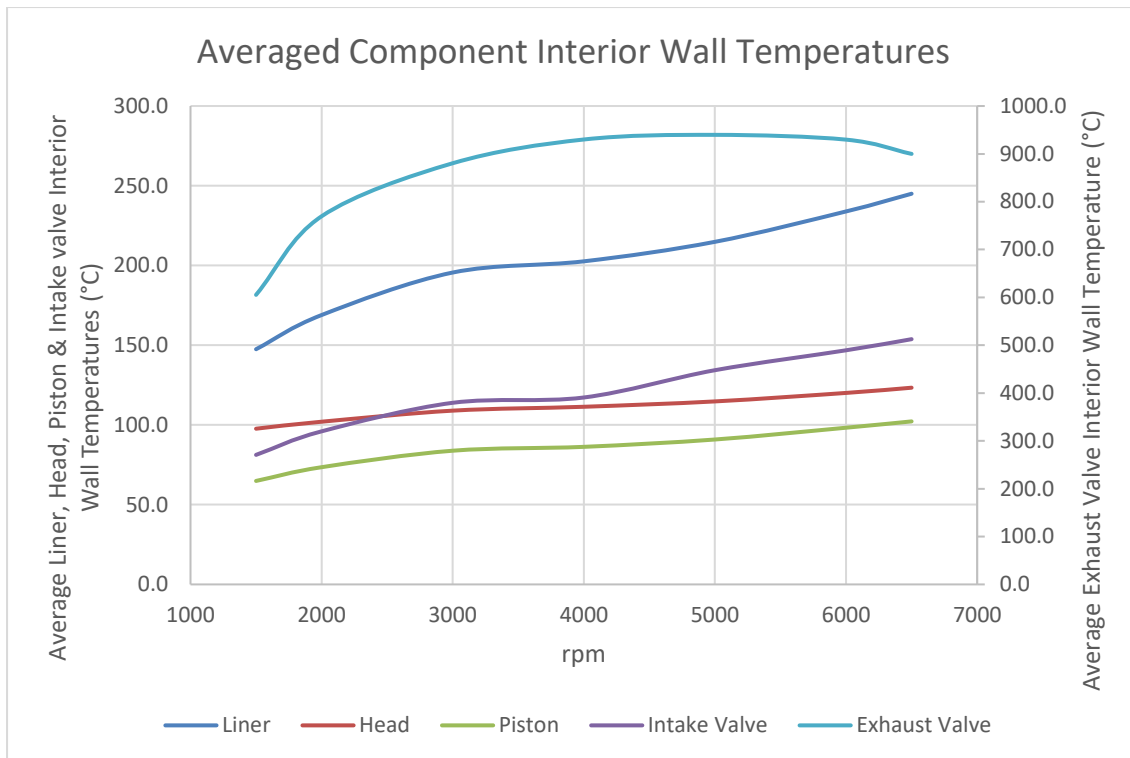


Figure 4-12: Averaged Component Interior Wall Temperatures

Figure 4-12 shows the component interior wall temperatures averaged over the compression and combustion/ expansion strokes. The average exhaust valve temperatures are higher than the 600°C - 700°C expected range (Heywood, 1988, p. 700). This could be due to the thermal coating applied to the head of the exhaust valves, as shown in Figure 4-13. The average



Figure 4-13: Exhaust Valve of The Ford Fox ICE

cylinder-head temperature at 2,000rpm is 102.0°C, which is arguably close to the expected ~130°C (Heywood, 1988, p. 699), considering the comparison is done on different engines. The averaged surface temperature of the piston crown at 5,000rpm is 90.9°C, which is much cooler than the expected ~260°C (Heywood, 1988, p. 700), even if the oil squirters are considered. This suggests the assumed T_{∞} value of piston to be too small. The temperature levels are greatly affected by the cooling temperature shown in Figure 4-14. The profiles on the other hand are primarily affected by the conductive heat transfer coefficient of the material, Cast Aluminium Alloy 195, Cast Iron and Carbon Steel 0.5C for Liner and Cylinder Head, Liner, Intake and Exhaust valves respectively.

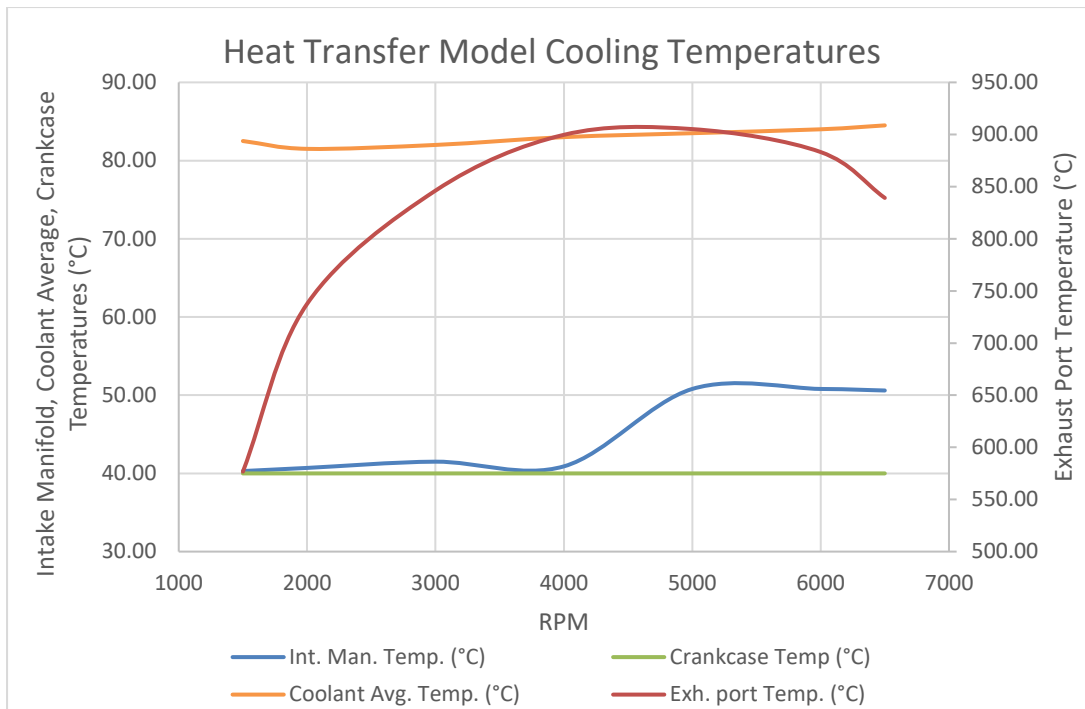


Figure 4-14: Heat Transfer Model Cooling Temperatures

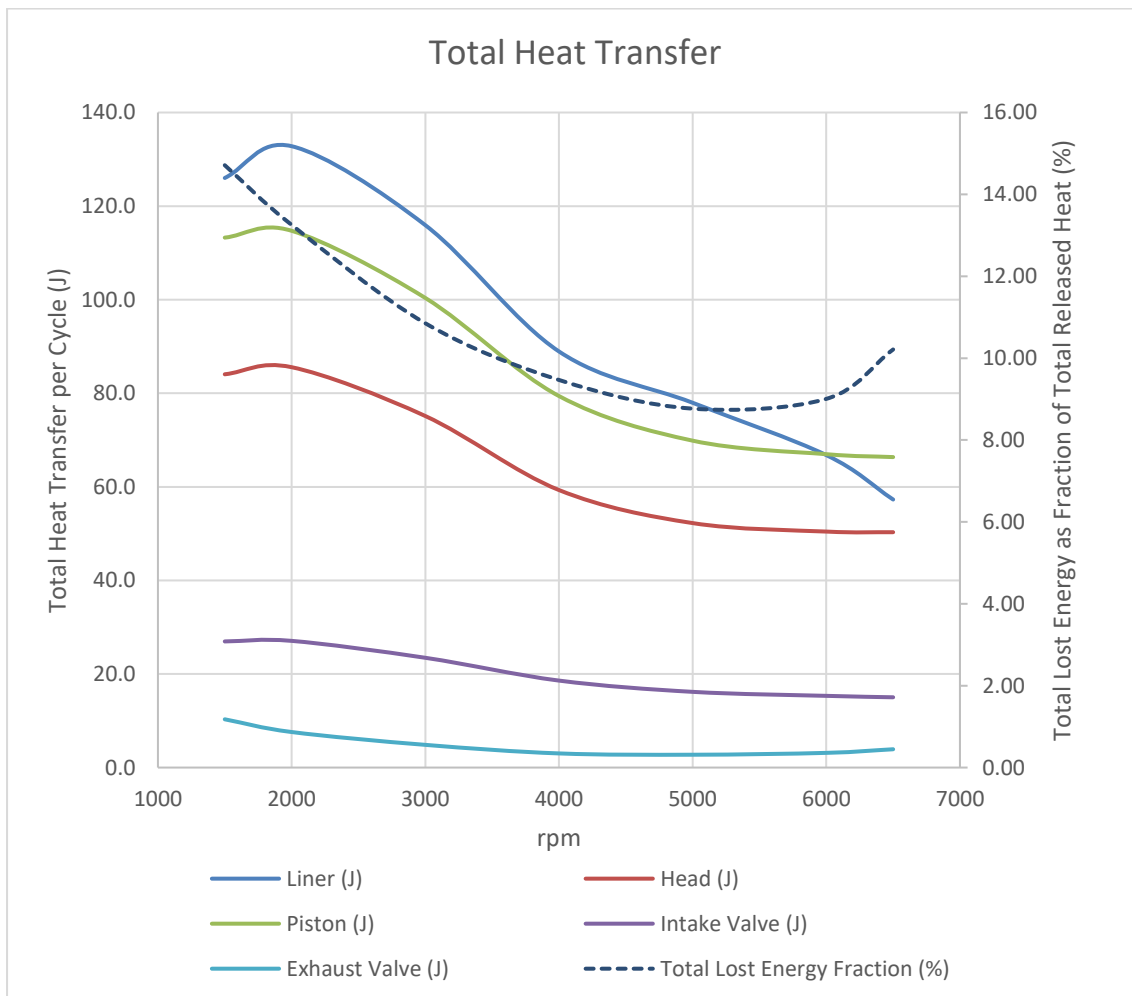


Figure 4-15: Total Heat Transfer

Figure 4-15 shows that the total transferred heat through component profiles are very similar, the difference being the total heat transferred, which is primarily due to the differences in areas and materials. The two components which display different behaviours are liner and exhaust valve. Former is due to the variable area and the retardation of SOC, causing smaller area to be present at the time of high gas temperatures. Latter is due to the varying exhaust gas temperatures shown in Figure 4-14. Figure 4-15 also shows that a total of 9% - 16% of the energy from fuel is lost due to heat transfer. This is lower than the expected 17% - 26% (Heywood, 1988, p. 674). However, the expected values are based on older, less efficient, naturally aspirated engines. Additionally, the heat transfer model proposed by author was used to calculate the heat transfer during compression and combustion/ expansion strokes only, making the direct comparison misleading.

Considering all of the mentioned points, author believes the developed heat transfer model to simulate very realistic and applicable results which are accurate enough to use in the rest of the polytropic index model.

4.4 HEAT RELEASE RATE

The heat release rate in ICE is equal to the sum of net heat absorbed by the gas in the cylinder and the lost heat due to heat transfer, as shown by Equation 10.

$$dQ_r = dQ_g + dQ_l$$

Equation 10: Heat Release Rate

The dQ_l is calculated via the already mentioned heat transfer sub-model, whereas dQ_g is calculated as shown in Equation 11.

$$dQ_{g_i} = \frac{\gamma_{avg_{i-1}} - n_{i-1}}{\gamma_{avg_{i-1}} - 1} * |P|_{i-1}^i dV_i$$

Equation 11: Net Heat into Gas

Author believes this method to be valid and applicable since the model bases the majority of inputs on well-known and easily calculable parameters such as, traditional polytropic index, cylinder pressure, change of volume etc. However, more challenging parameters such as ratio of specific heats and heat transfer are still used since author was not able to find a solution which would replace them, while retaining the accuracy and applicability of the model. This is the reason why author has made sure to lower the uncertainty and error associated with those parameters, as to retain the model integrity. It is also important to realise that the inaccuracy of the challenging parameters have relatively low effect on the overall accuracy of HRR, once ballpark values are achieved, due to their relative magnitudes, as shown in Figure 4-16.

This relatively un-orthodox method is required as the goal of the model is to accurately determine the more abstract polytropic index, which many models consider occurring every dC.A. during expansion but before pressure rises due to combustion. Therefore, the standard method/s could not be utilised since all of the researched techniques require the assumption of the very parameter which this model is trying to discover.

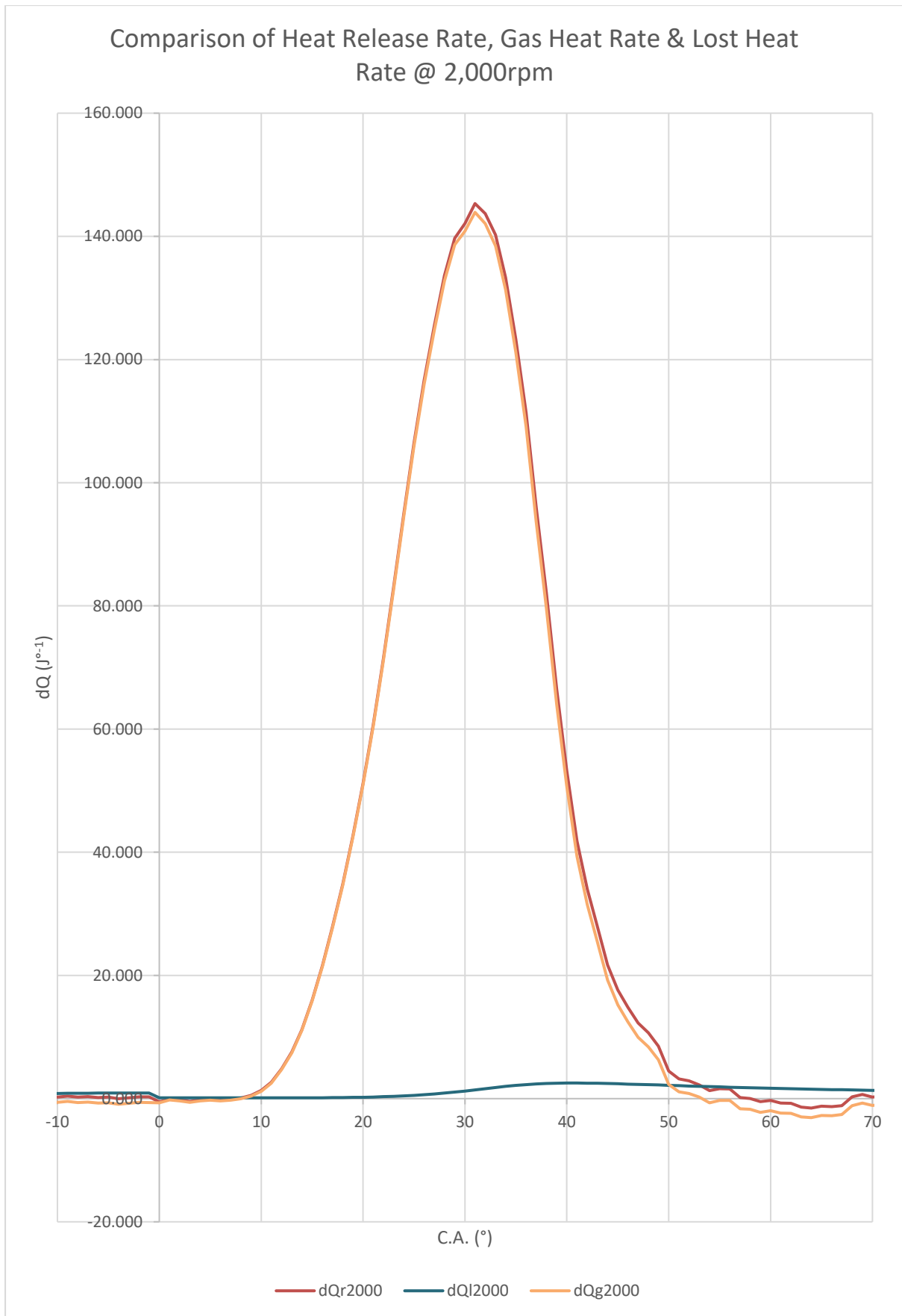


Figure 4-16: Comparison of Heat Release Rate, Gas Heat Rate & Lost Heat Rate @ 2,000rpm

4.5 2-ZONE COMBUSTION MODEL

To accurately determine the average ratio of specific heats, author used a 2-Zone 0D model, as it is believed that the separation of burnt and un-burnt zones leads to a great increase of accuracy, whereas 0D ensures the ease of calculation as well as zone averaged results.

Firstly, the MFB was determined as shown in Equation 12.

$$MFB_i = \frac{\sum_0^i dQr_i}{m_f * LHV * \eta_c}$$

Equation 12: Mass Fraction Burned

Author has considered the RRI content in the total mixture mass, as shown in Equation 13.

$$m_m = (m_f + m_a) * \left(1 + \frac{RRI\%}{100}\right)$$

Equation 13: Total Cylinder Mixture Mass (Tang, 2016)

Author has assumed adiabatic process in the un-burnt zone; therefore, the temperature after SOC was determined as shown in Equation 14, whereas before SOC, author assumed the un-burnt zone temperature to be equal to the mean cylinder gas temperature, calculated as shown in Equation 15.

$$T_{un-Burnt_i} = T_{un-Burnt_{i-1}} * \frac{P_i}{P_{i-1}}^{\frac{\gamma_{un-Burnt_{i-1}} - 1}{\gamma_{un-Burnt_{i-1}}}}$$

Equation 14: un-Burnt Zone Temperature

$$T_{avg_i} = \frac{P_i V_i}{m_m * R_i}$$

Equation 15: Mean Cylinder Gas Temperature

To determine the specific gas constant shown in Equation 17, author used the zone molecular weight shown in Equation 16.

$$M_x = \frac{\sum_i \text{mol}_i M_i}{\sum_i \text{mol}_i}$$

Equation 16: zone Molecular Weight

$$R_x = \frac{R_u}{M_x}$$

Equation 17: Specific Gas Constant

Where the instantaneous specific gas constant was calculated as shown in Equation 18.

$$R_i = R_{\text{Burnt}} * MFB_i + R_{\text{un-burnt}} * (1 - MFB_i)$$

Equation 18: Instantaneous Specific Gas Constant

The rearrangement of ideal gas law allows for the calculation of the un-burnt volume, as shown in Equation 19.

$$V_{\text{un-Burnt}_i} = \frac{(1 - MFB_i) m_m R_i T_{\text{un-Burnt}_i}}{P_i}$$

Equation 19: un-Burnt zone Volume

Determination of un-burnt volume allows for the calculation of burnt volume, as shown Equation 20.

$$V_{\text{Burnt}_i} = V_i - V_{\text{un-Burnt}_i}$$

Equation 20: Burnt zone Volume

Lastly, the rearrangement of ideal gas law can be used to determine burnt zone temperature once burnt volume is known, as shown in Equation 21.

$$T_{\text{Burnt}_i} = \frac{P_i V_i}{m_m R_{\text{Burnt}_i}}$$

Equation 21: Burnt zone Temperature

4.6 RATIO OF SPECIFIC HEATS IN UN-BURNT ZONE

Firstly, author has plotted the molar specific heat at constant pressure of all relevant species (Heywood, 1988, p. 131), as shown in Figure 4-17, the results of which were as expected (NIST, 2018).

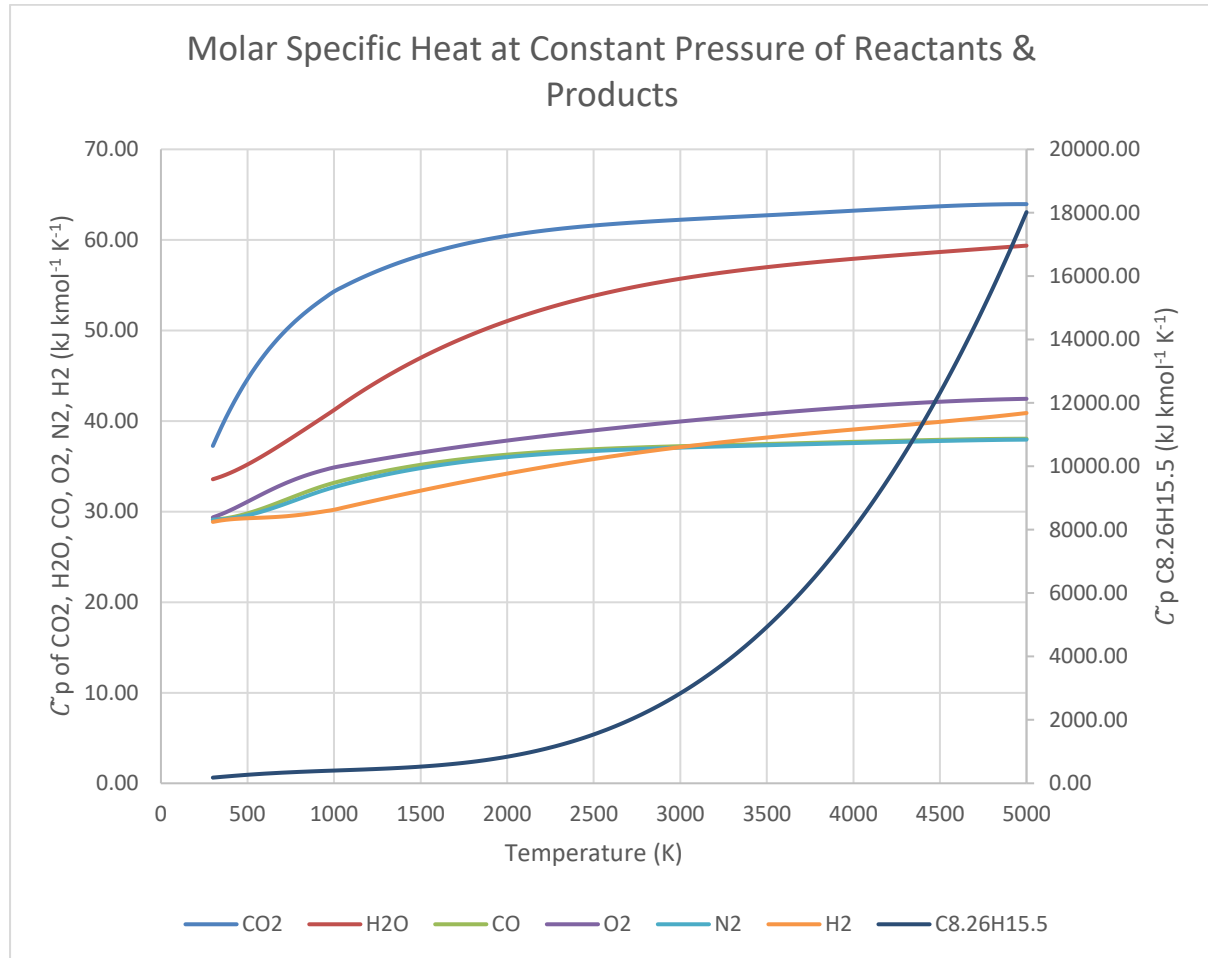


Figure 4-17: Molar Specific Heat at Constant Pressure of Reactants & Products

Figure 4-17 clearly shows that the molecular weight as well as the species complexity both have a primal effect on the specific heat capacity, as the CO and N2 both have a molecular weight of 28 kg kmol⁻¹ and as a result, very similar $\tilde{C}_p$. Whereas the fuel specie has 22.76 molecular bonds on average, which is 11.4 times more than the specie with the 2nd highest $\tilde{C}_p$, which is CO2. The validated $\tilde{C}_p$ can be used to calculate ratio of specific heats, as shown in Equation 22, the results are shown in Figure 4-18.

$$\gamma_x = \frac{|C_p|_x}{|C_p|_x - R_u}$$

Equation 22: Ratio of Specific Heats

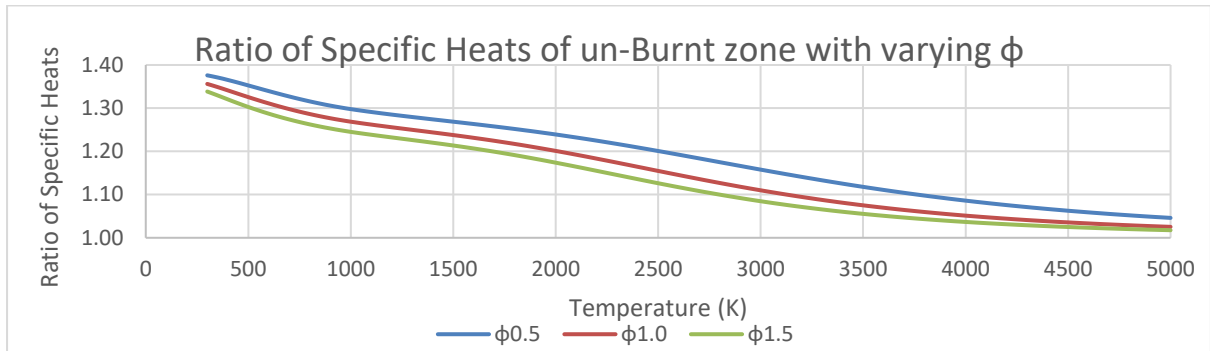


Figure 4-18: Ratio of Specific Heats of un-Burnt zone with varying ϕ

Figure 4-18 shows valid ϕ values (Heywood, 1988, p. 134), with a relatively linear negative correlation with the mixture temperature.

The validated method was then used to calculate the ratio of specific heats in the un-burnt zone, as shown in Figure 4-19, by using the previously calculated un-burnt zone temperatures.

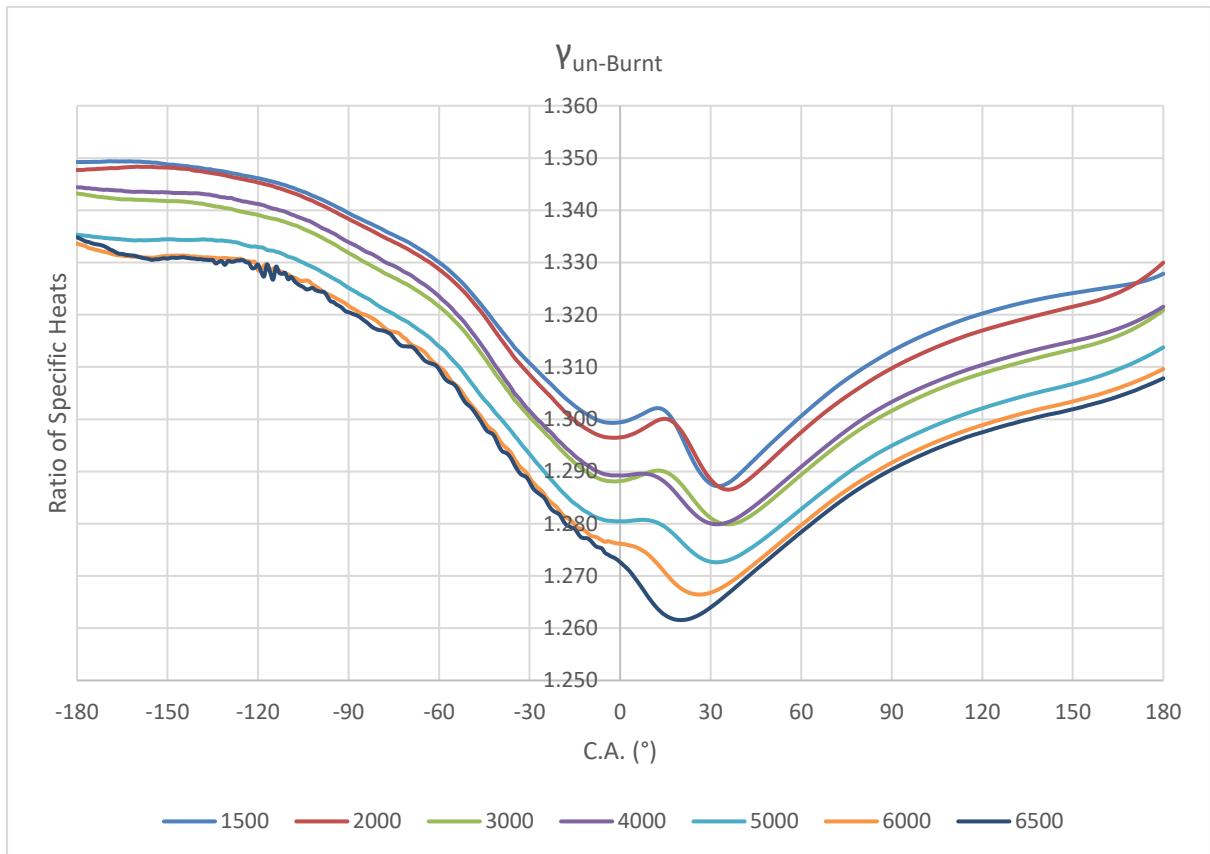


Figure 4-19: Ratio of Specific Heats in the un-Burnt Zone

Due to the mentioned correlation, the profile of the ratio of specific heats becomes the inverse of the un-burnt zone temperature. Because of the relatively low peak temperatures of $\sim 700\text{K}$ to $\sim 1,000\text{K}$, the minimal ratio of specific heats is only 1.29 to 1.26.

4.7 DISSOCIATED RATIO OF SPECIFIC HEATS IN BURNT ZONE

The basic burnt zone ratio of specific heats value has been calculated as in chapter: “Ratio of Specific Heats in un-Burnt Zone”. However, author had to account for the dissociation and the additional required energy associated with it, as the burnt zone temperatures exceed ~2,000K (Heywood, 1988). Dissociation is where molecule has enough energy (due to temperature) to break a bond which attaches two or more atoms together. The utilised dissociation model assumes that there is enough time for the forward and reverse reaction to come to equilibrium and only dissociation of $\text{CO}_2 \rightarrow \text{CO} + \text{O}$ and $\text{H}_2\text{O} \rightarrow \text{H}_2 + \text{O}$ were accounted for (Goodger, 1981), due to their relative quantities.

To determine the quantity of dissociated species, author has employed the equilibrium constant, which can be described as ratio of partial pressures (partial pressure equilibrium) or ratio of species concentration (concentration equilibrium) (Goodger, 1981, p. 284), as shown in Equation 23.

$$K_{x_p} = \frac{k_F}{k_R} = \frac{[x_p]^{x_p}}{\sum_i [x_{re_i}]^{x_{re_i}}}$$

Equation 23: Equilibrium Constant Defined as Molar Quantities of Product & Reactants

To determine the ratio of partial pressures of CO_2 and H_2O , the Gibbs free energy equation can be rearranged, as shown in Equation 24.

$$K_{x_p} = \exp\left(\frac{-\Delta G_T^\circ}{R_u T}\right)$$

Equation 24: Ratio of Partial Pressures (Turns, 2006, p. 390)

To determine the change of Gibbs free energy, author has plotted and calculated the equation of the line for CO , CO_2 & H_2O , as shown in Figure 4-20.

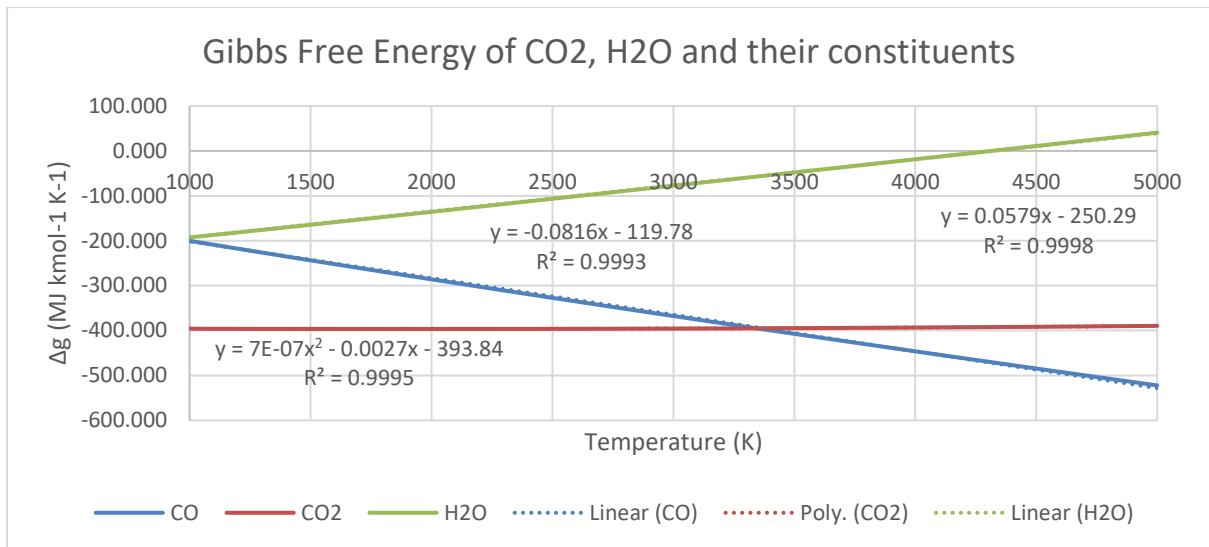


Figure 4-20: Gibbs Free Energy of CO₂, H₂O and their Constituents

The R² value of effectively 1.0 has been achieved for all three species, which has resulted in confident equilibrium constants, as shown in Figure 4-21.

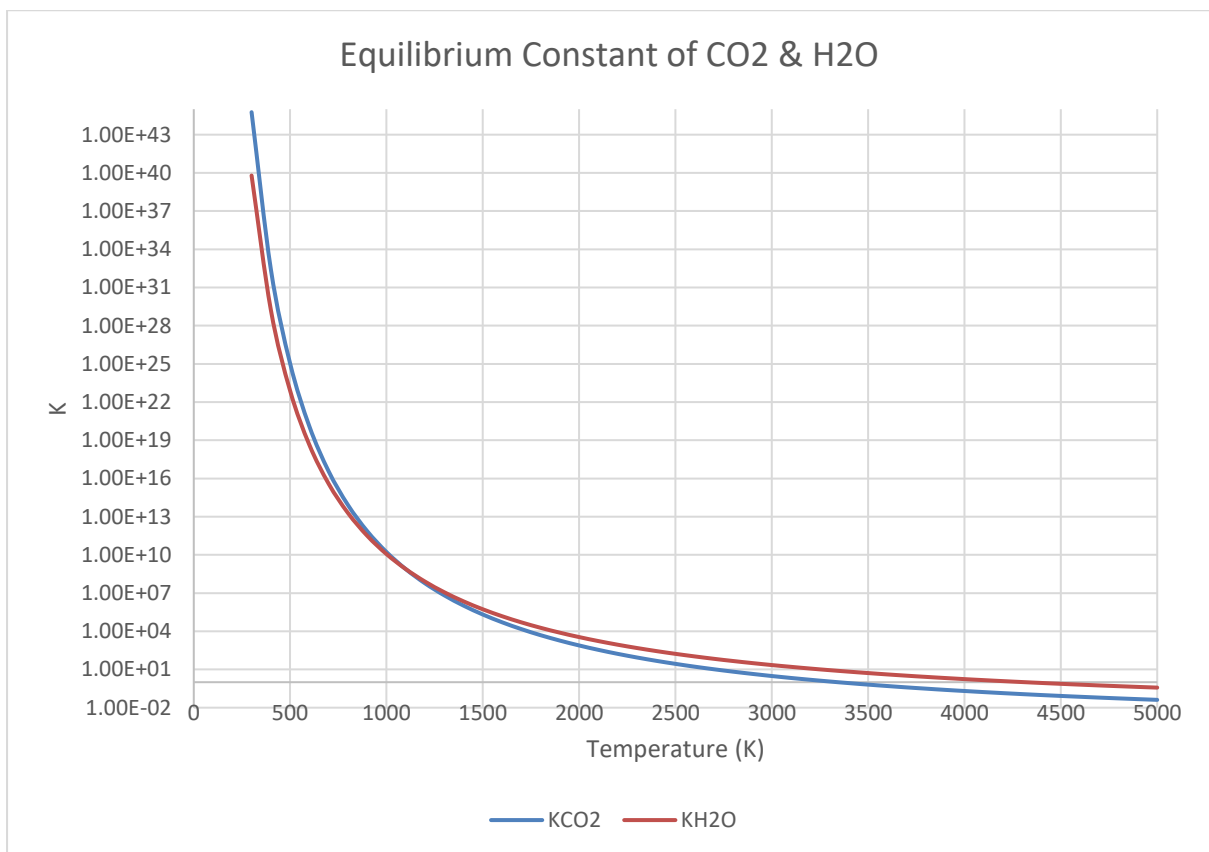


Figure 4-21: Equilibrium Constant of CO₂ & H₂O

The equilibrium constants have a logarithmic relationship with temperature, which is the cause of effectively no dissociation below ~2,000K and relatively high growth rate beyond that point.

Due to the number of unknown quantities of species, author had to employ an iterative method, which is as follows (Goodger, 1981, p. 286):

Assume the O₂ concentration, as shown in Equation 25.

$$[O_2] = Assumed[O_2]$$

Equation 25: Assumed O₂ Concentraion (Goodger, 1981, p. 286)

$$ppO_2 = ([O_2] * P)^{\frac{1}{2}}$$

Equation 26: Partial Pressure of Oxygen (Goodger, 1981, p. 286)

$$mol_{CO} = \frac{mol_C * \varphi}{K_{CO_2} * ppO_2 + 1}$$

Equation 27: Dissociated Moles of Carbon Monoxide (Goodger, 1981, p. 286)

$$mol_{CO_2} = mol_C * \varphi - mol_{CO}$$

Equation 28: Resultant Moles of Carbon Dioxide (Goodger, 1981, p. 286)

$$mol_{H_2} = \frac{0.5 * mol_H * \varphi}{K_{H_2O} * ppO_2 + 1}$$

Equation 29: Dissociated Moles of Dihydrogen (Goodger, 1981, p. 286)

$$mol_{H_2O} = 0.5 * mol_H * \varphi - mol_{H_2}$$

Equation 30: Resultant Moles of Water (Goodger, 1981, p. 286)

$$mol_{O_2} = \varphi \left(mol_C + \frac{mol_H}{4} \right) - mol_{CO_2} - 0.5(mol_{H_2O} + mol_{CO})$$

Equation 31: Resultant Dissociated Moles of Dioxygen (Goodger, 1981, p. 286)

$$mol_{N_2} = \frac{[N_{2air}]}{[O_{2air}]} * \left(mol_C + \frac{mol_H}{4} \right)$$

Equation 32: Moles of Dinitrogen (Goodger, 1981, p. 286)

$$mol_{Total} = 2mol_{CO_2} + 1.5(mol_{CO} + mol_{H_2O}) + mol_{H_2} + mol_{O_2} + mol_{N_2}$$

Figure 4-22: Total Moles of Combustion & Dissociation Products (Goodger, 1981, p. 286)

$$Real[O_2] = \frac{mol_{O_2}}{mol_{Total}}$$

Equation 33: Real Concentration of Dioxygen (Goodger, 1981, p. 286)

$$D.C.E. = \frac{Real[O_2] - Assumed[O_2]}{Real[O_2]} * 100$$

Equation 34: % of the Dissociation Calculation Error

To ensure valid results, author has written VBA code shown in Figure 4-24, to automate the MS Excel function: “Goal Seek”, which was used to iteratively compute the assumed O2 concentration so that the D.C.E. is ~0.00%. In practise, an accuracy of +/- 0.001% was achieved, as shown in Figure 4-23.

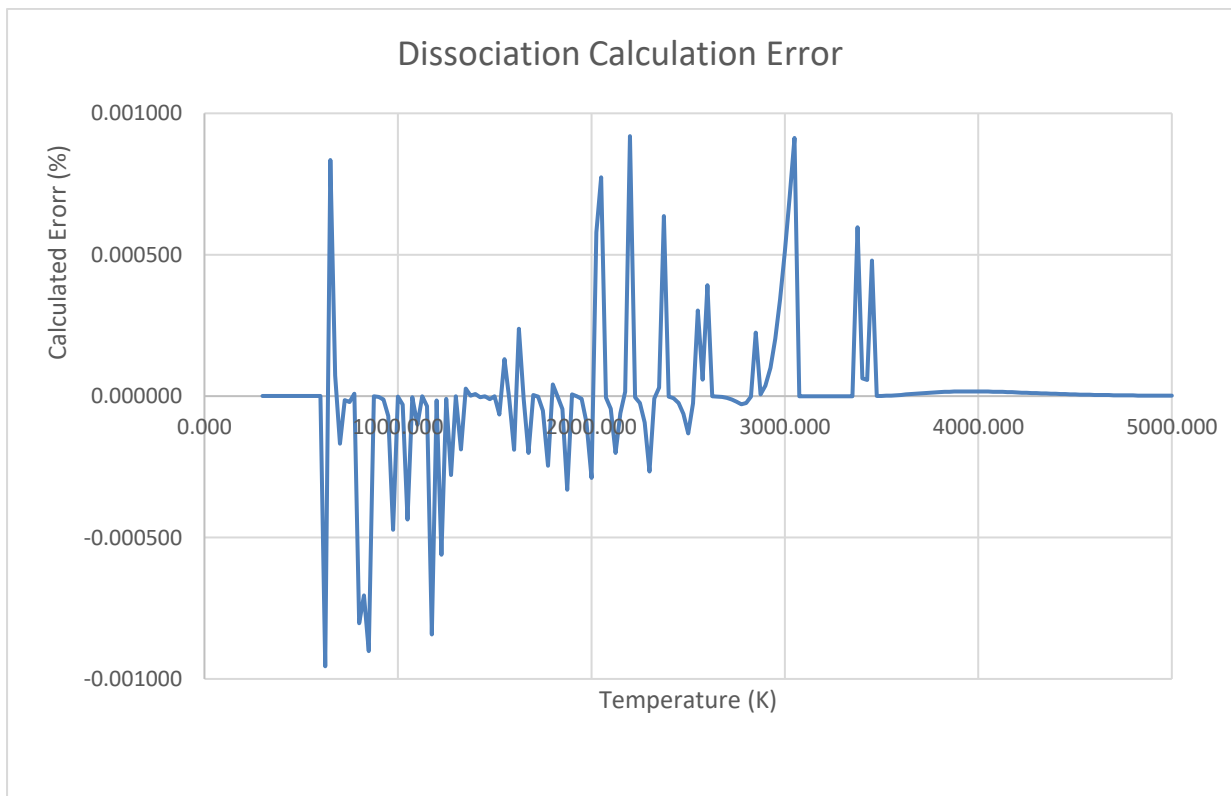


Figure 4-23: Dissociation Calculation Error

```

Sub Dissociation()
'
' Dissociation Macro Written by Kacper Kaczmarczyk
'
'
'
' SOURCE of the Macro Timer: www.TheSpreadsheetGuru.com/the-code-vault

Dim StartTime As Double
Dim MinutesElapsed As String

'Remember time when macro starts
    StartTime = Timer

' BEGINNING of AUTHOR's CODE:

Dim i 'Declare row variable
Dim n 'Declare column variable
Dim iter 'Declare iteration variable

iter = Range("C5") 'Make iteration equal to input value from worksheet

For n = 1 To iter 'Run it as many times as iteration value requires

If n = 1 Then 'On 1st iteration

Range("G5:G193") = 0.00001 'Change all assumed values

End If

For i = 0 To 188 'Go through all temperature points

    Cells(5 + i, 23).GoalSeek Goal:=0, ChangingCell:=Cells(5 + i, 7)
    'Find assumed value so that the Error is equal to 0

    Range("C6") = Cells(5 + i, 6) 'Display the current temperature point

Next i

Next n

' END of AUTHOR's CODE.

'Determine how many seconds code took to run
    MinutesElapsed = Format((Timer - StartTime) / 86400, "hh:mm:ss")

'Notify user in seconds
    MsgBox "This code ran successfully in " & MinutesElapsed & " minutes", vbInformation

End Sub

```

Figure 4-24: Dissociation Macro

To calculate the required energy to dissociate CO₂ and H₂O, author has utilised Equation 35. The required enthalpy of formation has been retrieved by plotting tabulated data (Turns, 2006) and determining equation of the line of all three relevant substances, as shown in Figure 4-25.

$$\begin{aligned}
 E_{Total\ Dissociation_i} &= \sum_i \Delta mol_{x_i} * \Delta h_{f_i} \\
 &= \left(mol_C - mol_{CO_{2i}} \right) * \Delta h_{f_{CO_{2i}}} + \left(\frac{mol_H}{2} - mol_{H_2O_i} \right) * \Delta h_{f_{H_2O_i}}
 \end{aligned}$$

Equation 35: Cumulative Energy due to Dissociation

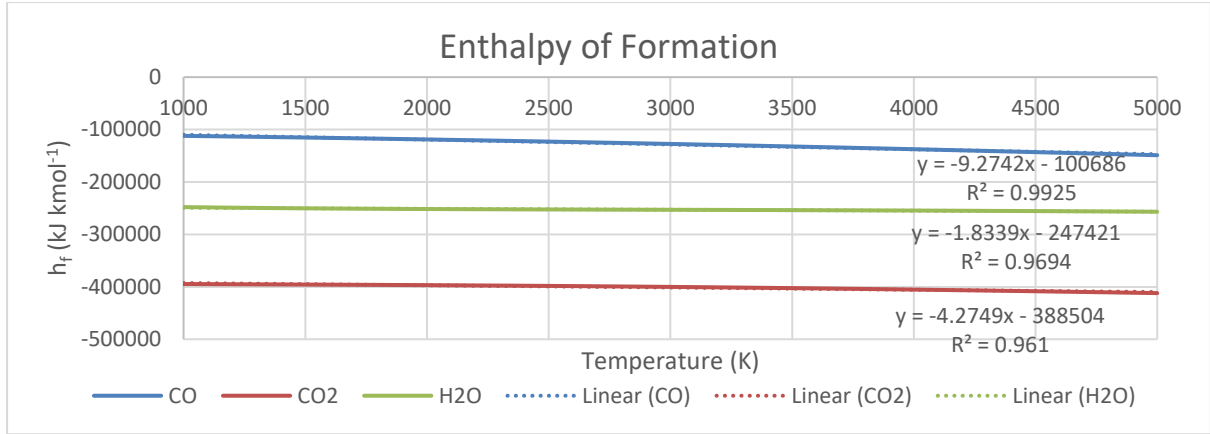


Figure 4-25: Enthalpy of Formation

Finally, to determine the additional specific heat capacity inside the cylinder due to dissociation, author has utilised Equation 36. Since the value of molar specific heat capacity at constant pressure is steady at given temperature, and as a result, unaffected by the dissociation in the past, author had to develop a method which picked the burnt zone temperature point of the negative energy term, to be closest to the current temperature. This has ensured that the change of dissociation energy is valid.

$$C_{p, \text{Dissociation}_i}^{\sim} = \frac{\Delta E_{\text{Total Dissociation}_i}}{\text{mol}_{\text{Total}} * \Delta T_{\text{Burnt}_i}} = \frac{E_{\text{Total Dissociation}_i} - E_{\text{Total Dissociation}_{\max(T_{\text{Burnt}}) < T_{\text{Burnt}_i}}}}{\text{mol}_{\text{Total}} * (T_{\text{Burnt}_i} - (\max(T_{\text{Burnt}}) < T_{\text{Burnt}_i}))}$$

Equation 36: Additional Molar Specific Heat Capacity at Constant Pressure due to Dissociation

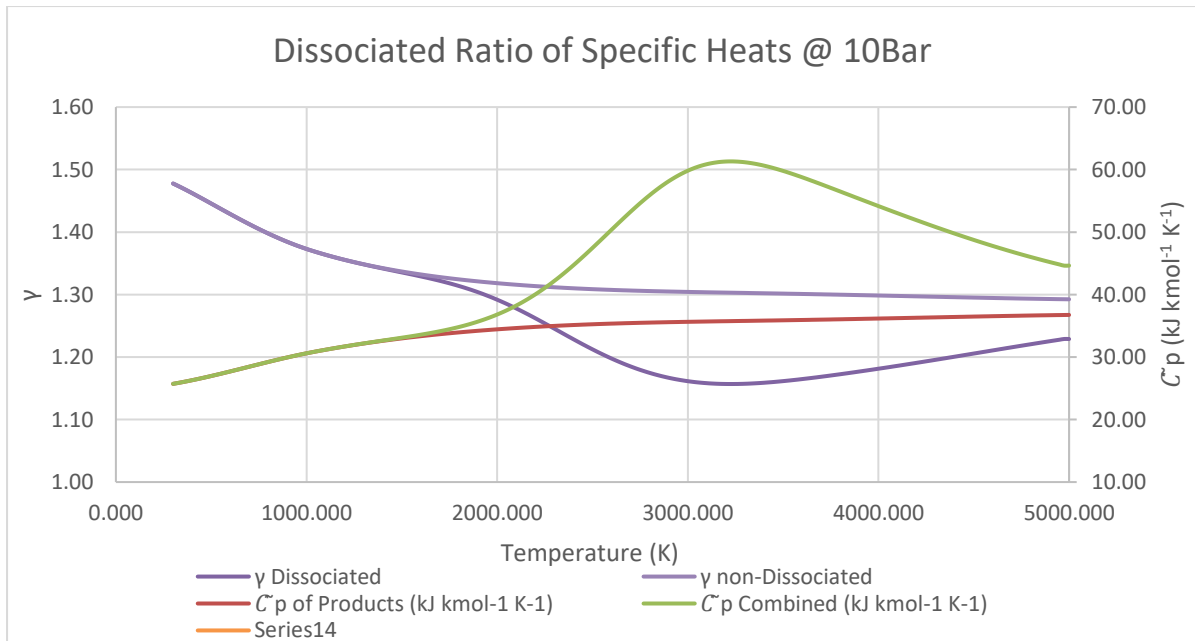


Figure 4-26: Dissociated Ratio of Specific Heats @ 10Bar

Figure 4-26 shows that the dissociated ratio of specific heats at 3,200K is 11.2% lower than non-dissociated. Author believes this difference to be very significant, considering the model's reliance on the value.

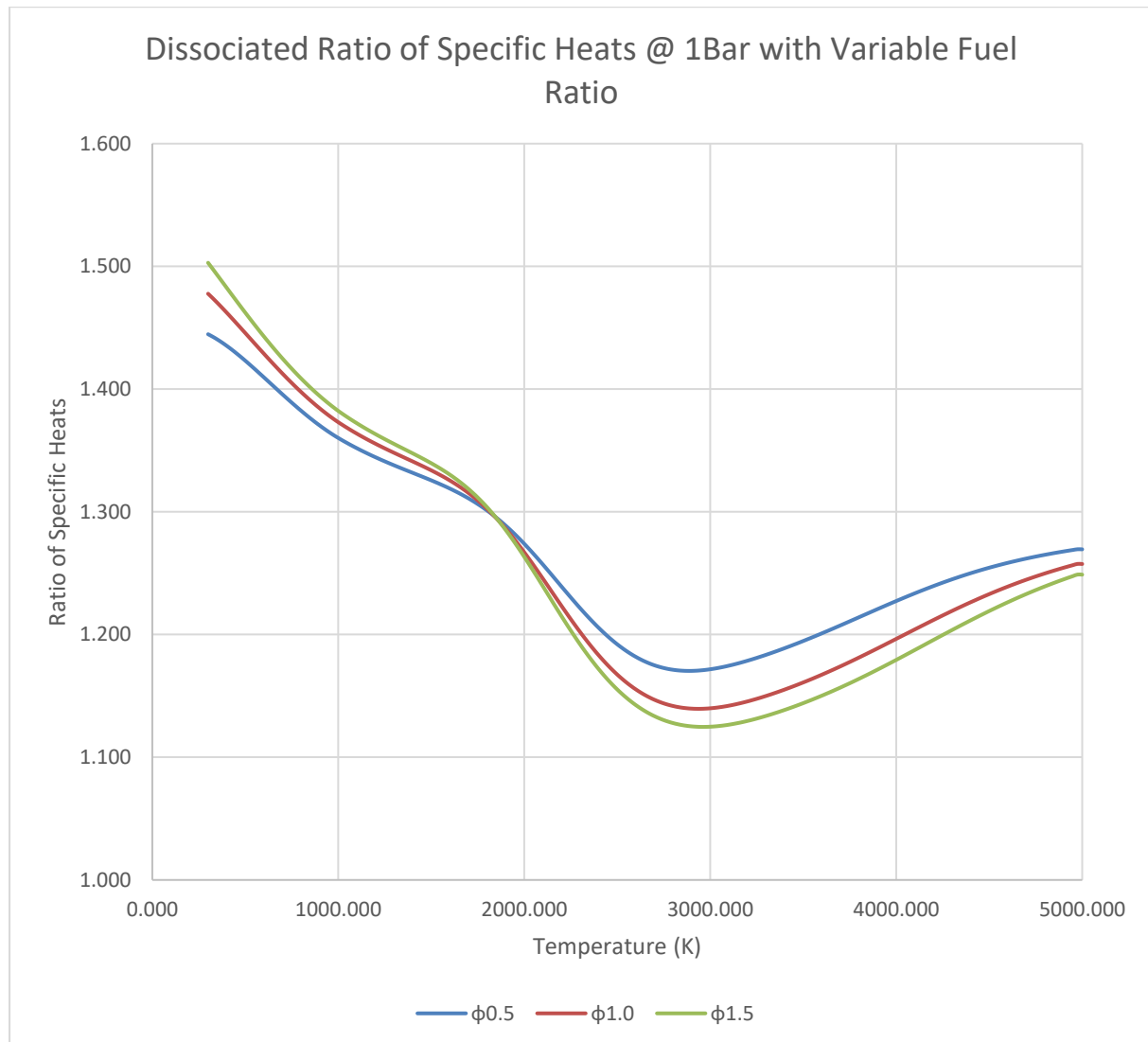


Figure 4-27: Dissociated Ratio of Specific Heats @ 1Bar with Variable Fuel Ratio

Figure 4-27 shows the calculated ratio of specific heats of iso-Octane fuel at varying fuel air ratios. They have proven to agree with the expected results (Heywood, 1988, p. 139) and as a result, author has deemed the method to be valid, which is why it has been implemented into the main model.

However, due to the method required to calculate the C_p due to dissociation, Author had to assume constant pressure of the midpoint between SOC and peak pressure, to determine the partial pressure of O₂. This is because the C_p method would not work with instantaneous cylinder pressures, as that causes less dissociation as pressure increases.

4.8 THERMAL EQUILIBRIUM ERROR CORRECTION

Quasi-static or “quasi-equilibrium” process in thermodynamics is one which occurs at slow enough rate so that equilibrium states such as: Thermal, Mechanical, Phase and Chemical are achieved before and at the end of the process (Turns, 2006, pp. 21-23).

Author has come to the realisation that the considered quasi static assumption is invalid. Author believes that Thermal and Chemical equilibrium states are not achieved in the investigated ICE. By definition, thermal equilibrium inside the cylinder is not achieved at any instantaneous C.A. due to the temperature gradients between the mixture and cylinder boundaries, as previously shown in Heat Transfer Model and 2-Zone Combustion Model chapters. Dynamic chemical equilibrium; where substance concentrations/ ratio of reaction rates becomes constant over time, is initially assumed when simulating dissociation. However, due to the very low time duration at each C.A., author believes that the reaction doesn't have the sufficient time to achieve chemical equilibrium state.

Therefore, author has employed the following error correction multipliers:

- Heat Transfer Correction Multiplier Compression (HTCMC) – adjusts component heat transfer during compression stroke
- Heat Transfer Correction Multiplier Expansion (HTCME) – adjusts component heat transfer during expansion stroke
- Dissociation Completion Correction Multiplier (DCCM) – adjusts the dissociated quantity of substances

Since the net heat flow outside of combustion is primarily driven by heat transfer, HTCMC and HTCME are adjusted so that on average, $n(s)$ matches $n(g)$, the accuracy of which is shown in Figure 4-28. The DCCM values are adjusted so that the combustion efficiency of the model equals the results calculated in Combustion Efficiency chapter.

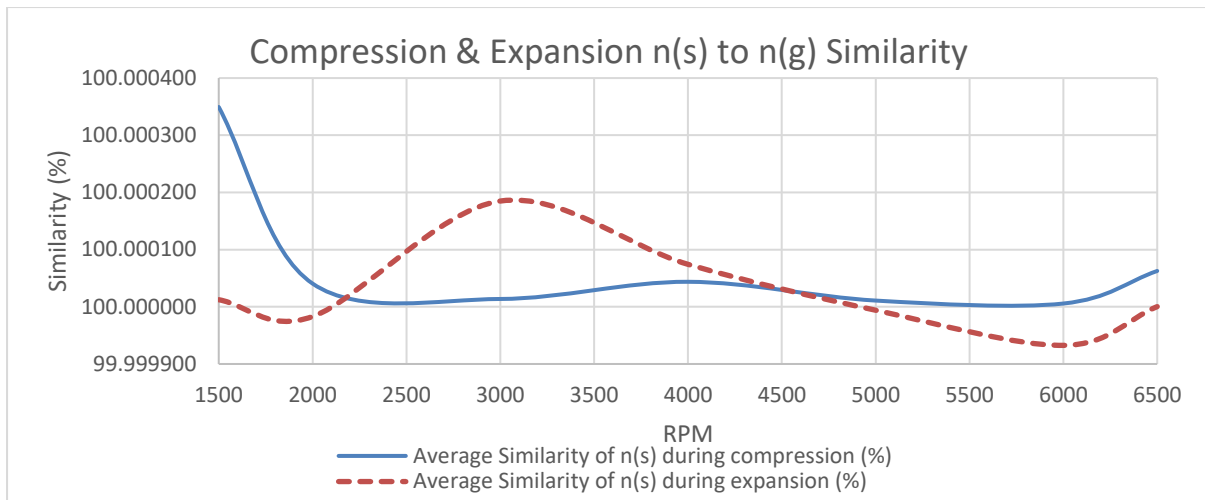


Figure 4-28: Compression & Expansion $n(s)$ to $n(g)$ Similarity

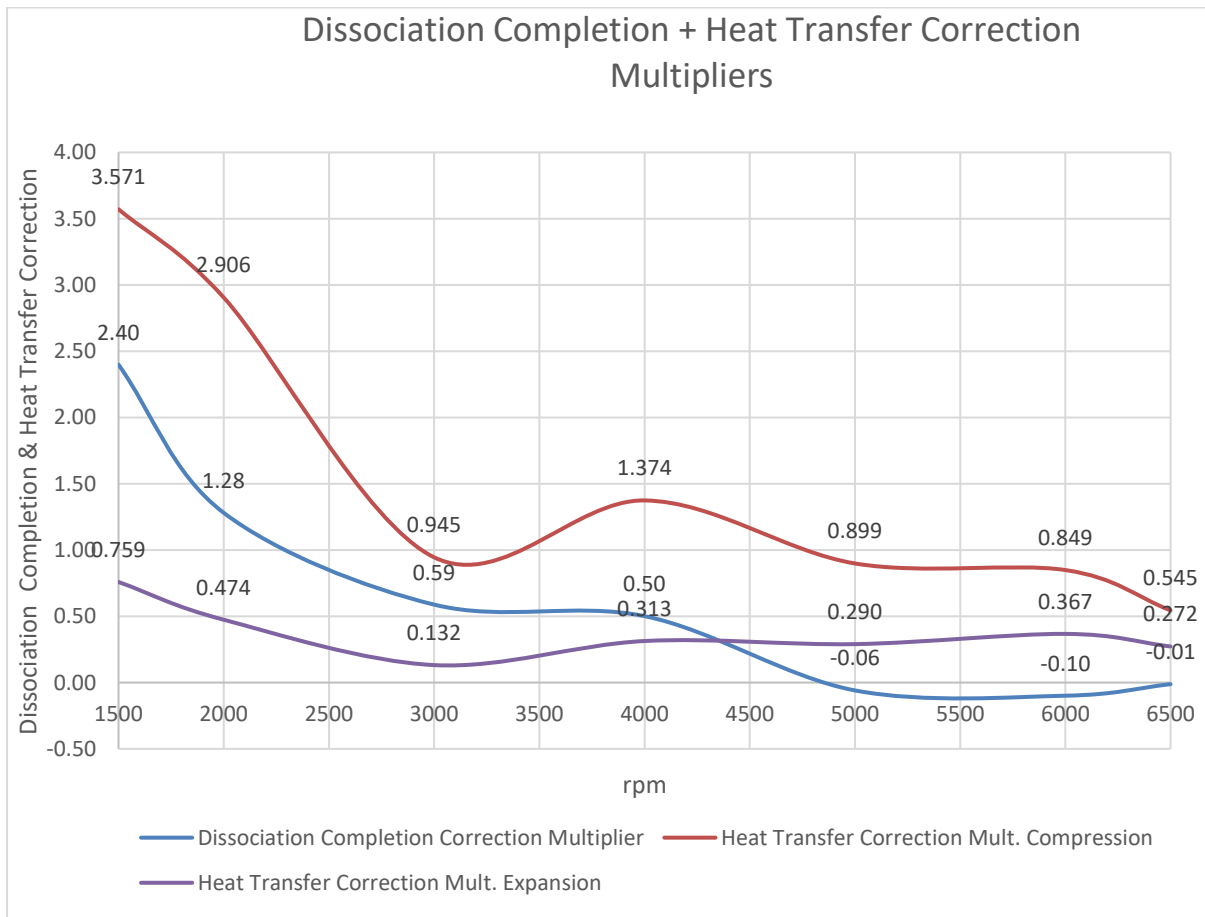


Figure 4-29: Dissociation Completion + Heat Transfer Correction Multipliers

Figure 4-29 shows that at all rpm the required HTCME values are unproportionally larger than the relative HTCME values, causing heat transfer during compression to be much more similar in magnitude to that during expansion. Author believes this problem to be caused by model's inability to capture the phenomena where heat transfer during compression fluctuates between positive and negative, as the relation between $n(g)$ and γ suggests.

The HTCME values on the other hand are relatively consistent, which suggests that author's method has adjusted Woschni type heat transfer model to the specific engine which has been investigated. The caused decrease of heat flux is drastic but still plausible (Johannes Michl, 2015). However, this has resulted in very unrealistic interior wall temperatures, suggesting either a methodological mistake or the lack of consideration of crucial phenomena in the heat transfer model. The DCCM values have developed a relatively consistent negative correlation with rpm, suggesting the initial 'dissociation completion hypothesis' to be possible.

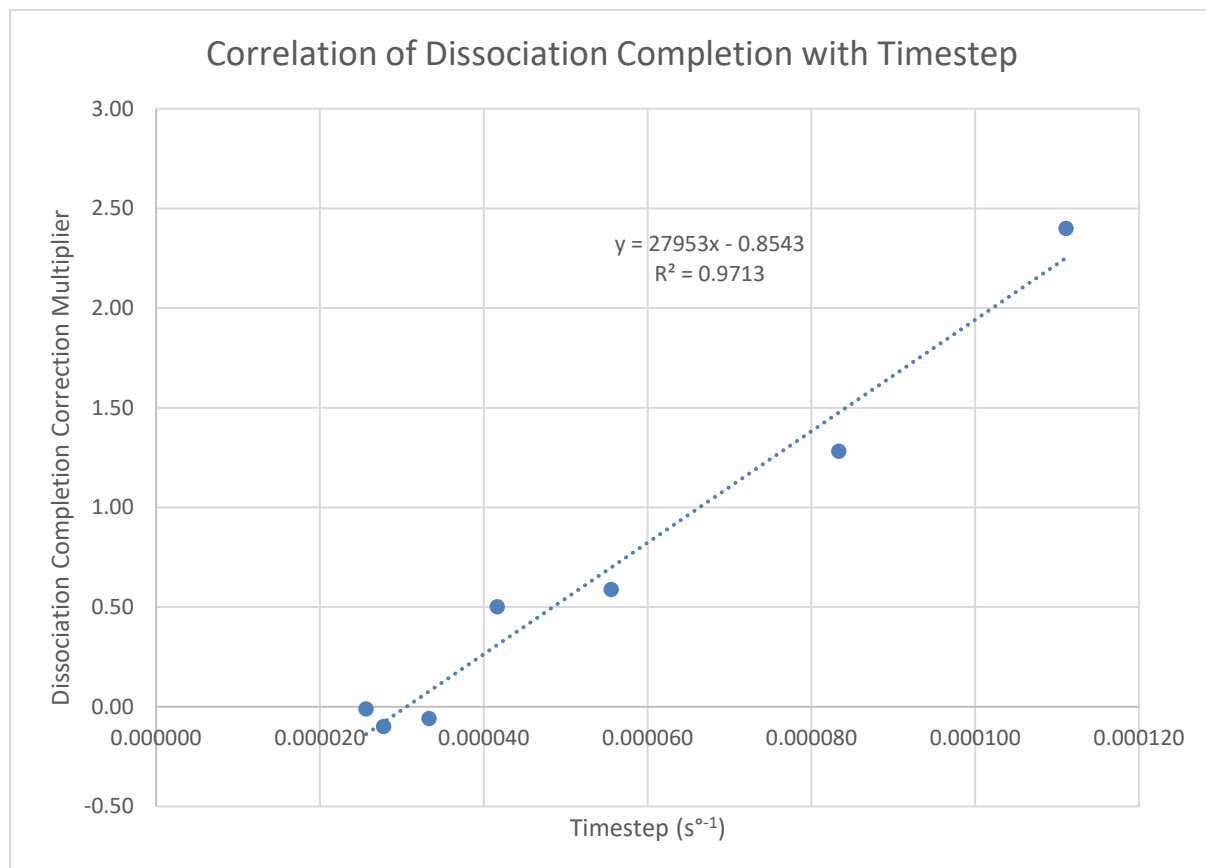


Figure 4-30: Correlation of Dissociation Completion with Timestep

Figure 4-30 shows that a very good correlation, with an R^2 value of ~ 0.95 , exists between the DCCM and timestep (time duration per ° of C.A.), making author very confident with the particular method.

The resultant correction multipliers show that author's original model is imperfect, suggesting lack of consideration of important effects which occur in real life. However, due to the methodology, mistakes committed by the model are accounted for and corrected, making the final HRR values, in author's opinion, more accurate and trustworthy than the traditional comparable techniques.

4.9 POLYTROPIC INDEX DURING COMBUSTION

Once the D.C.E < 0.1% and correction multipliers are finalized, the calculated heat release rate is used to determine the rise of pressure due to combustion, as shown in Equation 37.

$$\Delta P_i = \frac{dQr_i * (\gamma_{avg,i} - 1)}{V_i}$$

Equation 37: Rise of Pressure due to Combustion

Lastly, the calculation of polytropic index without combustion is carried out, as shown by Equation 38.

$$n_{(s)i} = \frac{\log\left(\frac{P_i - \Delta P_{i-1}}{P_{i-1}}\right)}{\log\left(\frac{V_{i-1}}{V_i}\right)}$$

Equation 38: Polytropic Index Without Combustion

Author distinguishes between the two polytropic indices as follows:

- $n(g)$ – polytropic index of gas inside the cylinder – considered as ‘nett’ index, as it includes combustion. It is the gradient of the logP-logV diagram.
- $n(s)$ – polytropic index of the system – considered as the ‘gross’ index, as it doesn’t include combustion. It dictates the pressure drop due to expansion during the combustion process.

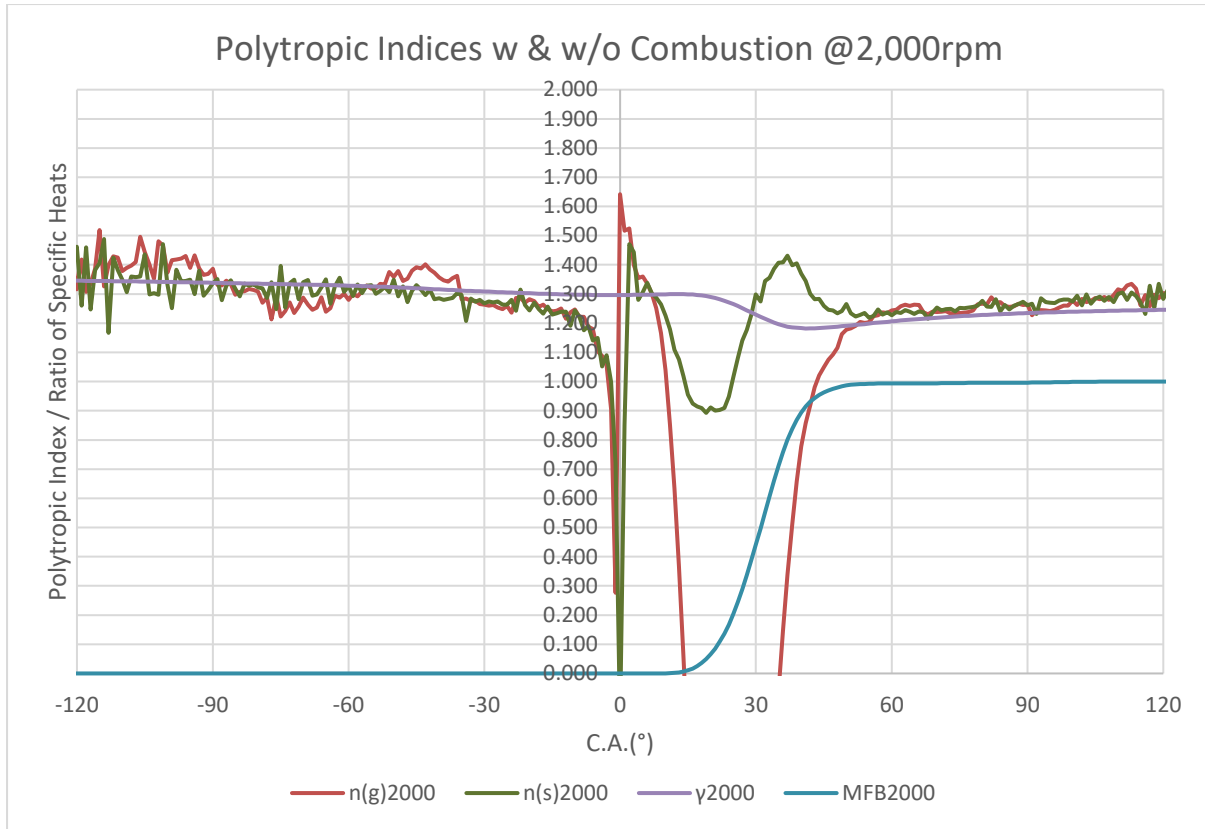


Figure 4-31: Polytopic Indices w & w/o Combustion @2,000rpm

Polytropic index $n(s)$ describes the thermodynamic process of the system if combustion ended 1° before the investigated point. Therefore, while discussing the instantaneous $n(s)$, the assumption is that during expansion, the cylinder pressure and temperature have dropped from their corresponding values 1° before the analysed point.

Figure 4-31 shows that between MFB0 and MFB10, $n(s)$ is decreasing and so the process becomes isothermal and 10% isobaric at the trough. Equation 11 implies a net heat input into the system. Since $n(s)$ doesn't consider combustion, for this to be true the gas temperature must be lower than the interior wall temperature. Similarly, between MFB10 and MFB50 the $n(s)$ increases, suggesting the rise of gas temperature to be greater than rise of interior wall temperature, supposedly due to heat transfer. At MFB50, $n(s)$ and γ come to equilibrium, suggesting adiabatic process which equates to equal gas and wall temperatures. Between MFB50 and MFB80, the $n(s)$ rises further and becomes greater than γ , suggesting interior walls becoming cooler than the gas, resulting in system losing heat. Between MFB80 and MFB100, the $n(s)$ decreases, resulting in the decrease of the temperature gradient. At MFB100, the interior walls come to a dynamic thermal equilibrium with the gas, which indicates relatively small net loss of heat.

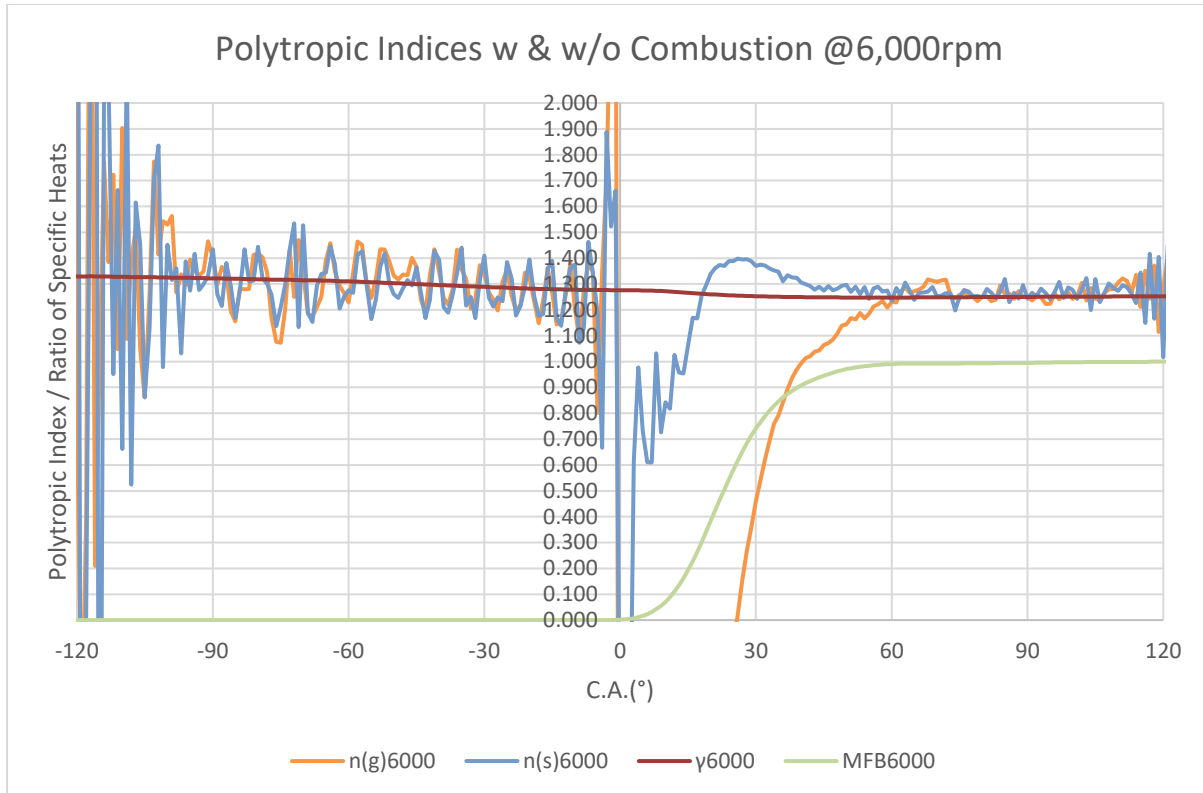


Figure 4-32: Polytopic Indices w & w/o Combustion @6,000rpm

Figure 4-32 shows the same correlations occurring at higher rpm. However, due to earlier SOC, the previously described MFB points shifted 9° closer to TDC, which is equal to the difference in SOC.

Author believes the developed model to be dependable, considering the availability of data, or lack thereof. However, author is sceptical of the $n(s)$ results during the initial part of combustion. This is because those results suggest one of the following:

- a) System experiences a source of heat other than combustion
- b) Interior wall temperatures are initially far greater than the gas

Author doesn't believe either of the proposed hypotheses to be plausible, since to author's knowledge, the investigated ICE doesn't have an auxiliary heat source which is perfectly in sync with the initial part of combustion; this cannot be the ignition spark since that would have caused the drop of $n(s)$ to occur earlier than SOC, making a) not possible. Additionally, author acknowledges the effect heat soak has on the component temperatures. However, for b) to be true, the component heat soak would have to come in a perfectly timed 'wave' which would increase the wall temperatures from and beyond SOC, as the $n(s)$ results suggest a rapid increase of temperature gradient from SOC, not before it.

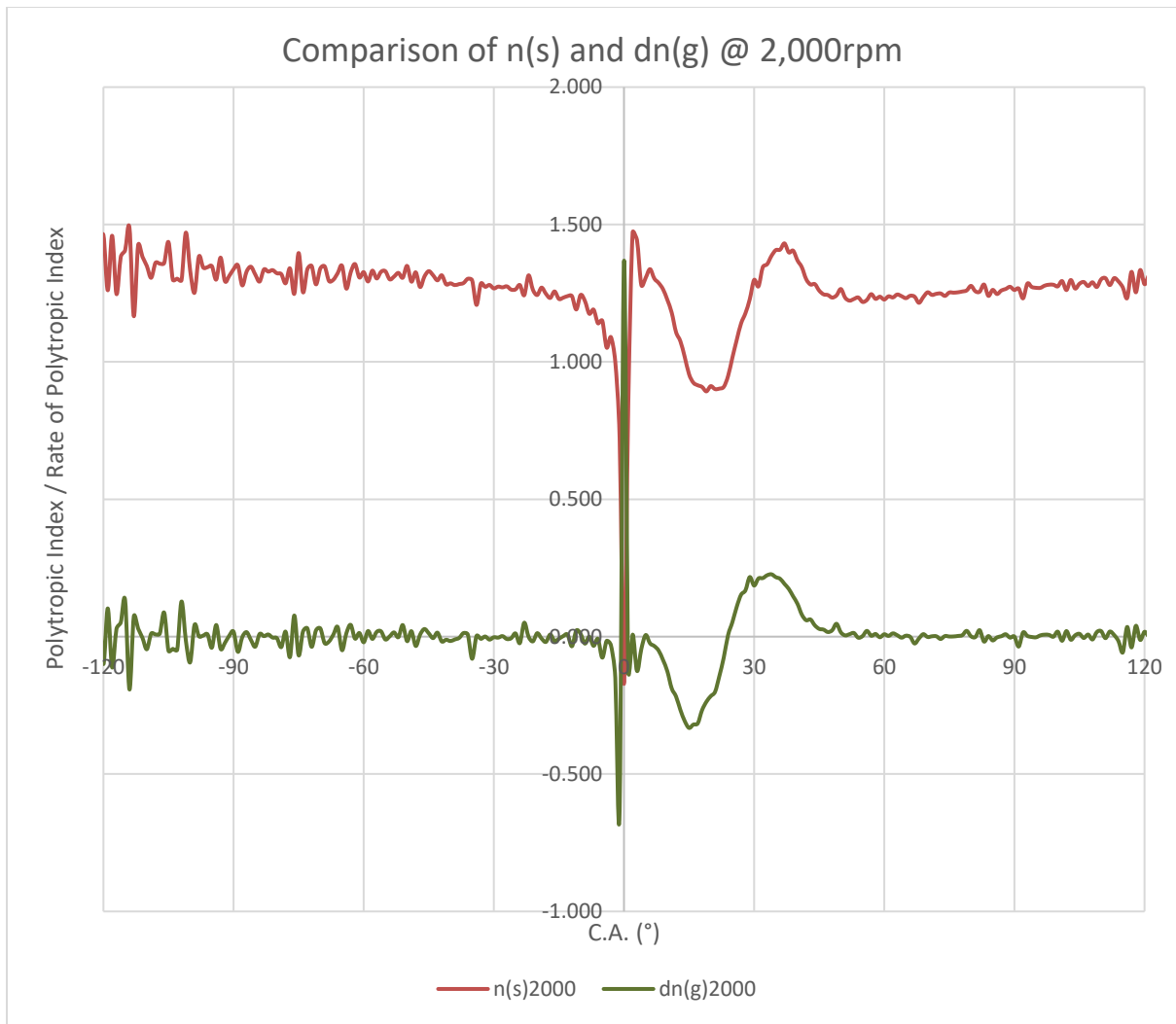


Figure 4-33: Comparison of $n(s)$ and $dn(g)$ @ 2,000rpm

Interestingly, Figure 4-33 shows a striking resemblance between $n(s)$ and $dn(g)$, which was observed at all engine speeds. The differences in profiles are believed to be caused by systematic errors in the data and the method, as well as the heat resistivity of the walls which introduce time delay in heat transfer. Despite this, author's opinion is that the resemblance is very clear and valid due to the alignment and relative magnitudes of peaks and troughs, even though the direct correlation was calculated to have an R^2 value below 0.4.

Naturally, $n(s)$ is an abstract which defines the change of pressure before combustion heat is appended, possibly making the task of $n(s)$ rationalisation flawed. However, author's findings suggest $n(s)$ to be closely related to the 'velocity' of heat transfer, which if true, would greatly improve the understanding and possibilities of engine modelling from cylinder pressure data.

However, due to the requirement of additional data and evaluation, author was not able to confirm nor deny these findings.

4.10 POLYTROPIC INDEX DURING COMBUSTION: CONCLUSION

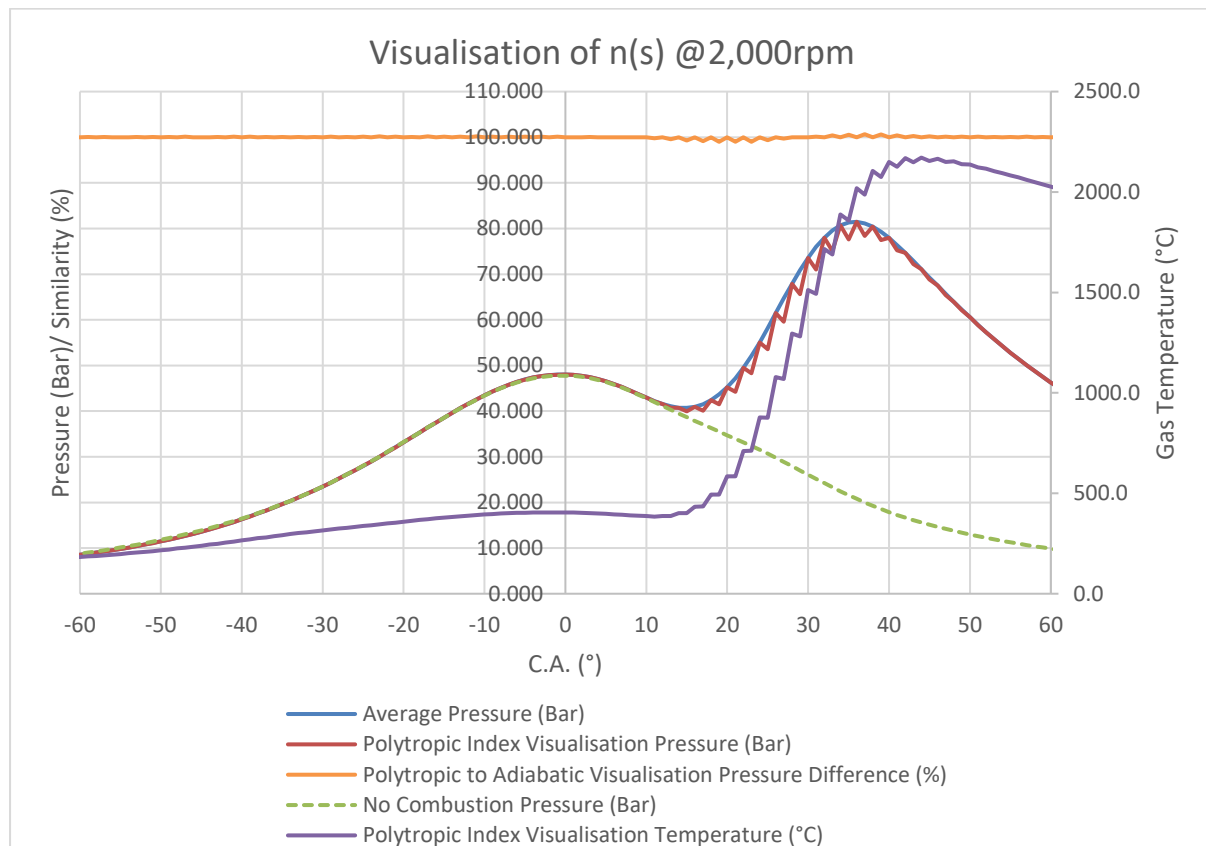


Figure 4-34: Visualisation of $n(s)$ @2,000rpm

Figure 4-34 shows the cylinder pressure and temperature if combustion was ‘turned off and on’ every 1° of C.A. This visualises the effect $n(s)$ has on the investigated ICE.

The Polytypic Index Visualisation Temperature shows that the mean cylinder temperature would not decrease below the estimated interior wall temperatures, making hypothesis b) even more improbable.

Most importantly, the difference in adiabatic and $n(s)$ pressure drop is shown to be less than 1%. Therefore, if the calculated $n(s)$ values are to be believed, then the assumption of adiabatic process during combustion is acceptable, due to the ineffective difference. This however is not supported by the heat transfer research (Johannes Michl, 2015). Due to this, author personally believes the difference between real $n(s)$ and γ to be relatively constant and comparable to the difference between $n(g)$ and γ after EOC. Thus, more work and most importantly data is required to find real $n(s)$ values. Despite this, author also believes that the work showcased in this project is a relatively good base to start of such research, despite the inability to draw concrete conclusions.

5 MEASUREMENTS & EXPERIMENTS

5.1 GEOMETRICAL ACQUISITION

Author has collected additional data in order to expand the modelling possibilities and to carry out validation.

5.1.1 Engine Components

The ports and combustion chamber were silicone cast and scanned in using traditional surface optical scanner. The same scanner was used to acquire surface data of the piston crown. The resultant point clouds were then repaired and converted into surface meshes, which were then used to create 3D CAD solid models. Non-organic geometries such as valves or spark plug, were measured and created in CAD utilising 'traditional' techniques. A microscope was used to indirectly measure the fuel injector nozzle and chamber bores. All of the components were then assembled and converted into a single surface body, as shown in Figure 5-1.



Figure 5-1: Rendering of the Finished Ford Fox GTDI Surface Assembly

5.1.2 Valve Lift Profiles

The camshaft lift profiles were acquired via mounting the camshafts in a manual degree lathe and placing the dial indicator on the camshaft lobe, as shown in Figure 5-2. Author has taken lift measurements every degree of the camshaft rotation.

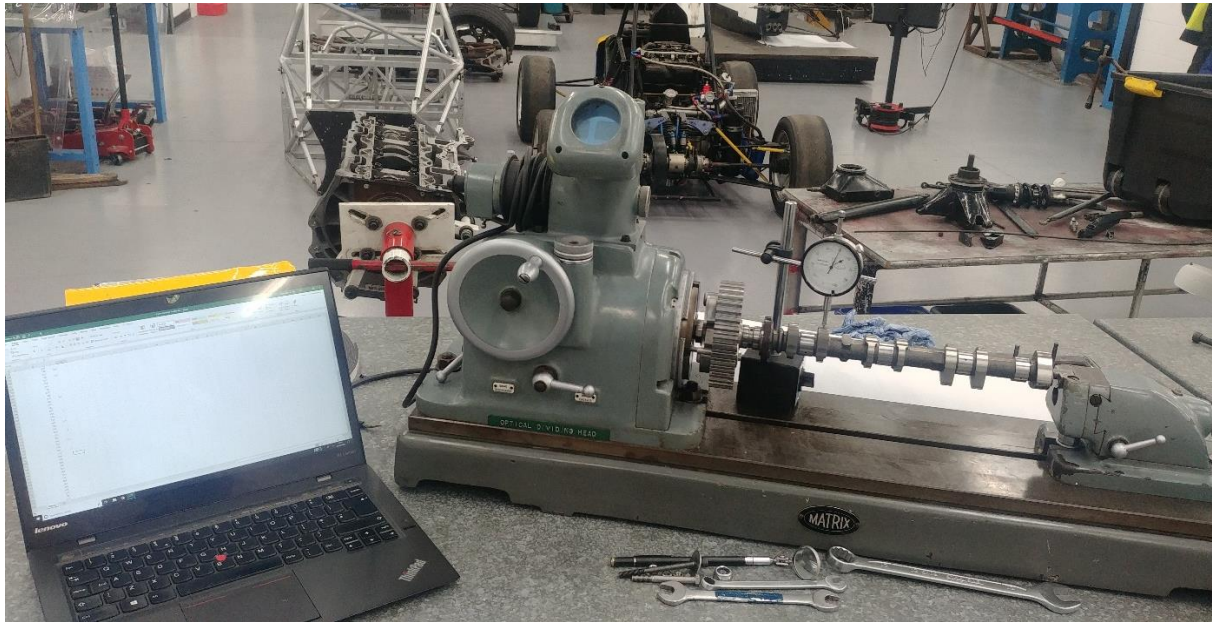


Figure 5-2: Ford Fox GTDI Intake Camshaft Mounted in a Manual Degree Lathe

The camshaft lift profiles were then converted to valve lift using traditional method, as shown in Figure 5-3.

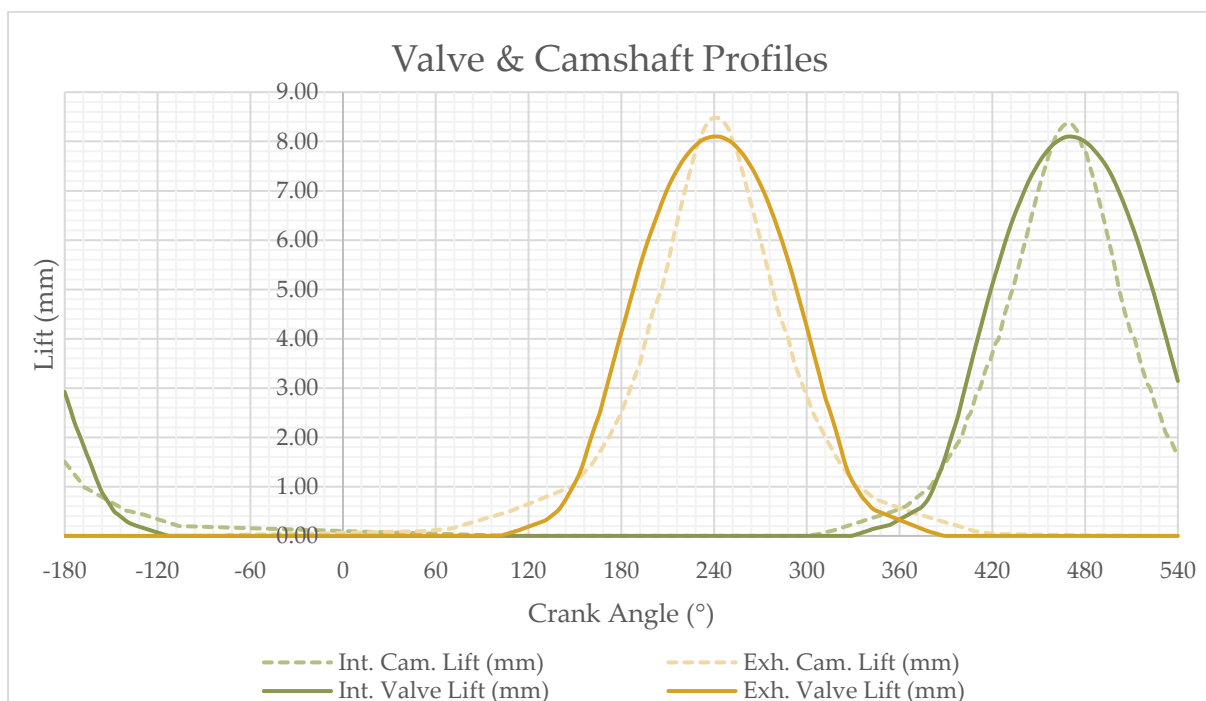


Figure 5-3: Valve & Camshaft Profiles of the Ford Fox GTDI Engine

5.2 FLOW-BENCH EXPERIMENT

Author has used a flow-bench to measure the forward and reverse flow through intake and exhaust ports of the Ford Fox GTDI engine, the results were then used to calculate the flow coefficient, of which effective flow diameter was determined to be the minimal diameter at the valve seat, minus the valve stem area and the additional area due to the radius between valve stem and head. This method accounts for the system bottleneck, making the C_d values in author's opinion, more valid than taking the flow area to be that of the valve diameter.

5.2.1 Method

Cylinder-head was mounted on the flow-bench as shown in Figure 5-4.

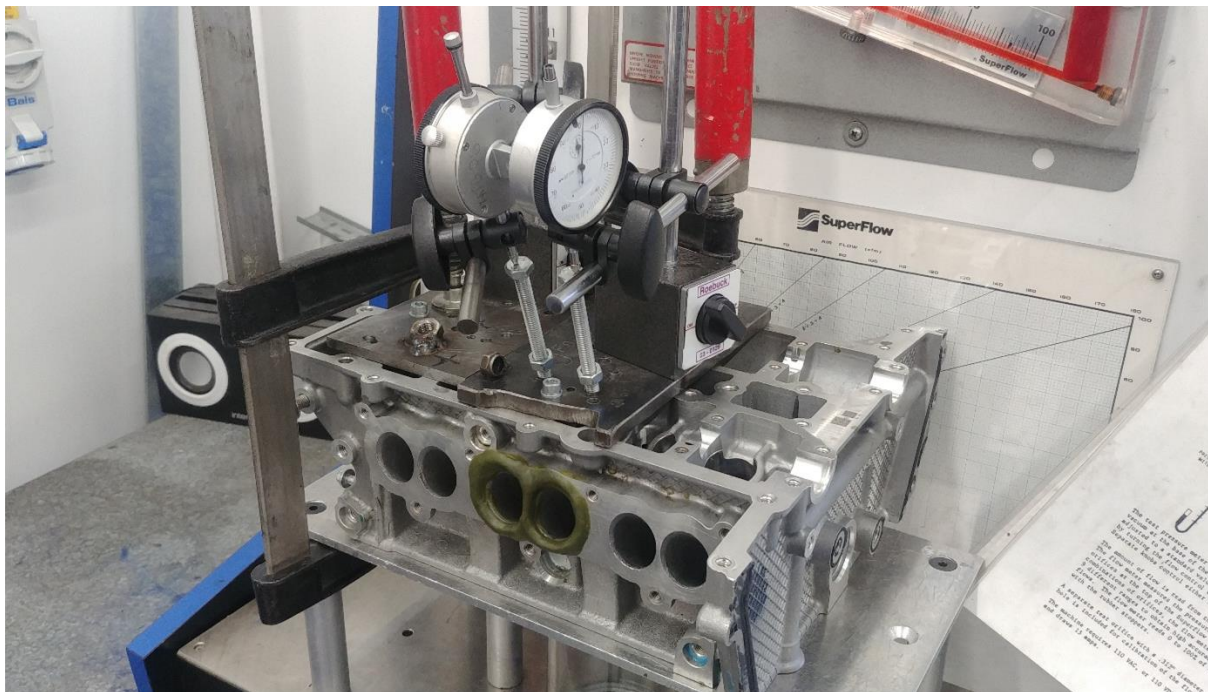


Figure 5-4: Ford Fox GTDI Cylinder-head Mounted in a Intake Flowing Direction on a Super-Flow flow-bench

An acrylic cylinder was placed in-between the cylinder-head and the flow-bench, to act as the engine liner. Author has used modelling clay at the port openings to prevent turbulence and losses. At the time, author had only access to a relatively small flow-bench. Therefore, the pressure drop between atmosphere and the flow-bench was set to 10" drop of water or 2,484 Pa. Two dial gauges were mounted on the bolts which depressed the valves, to accurately measure the valves lift. The measurements were taken every 1.0mm of valve lift up to maximum value of 12.0mm, except of initial 0.5mm lift.

5.2.2 Results

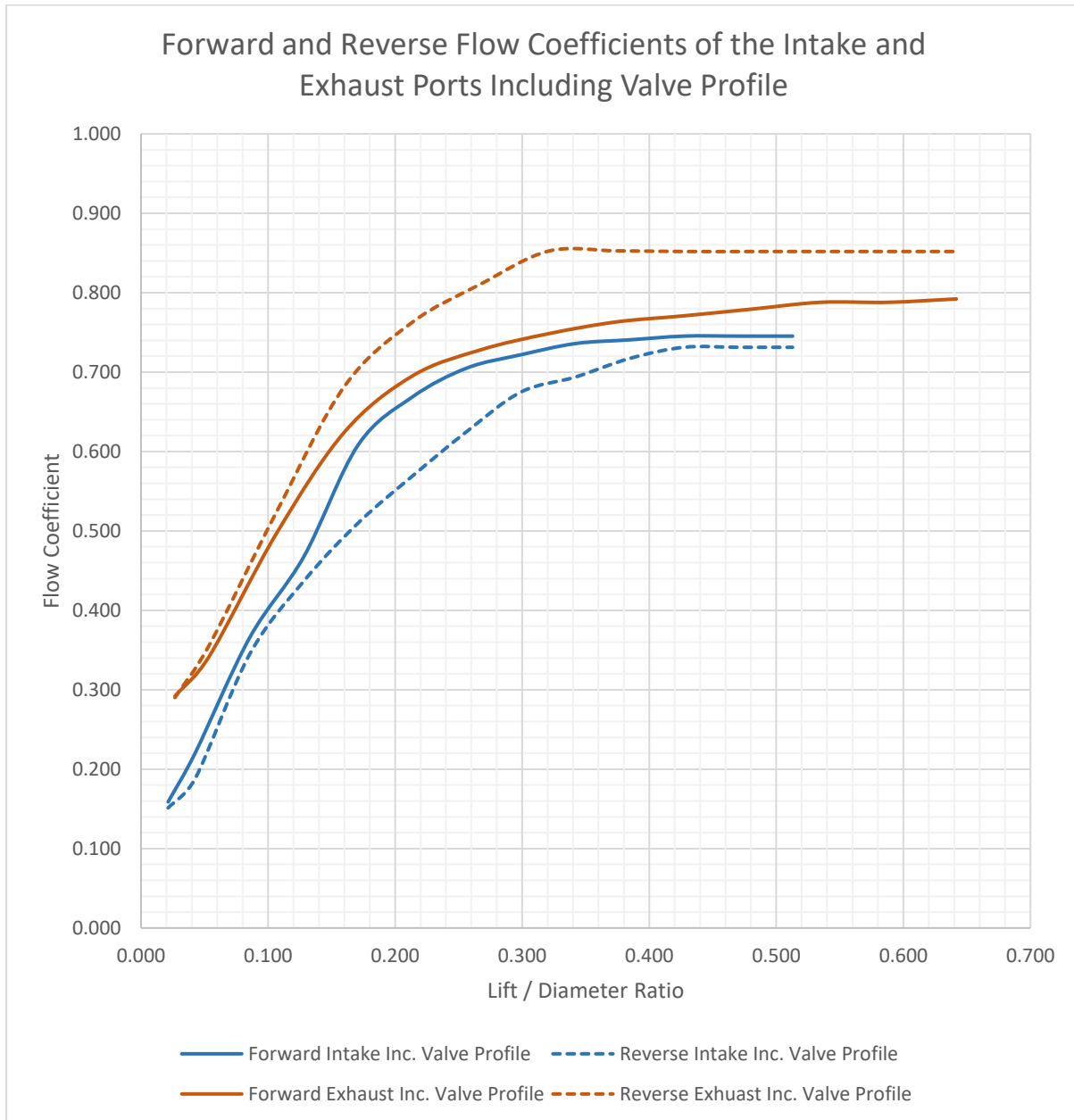


Figure 5-5: Forward and Reverse Flow Coefficients of the Intake and Exhaust Ports Including Valve Profile

Figure 5-5 shows the calculated C_d . It is clear that the ports flow more efficiently when the direction of flow is from atmosphere into the flow-bench. It is also clear that the exhaust ports flow much more efficiently than the intake ports. Author believes this to be because intake ports have been designed to induce in-cylinder turbulence, especially tumble, since it is crucial for the homogenization of the intake charge in DI engines. Lastly, author believes the C_d magnitudes to be higher compared to expected results due to the relatively low-pressure difference, as it decreases the flow velocity and therefore turbulence, allowing for more fluid to pass through the system unaffected.

5.2.3 Flow Turbulence Utilising Pyrotechnics

Author has attempted to visualize the in-cylinder turbulence utilising pyrotechnic devices which produced coloured smoke as a result of exothermic reaction. The produced smoke was trapped in a vessel, which directed the smoke into the intake ports. The experiment was carried out with already mentioned pressure difference and 4.0mm lift. The setup is shown in Figure 5-6.



Figure 5-6: In-Cylinder Turbulence Visualization Experiment Setup



Figure 5-7: Frame @ 3:30 from the Recording of the In-Cylinder Turbulence Experiment

However, despite author's best efforts, all 4 attempts have been unsuccessful. Figure 5-7 shows the most 'telling' frame from the recording of the experiment. Author believes that only single conclusion could be taken from the experiment, which is that majority of the flow through the acrylic tube occurs at and around highlighted regions in Figure 5-7, as author believes that areas of low flow/ stagnation would have more visible low velocity smoke. Naturally, this experiment has proven to have too many flaws and so, the results should not be taken as absolute.

5.3 FLOW-BENCH 3D MODEL VALIDATION

5.3.1 Method

The aim of simulating air flow through the intake ports was to validate the Converge model against previously collected flow-bench data. The surface body from Geometrical Acquisition chapter was modified so that it was equivalent of the real life flow-bench setup, as shown in Figure 5-8. Table 5-1 shows important simulation setup parameters and corresponding values. The case was run at valve lift of 1.0mm, 4.0mm and 8.0mm to cover low, medium and high flow scenarios respectively, in the OEM valve lift profile.

Table 5-1: Forward Intake Port Flow Simulation Setup

VARIABLE	VALUE
EQUATION OF STATE	Redlich-Kwong
REAL GAS PROPERTIES	Temperature only
GLOBAL PRANDTL & SCHMIDT VALUES	0.9 & 0.78
SOLVER TYPE	Steady State
SIMULATION MODE	Full Hydrodynamic
SOLVE MOMENTUM	Yes
ENERGY SOLVER	Internal Energy
INLET TO OUTLET PRESSURE GRADIENT	2,484.26 Pa
TURBULENCE MODEL	RNG k- ϵ
BASE MESH	4 x 4 x 4 mm
GLOBAL VELOCITY AMR, EMBEDDING LEVEL & CRITERION	5 & 1
MAXIMUM CELLS	600,000

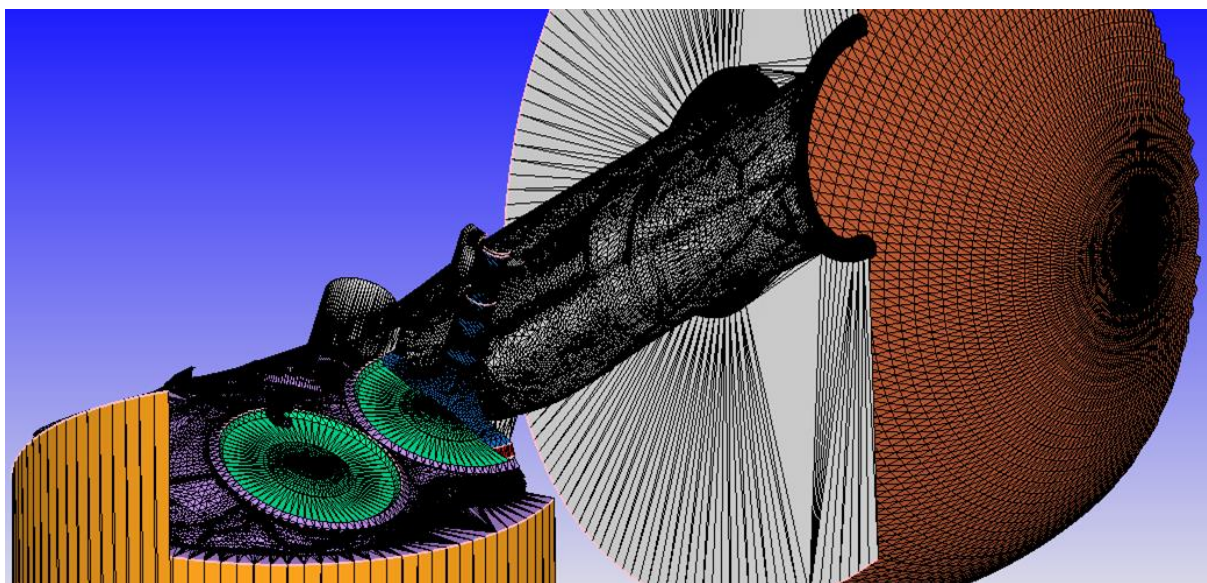


Figure 5-8: Surface Mesh in Converge of the Cylinder-Head on Flow-Bench Case

5.3.2 Validation

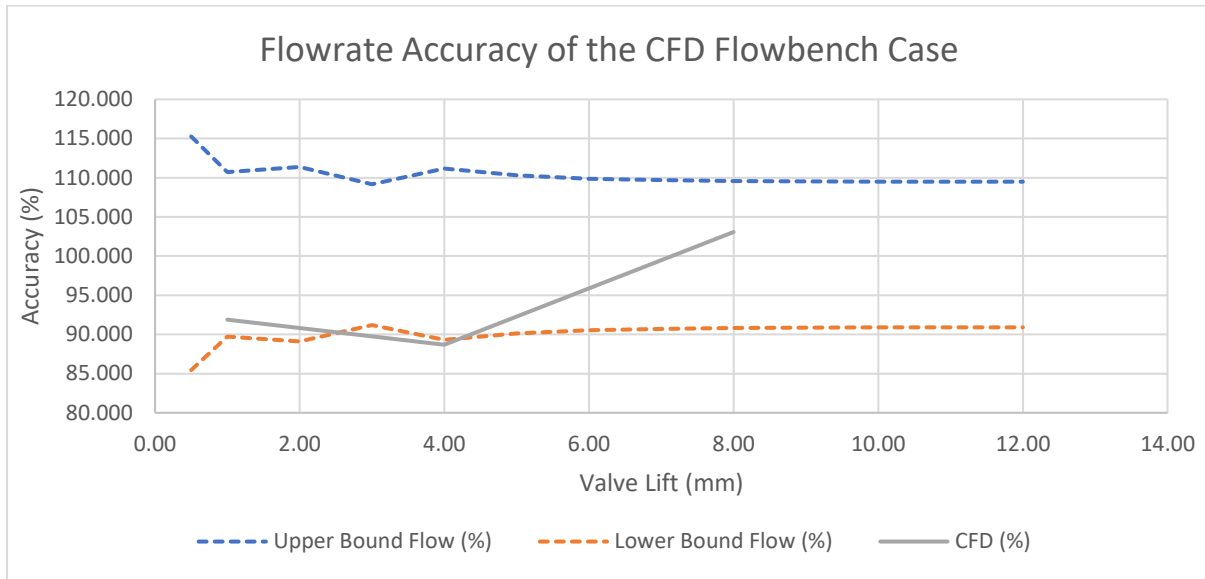


Figure 5-9: Flowrate Accuracy of the CFD Flowbench Case

Figure 5-9 shows the flowrate accuracy of the CFD results, as well as the accuracy bounds which show the tolerance of the experiment results. All three CFD results were inside the accuracy bounds, although at 4.0mm lift, the CFD accuracy was at the tolerance limit. The variation of accuracy suggests that the CFD results over-estimate the turbulence, of which there is more at lower valve lifts. Furthermore, the inconsistency of CFD accuracy suggests that author wasn't able to capture a real-life variable which has big enough effect to skew the results. The possible variables could be humidity, increased flow-bench temperature, component sealing proficiency etc. However, author wasn't able to proceed with improving the experiment due to lack of equipment, as the biggest factor effecting flowrate is turbulence in the studied case and as already mentioned, author was unsuccessful at collecting turbulence data.

Despite this, the CFD flow was deemed to be accurate enough to proceed with further modelling, due to CFD accuracy appearing inside tolerance bounds. Furthermore, due to the very strong relation between flowrate and turbulence kinetic energy, the CFD results gave author more confidence in the validity of the turbulence model.

However, author acknowledge the limitation of this validation as the dynamic characteristics in flow-bench case are far different to that inside of operating ICE. Additionally, author has only included the instrumental tolerances in the calculation of bounds, therefore it is very likely that author has underestimated them.

5.4 SPRAY EXPERIMENT

Author has carried out a spray experiment where fuel injector from the Ford Fox GTDI engine was spraying H₂O into vessel with ambient as well as 1 Bar gauge pressures, as shown in Figure 5-10. The aim of this experiment was to validate Converge spray model.

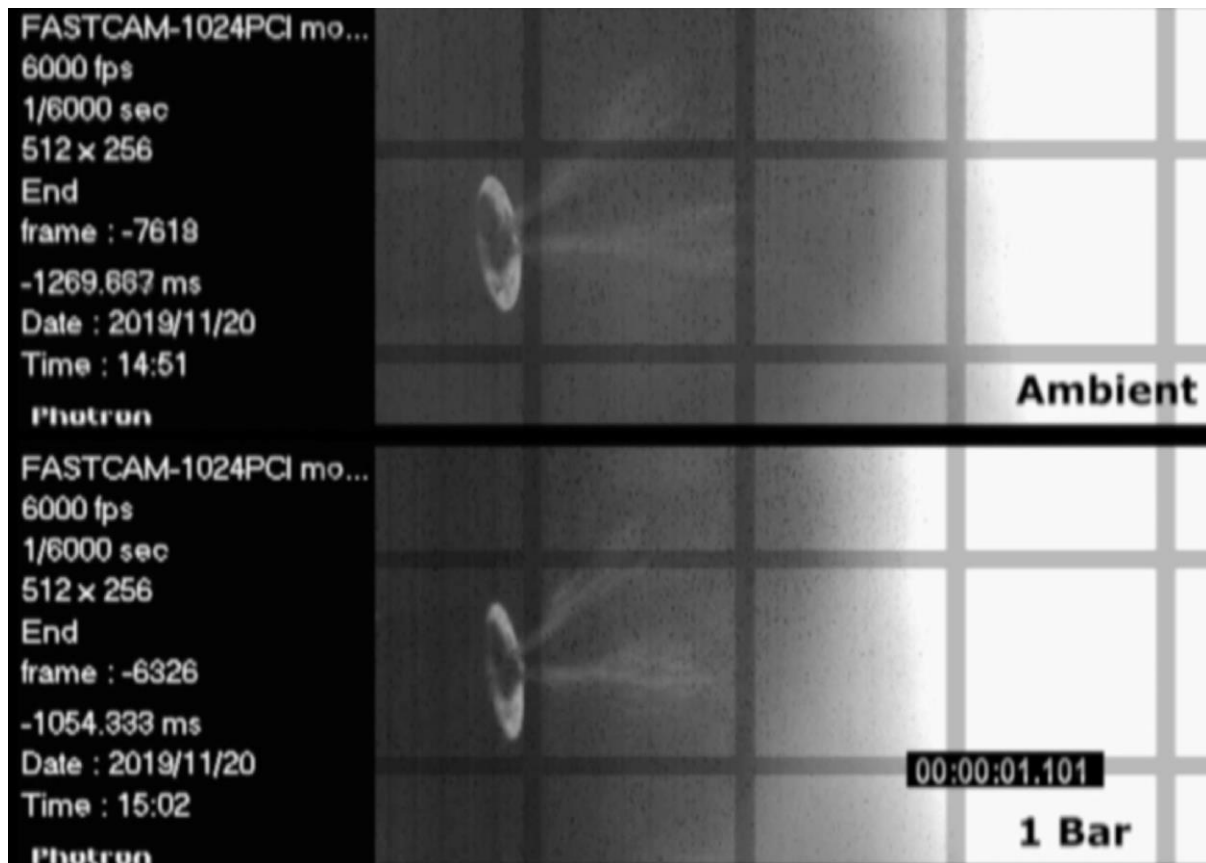


Figure 5-10: Frame @ 1.101ms from the Spray Experiment Recording

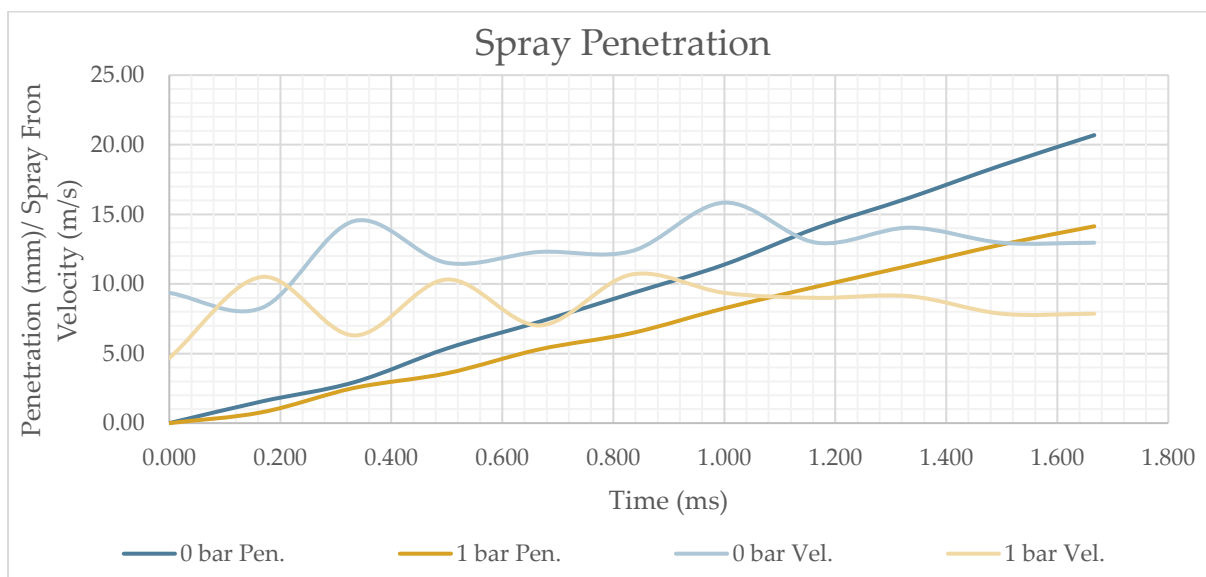


Figure 5-11: Spray Penetration of the Spray Experiment

Figure 5-11 shows that as expected, the spray front velocity of the case with ambient vessel pressure was higher, due to higher pressure gradient. The noise in velocity suggests the timestep to be too coarse and/ or, the penetration measurement to be inconsistent. Author believes that in order to achieve somewhat usable data, the experiment would have to be recorded at 10,000fps. Also, linearity of spray penetration shows that not enough distance parallel to spray direction was measurable, since the penetration velocity should decrease at certain distance due to dissipation of kinetic energy. The combination of required fps and wider screen capture has made it impossible for the author to collect usable data.

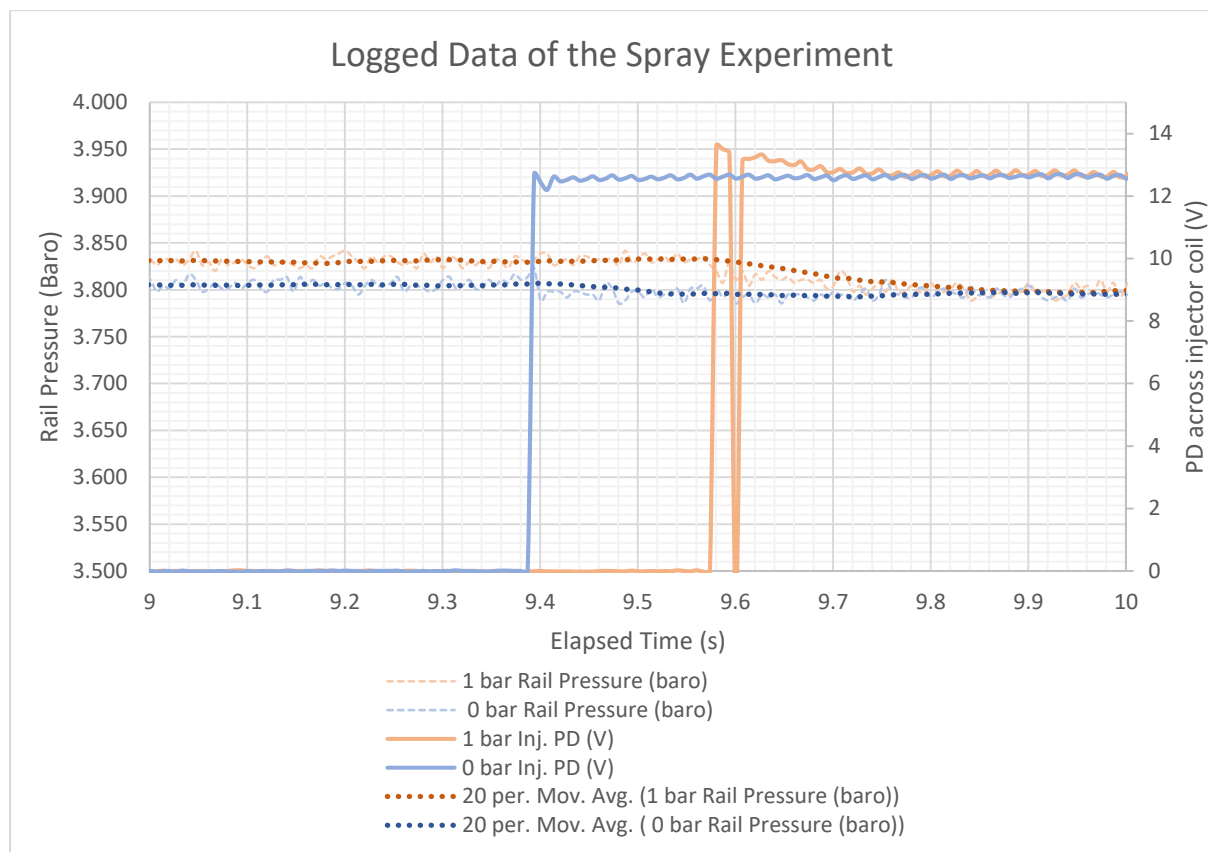


Figure 5-12: Logged Data of the Spray Experiment

Figure 5-12 shows the logged sensor data of the spray experiment. The PD profiles indicate the start of spray. At elapsed time of 9.6, the PD is momentarily lost, showing the system to have unreliable trigger. The initial rail pressure shows to be different in both cases, despite the same setup, making the results incomparable.

All of the mentioned issues as well as the computationally expensive spray model setup required unavailable equipment, forcing author to cease the work on spray modelling.

6 3-DIMENSIONAL ENGINE MODELLING

6.1 MODELLING ORIGINAL FORD FOX GTDI ENGINE

6.1.1 Case Setup

Author has decided to focus on modelling the engine at single engine speed to reduce the computational time. 4,000rpm was chosen, due to highest net thermal efficiency, as shown in Figure 6-1. Oscillations in thermal efficiency were caused by changing AFR.

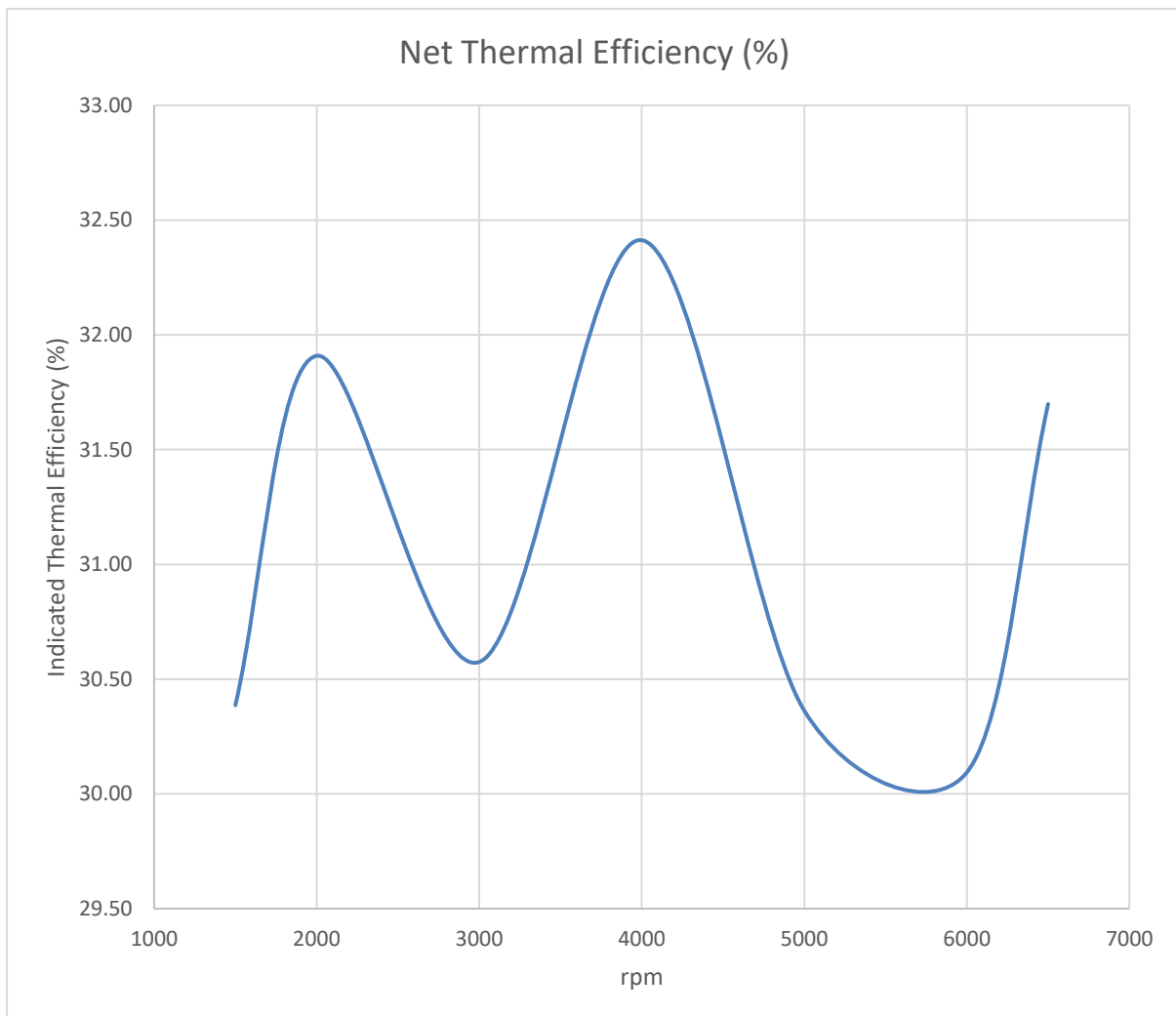


Figure 6-1: Net Thermal Efficiency

Surface body from Geometrical Acquisition chapter was used to create the surface mesh. Despite having enough data to simulate the engine through all 4 strokes, author has decided to focus on the combustion/ expansion process, in order to reduce the computational time, as the equipment available to the author was severely limited in computational power.

Author has adjusted certain simulation parameters in order to replicate the real Ford Fox engine as best as possible with the available data and equipment. Table 6-1 shows important simulation parameters used in the final simulation of combustion in stock Ford Fox ICE.

Table 6-1: Stock Ford Fox GTDI Engine Combustion Simulation Setup

VARIABLE	VALUE
SOLVER TYPE	Transient, crank angle based
EQUATION OF STATE	Redlich-Kwong
REAL GAS PROPERTIES	Temperature only
GLOBAL PRANDLT & SCHMIDT VALUES	0.9 & 0.78
REACTION MECHANISM	By Dalian University of Technology (2011), 44 species and 139 reactions for PRF, 4 species and 13 reactions for NOx
FUEL TYPE	IC8H18
SIMULATION MODE	Full Hydrodynamic
GAS FLOW SOLVER	Compressible
LIQUID FLOW SOLVER	Incompressible
SOLVE MOMENTUM	Yes
ENERGY SOLVER	Solve Internal Energy
REREAD INPUTS EACH TIME-STEP	Yes
SOLVE SPECIES	Yes
START TIME	-35.0 deg.
END TIME	180.0 deg.
TIME-STEP SELECTION	Variable time-step algorithm
INITIAL TIME-STEP	5e-7s
MINIMUM TIME-STEP	1e-8s
MAXIMUM TIME-STEP	5e-6s
CONVECTION CFL LIMIT	5.0
DIFFUSION CFL LIMIT	2.0
MACH CFL LIMIT	40.0
CHEMICAL TIME-STEP CONTROL MULT.	0.5
MOVING BOUNDARY TIME-STEP MULT.	0.5
WALL TEMPERATURE BOUNDARY CONDITION (ALL)	Law of Wall
WALL ROUGHNESS (ALL)	0.0
PISTON TEMPERATURE	450K
LINER TEMPERATURE	450k
HEAD TEMPERATURE	450K
SPARK PLUG TEMPERATURE	550K
INTAKE PORTS TEMPERATURE	425K
EXHAUST PORTS TEMPERATURE	500K
INFLOW TEMPERATURE & PRESSURE	314K & 234,530.0Pa

OUTFLOW TEMPERATURE & PRESSURE	1200K & 290,800.0Pa
IV STEM, SEAT & HEAD TEMPERATURE	480K, 480K & 480K
EV STEM, SEAT & HEAD TEMPERATURE	525K, 525K & 525K
CYLINDER REGION INITIALIZATION: TEMPERATURE, PRESSURE, [IC8H18], EGR, [N2]/[O2]	672K, 2038,500.0Pa, 0.07164731, 2.2%, 2.855
COMBUSTION TEMPERATURE CUTOFF	900K
COMBUSTION MINIMUM HC SPECIES MOLE FRACTION	1e-14
EMISSIONS MODEL	Extended Zeldovich with equilibrium assumption
COMBUSTION MODEL	Sage Detailed Chemistry Solver with Adaptive Zoning
REACTION MULTIPLIER	0.8
COMBUSTION SOLVER TYPE	Constant volume
TURBULENCE MODEL	RNG k- ϵ
WALL HEAT TRANSFER MODEL	O'Rourke and Amsden
START OF IGNITION	-1.0 deg.
BASE MESH	4 x 4 x 4 mm
CYLINDER VELOCITY & TEMPERATURE, EMBEDDING, CRITERION	3, 1 & 3, 2.5
MAXIMUM CELLS	500,000

The major assumptions in the simulation are as follows:

- Since the simulation begins close to TDC, in-cylinder turbulence due to gas exchange process isn't modelled. However, other phenomena such as squish are present.
- Since model doesn't simulate the gas exchange process and fuel mixing, the trapped charge in cylinder is assumed to be perfectly homogenous at the start of simulation.
- Due to lack of computational power, author wasn't able to take advantage of the conjugate heat transfer model, therefore the interior wall temperatures were assumed to be constant and the applied values were that of the Converge example GDI engine.
- The source of ignition was represented as a sphere of 0.9mm in diameter, into which energy was artificially applied.

6.1.2 Model Validation

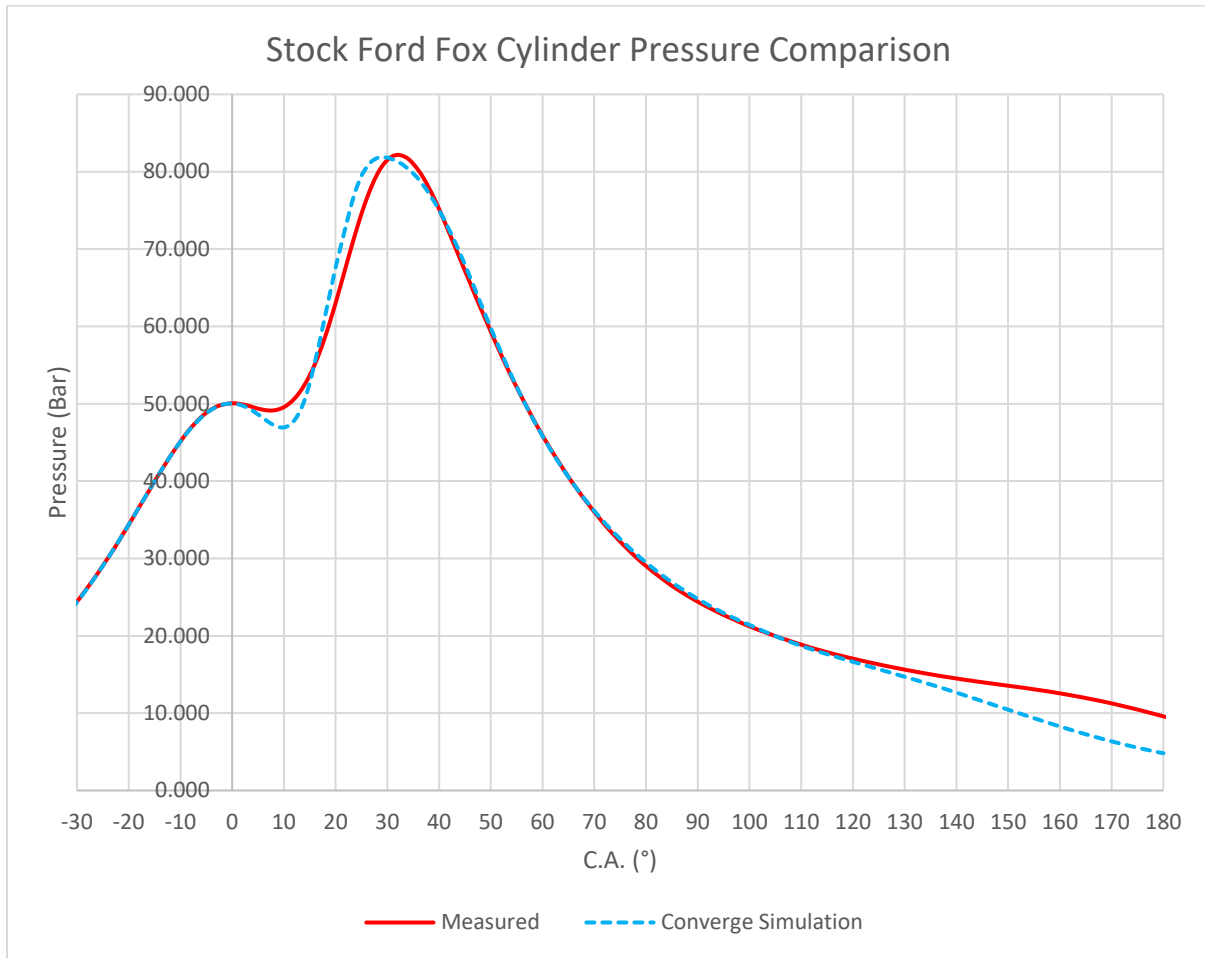


Figure 6-2: Stock Ford Fox Cylinder Pressure Comparison

Figure 6-2 infers that in the simulation, the pressure rise due to combustion occurs at later C.A., causing maximum deviation of 3.0Bar at 10° ATDC. Author believes this to be caused by the lack of tumble in the simulation, since apart from mixing, it also aids in the acceleration of initial combustion, as the combustion zone is spread. Once combustion zone is established, the rate of rise of pressure due to combustion is higher than in real engine. This has been artificially adjusted by the author so that accurate peak pressures are achieved, improving the mean accuracy. The required reaction multiplier to obtain correct peak pressure was 0.8, causing 20% reduction in reaction rate from standard. Due to requirement of artificially fast combustion, author believes that the utilised reaction rate is higher than in reality. This inaccuracy is considered to be caused by the reaction mechanism file; however, mechanism tuning is outside the scope of this project. After peak pressure, the simulation is practically identical to real values, considering the extent of inaccuracies in the model setup. However, deviation develops 120° ATDC. The cause is believed to be due to incorrect EVO timing.

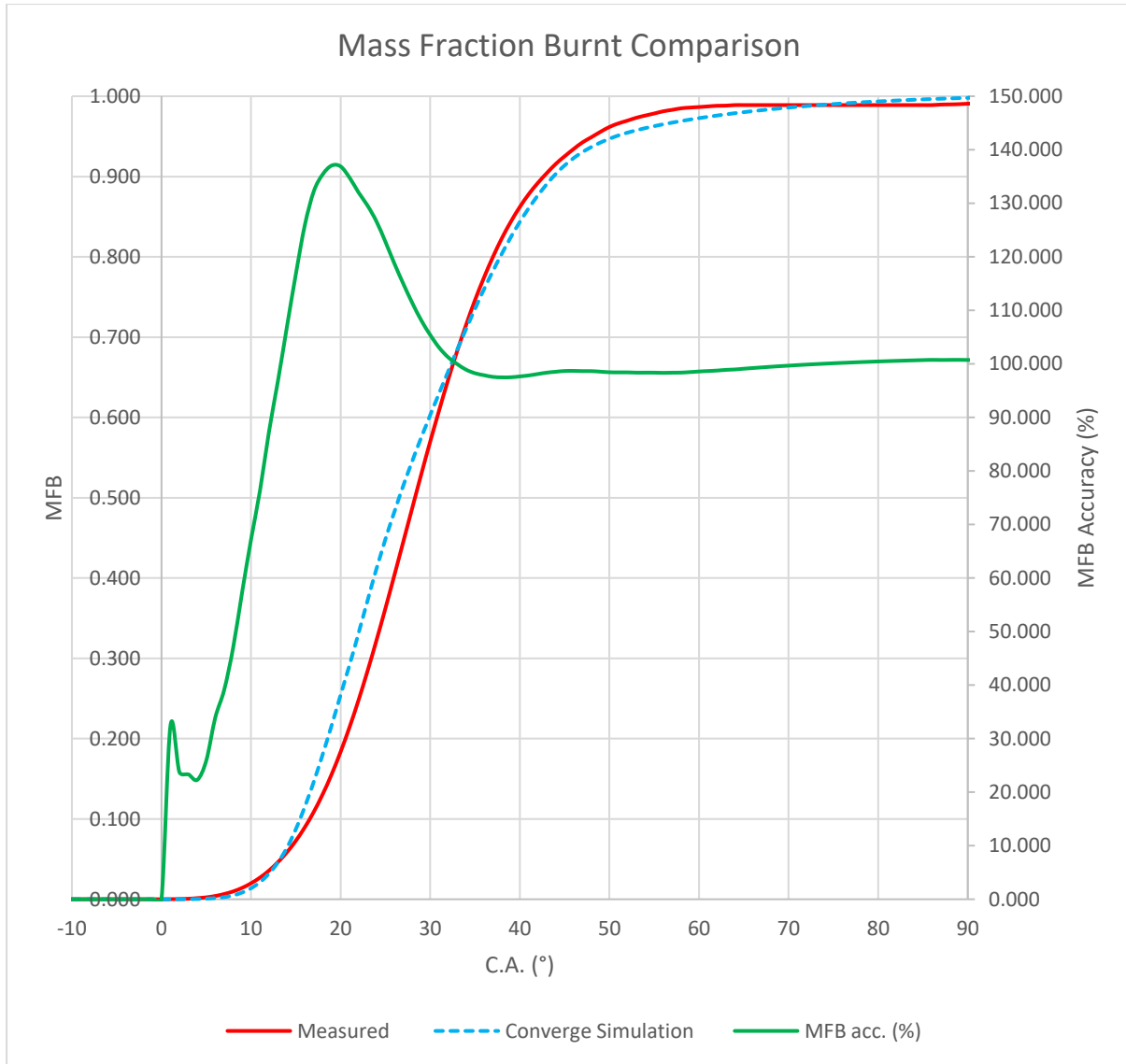


Figure 6-3: Mass Fraction Burnt Comparison

Figure 6-3 shows that maximum MFB inaccuracy of 82% occurred at 4° ATDC, although the accuracy is very sensitive during initial combustion due to low magnitudes. This proves that deviation in cylinder pressure was caused by 'slow' combustion, especially since change of volume close to TDC is minimal and so, relatively little energy is required to achieve the real pressures. Another inaccuracy peak of 37% occurred at 20° ATDC. As already mentioned, this was caused by adjusted combustion rate. Considering this, author believes the MFB inaccuracy to be surprisingly low, during the most vital section of MFB. Lastly, once MFB80 is achieved, the combustion simulation shows to be in good agreement with real results. On average, the simulated MFB was 97.2% accurate during the combustion process, although that statistic includes MFB80 – 100, which has relatively long duration and good accuracy, skewing the result in favour of the simulation.

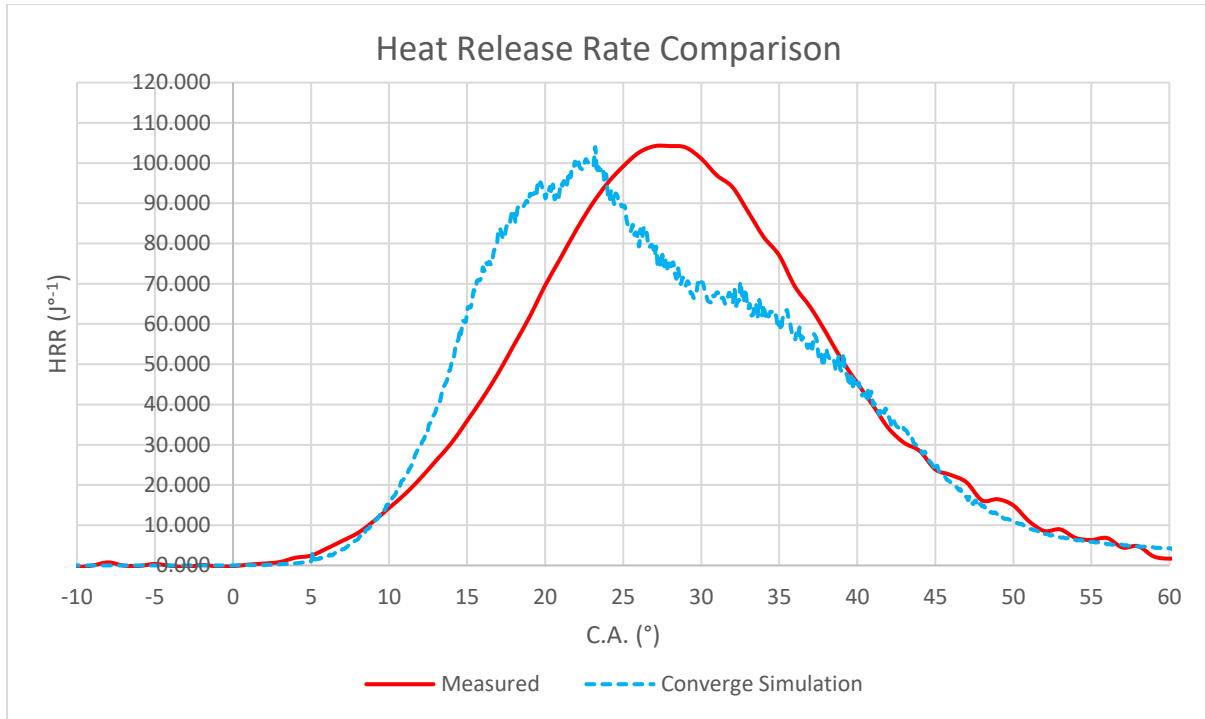


Figure 6-4: Heat Release Rate Comparison

Figure 6-4 shows that peak HRR magnitude is relatively accurate 96%. Naturally, the position of it isn't as already discussed. The simulated HRR profile is of very similar shape, although the combustion rate skews the gradient. However, HRR profile is in poor agreement with real values after the peak. Firstly, HRR abruptly decreases shortly after the peak is established. Secondly, at 30° ATDC, a second 'wave' of combustion occurs.

The relatively poor agreement could be caused by multitude of reasons, author believes the following to be most plausible:

1. The lack of tumble changes the burnt zone geometry, causing the geometrical limitation of combustion rate to occur at different times and severity.
2. Real mixture is likely to be very much more stratified, altering combustion rate as the combustion zone propagates through richer and leaner zones.
3. Reaction mechanism could be severely underestimating the energy output of reactions occurring between 24° and 30° ATDC.
4. At 30° ATDC, mean cylinder temperature of 2,200K is achieved, causing dissociation, of which products could be responsible for the additional HRR. However, this wasn't observed in the [HC].

The lack of equipment and data prevented author from perusing more accurate HRR results.

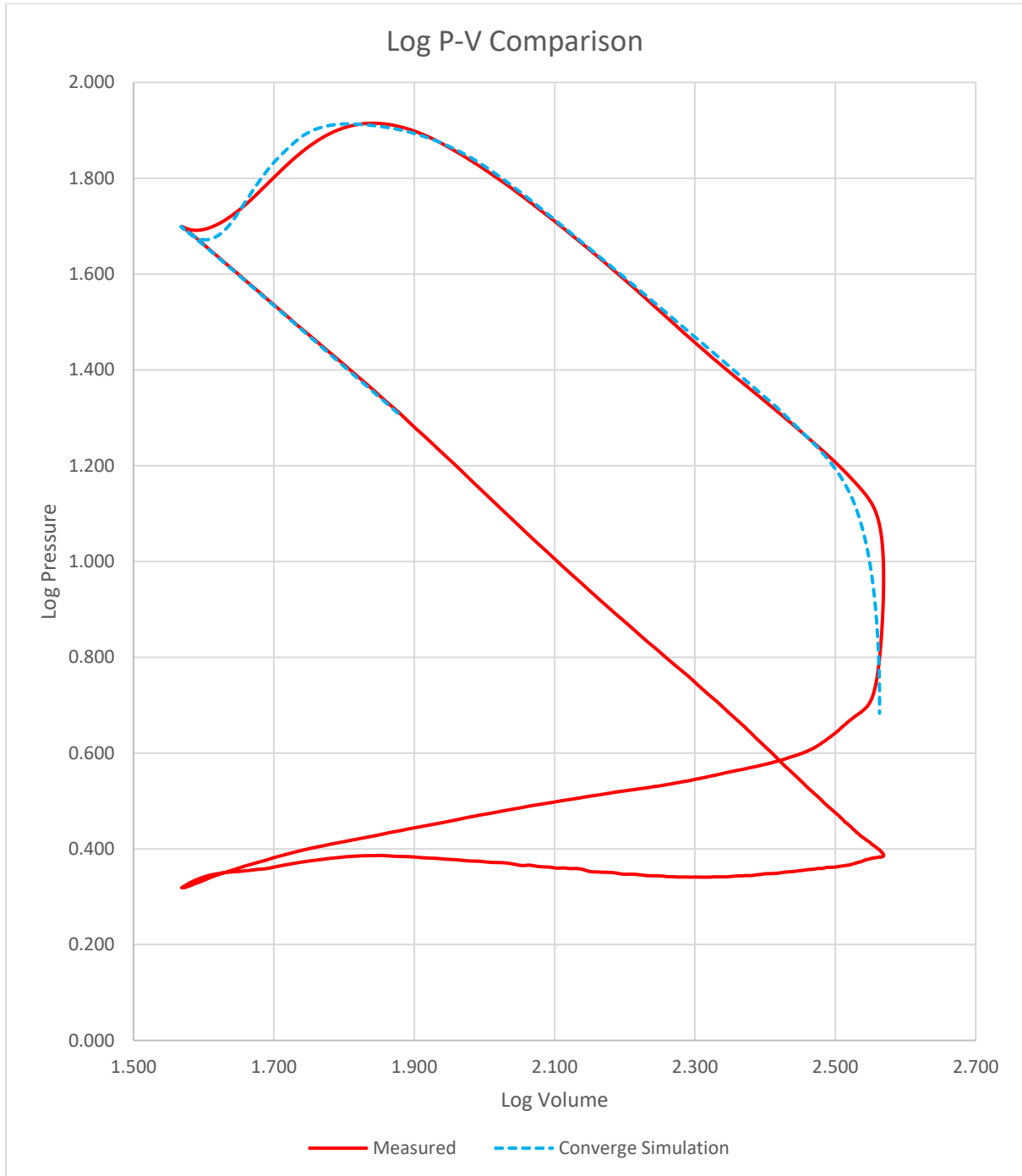


Figure 6-5: Log P-V Comparison

Figure 6-5 shows good agreement of simulated results with real data during compression and expansion, suggesting the achievement of accurate polytropic index and as a result, correct level of heat transfer throughout the stroke. The previously mentioned pressure discrepancy at the end of the expansion stroke was also observed, of which profile suggests incorrect exhaust flow simulation even after BDC. This was most likely caused by static outflow pressure; however, simulation of exhaust flow is outside the scope of this project.

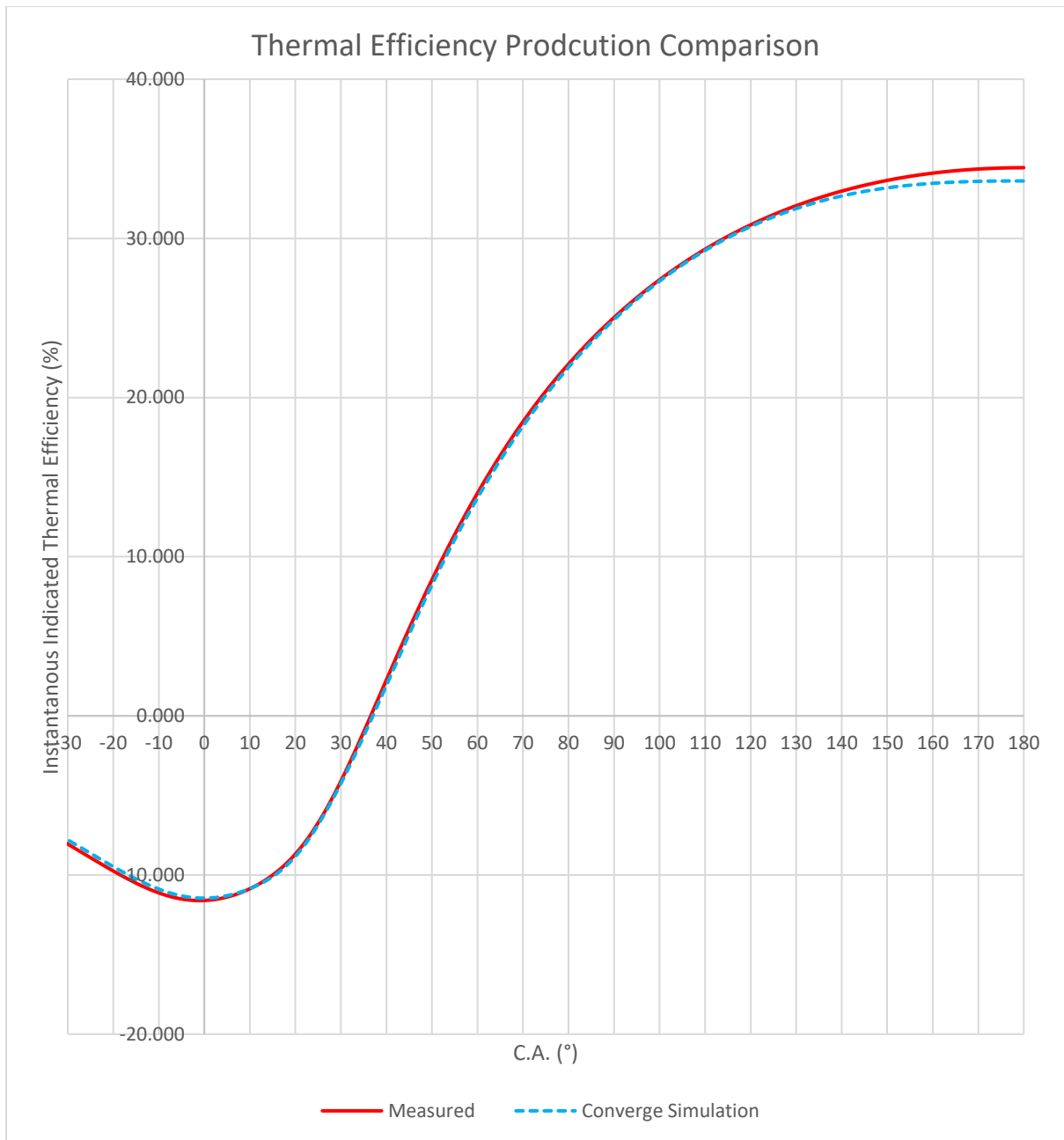


Figure 6-6: Thermal Efficiency Production Comparison

Figure 6-6 shows that despite the differences in LHV of fuels as well as in cylinder pressures, the simulated indicated thermal efficiency is very accurate throughout the modelled duration. The results indeed do start deviating at 140° ATDC, presumably due to the issue with exhaust flow. However, it is too little to make a practical effect on the final efficiency, which was 97.6% at BDC.

Given the carried-out validation, as well as challenges with lack of equipment and data, author has determined the simulation results to be of sufficiently accurate to progress with TJI development.

6.2 MODELLING TURBULENT JET IGNITION

6.2.1 Aims and Limitations

Author's approach to TJI development was to improve the environmental performance of the Ford Fox ICE, without an adverse effect on the power, reliability and manufacturing costs, which if achieved, would make the developed system appealing to the industry.

As such, the following objectives have been established:

1. Increase indicated thermal efficiency to 50.0%
2. Reduce NO_x concentration at EVO point by 50.0%

To ensure feasibility of the system, following limitations have also been set:

1. Peak pressure of standard ICE cannot be exceeded
2. Power output must not be reduced
3. Required modifications must be kept to minimum

6.2.2 Determining the Case Specifications & Simulation Results

The TJI system wasn't well understood in academia at the time of the project being carried out, as the nature is of a 'novel' idea. However, due to the complexity of system, author has tried to define as many parameters as possible before considering development.

According to academic sources, the optimal Pch volume was between 2% (Gerald Gentz, 2015) and 5% (Chinnathambi, 2015) of the clearance volume. Many sources which tried to optimise the Pch volume have concluded that smaller volume is preferred due to the decrease of ignition delay and NO_x. However, author believes that the additional ignition energy which larger volume offer should increase the reliability of the system, particularly when the chamber charge purity is considered. Due to those concerns, author has decided to utilise the 5% Pch volume as it is believed to be the safer option in industrial sense.

Many sources have concluded the optimal nozzle diameter to be in the ballpark of 1.0mm (Bryce Thelen, 2016), which author choose to be the initial value at beginning of the development. However, due to the variability in the fuels as well as equipment utilised in research, author has decided to test 0.5mm (Ashish Shah, 2015) and 2.0mm (Gerald Gentz, 2017) nozzles as well.

Author found little research about nozzle lengths but has compared the nozzle illustrations and found 3.0mm (Gerald Gentz, 2015) to be in the ballpark.

It was also found that a relatively strong conclusion has been made about positioning the source of ignition in the Pch, to be as far away from the nozzle as possible (Bryce Charles Thelen, 2016). However, contradicting conclusions have been found about the Pch geometry. One source concluded the wide and short geometry to be preferred (AbdoulAhad Validi, 2017), whereas another concluded the opposite (Masumeh Gholamisheeri, 2017). Therefore, author has decided to test each suggested chamber geometries.

Author was unable to find research regarding the effect of nozzle geometry on the jet formation and combustion and so decided to test a 5° diverging cone in the nozzle.

Research have shown that multiple nozzles provide the best performance up to certain count, but only if well designed (Gerald Gentz, 2017). Therefore, in order to retain simplicity it was decided to optimise single nozzle first, after which author simulated double nozzle design with 70° included angle and equal total flow area as the single nozzle design.

Lastly, author has calculated in order to achieve the efficiency goal and retain equal power, the required λ in the Mch to be 1.51 by mass. Initially, λ 1.0 has been kept in the Pch, but

Each design has been associated with a letter, as shown in Table 4-1.

Table 6-2: Specifications of the TJI Cases

Case Name	Nozzle Diameter & Type (mm)	Pre-chamber geometry	Pre-Chamber λ	Main-Chamber λ	Nozzle Length (mm)
A	1.0 - straight	Square	1.0	1.51	3.0
B	1.0 - straight	Cone	1.0	1.51	3.0
C	1.0 - straight	Over-Square	1.0	1.51	3.0
D	2.0 - straight	Cone	1.0	1.51	3.0
E	0.5 - straight	Cone	1.0	1.51	3.0
F	1.0 – 10° inc.	Cone	1.0	1.51	1.0 std. 2.0 div.
G	1.0 - straight	Cone	0.8	1.51	3.0
H	2x 0.7 - straight	Cone	0.8	1.51	1.0

Parameters from Table 6-1 have been used in the simulation of all cases, apart from IT of 15° BTDC, assumed Pch wall temperature of 500K and values from Table 6-2.

6.2.3 Comparison of Case Results

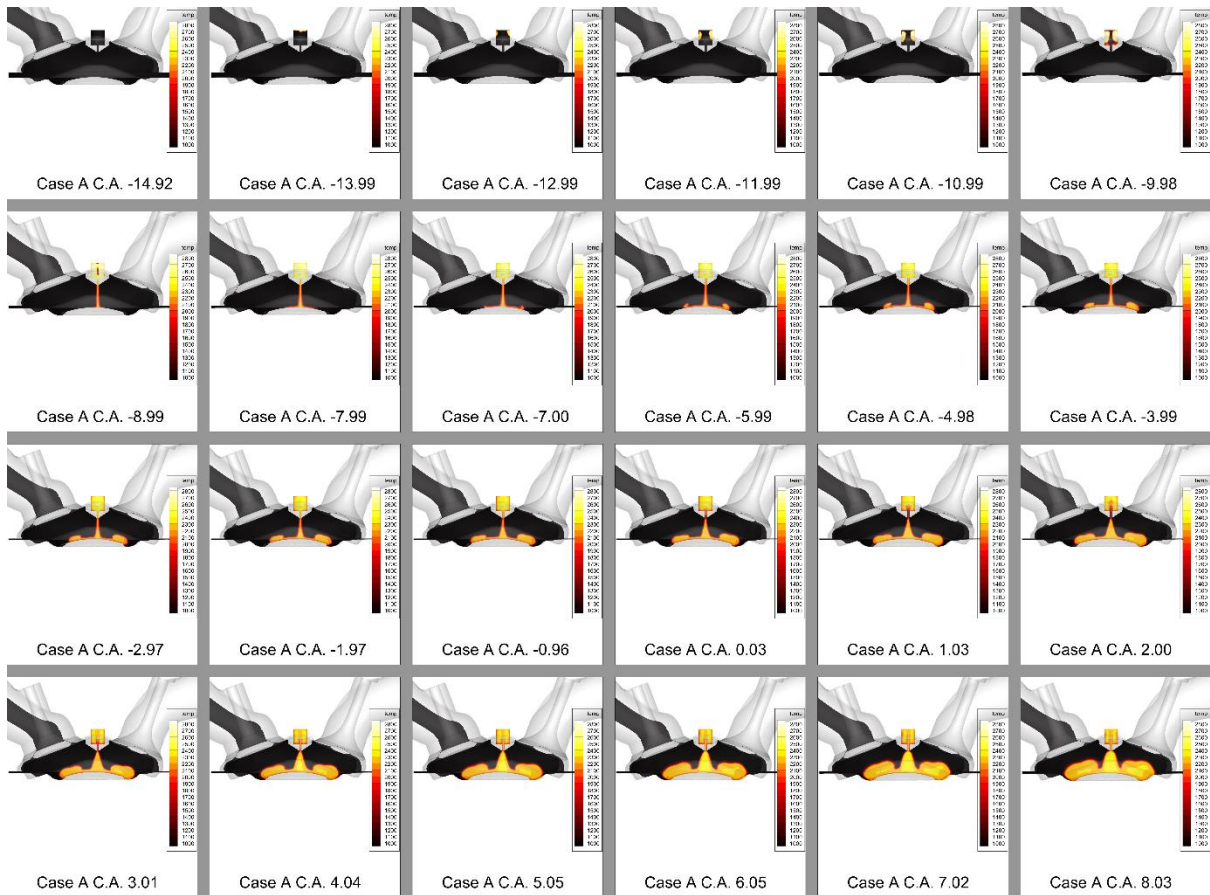


Figure 6-7: Case A Temperature Contour Side View

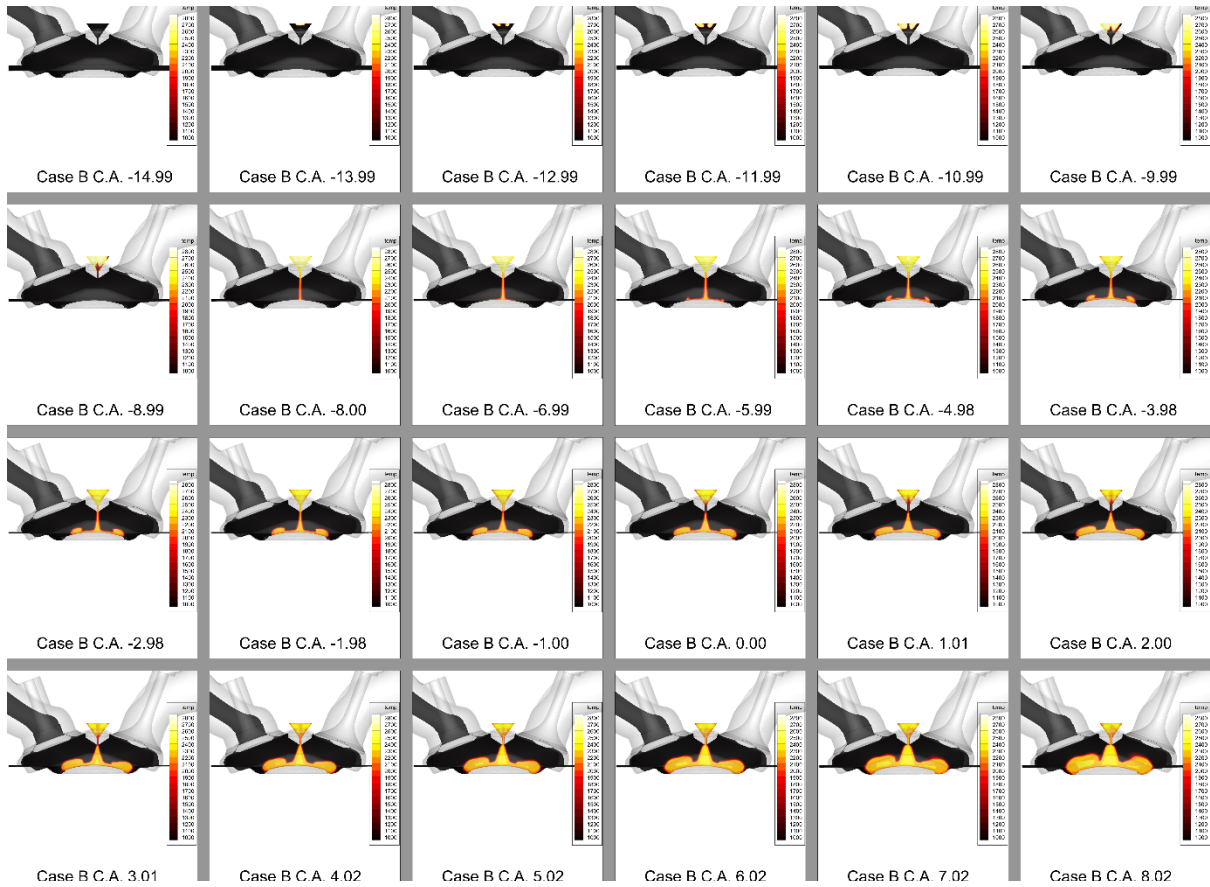


Figure 6-8: Case B Temperature Contour Side View



Figure 6-10: Case C Temperature Contour Side View

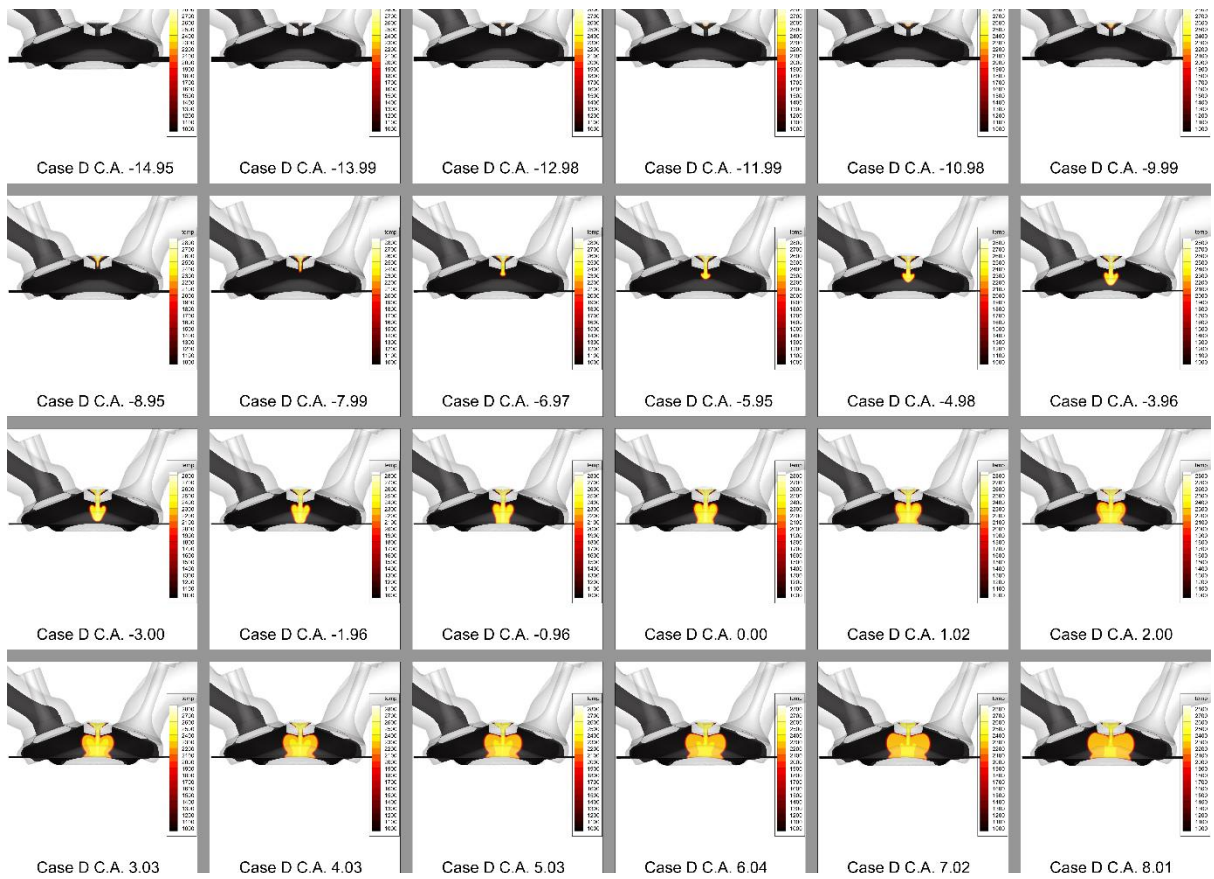


Figure 6-9: Case D Temperature Contour Side View

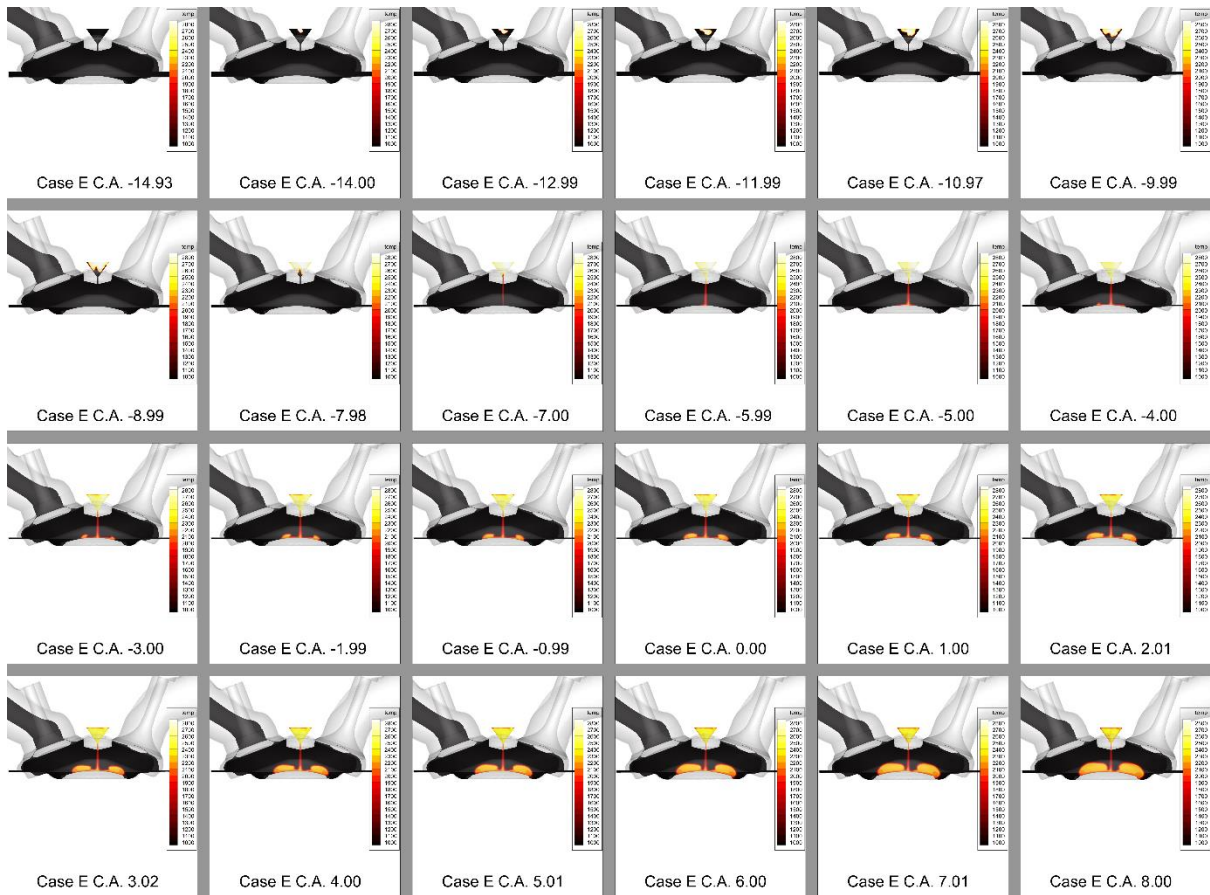


Figure 6-12: Case E Temperature Contour Side View

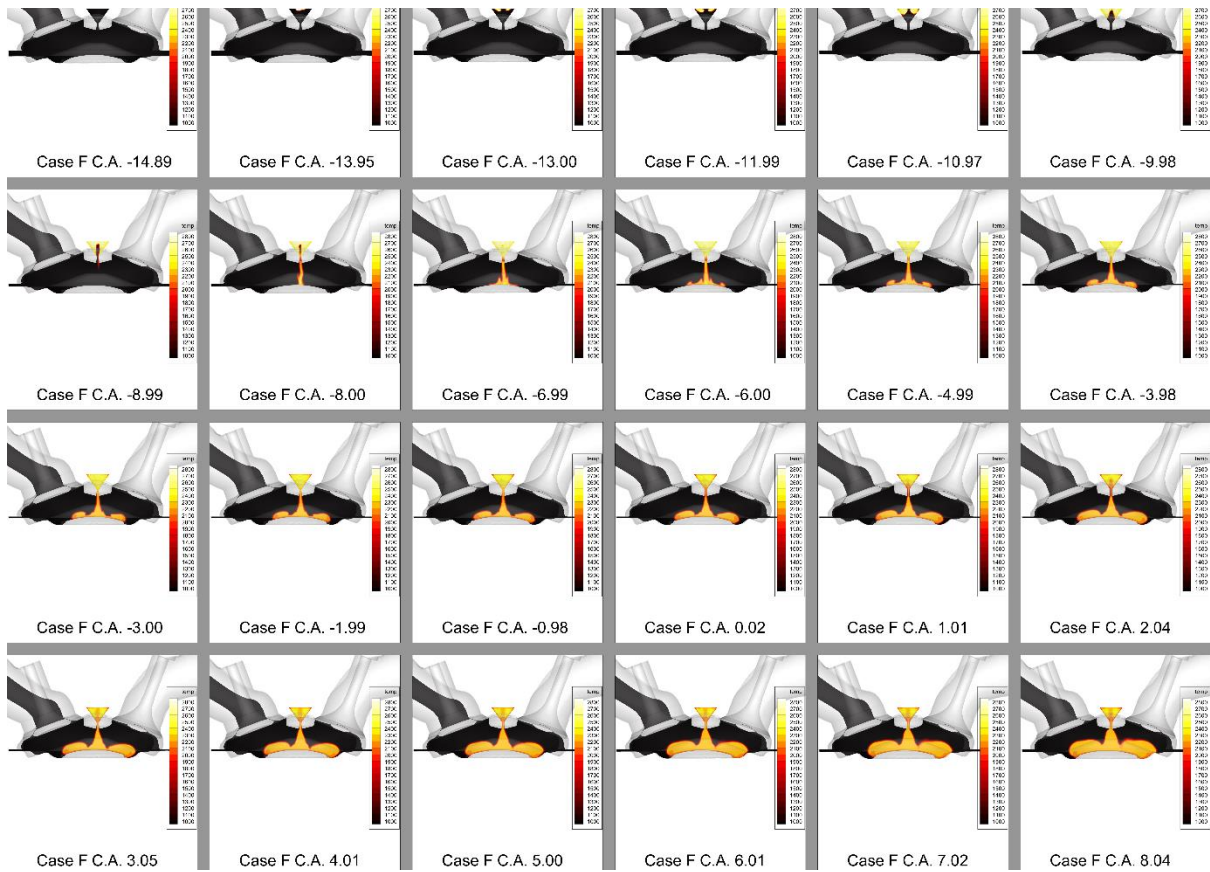


Figure 6-11: Case F Temperature Contour Side View

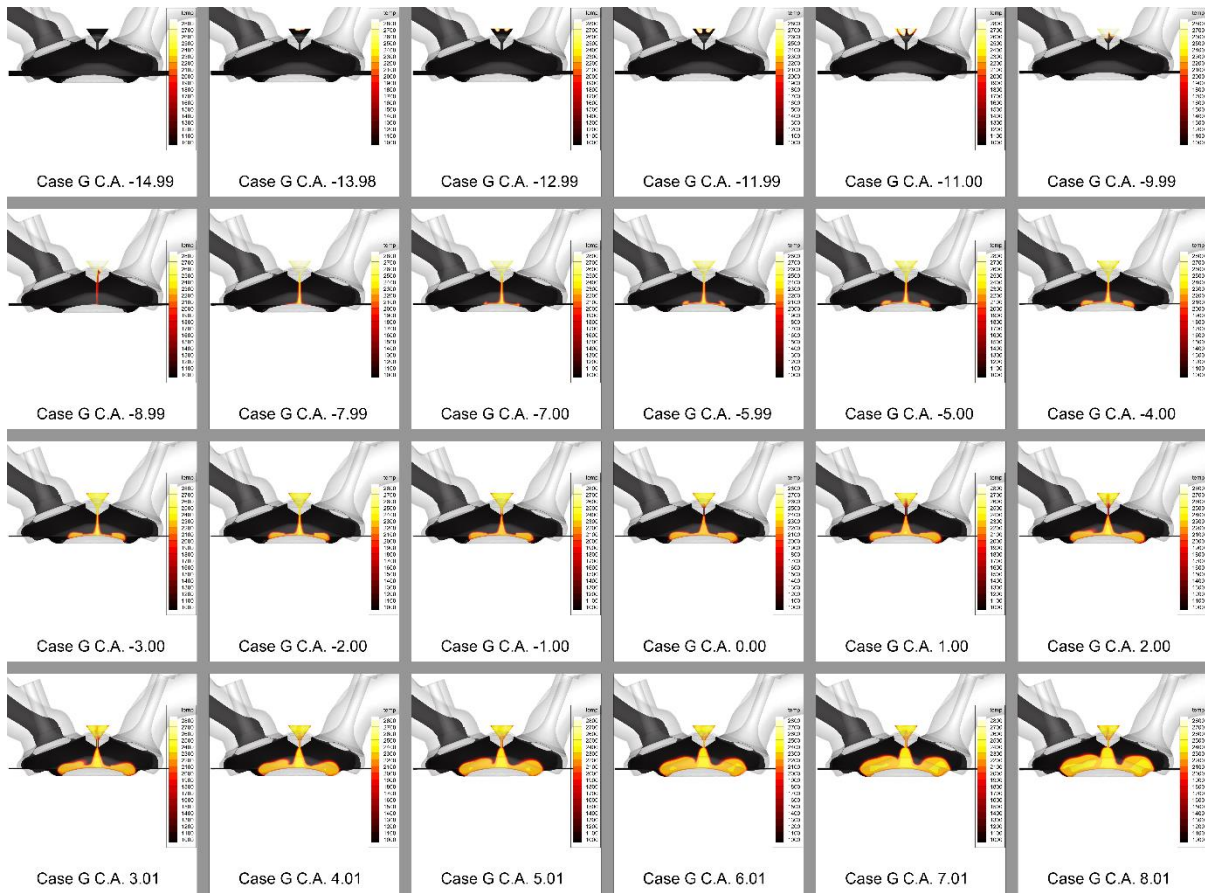


Figure 6-14: Case G Temperature Contour Side View

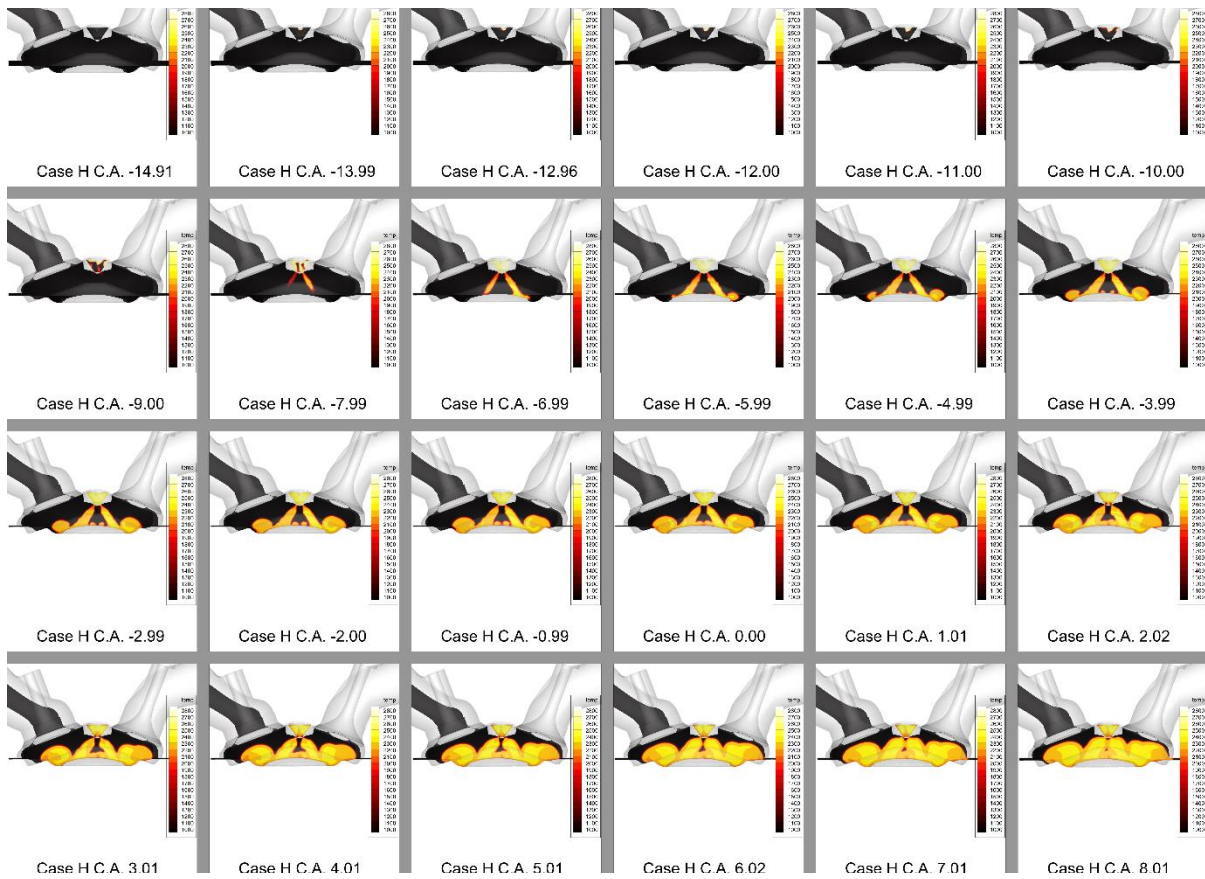


Figure 6-13: Case H Temperature Contour Side View

6.2.3.1 Pre-Chamber Geometry: A, B & C

The dimensions of pre-chambers tested are shown in Table 6-3.

Table 6-3: Pre-Chamber Case Dimensions

Case Names	Pre-Chamber Type	Top Diameter (mm)	Bottom Diameter (mm)	Length (mm)
A	Cylinder	6.0	6.0	6.54
B	Cone	10.0	1.0	6.37
C	Cylinder	10.0	10.0	2.36

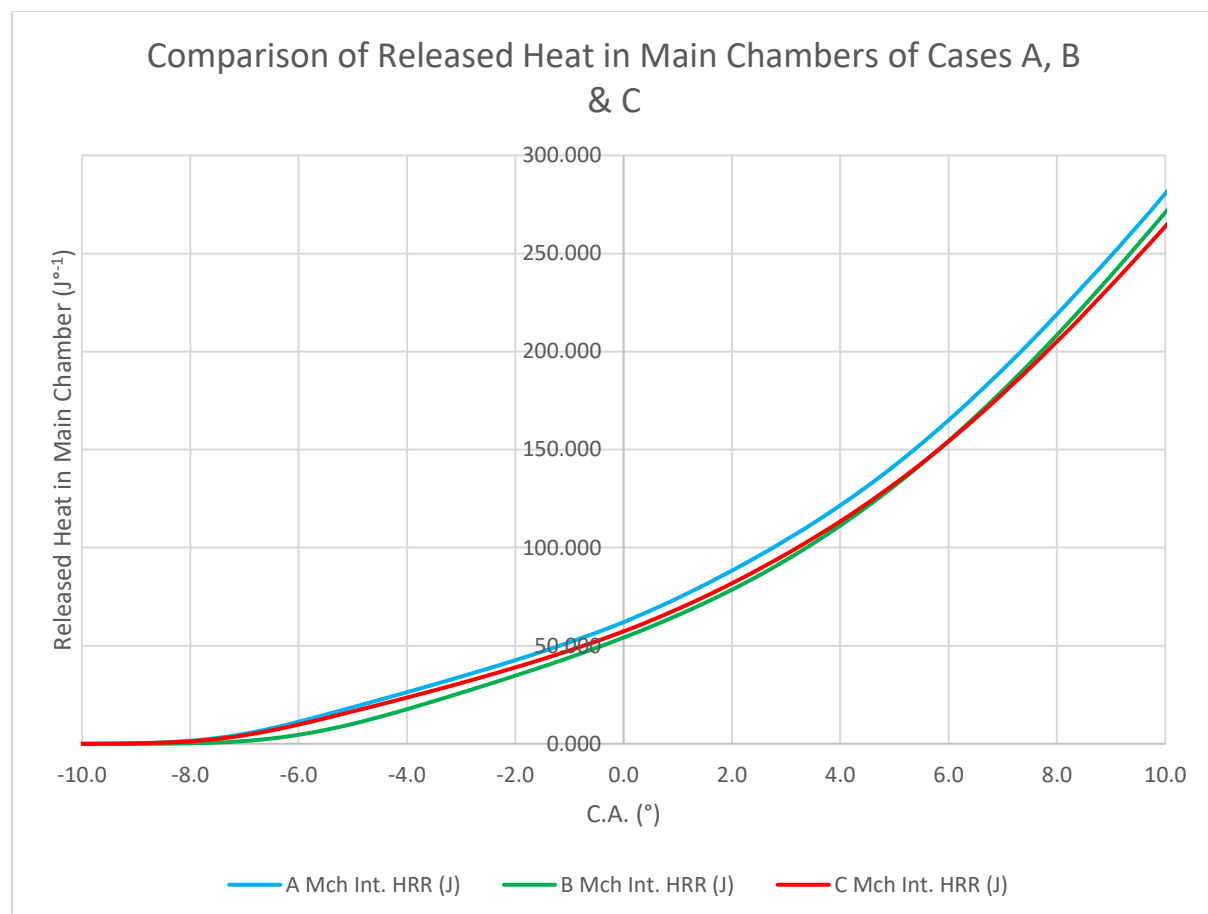


Figure 6-15: Comparison of Released Heat in Main Chambers of Cases A, B & C

Figure 6-15 shows that quicker Mch combustion occurred in Case A compared to Case C. This was because the Case A geometry achieved much more complete combustion in the Pch before the formation of a jet, which caused higher pressure built up in the Pch, as shown in Figure 6-16. This has resulted in higher jet exit temperature, as shown in Figure 6-17: note that drop of exit temperature ATDC is caused by flow reversal of surrounding colder mixture from Mch into Pch. Consequently, Case A jet initialized combustion in the Mch quicker and at many more points due to delivering higher ignition energy.

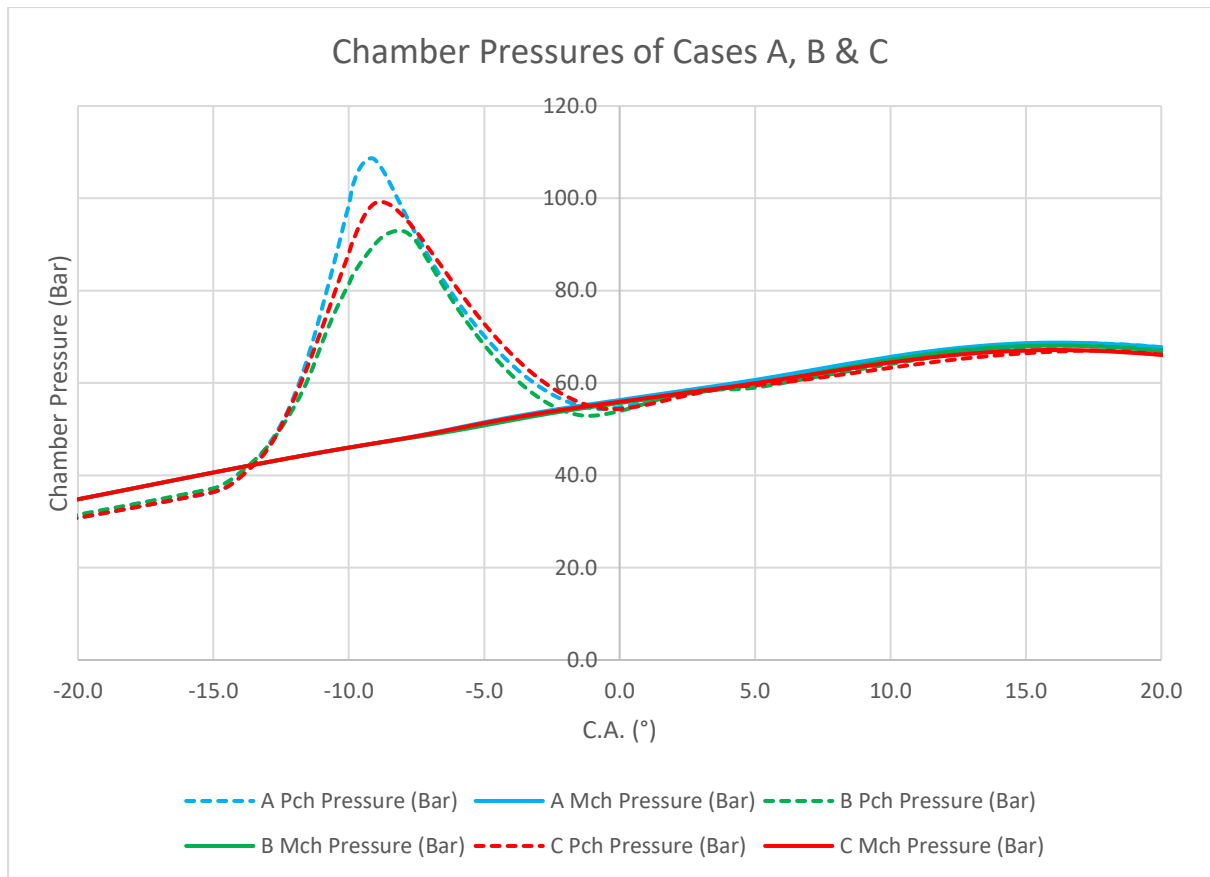


Figure 6-16: Chamber Pressures of Cases A, B & C

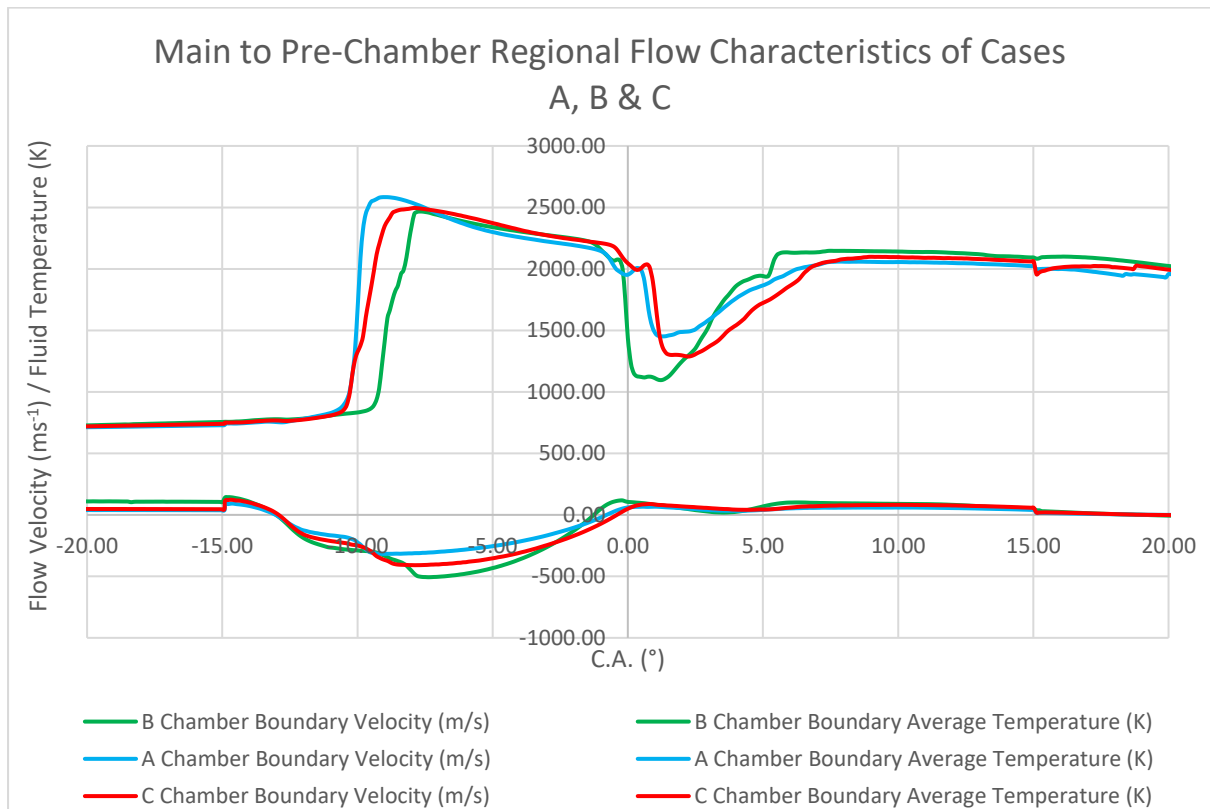


Figure 6-17: Main to Pre-Chamber Regional Flow Characteristics of cases A, B & C

However, calculation of MFB0-10 shows that Case B has performed the best, as the initial combustion period was shortened by 5.2% compared to Case A, as shown in Table 6-4.

Table 6-4: MFB0-10 Durations for Cases A, B & C

Case Name	MFB0-10 Duration (C.A.)
A	15.5
B	14.7
C	15.8

This was due to even more complete combustion occurring in the Pch and the decrease of turbulence at the entrance of the nozzle, which resulted in higher C_d , increasing exit velocity and interestingly, decreasing Pch pressure. The additional velocity delivered the heat in the jet at quicker rate, condensing the ignition energy density and inducing more turbulence in the Mch and thus, creating more combustion zones during the MFB0-10. However, geometry was restricting the combustion rate as the area was decreasing towards the nozzle entrance, which delayed formation of the jet, causing Mch ignition to occur later in the stroke and so, making results in Figure 6-15 initially misleading.

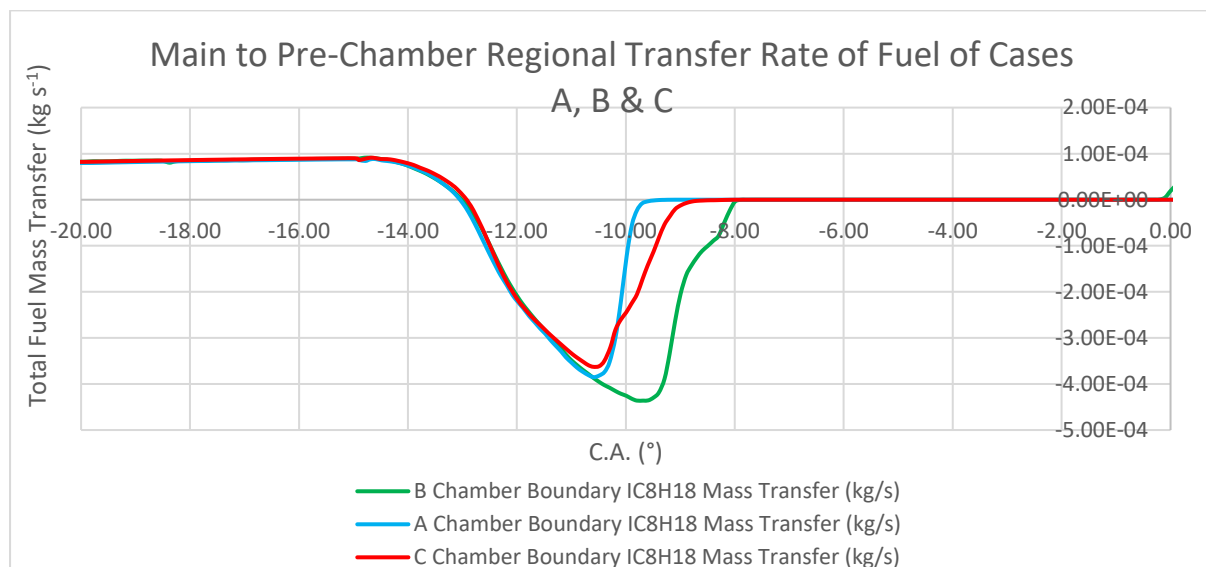


Figure 6-18; main to Pre-Chamber Regional Transfer Rate of Fuel of Cases A, B & C

Figure 6-18 shows that another factor which could be aiding Case B is the action of fuel transfer from Pch to Mch, as this causes richer region to form in a very lean chamber and therefore, the jet is able to use that region as a form of 'kindling'.

Due to the mentioned reasons, as well as the ability to house standard Ford fox spark plugs, author has determined the Case B to be the most optimal tested geometry.

6.2.3.2 Nozzle Diameter: B, D & E

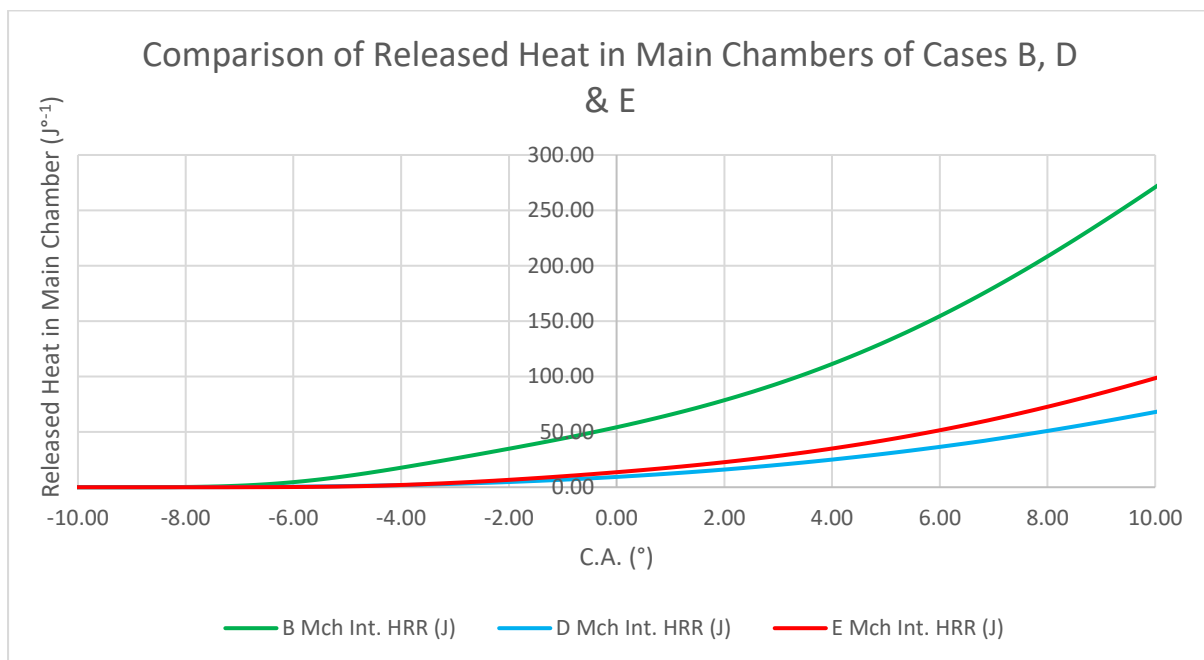


Figure 6-19: Comparison of Released Heat in Main Chambers of Cases B, D & E

Figure 6-19 clearly shows that only Case B performed satisfactorily. The other Cases failed due to two separate issues created when nozzle in TJI system is too small or too large.

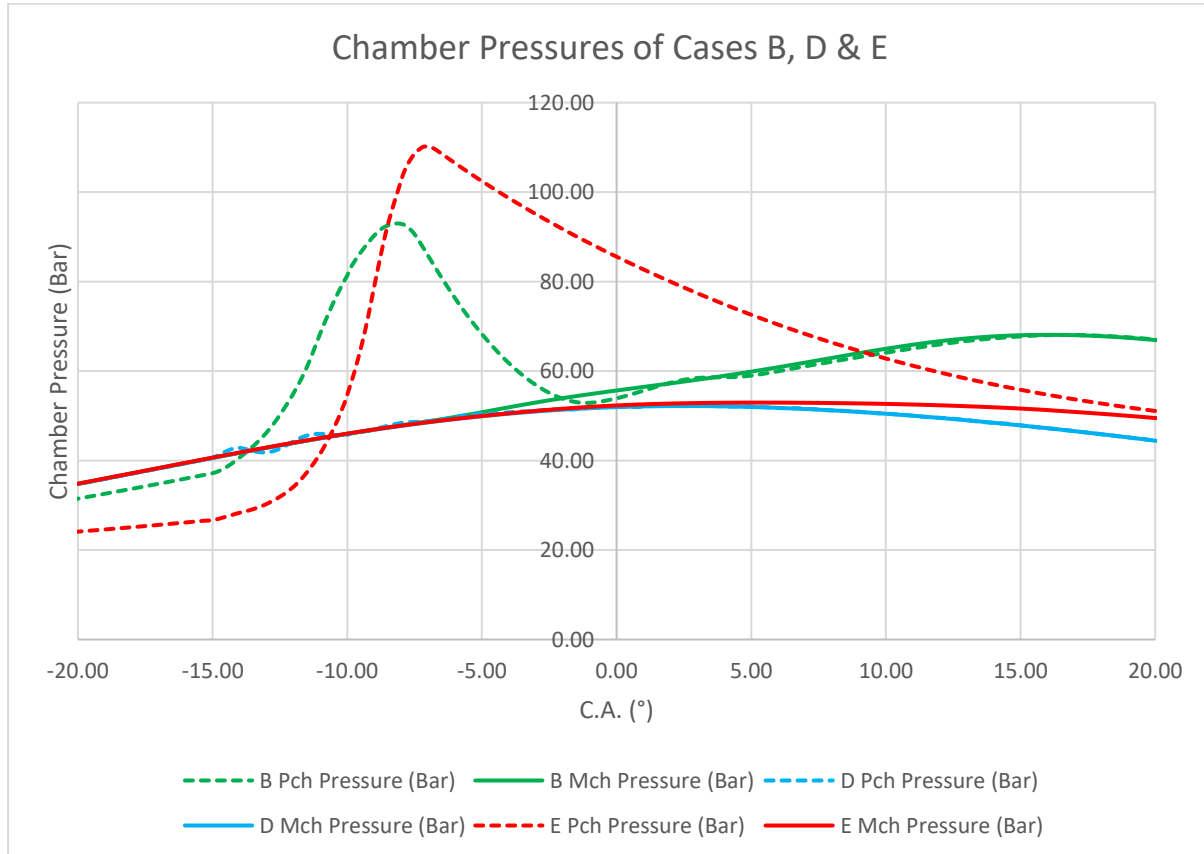


Figure 6-20: Chamber Pressures of Cases B, D & E

Figure 6-20 shows the reasons for the shortcomings of Cases D & E:

- Due to the very large nozzle in case D, pressure in the Pch didn't built up and as a result, the combustion in the Mch occurred very much like in standard SI ICE.
- Due to the very little nozzle in Case E, the flow between chambers was too restrictive. Initially resulting in the Pch mixture not being compressed by the piston. Later, the restrictive nozzle prevent fluid from entering the Mch, causing the Pch pressure to be slowly 'bleed' off.

6.2.3.3 Nozzle Geometry: B & F

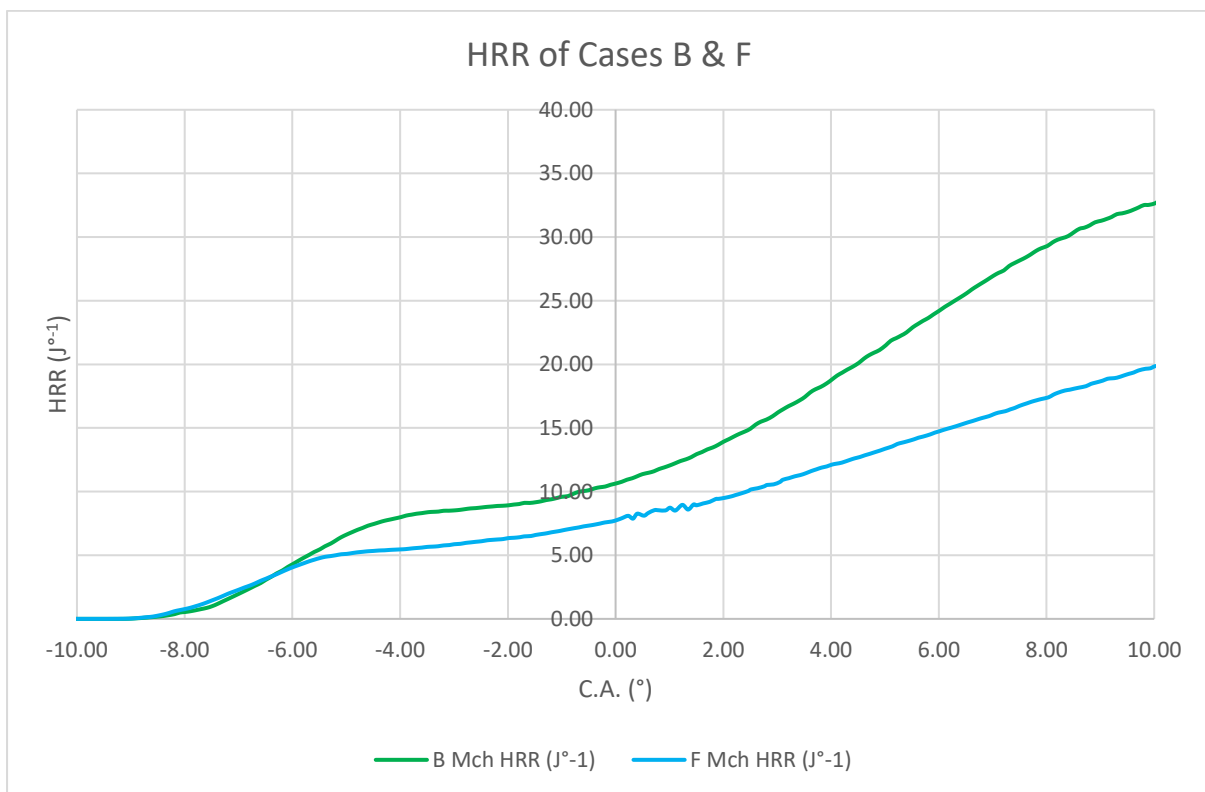


Figure 6-21: HRR of Cases B & F

Figure 6-21 shows very similar HRR of Cases B and F in the Mch up until $\sim 6.0^\circ$ BTDC, after which combustion in Case F slows down. The design has been relatively successful at expanding jet area; the initial jet diameter has been roughly doubled at the piston crown point. However, the broadening of the jet caused the temperature to decrease, resulting in the slower combustion rate. This, as well as the initially distorted jet formation suggests the nozzle diameter to be too large for diverging nozzle design, as similar observations have been made in Case D. Due to additional manufacturing and design complexity, author has decided not to pursue this design, although it is likely to provide benefits if well designed.

6.2.3.4 Pre-Chamber Mixture: B & G

Results in Pre-Chamber Geometry: A, B & C chapter suggested the action of pushing fuel out of the Pch and forming richer region to be beneficial. As such, author has decided to investigate this effect by creating 20% richer Pch.

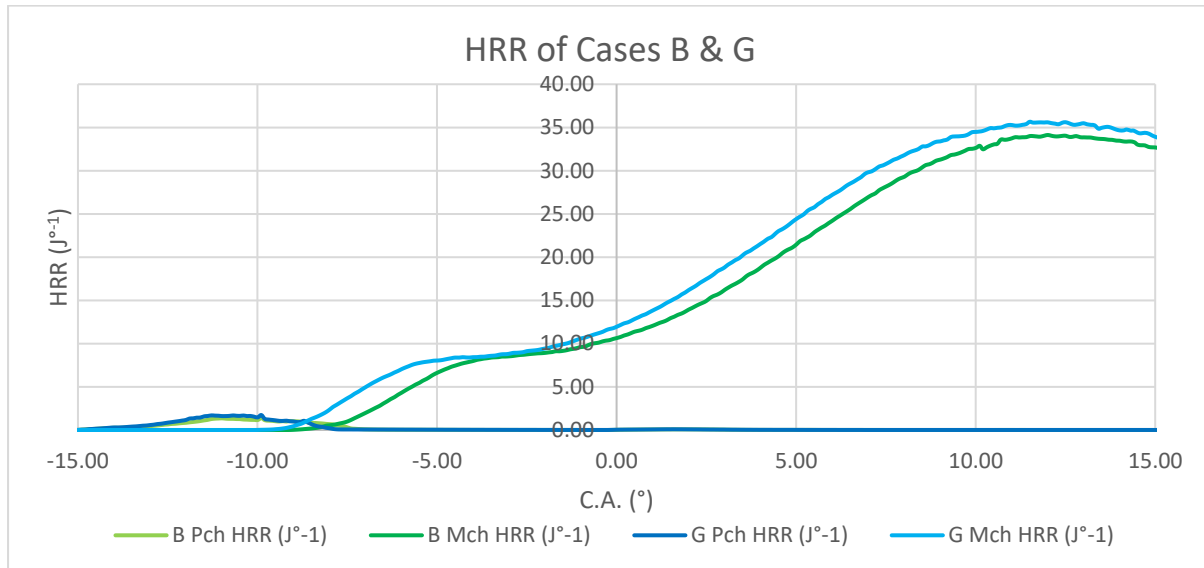


Figure 6-22: HRR of Cases B & G

Figure 6-22 shows Case G to have had faster combustion rate, especially during initial combustion phase. However, the combustion in the Pch was also accelerated and so the combustion completed faster than in Case B, despite the additional fuel mass which had to be combusted. This has caused much elevated Pch pressures shown in Figure 6-23, despite only releasing additional $\sim 1.0\text{J}$.

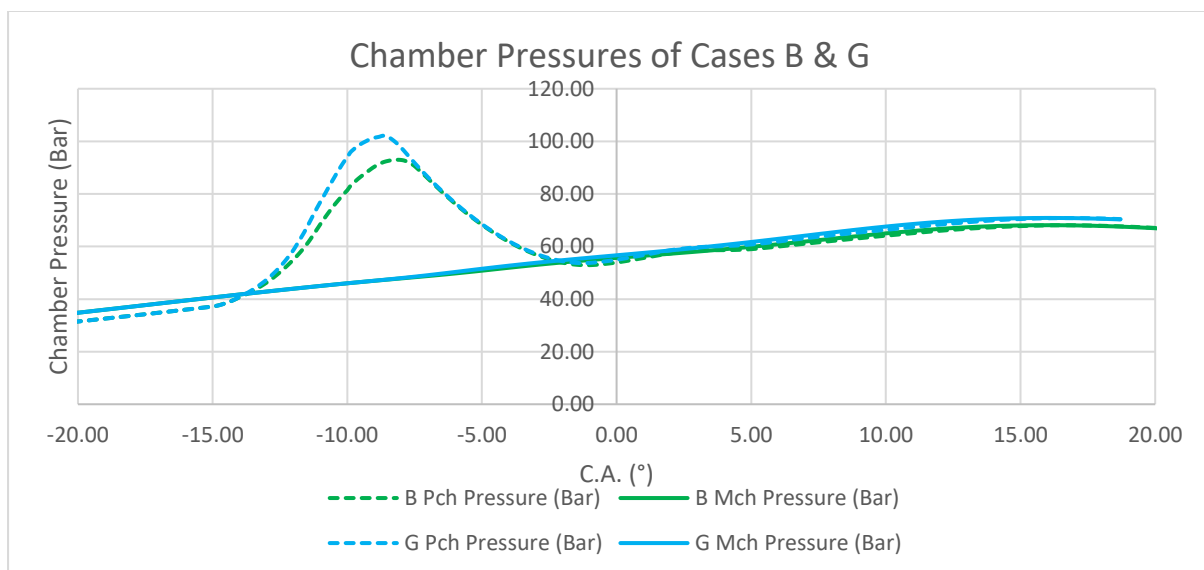


Figure 6-23: Chamber Pressures of Cases B & G

The additional pressure increased the exit temperature and velocity, shown in Figure 6-24, resulting in more ignition energy being transferred into the Mch, speeding up the combustion rate. The exit temperature also shows that the jet was formed 1 C.A. earlier, decreasing the ignition delay and starting combustion in the Mch earlier. However, not all of the success can be accredited to reduction of ignition delay, as the peak HRR has increased by 5%.

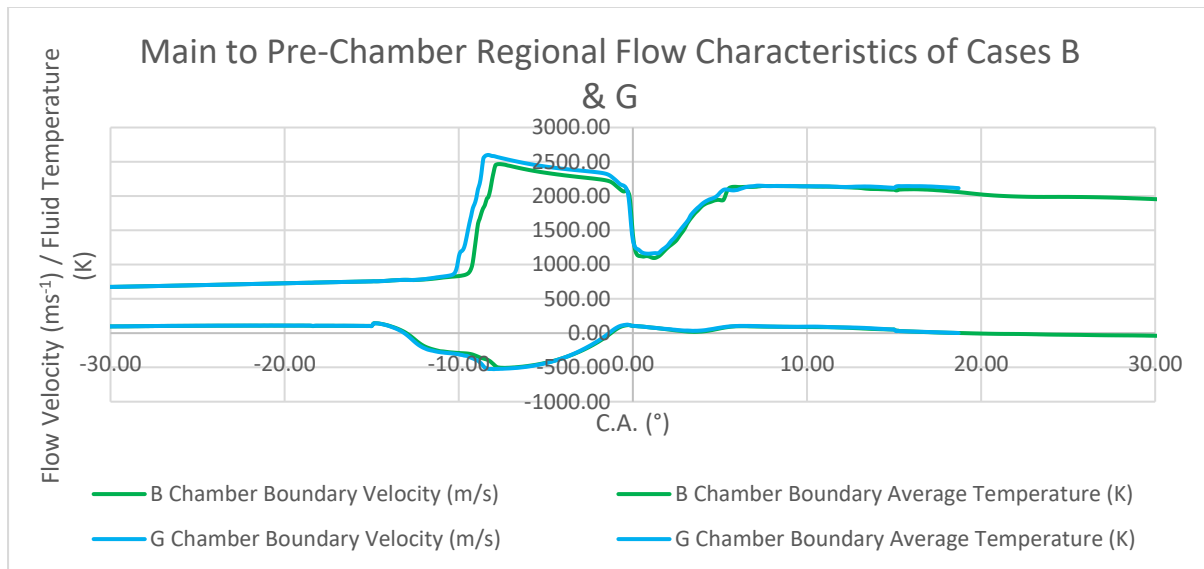


Figure 6-24: Main to Pre-Chamber Regional Flow Characteristics of Cases B & G

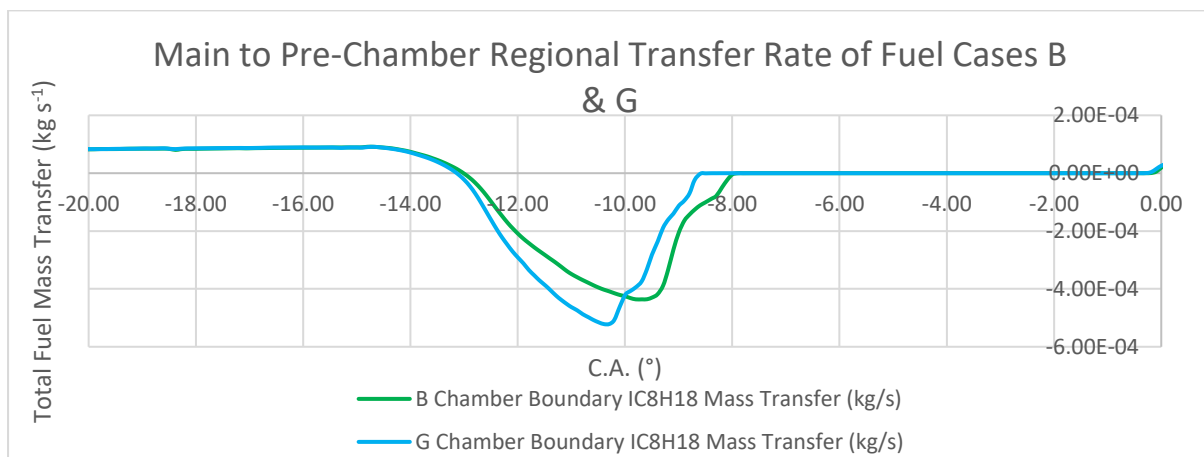


Figure 6-25: Main to Pre-Chamber Regional Transfer Rate of Fuel Cases B & G

Figure 6-25 shows that more fuel was transferred into the Mch in Case G.

However, due to the inability to separate the fuel transfer from accelerated combustion in the Pch, author was unable to confidently conclude the benefits of such action. Instead, author has determined richer Pch mixture to be beneficial itself, as a clear combustion acceleration occurred.

6.2.3.5 Nozzle Count: G & H

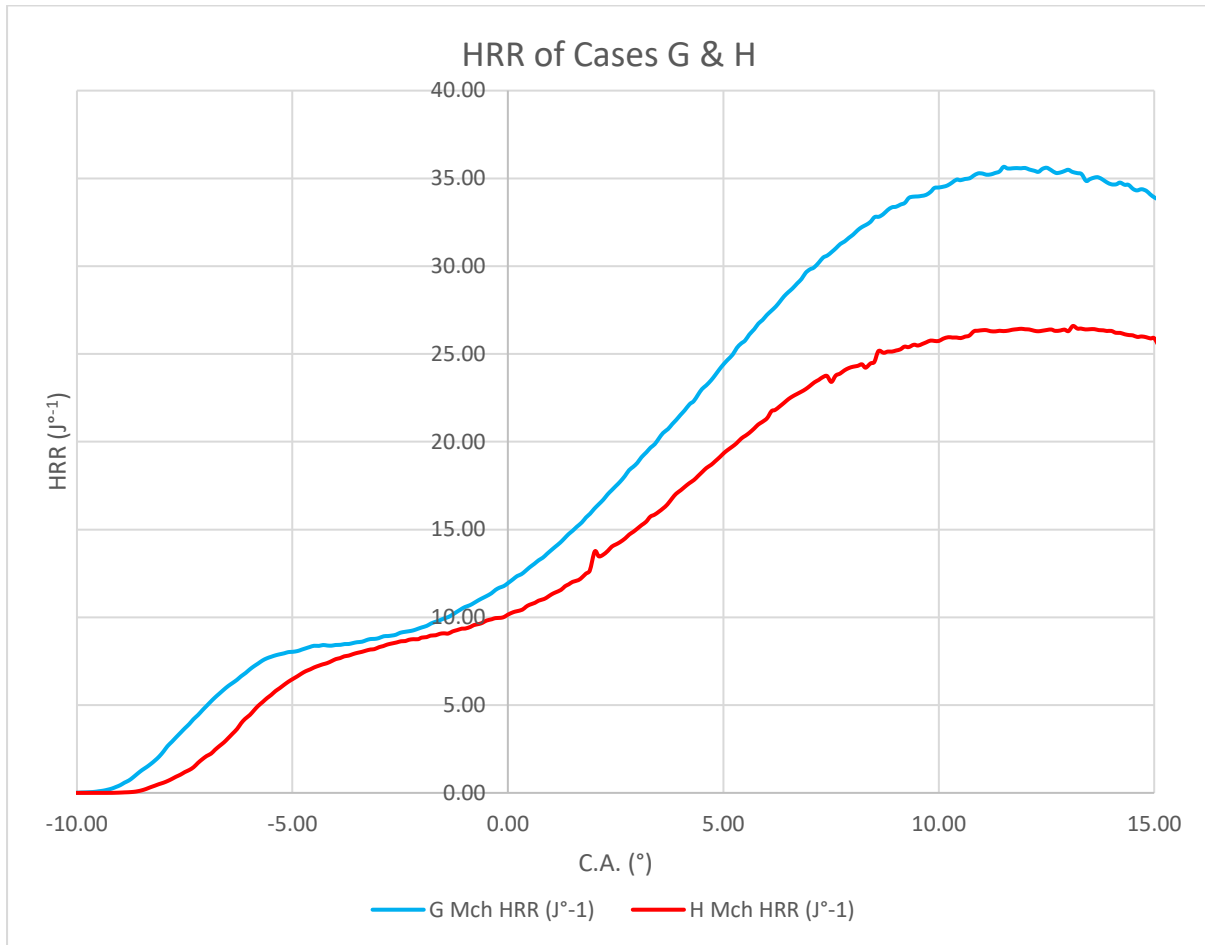


Figure 6-26: HRR of cases G & H

Figure 6-26 shows that double nozzle design had a negative effect on the combustion rate in the Mch. The Figure 6-13 and Figure 6-14 show the opposite to be true, as the Case H showed to produce wider jets and induce more ignition sources which caused larger combustion zones in comparison to Case G. This however was due to the shown plane which favoured Case H, Figure 6-27 and Figure 6-28 visualize perpendicular planes, which clearly show very poor combustion in Case H across the bore. Pch combustion in Case H was also slower in all planes, as the incoming fluid wasn't directed to the ignition source, like in Case G, which was the cause of additional delay. However, the decreased jet length (1.0mm) which was due to packaging concerns, has shown to produce much larger jets, which was the reason for faster combustion Case H plane.

Due to added complexity and lack of time, author has decided to choose Case G as the final design, although it is believed that further investigation of nozzle count and nozzle lengths would have very beneficial effects.



Figure 6-28: Case G Temperature Contour Front View



Figure 6-27: Case H Temperature Contour Front View

6.2.4 Final TJI Setup

The final TJI setup which became the GTTJI in this project, was the same as in Case G except the Mch mixture was set to 1.29λ , making the IC8H18 mass 4×10^{-5} kg, resulting in equal total WD output as the SI variant, if 50% indicated thermal efficiency was achieved.

Due to lack of equipment author was unable to validate the jet formation. However, research has shown that accurate cylinder averaged results can be achieved with RANS turbulence model, as used in this project. Though eddy-based turbulence models such as LES or DES are preferred when investigating the accuracy of the jet formation (Masumeh Gholamisheeri, 2017).

6.2.4.1 Comparison of Final TJI System



Figure 6-29: Original GTDI Temperature Contour Side View

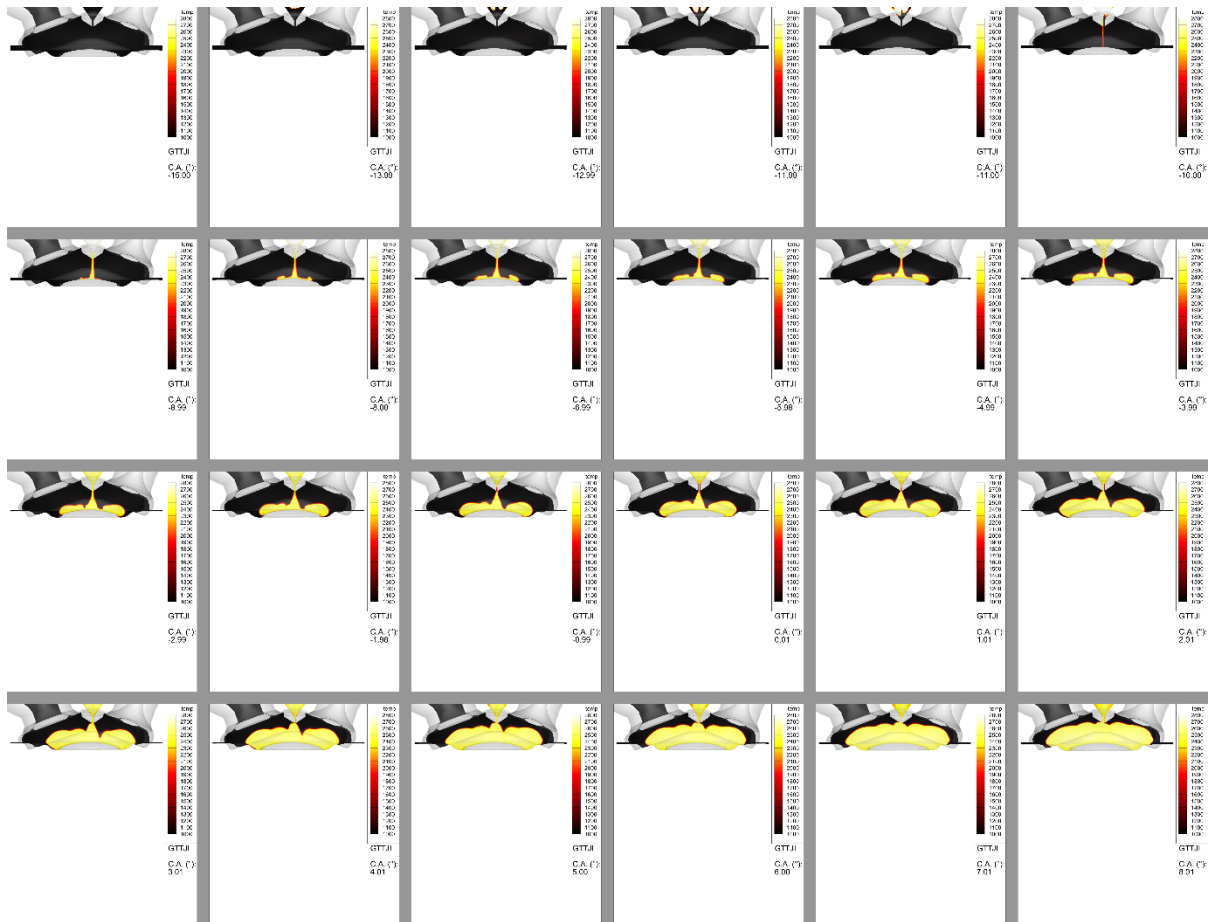


Figure 6-30: Final GTTJI Temperature Contour Side View

6.2.4.1.1 Cylinder Pressure

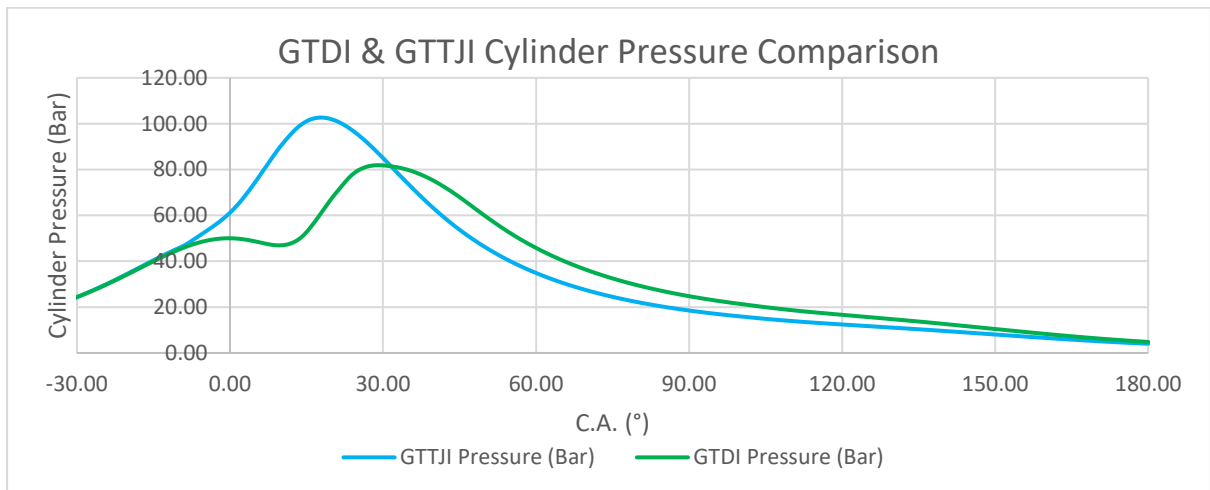


Figure 6-31: GTDI & GTTJI Cylinder Pressure Comparison

Figure 6-31 shows that the peak pressure limitation hasn't been met. This would be relatively easy to mitigate by retarding the ignition timing by $\sim 10^\circ$, which would have limited effect on WD output and thermal efficiency since the pressure would be reduced close to TDC. However, author wasn't able to simulate this due to lack of time.

6.2.4.1.2 Mass Fraction Burned & Burn rate

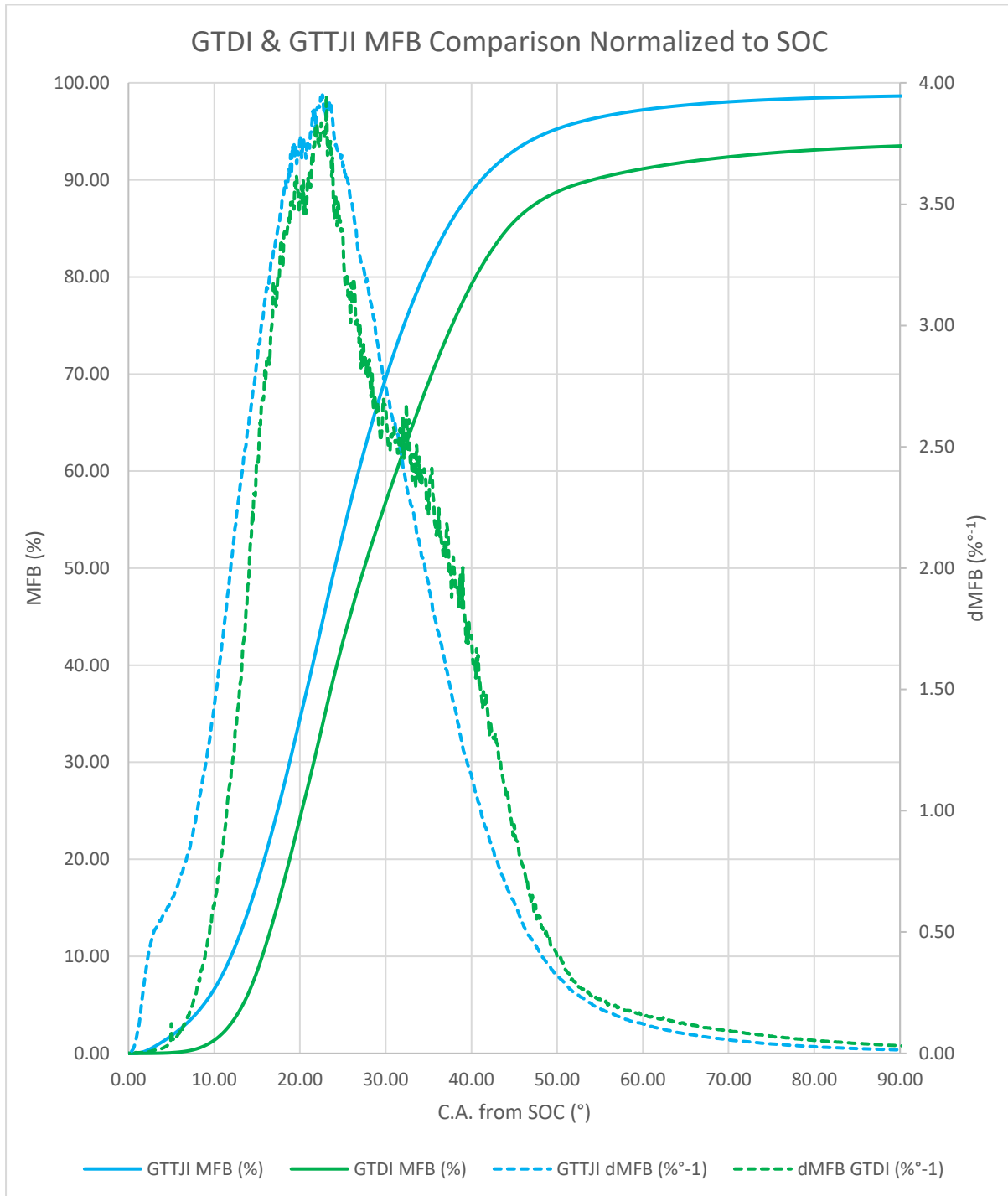


Figure 6-32: GTDI & GTTJI MFB Comparison Normalized to SOC

Figure 6-32 shows that the jet ignition has caused considerable increase in combustion rate, especially during first 3° of combustion, asserting dominance over SI up until 32° after the SOC, due to much lower HC levels at that point. The much faster combustion has resulted in astonishing 23.9% reduced MFB0-90 duration, while utilising 33.1% less fuel. The combustion efficiency also increased by 5.0% due to much leaner conditions.

6.2.4.1.3 Thermal Efficiency

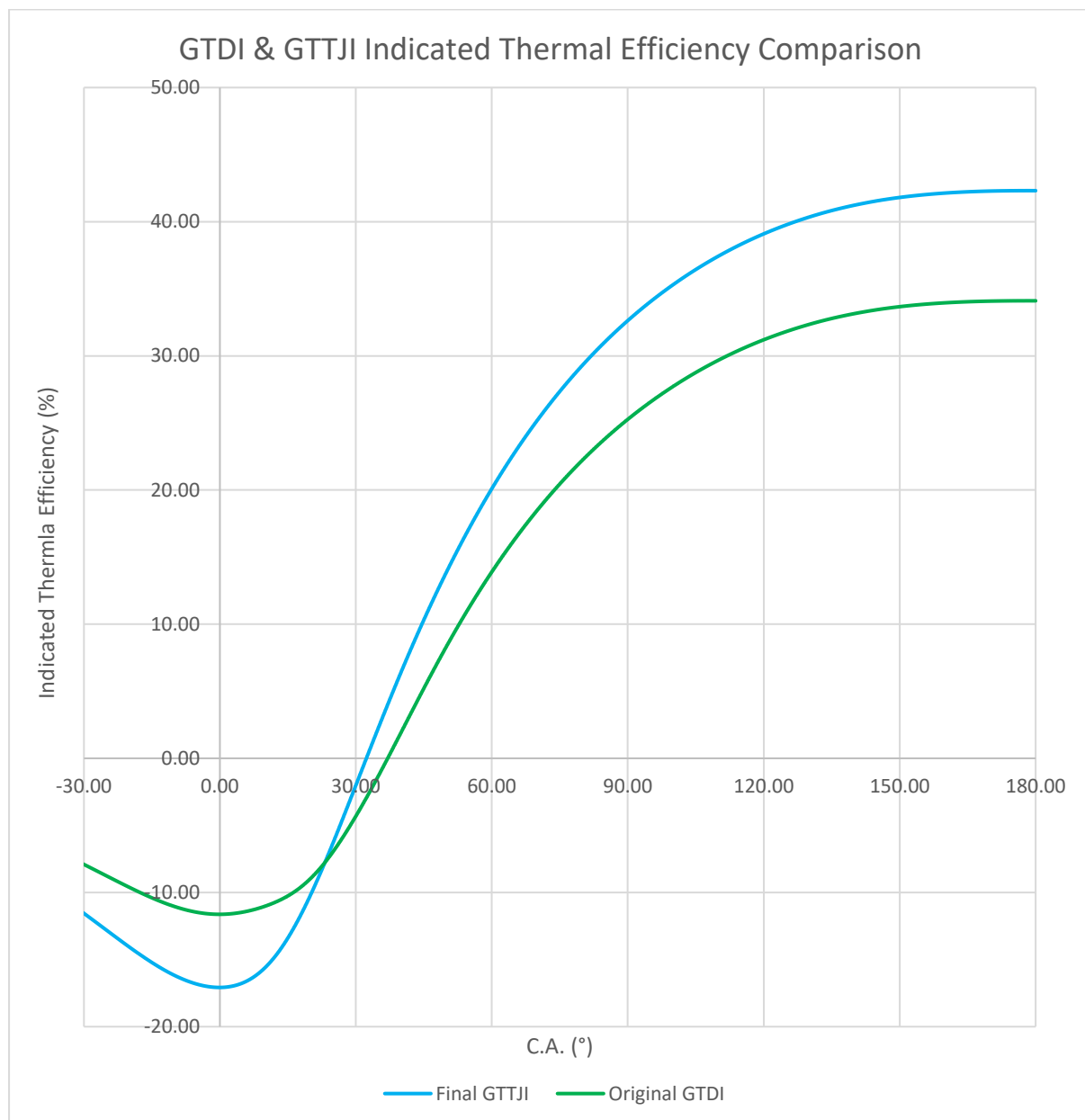


Figure 6-33: GTDI & GTTJI Indicated Thermal Efficiency Comparison

As the lower GTTJI pressures after EOC in Figure 6-31 suggested, the GTTJI ICE didn't achieve the 50% thermal efficiency target, as shown in Figure 6-33. However, the indicated thermal efficiency was increased by 24.1%, from 34.1% to 42.31%, which equates to equal fuel consumption reduction, a benefit which alone should be enough to spark major interest in the industry.

Author believes that the additional 7.7% required to achieve the efficiency target is achievable if further investigation is carried out, as the Comparison of Case Results chapter, literature and relatively recent advancements in motorsport suggest.

6.2.4.1.4 NO_x Production, Temperatures & O₂ Levels

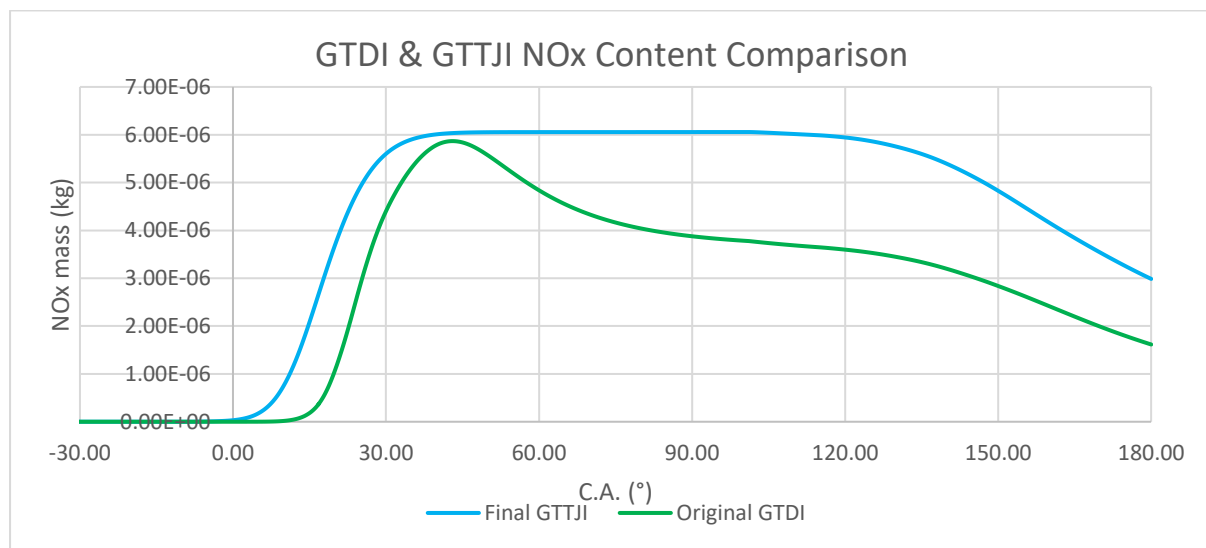


Figure 6-34: GTDI & GTTJI NO_x Content Comparison

Figure 6-34 shows that NO_x levels have increased in GTTJI ICE, as the dynamic chemical equilibrium was reached at magnitude little over the GTDI peak. It is believed that reverse reactions didn't take over due to 1.29λ ; as even though the mean temperatures have been reduced by ~500K, the maximum temperatures stayed relatively constant after EOC, as shown in Figure 6-35 and O₂ levels have been tremendously increased, as shown in Figure 6-36. This combination caused the new dynamic equilibrium to be increased by ~65%.

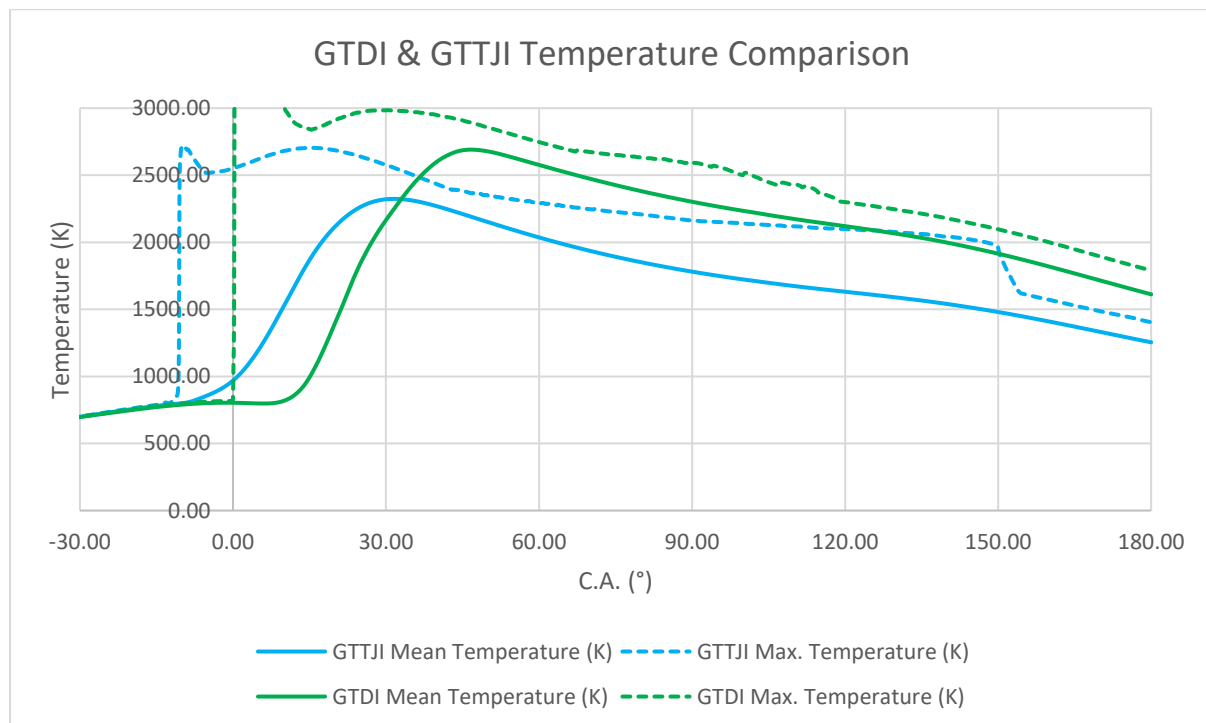


Figure 6-35: GTDI & GTTJI Temperature Comparison

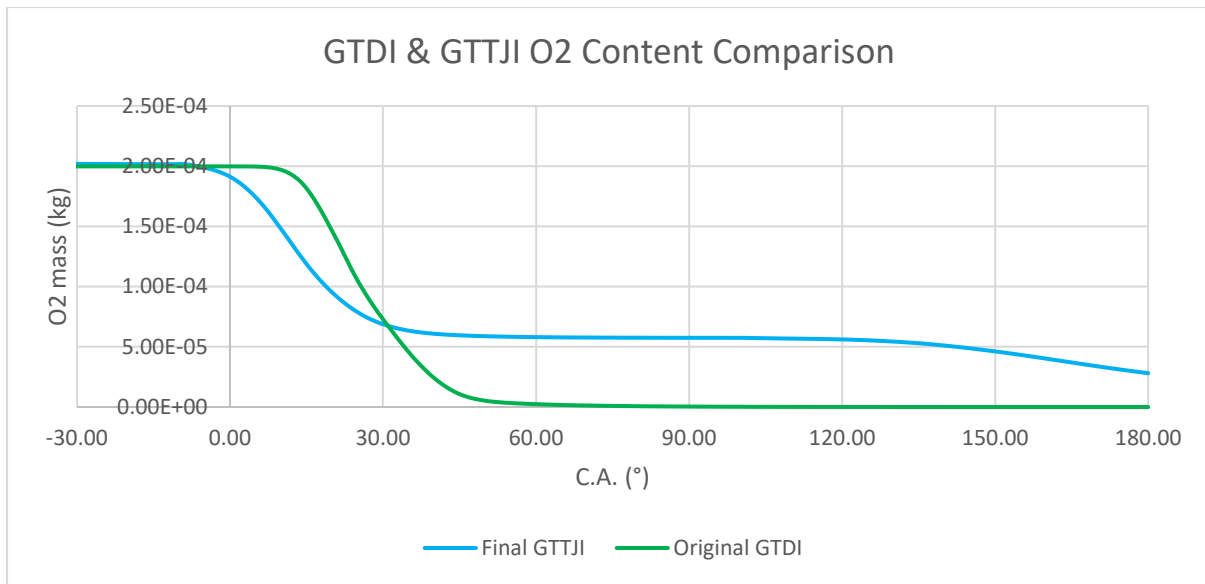


Figure 6-36: GTDI & GTTJI O2 Content Comparison

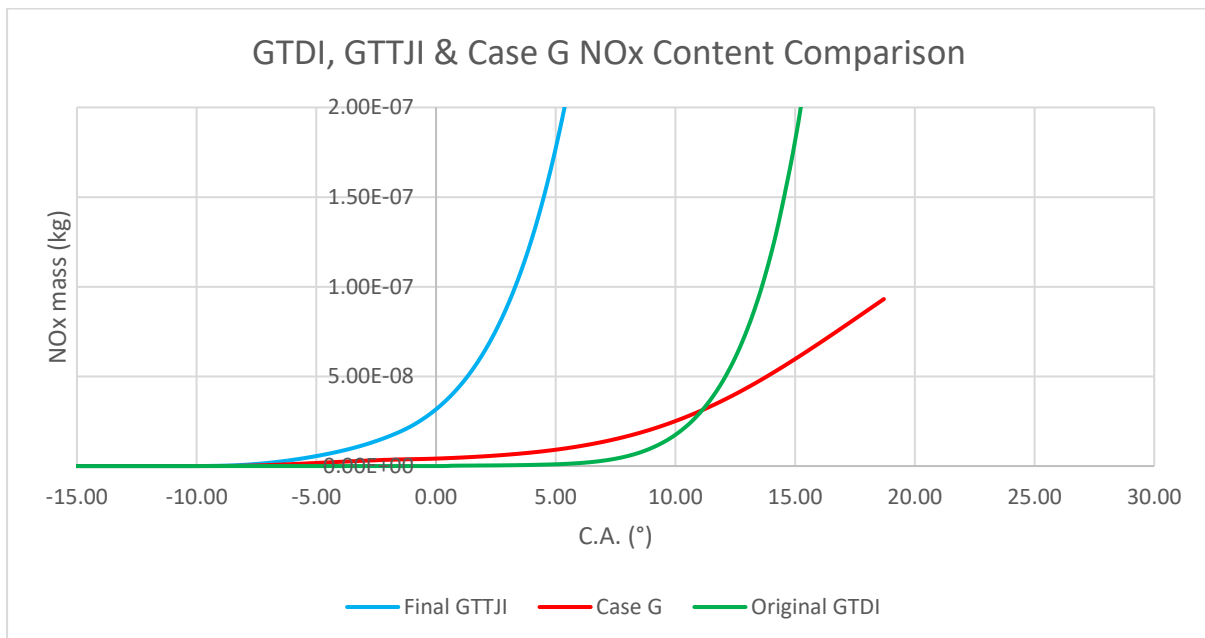


Figure 6-37: GTDI, GTTJI & Case G NOx Content Comparison

However, Figure 6-37 has shown that at 1.51λ , the NOx production can be reduced to practically nothing.

Naturally, further investigation would have to be carried out in order to find the TJI design which optimises the thermal efficiency and NOx production in a commercial ICE. Based on the showed results author suggested to utilise highly lean conditions $\sim 1.5\lambda$, during low load and utilise high amounts of EGR ($\sim 30\%$) along with more stoichiometric mixtures during high loads, to achieve the previously set NOx and power targets, as EGR would greatly reduce the O2 content required to produce NOx.

7 CONCLUSION

Author has developed a novel 0D 2-zone combustion model which is self-correcting inaccuracies regarding heat transferred and absorbed by the gas, by creating assumptions which author believes to be valid and applicable. The model was based around the combustion efficiency, which was retrieved from the analysis of exhaust gasses and have shown very good correlation with AFR as well as literature (Heywood, 1988). A quasi-static 1D heat transfer model has been developed based on classical techniques (Turns, 2006) and so included convection, conduction and radiation. The results have shown to be in very good agreement with research (Johannes Michl, 2015). The correction of heat transfer rate has caused the interior wall temperatures to become unrealistic, heat flux on the other hand remained plausible, suggesting the heat transfer sub-model to be uncomprehensive. The 2-zones allowed for accurate calculation of combusted temperature (Heywood, 1988), which was utilised to calculate the ratio of specific heats, including the dissociation of CO₂ and H₂O (Goodger, 1981), of which completion fraction was adjusted by the self-correction feature, showing good correlation between it and real time. The combination of corrected heat absorbed and transferred by the gas resulted in comprehensive HRR, which allowed accurate calculation of the polytropic index during combustion. The cause of the resultant profile has shown to be very abstract but physically linkable back to the data, although lack of equipment has unabled author to further investigate the matter, preventing confirmation of the findings. Most importantly, the polytropic comparison has shown the difference between adiabatic and polytropic process to be negligible and so, if the results are to be believed, author recommends assuming expansion polytropic index during the combustion phase, when modelling combustion by utilising classical methods. The results have been very thought provoking, ultimately extending the understanding of the ICE.

Combination of optical surface scanning and traditional measurement techniques were used to acquire a very detailed CAD model of the Ford Fox GTDI ICE. The method utilised to acquire organic ICE geometries have produced excessive challenges when being used in Converge CFD package. The improvements could be relatively easily implemented, such as: utilising more accurate scanner, mixing pigment into the silicone mixture, acquiring stiffer

castable silicone and most importantly, replacing the automatic point cloud to solid conversion with manual CAD features, as that would produce a much more uniform mesh.

Two experiments were carried out as an effort to validate the Converge CFD model:

1. Cylinder-head on a flow bench - the real-life setup has been replicated in Converge CFD. The results were as accurate as the experiment's tolerance, making the simulation of flow validated, although the trend suggested a potential accuracy issue.
 - a. Turbulence visualisation was also attempted, results weren't conclusive due to poor visualisation of eddy formations. However, the results have suggested formation of stagnation region/s, which have been present in CFD results.
2. Fuel Injector in Pressurised Vessel – spray of H₂O recorded at high speed. Author lacked the required equipment to record the spray at wide enough view to notice energy dissipation and time resolution to calculate usable penetration velocities. This, as well as the inability to accurately model spray due to lack of computational power, has forced the author to completely abandon spray modelling and validation.

The 3D combustion in stock Ford Fox GTDI ICE was modelled using Converge CFD. Overall, results have shown to be in good agreement with real life data, especially the formation of indicated thermal efficiency, despite utilising IC8H18. However, the pressure trace profile differed, which is believed to have been caused by lack of tumble and too fast reaction rates. The lack of computational power prevent author from improving this model.

Lastly, extensive TJI research has been carried out which allowed author to create eight different TJI designs (Gerald Gentz, 2015), all of which were simulated in Converge (Masumeh Gholamisheeri, 2017). The combustion performance was compared and so the optimal design was created, which was then used in the final simulation, which has shown very promising and comparable results to literature (Michael Bunce, 2016), such as: 42% thermal efficiency and 500K temperature reduction. Based on the simulated results, author was able to create a rudimentary fuelling strategy which would greatly reduce NO_x production while retaining the power and fuel consumption benefits. Results suggested that the TJI design can be greatly improved, benefiting the ICE industry even greater. However, further investigation must include the gas exchange process and fuel spray in the Pch, as the charge purity and homogenization are likely to have extensive effect on the TJI performance.

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9 APPENDIX

Table 9-1: Approximated Durations Spent on Major Activities

Activity Name	Time Duration	Quantity
3D Combustion Simulation	~30h, most prematurely stopped	+100
3D ICE Flow + Spray Simulation	~5 Days	2
3D Flow-bench Flow Simulation	~5h	5
3D Spray Vessel Simulation	~12h	1
Surface Scanning	~12h	5
Converting Point Cloud to Usable Format	~3h	5
CAD Modelling	1 Day	5
Flow-bench Experiment, Fabrication & Preparation	1 Day	5
Flow Turbulence Experiment	1 Day	1
Spray Vessel Experiment	Week	1
Nozzle Measurements	1 Day	1
Camshaft Measuring	1 Day	3

9.1 HEAT TRANSFER MODEL

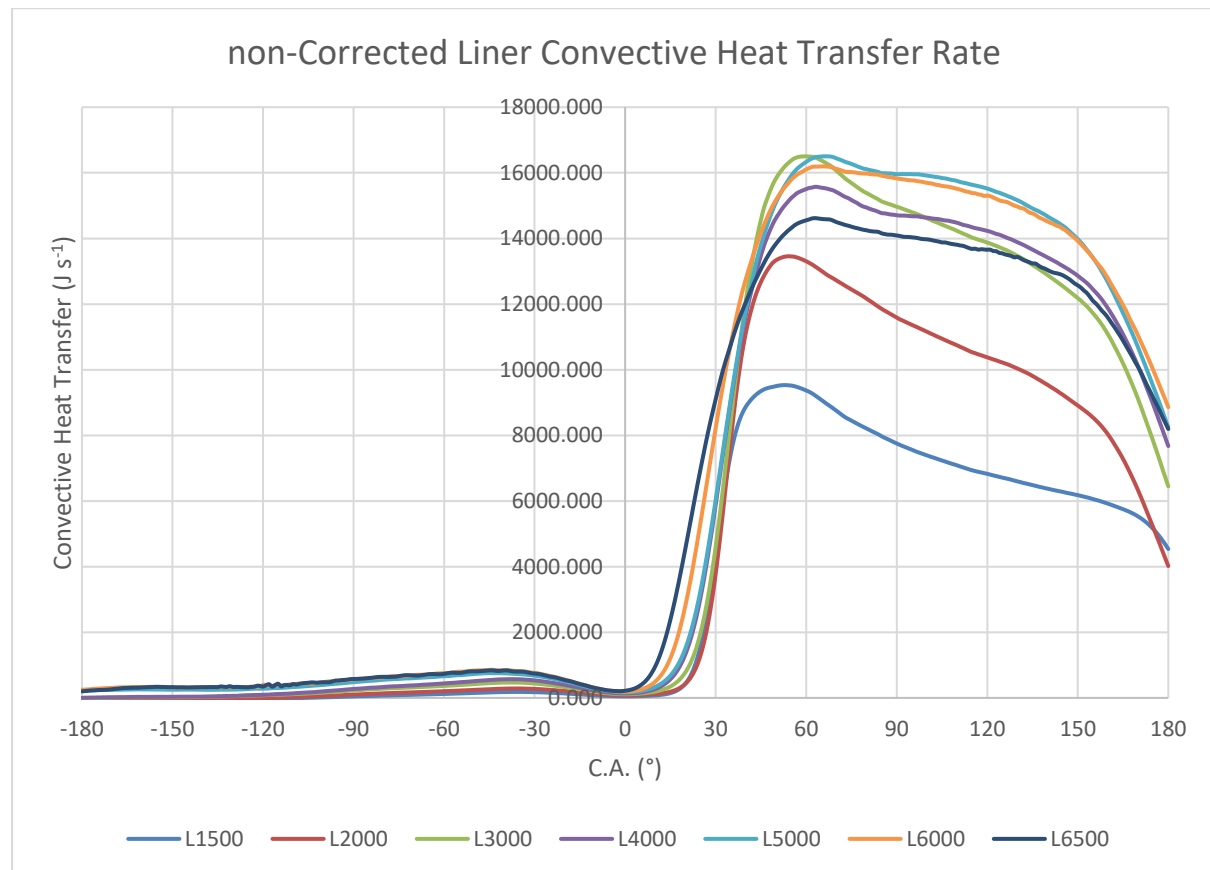


Figure 9-1: non-Corrected Liner Convective Heat Transfer Rate

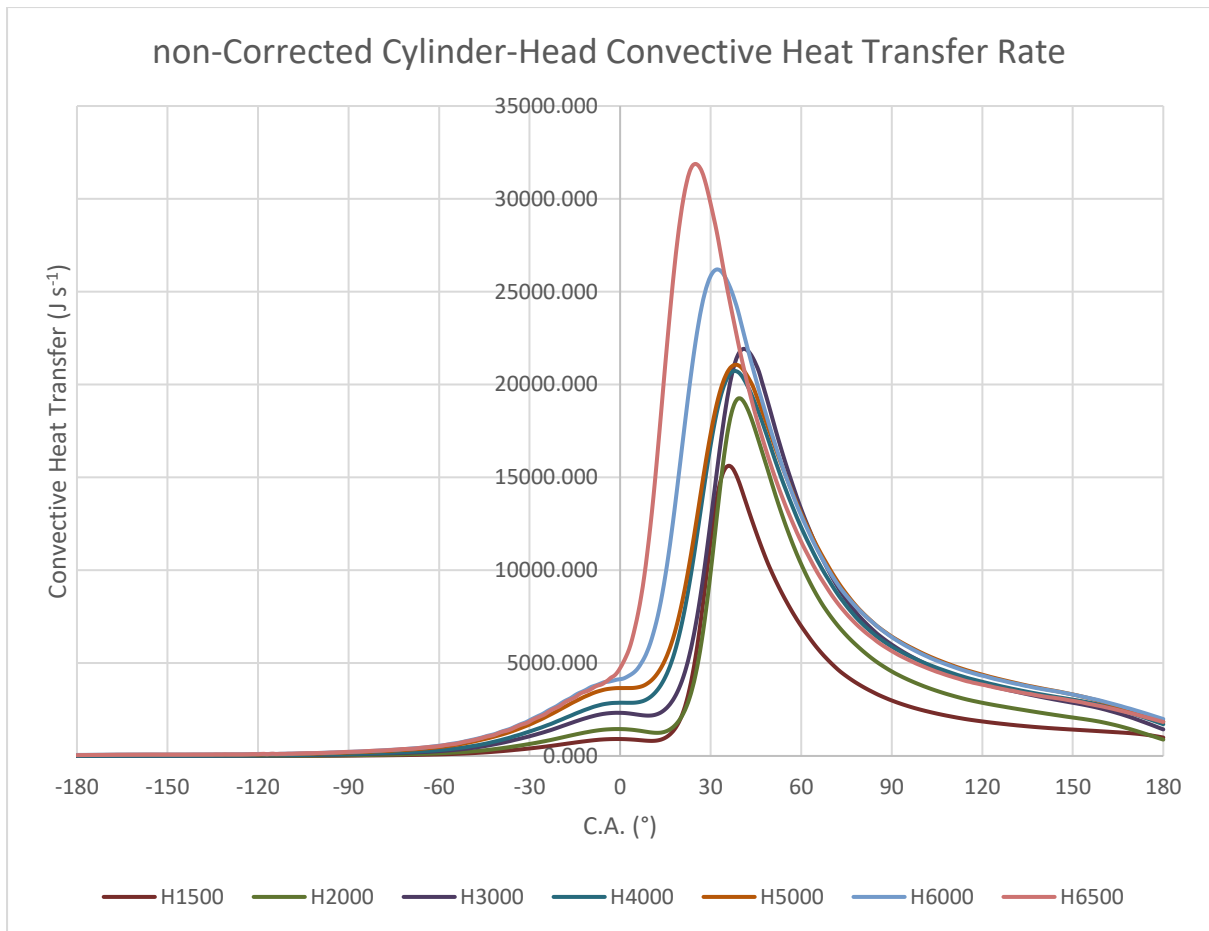


Figure 9-2: non-Corrected Cylinder-Head Convective Heat Transfer Rate

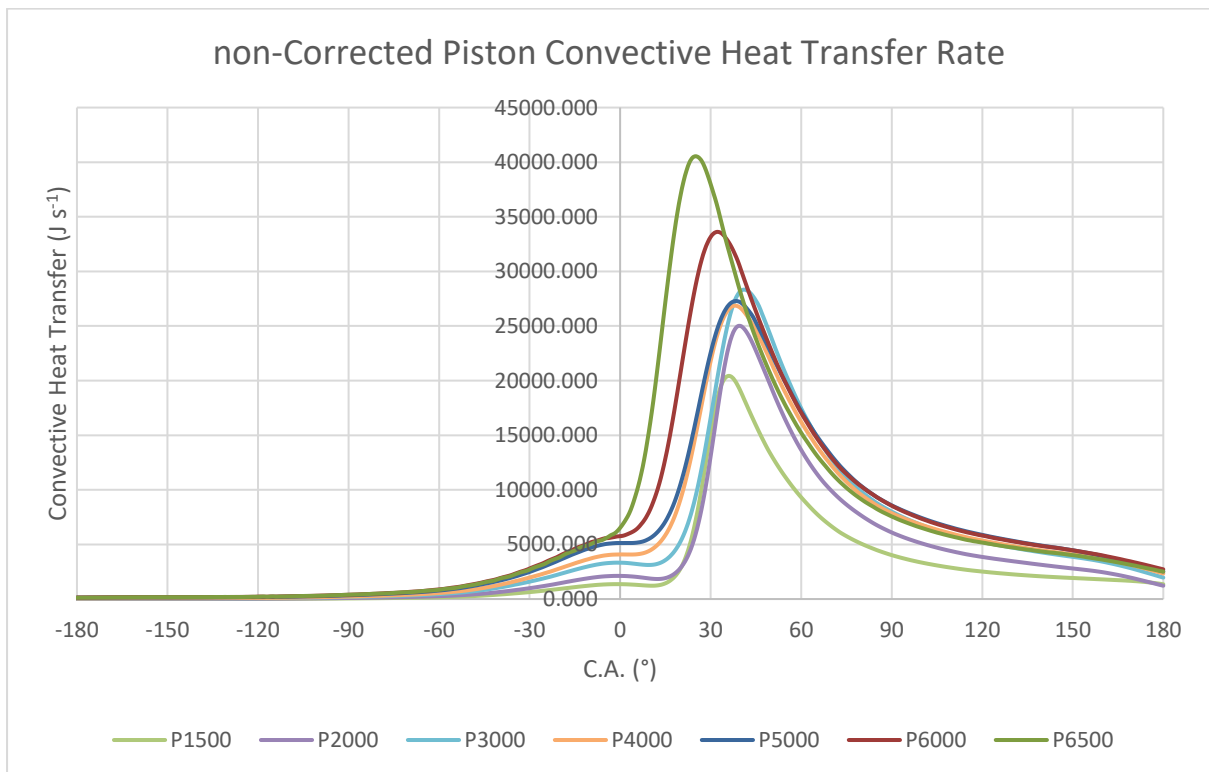


Figure 9-3: non-Corrected Piston Convective Heat Transfer Rate

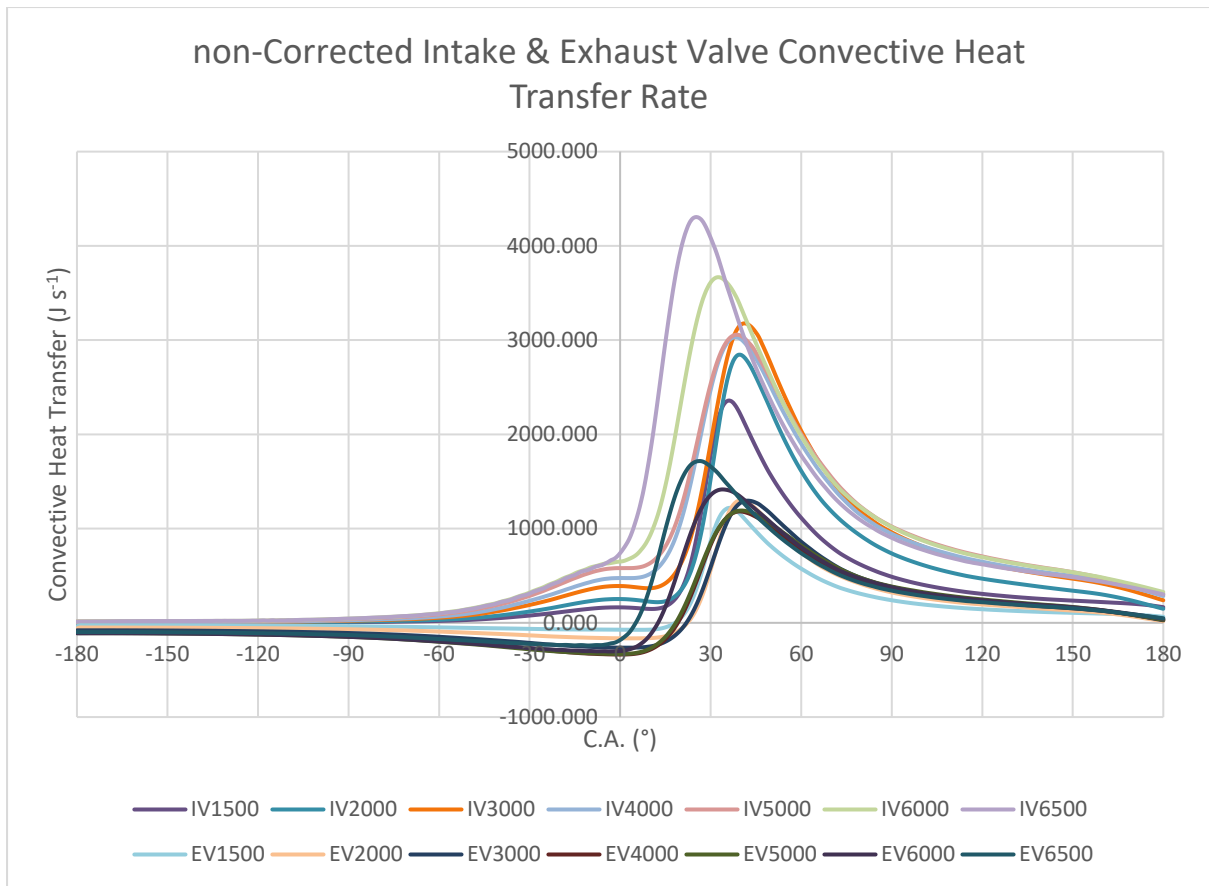


Figure 9-4: non-Corrected Intake & Exhaust Valve Convective Heat Transfer Rate

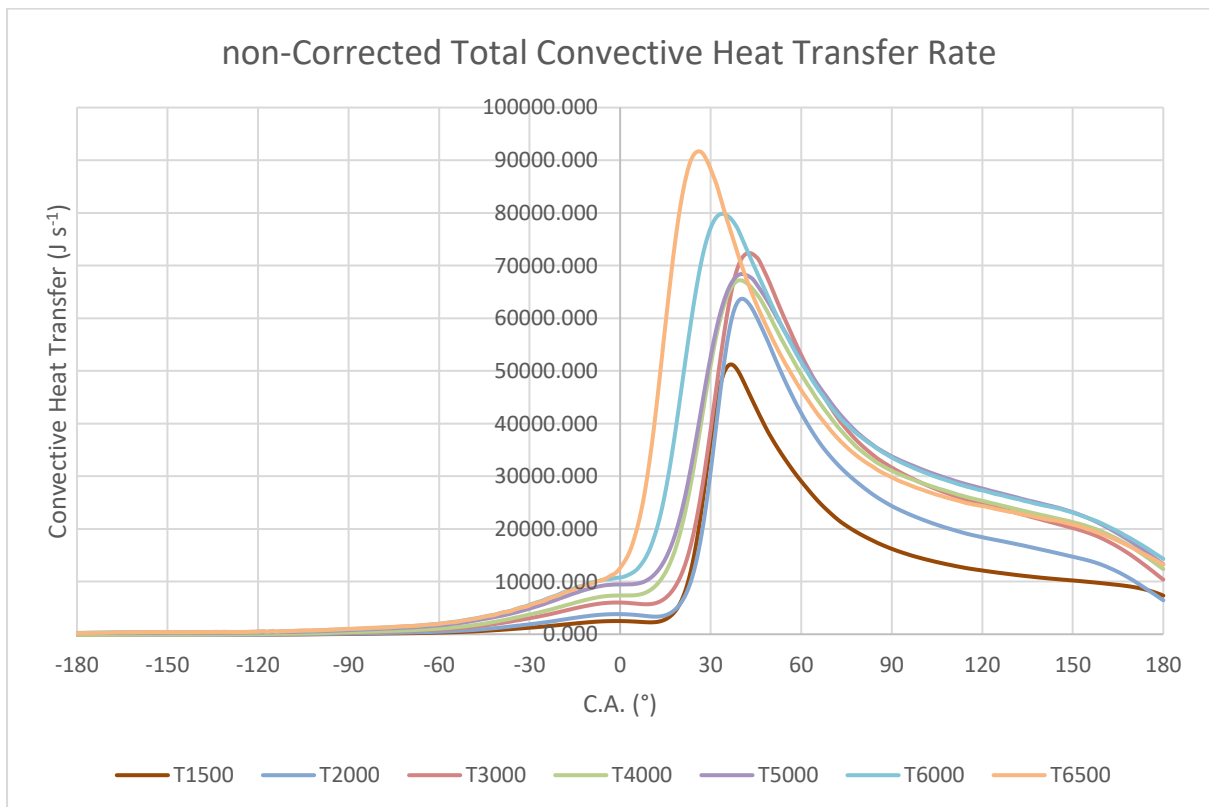


Figure 9-5: non-Corrected Total Convective Heat Transfer Rate

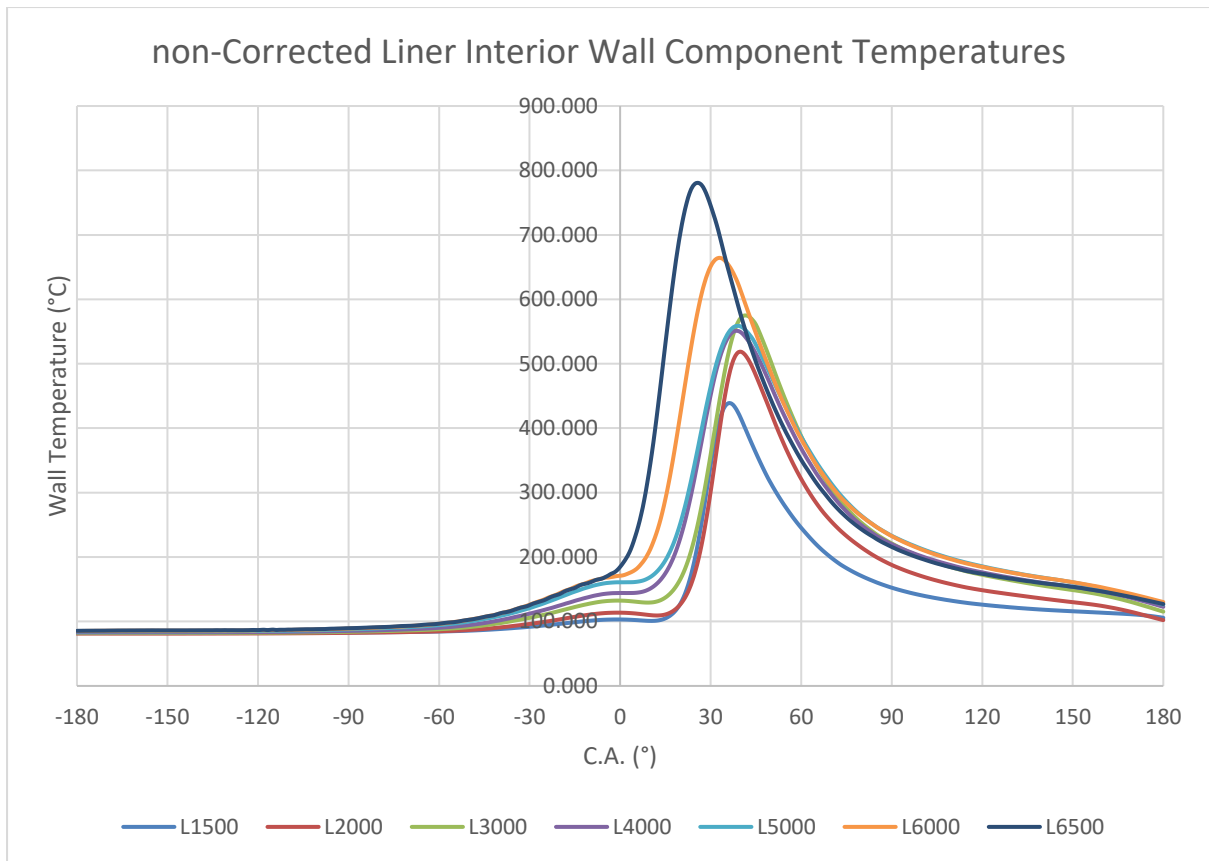


Figure 9-6: non-Corrected Liner Interior Wall Component Temperatures

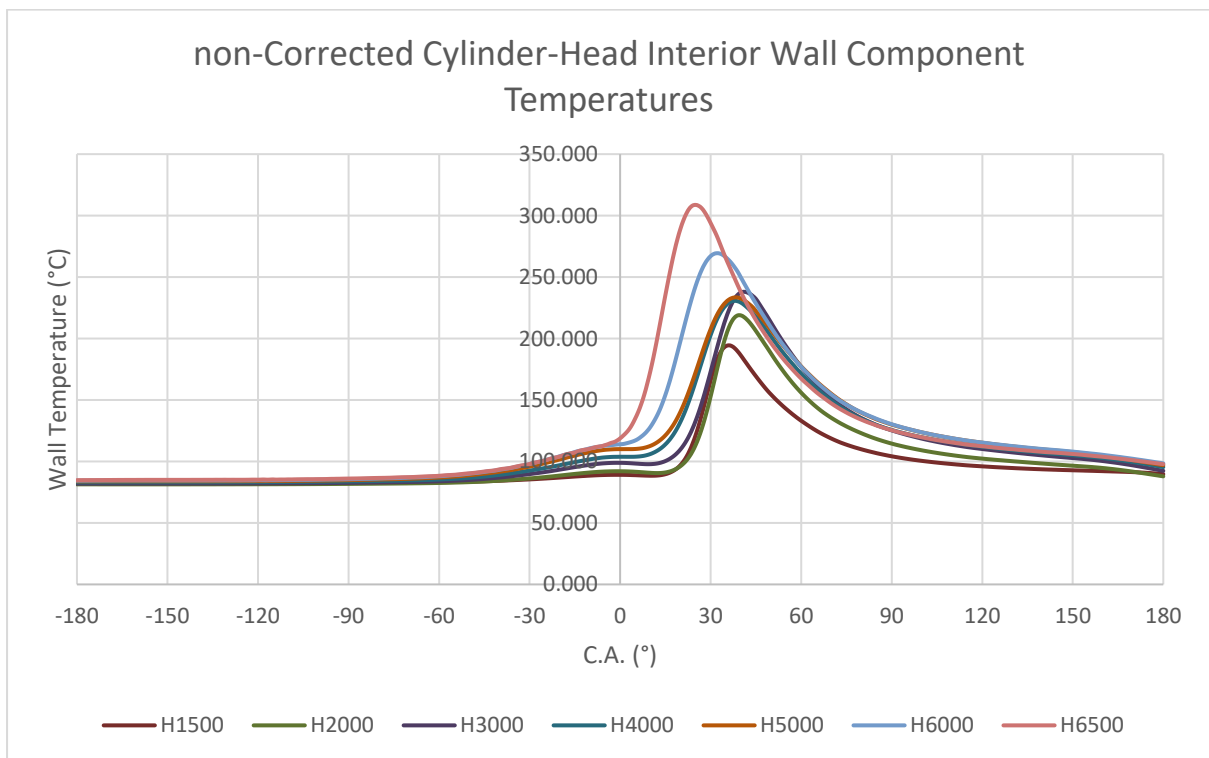


Figure 9-7: non-Corrected Cylinder-Head Interior Wall Component Temperatures

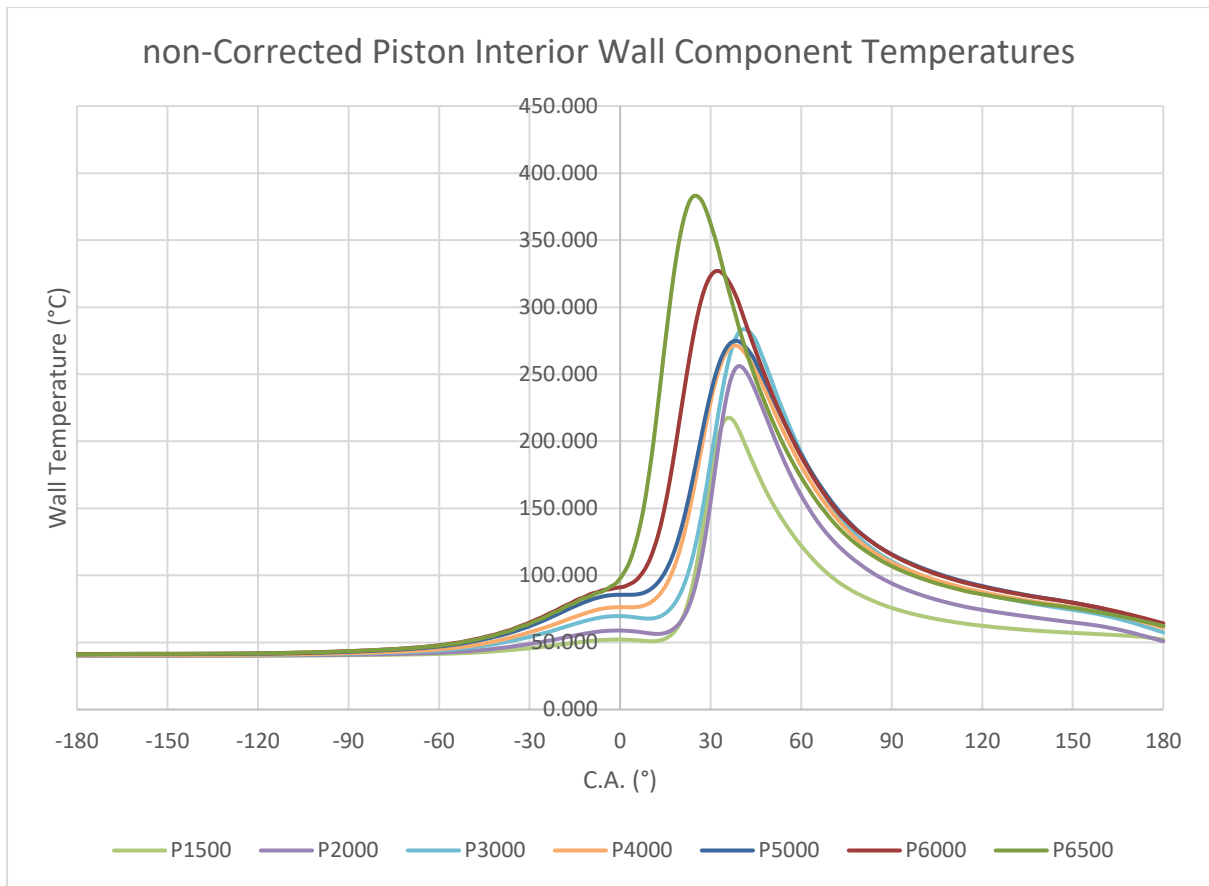


Figure 9-8: non-Corrected Piston Interior Wall Component Temperatures

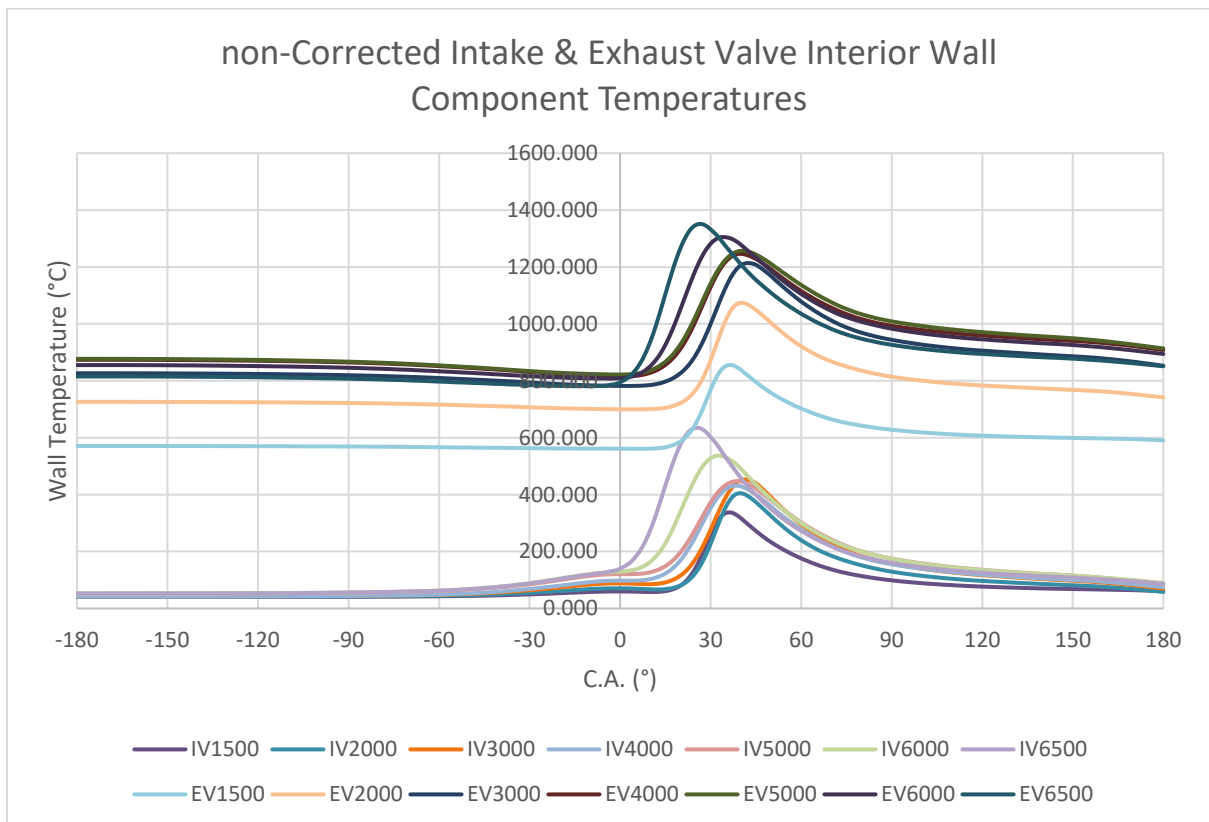


Figure 9-9: non-Corrected Intake & Exhaust Valve Interior Wall Component Temperatures

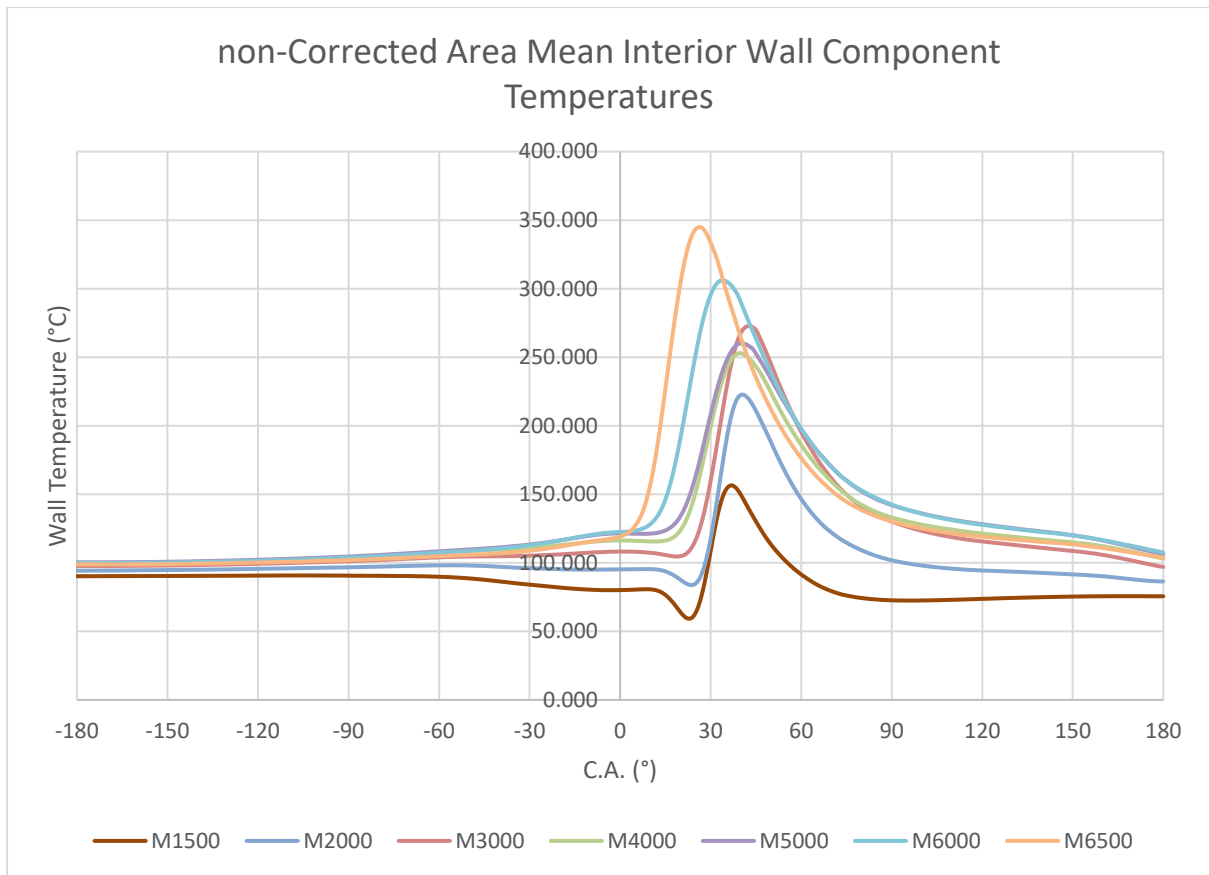


Figure 9-10: non-Corrected Area Mean Interior Wall Component Temperatures

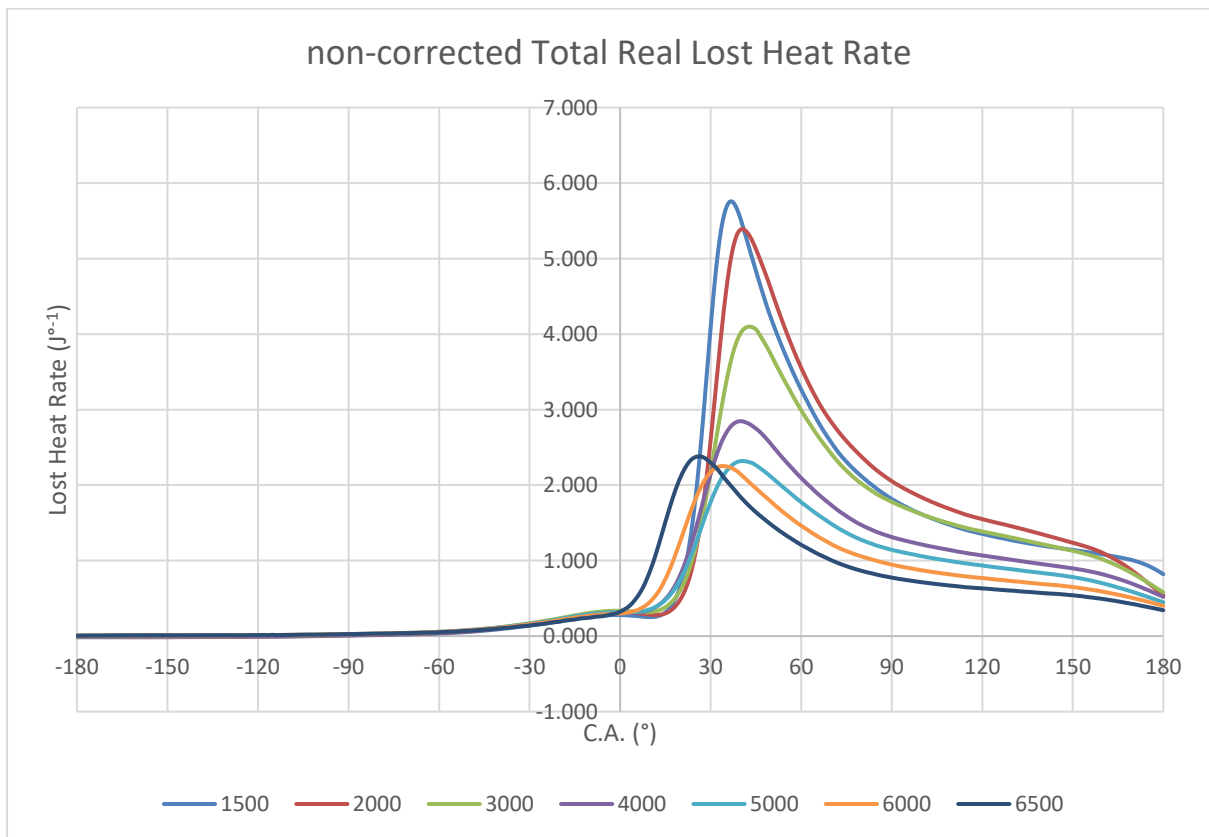


Figure 9-11: non-corrected Total Real Lost Heat Rate

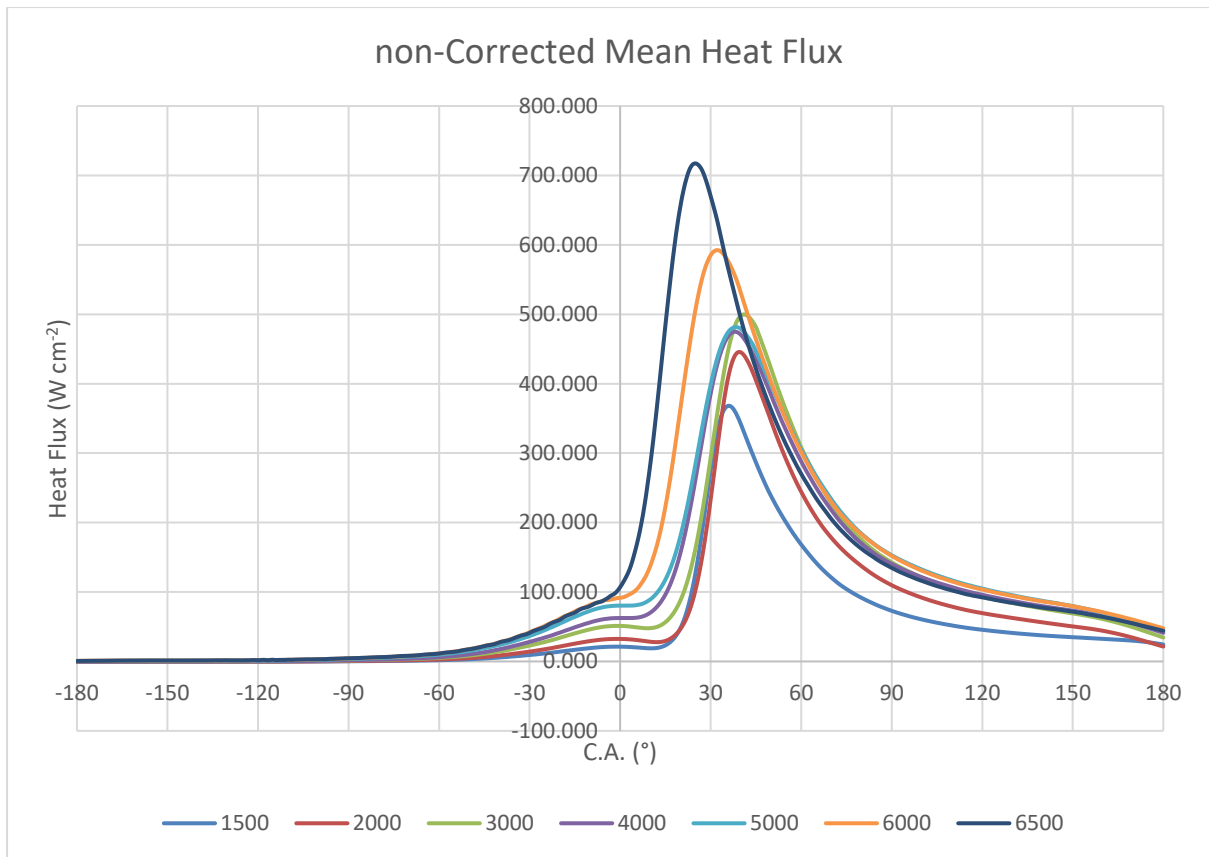


Figure 9-12: non-Corrected Mean Heat Flux

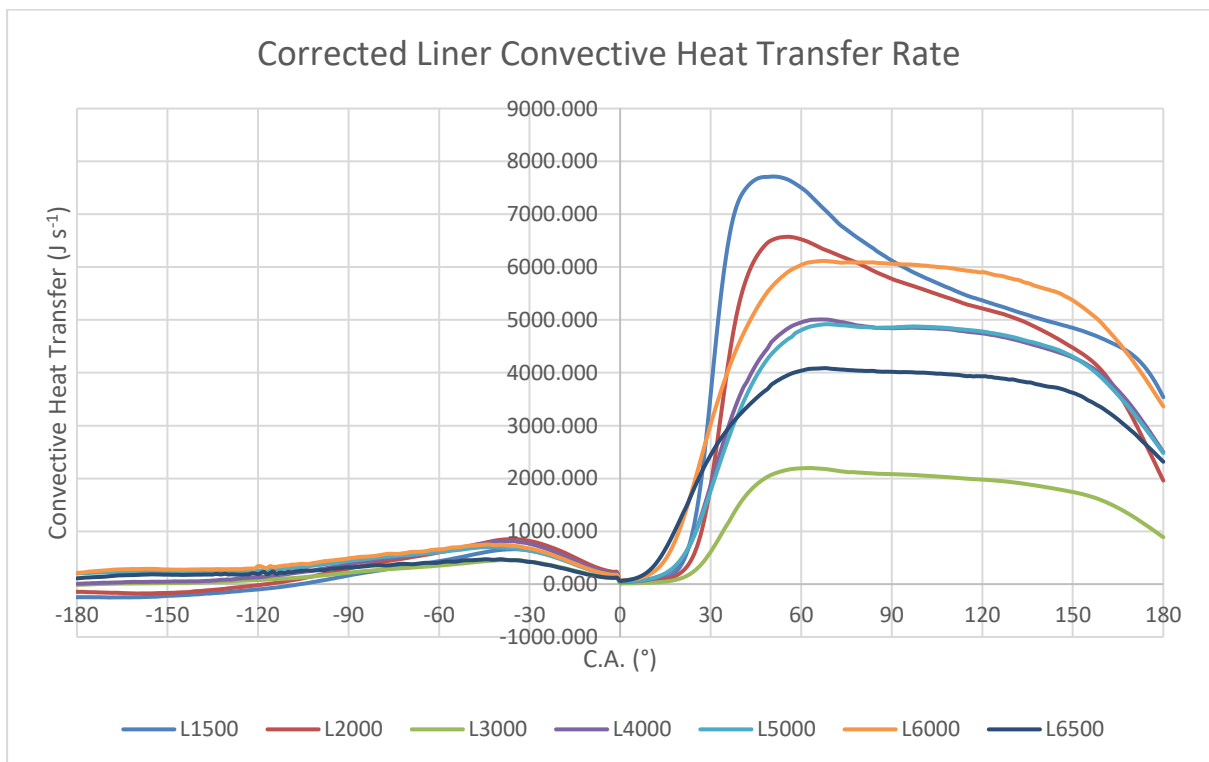


Figure 9-13: Corrected Liner Convective Heat Transfer Rate

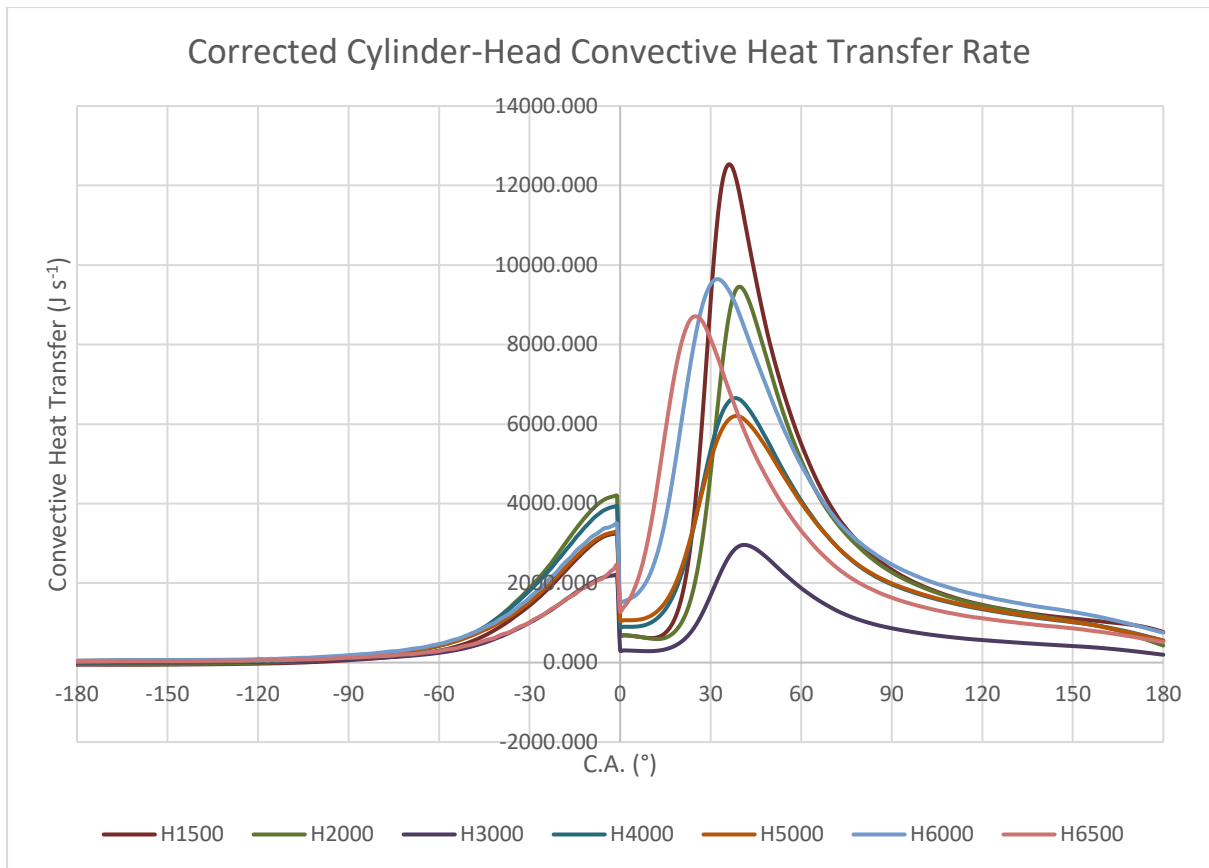


Figure 9-14: Corrected Cylinder-Head Convective Heat Transfer Rate

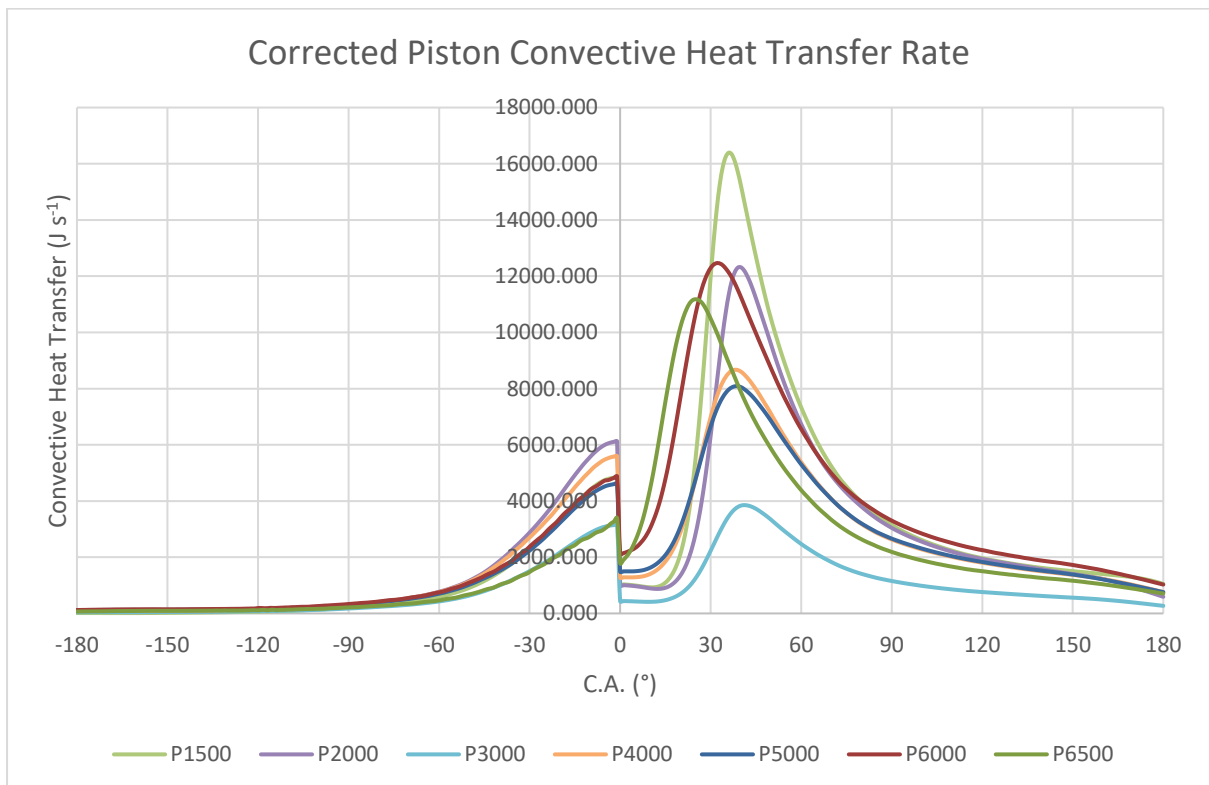


Figure 9-15: Corrected Piston Convective Heat Transfer Rate

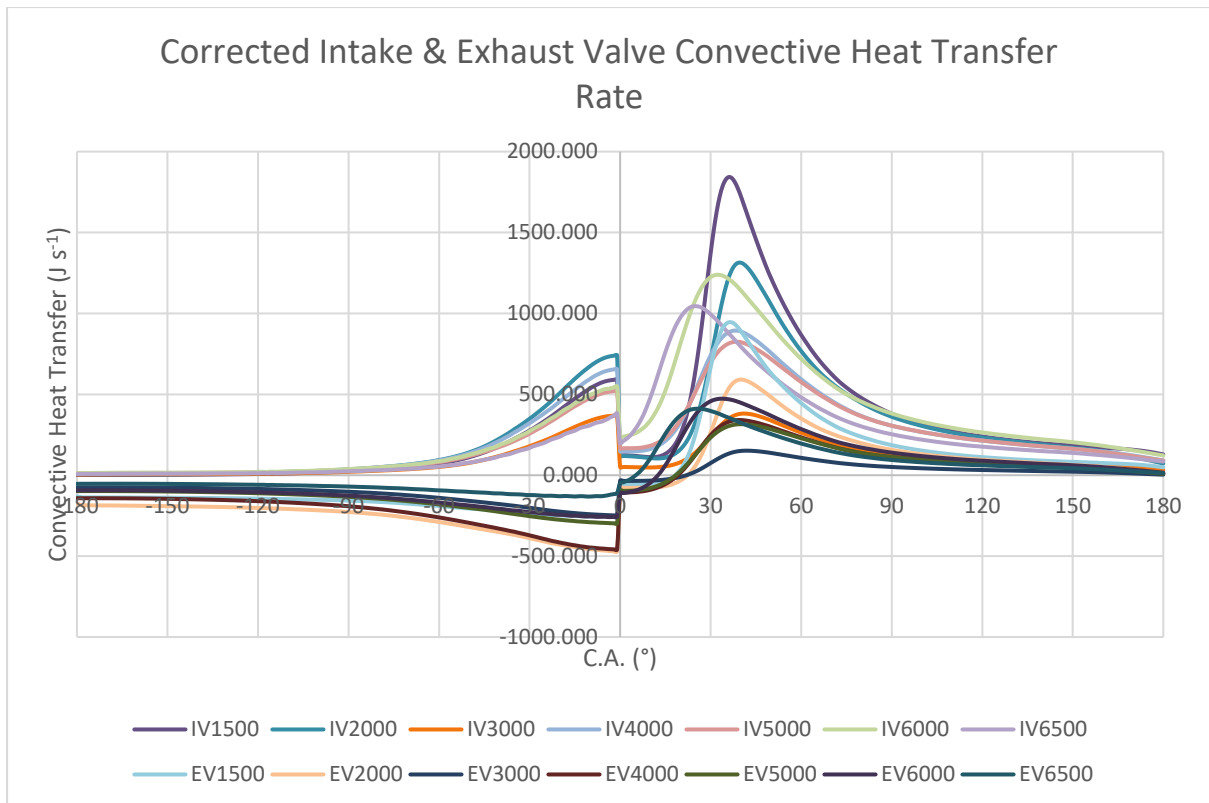


Figure 9-16: Corrected Intake & Exhaust Valve Convective Heat Transfer Rate

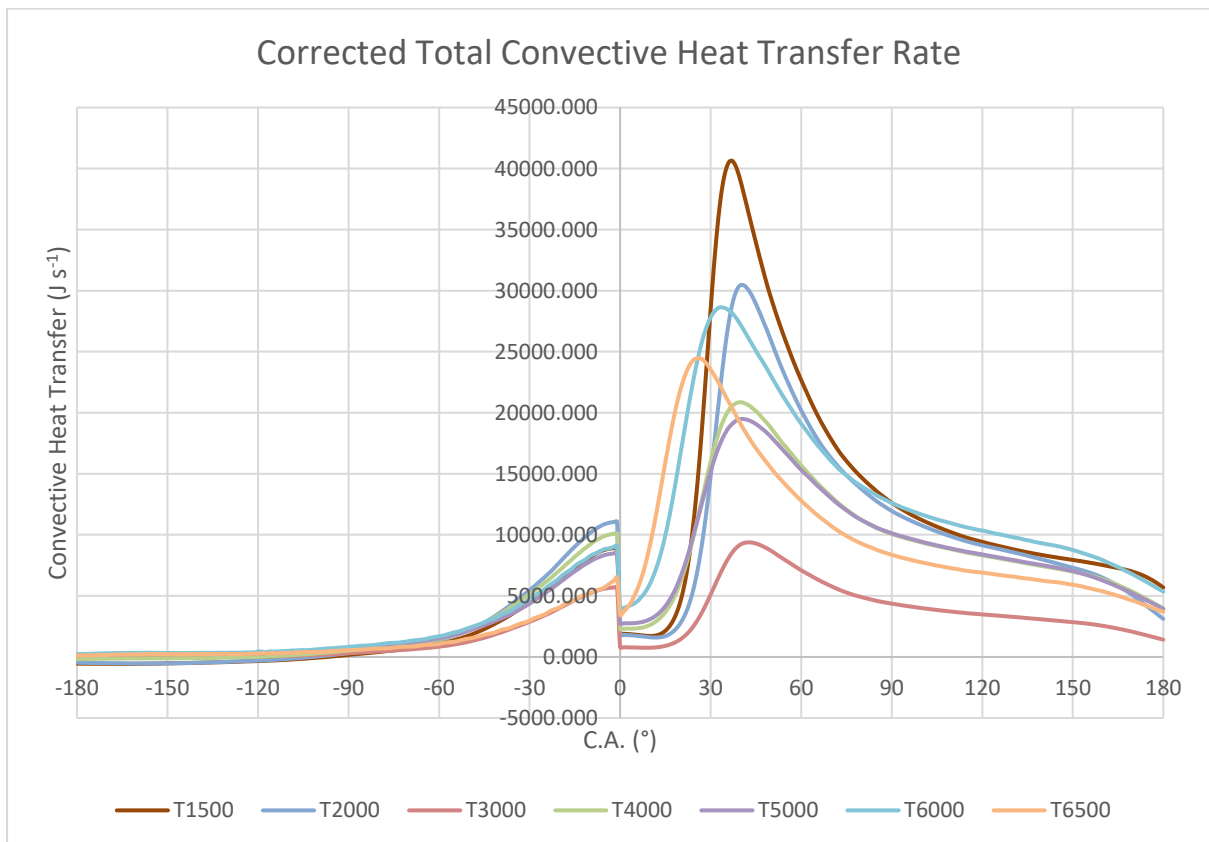


Figure 9-17: Corrected Total Convective Heat Transfer Rate

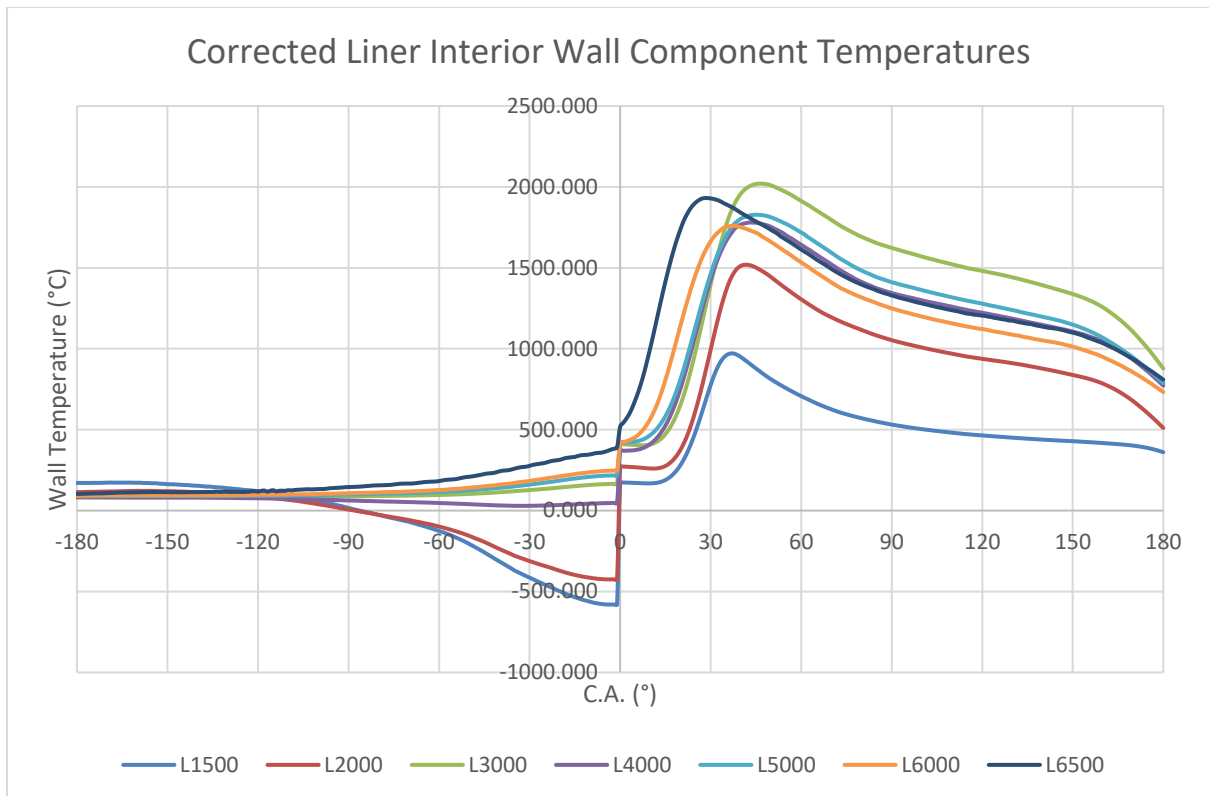


Figure 9-18: Corrected Liner Interior Wall Component Temperatures

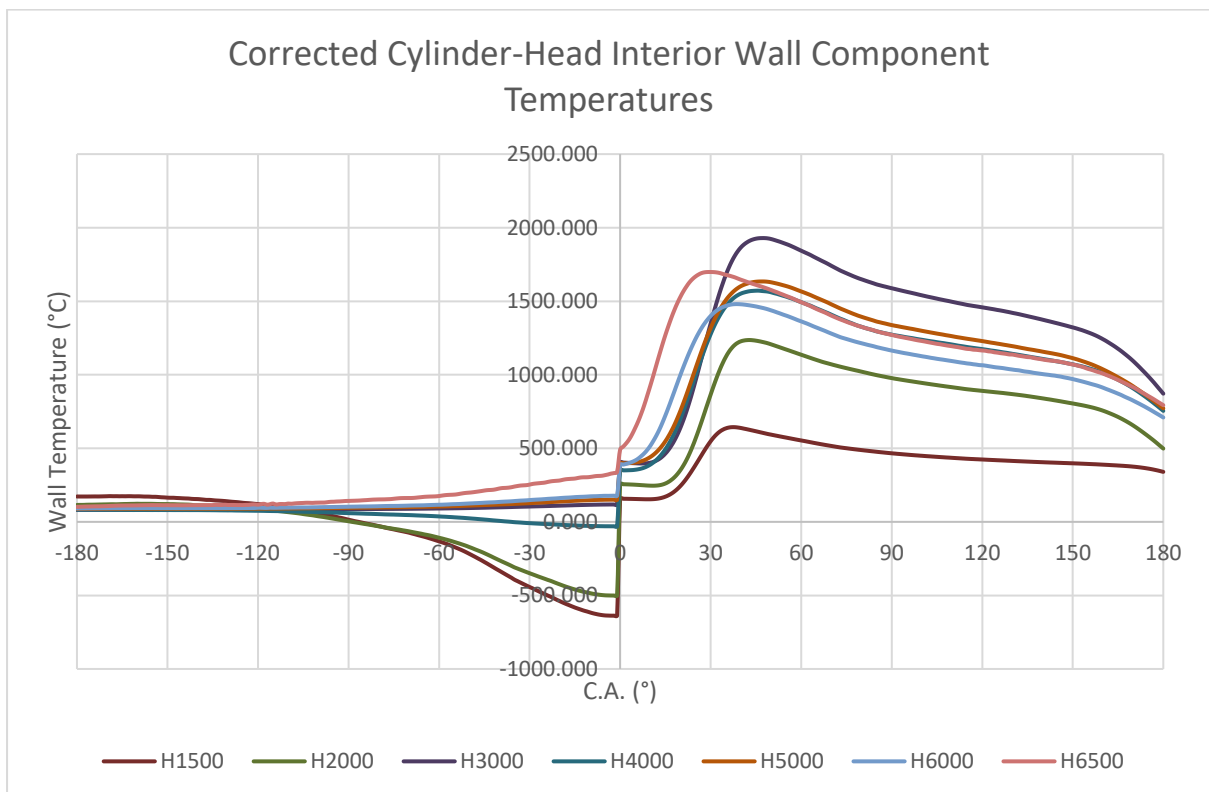


Figure 9-19: Corrected Cylinder-Head Interior Wall Component Temperatures

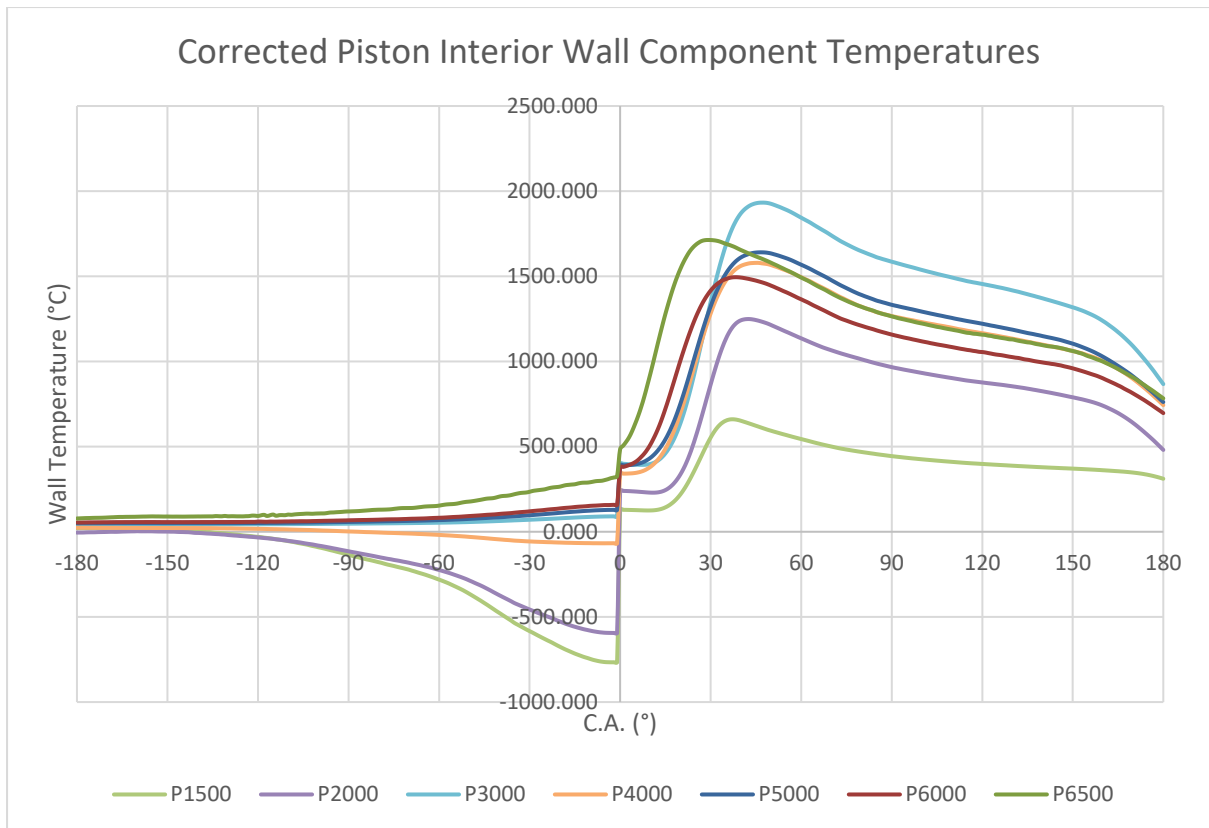


Figure 9-20: Corrected Piston Interior Wall Component Temperatures

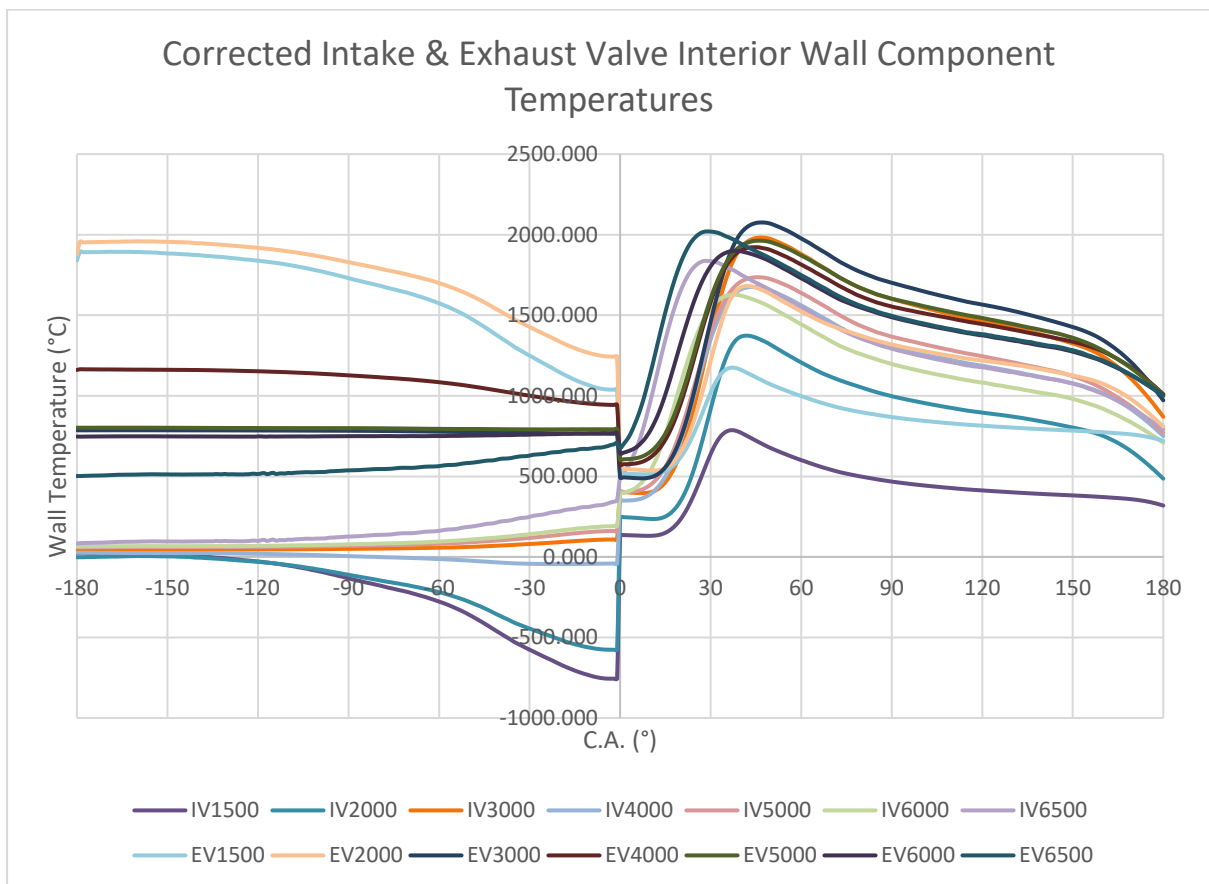


Figure 9-21: Corrected Intake & Exhaust Valve Interior Wall Component Temperatures

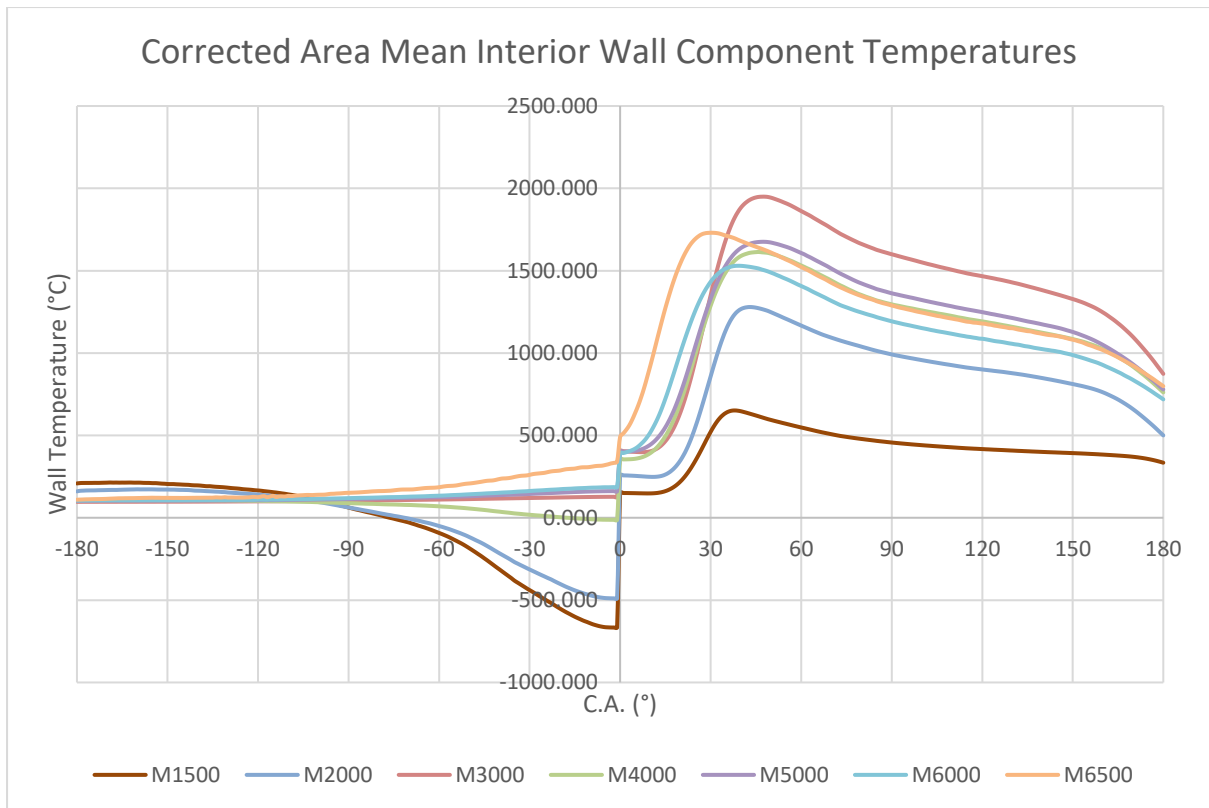


Figure 9-22: Corrected Area Mean Interior Wall Component Temperatures

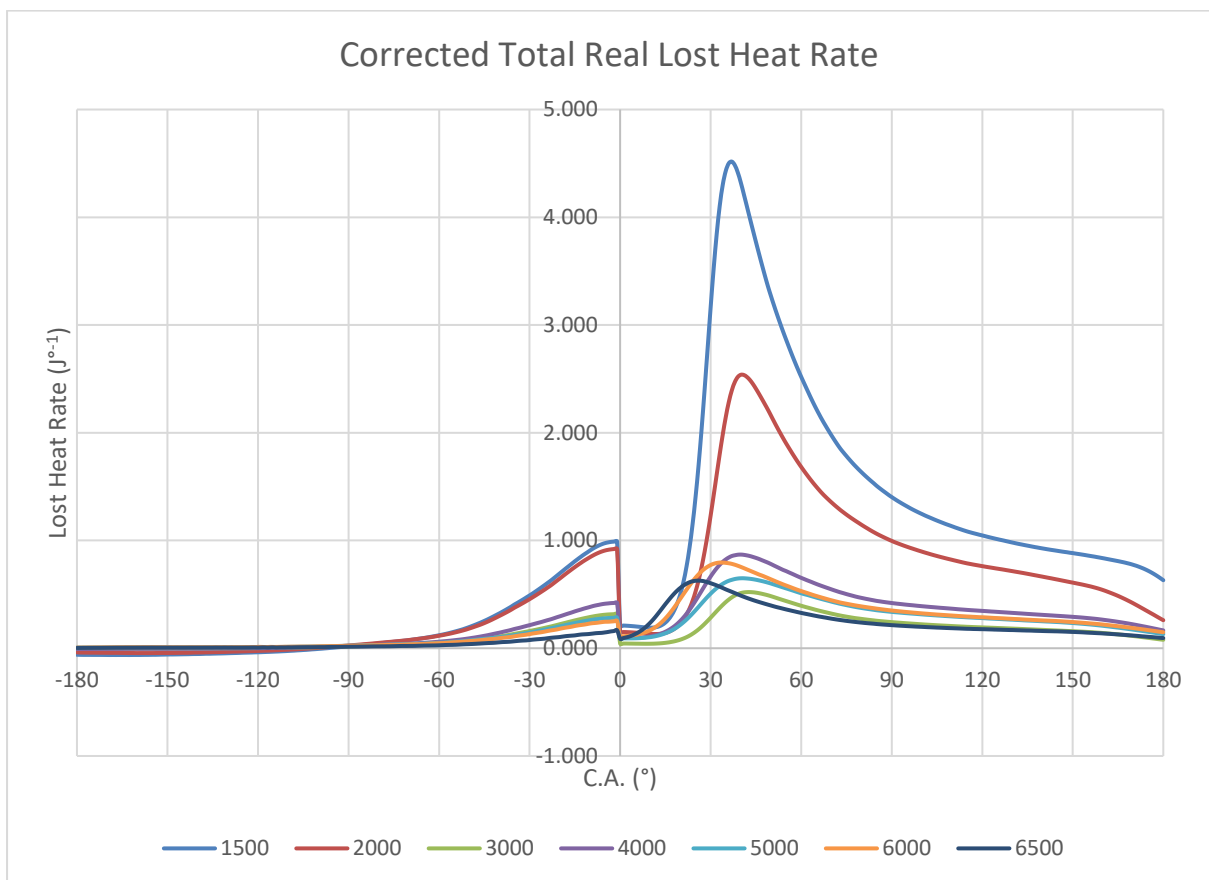


Figure 9-23: Corrected Total Real Lost Heat Rate

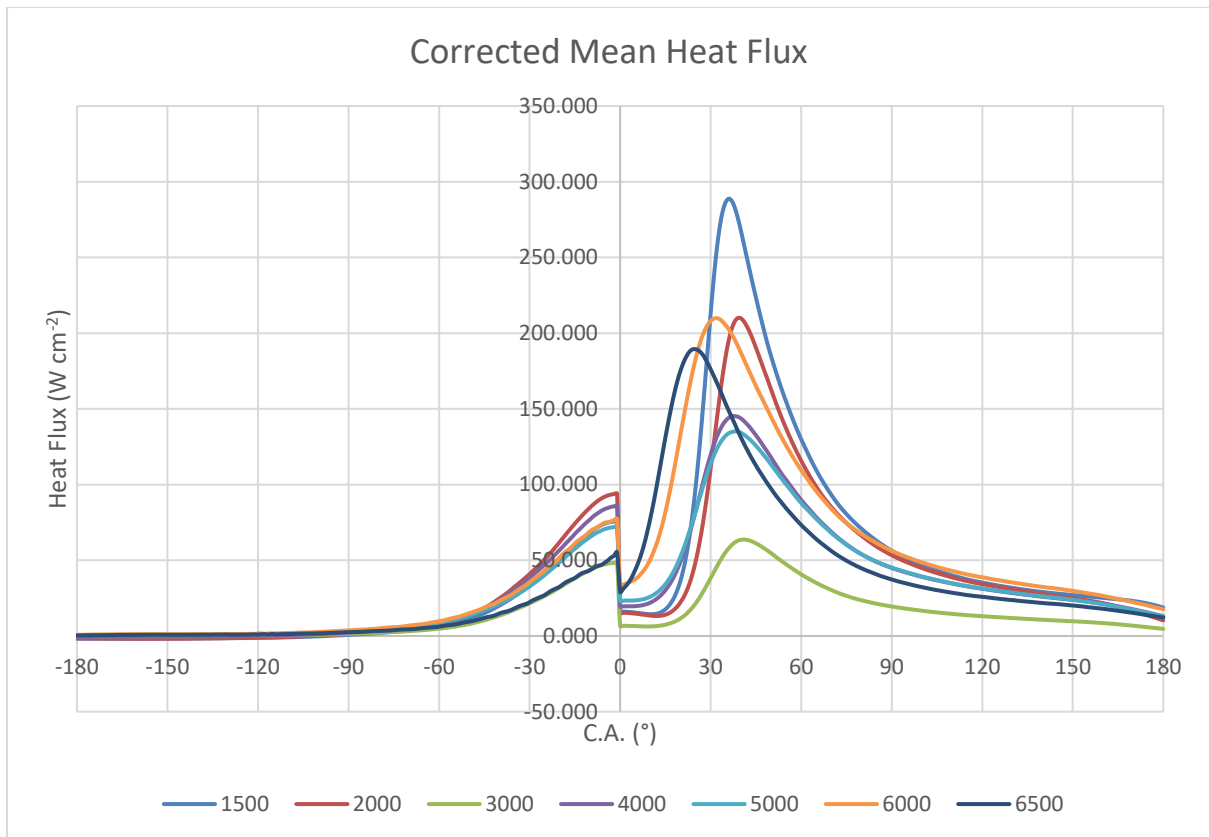


Figure 9-24: Corrected Mean Heat Flux

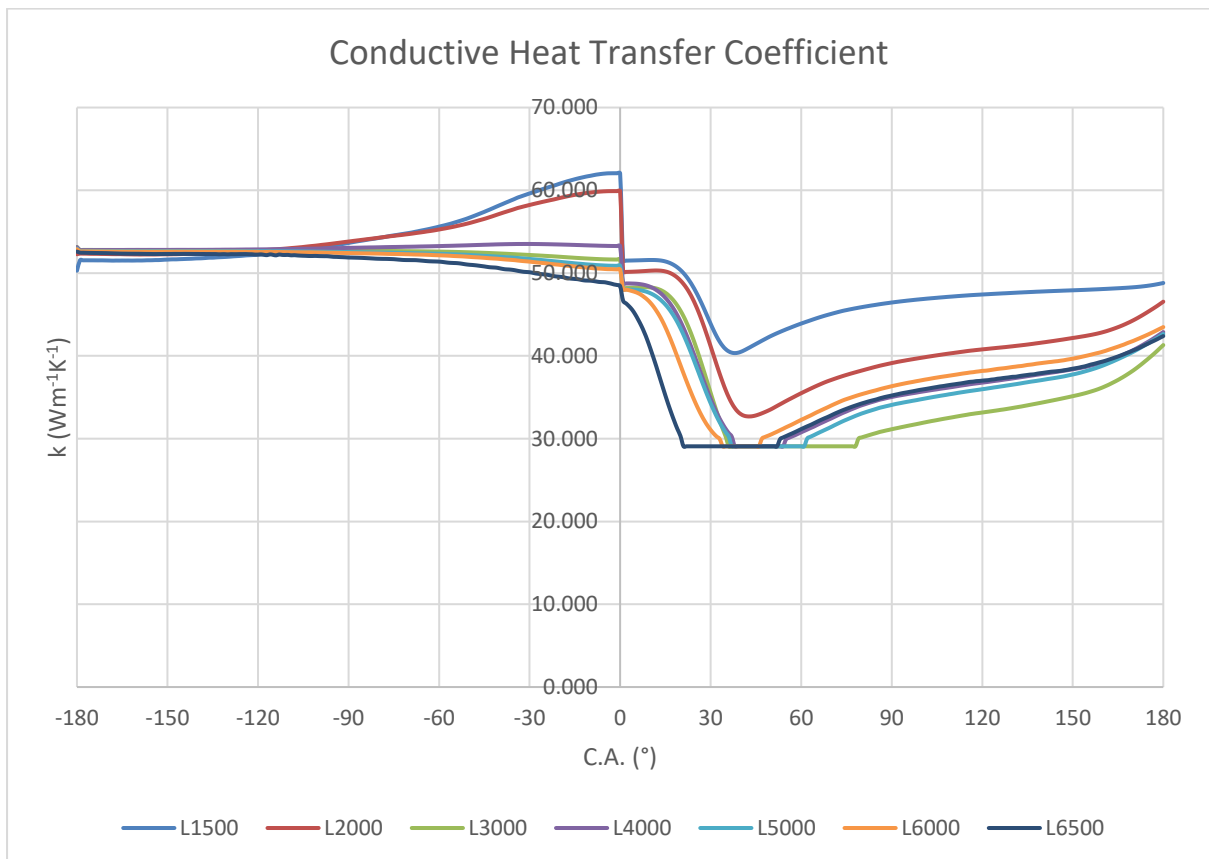


Figure 9-25: Conductive Heat Transfer Coefficient

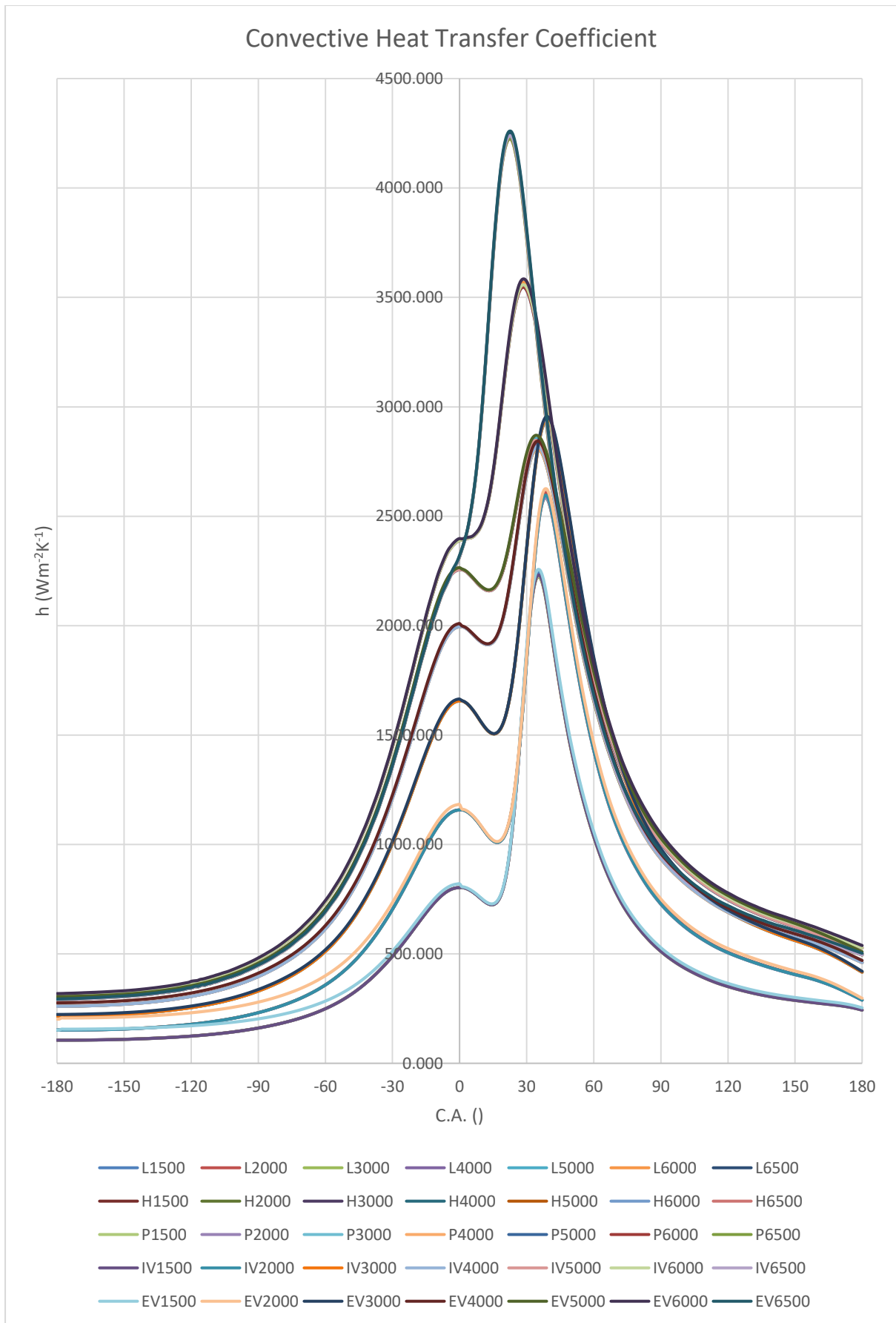


Figure 9-26: Convective Heat Transfer Coefficient

9.2 2-ZONE COMBUSTION MODEL

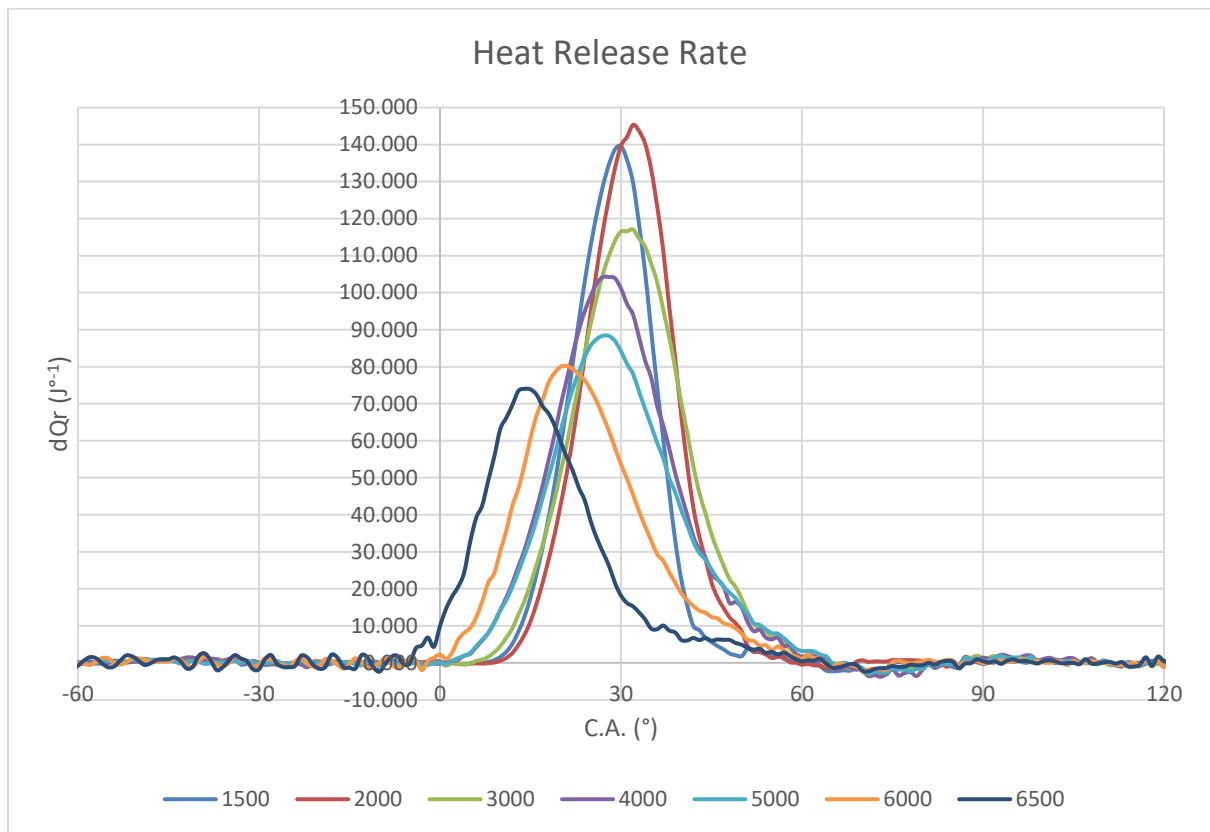


Figure 9-27: Heat Release Rate

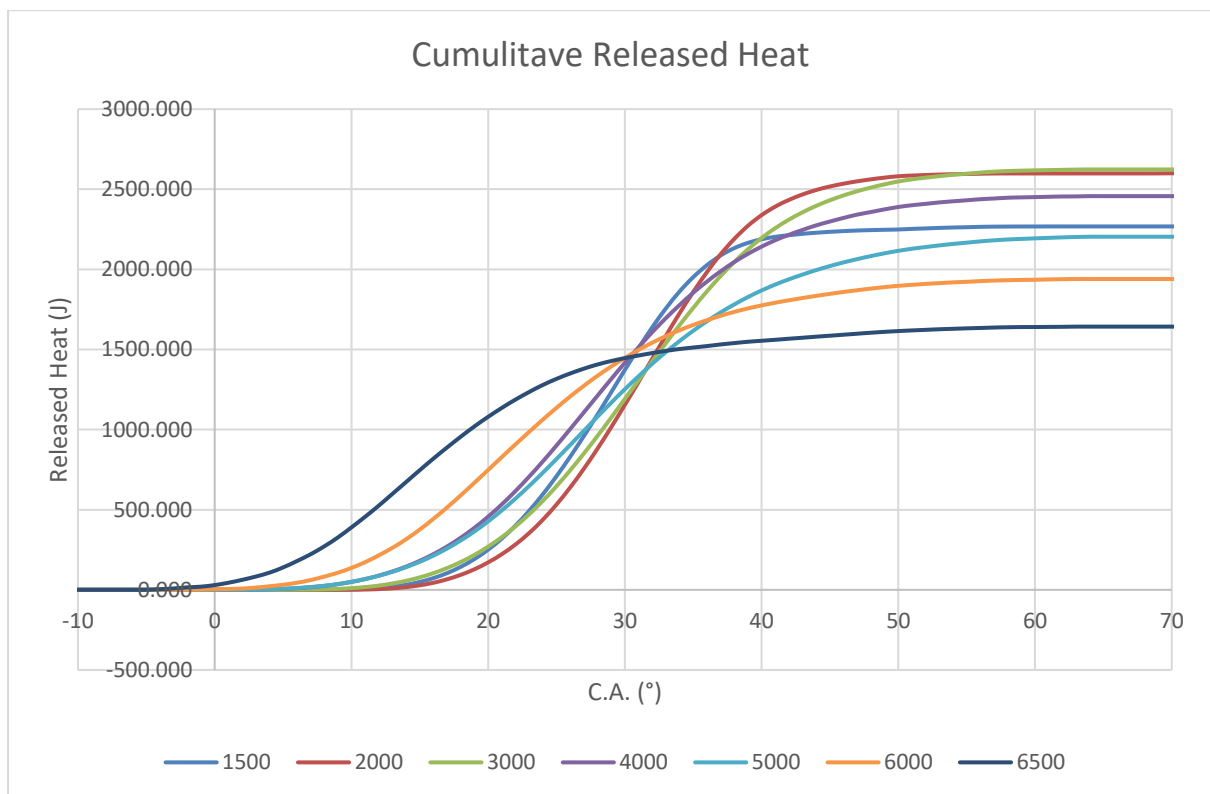


Figure 9-28: Cumulative Released Heat

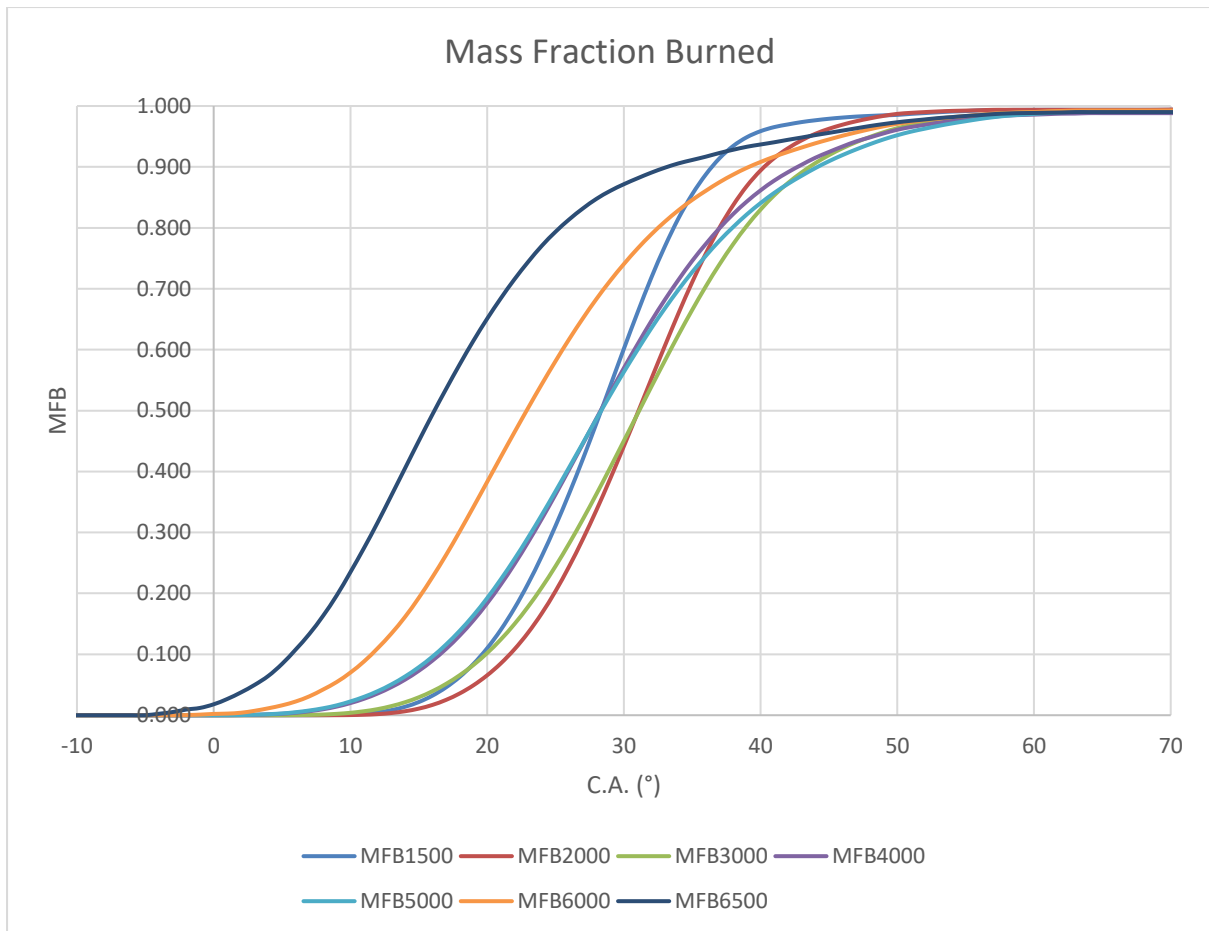


Figure 9-29: Mass Fraction Burned

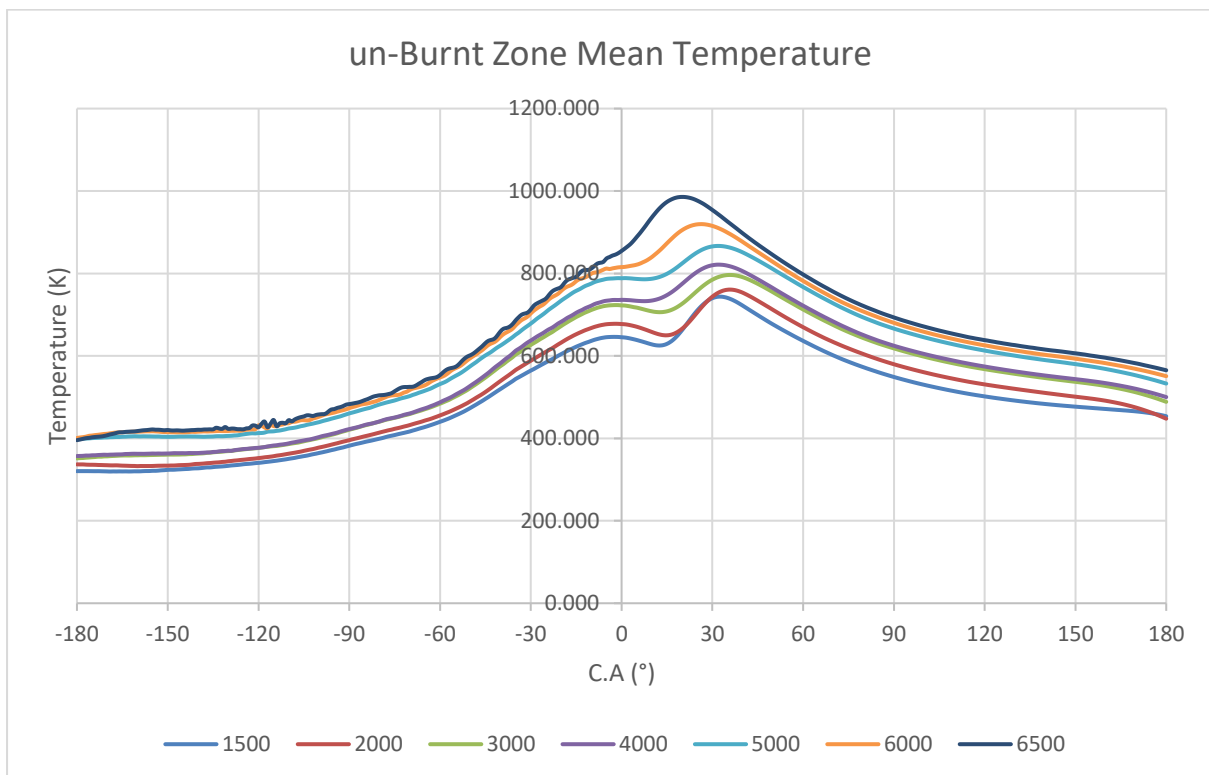


Figure 9-30: un-Burnt Zone Mean Temperature

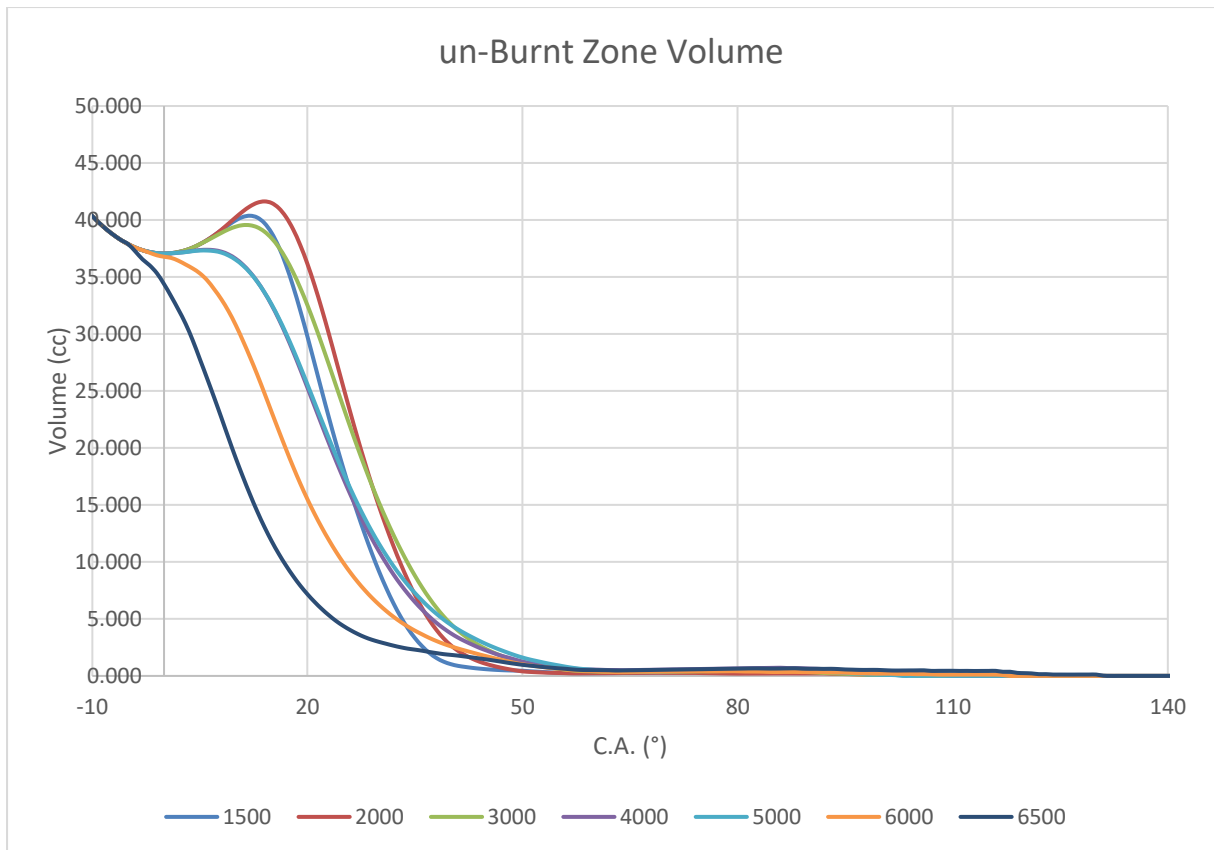


Figure 9-31: un-Burnt Zone Volume

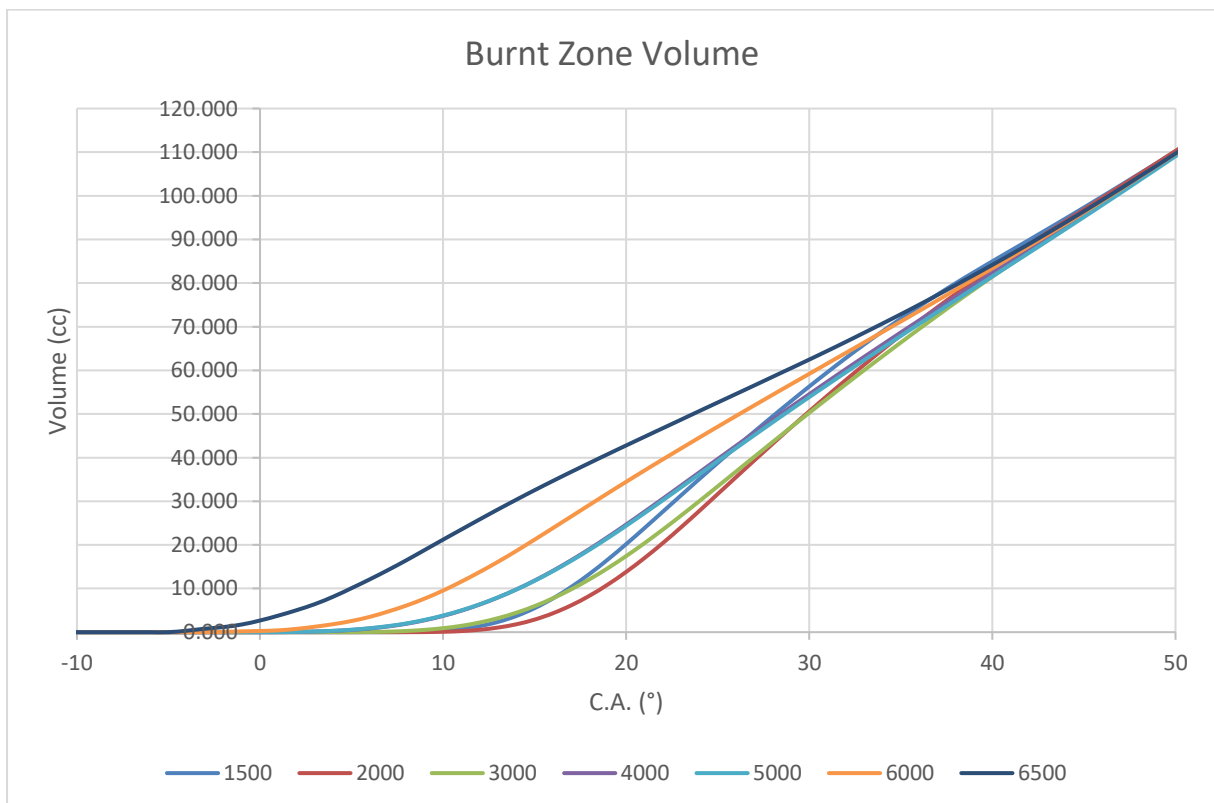


Figure 9-32: Burnt Zone Volume

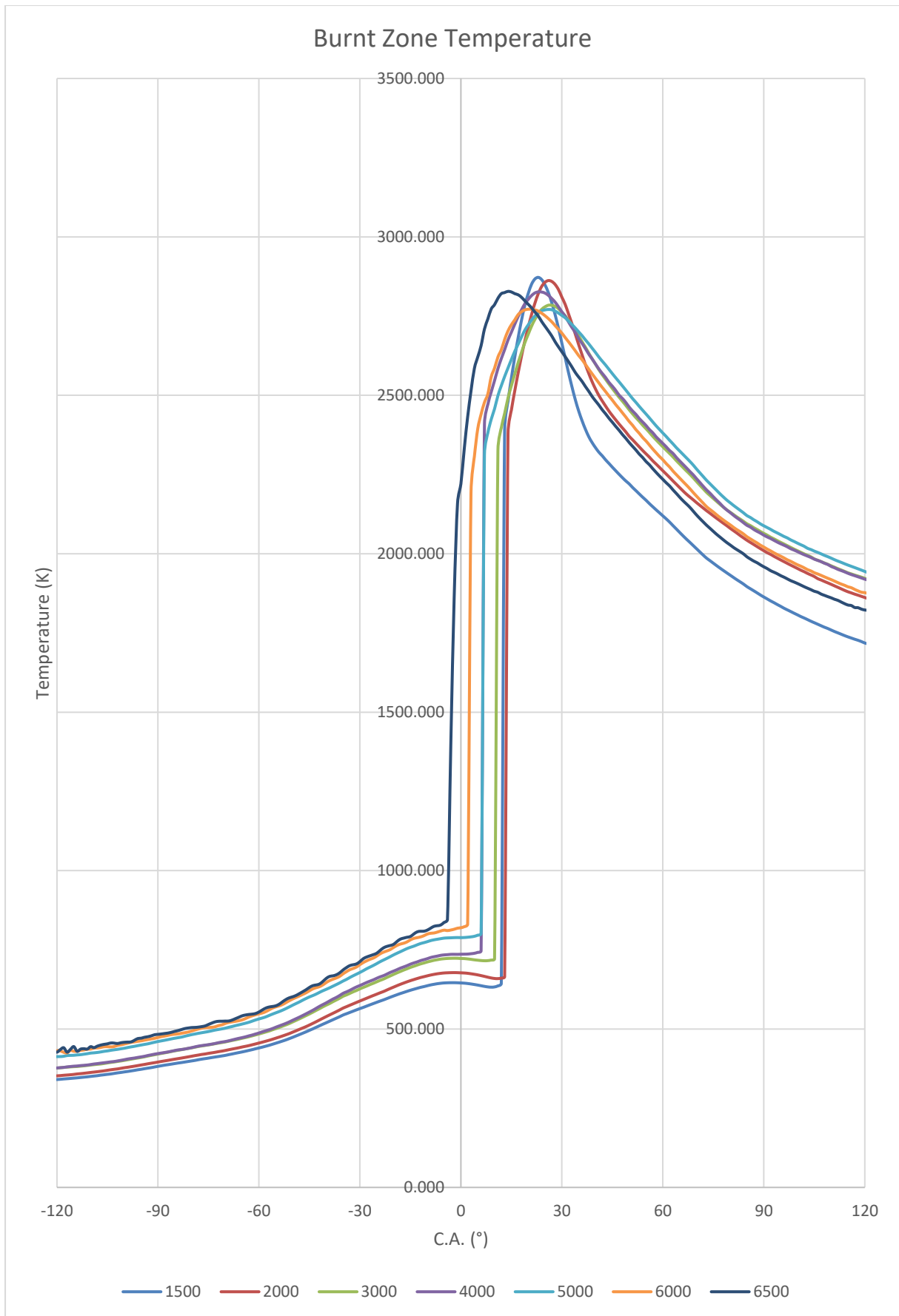


Figure 9-33: Burnt Zone Temperature

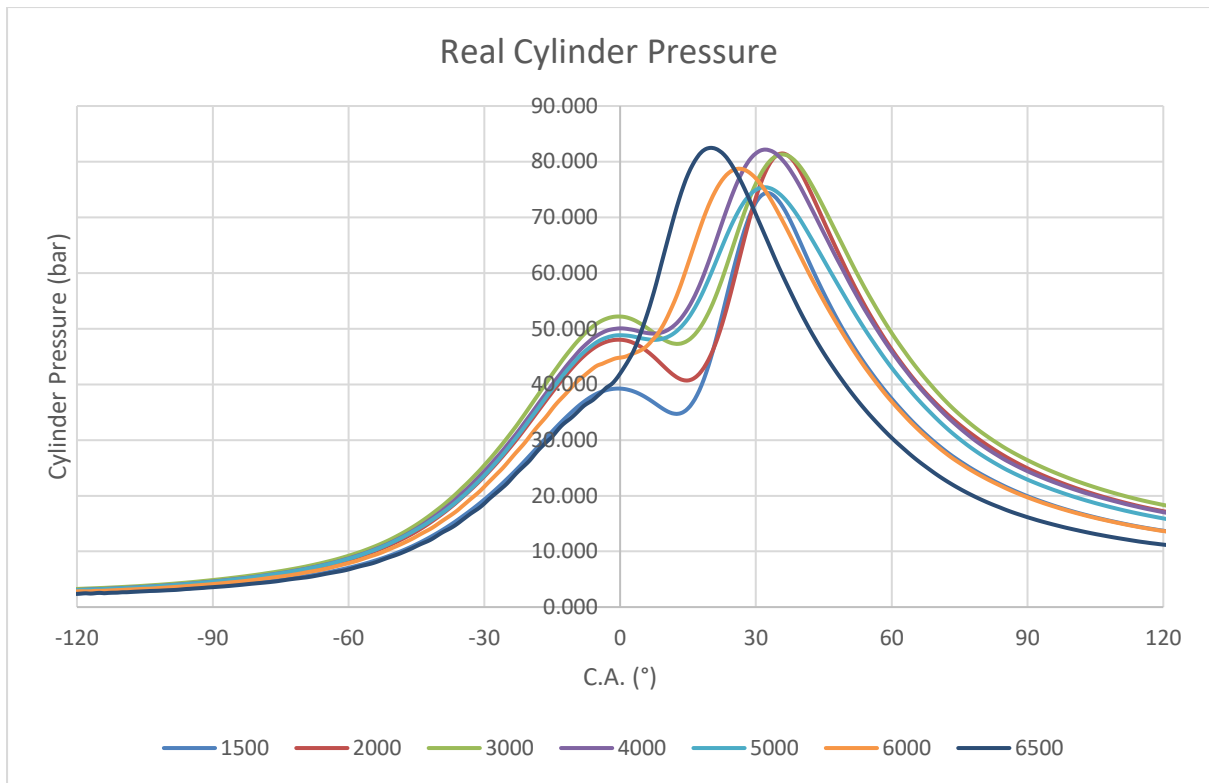


Figure 9-34: Real Cylinder Pressure

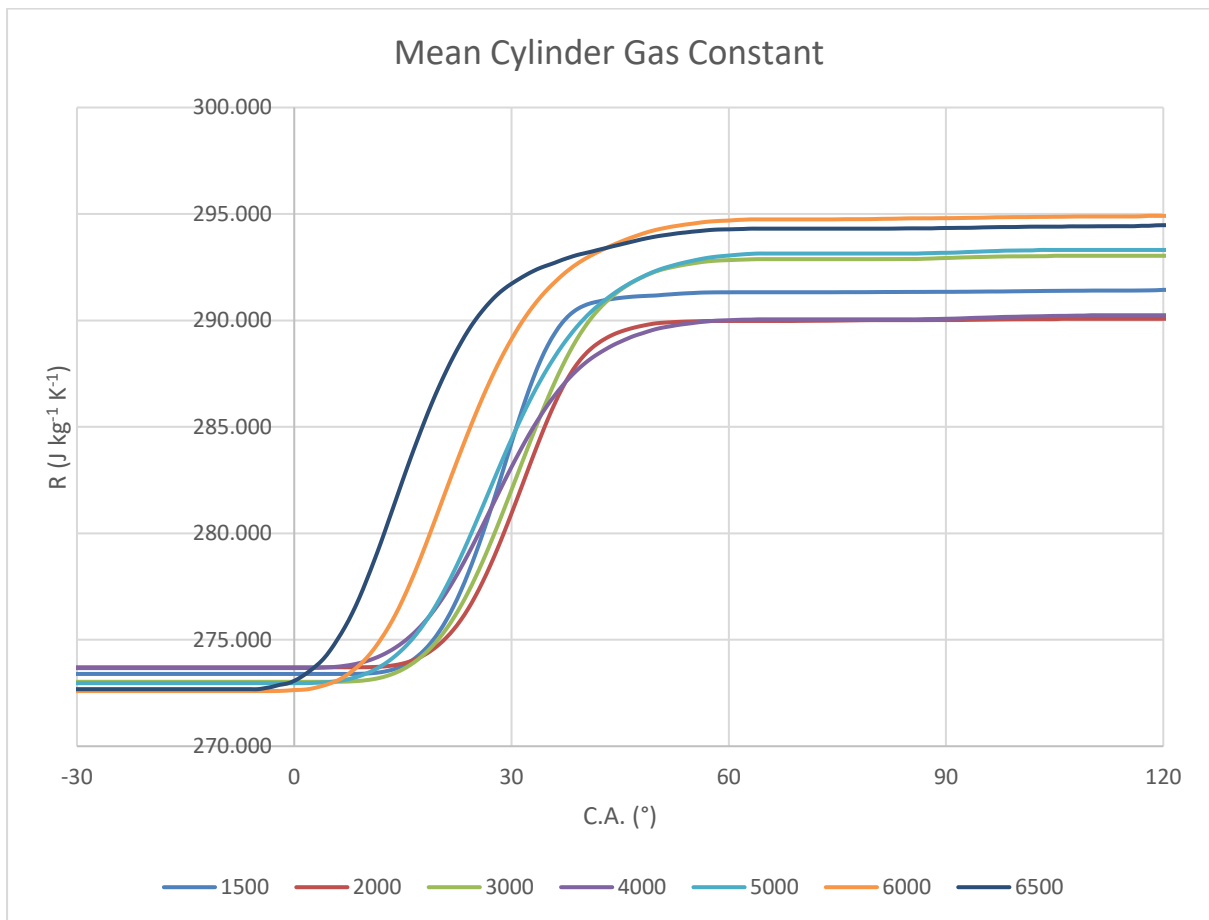


Figure 9-35: Mean Cylinder Gas Constant

9.3 RATIO OF SPECIFIC HEATS

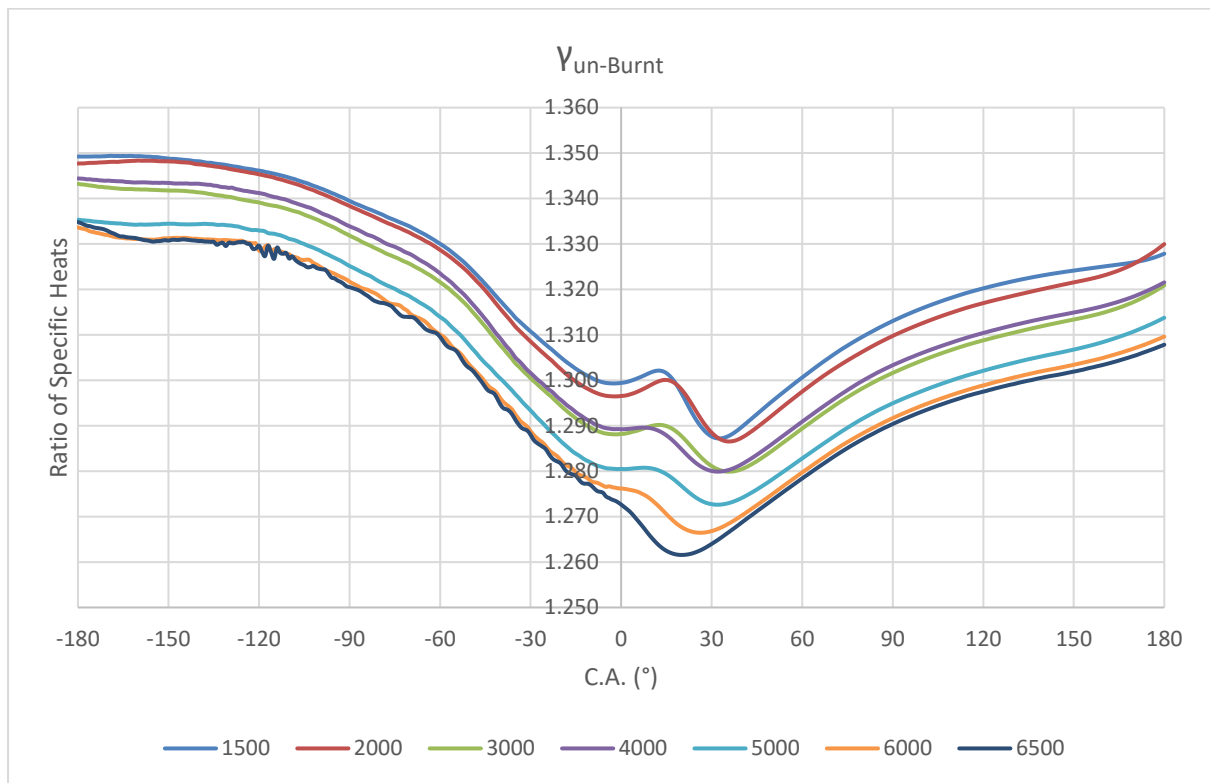


Figure 9-36: $\gamma_{un-Burnt}$

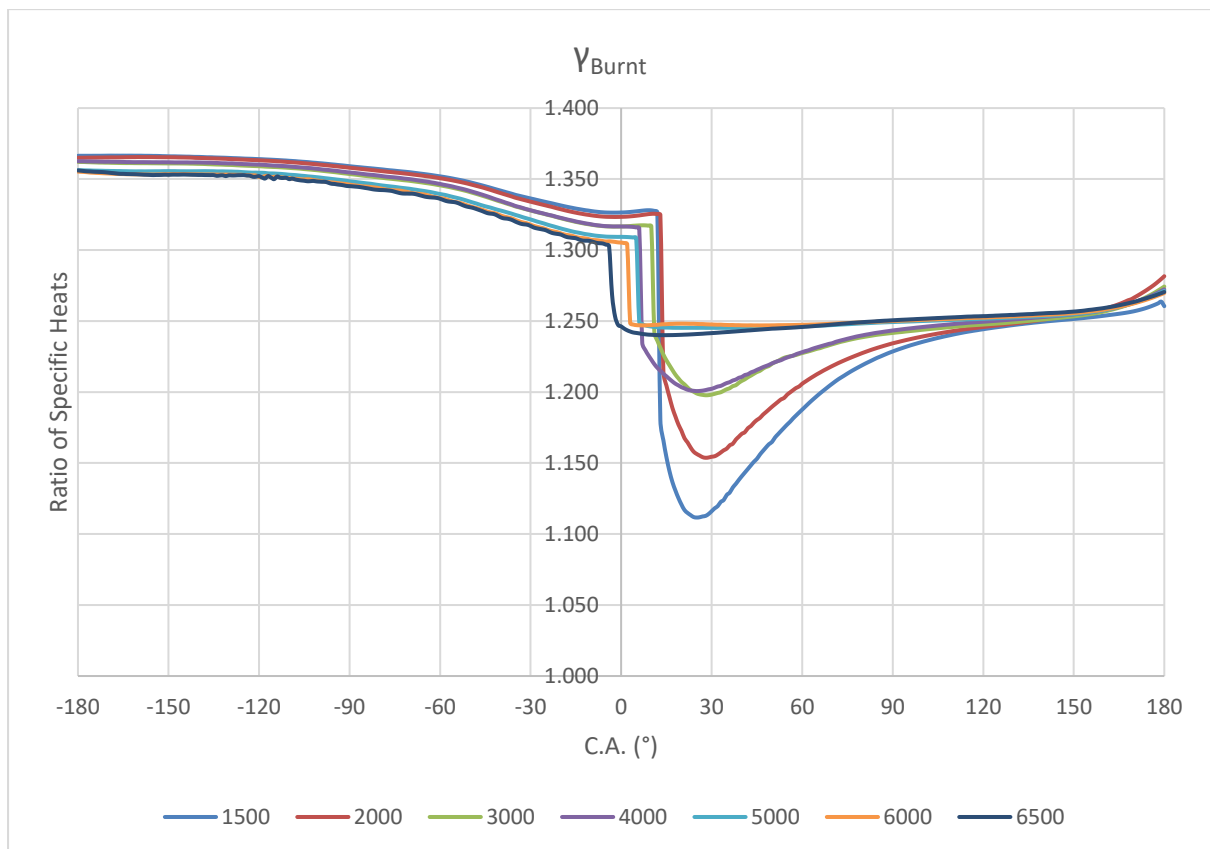


Figure 9-37: γ_{Burnt}

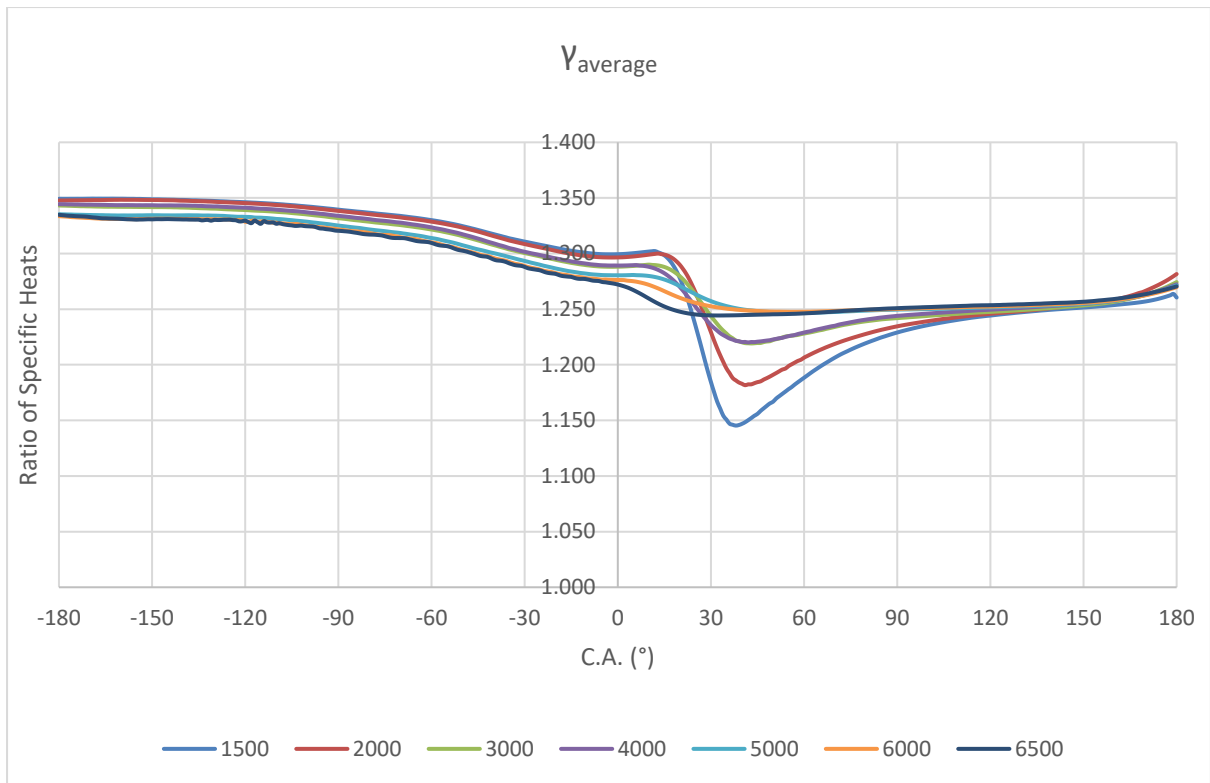


Figure 9-38: γ_{average}

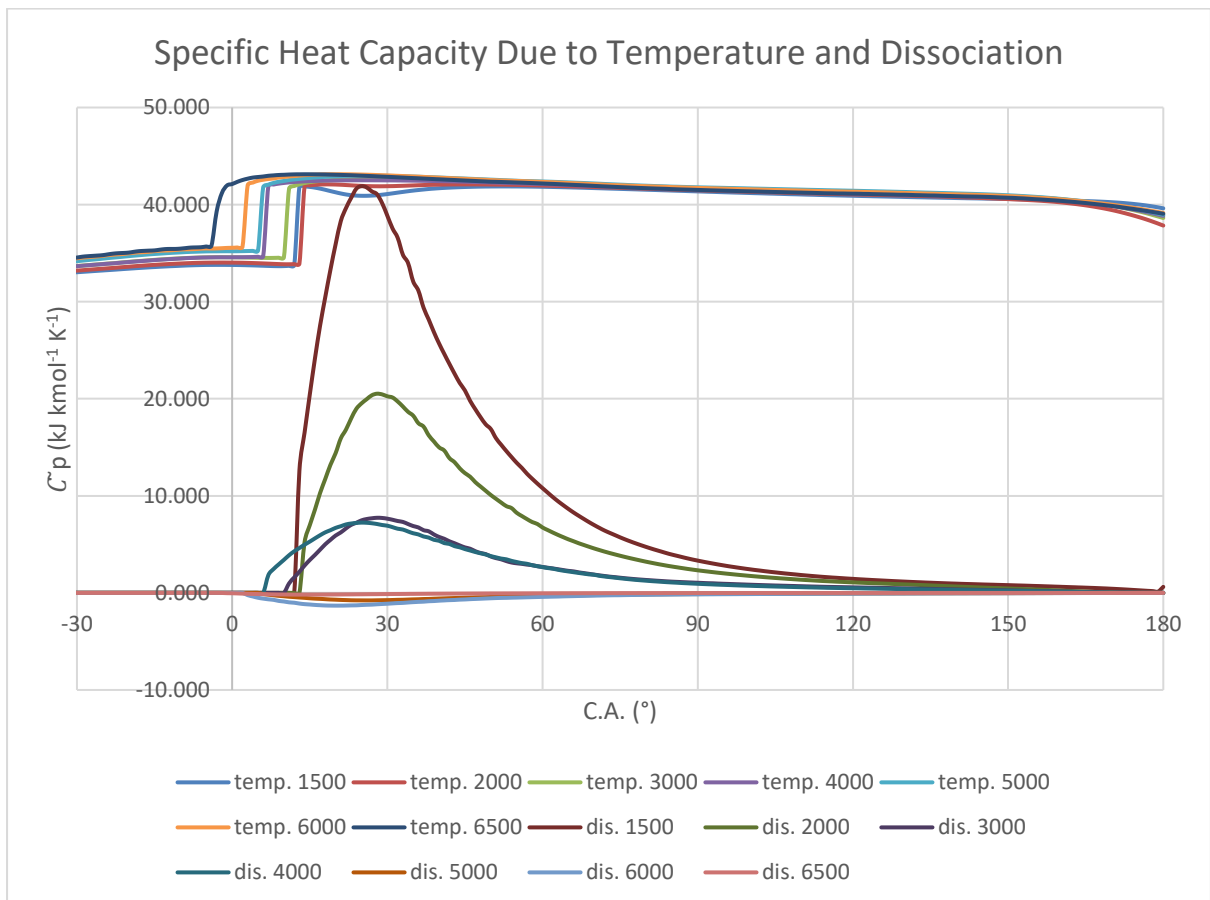


Figure 9-39: Specific Heat Capacity Due to Temperature and Dissociation

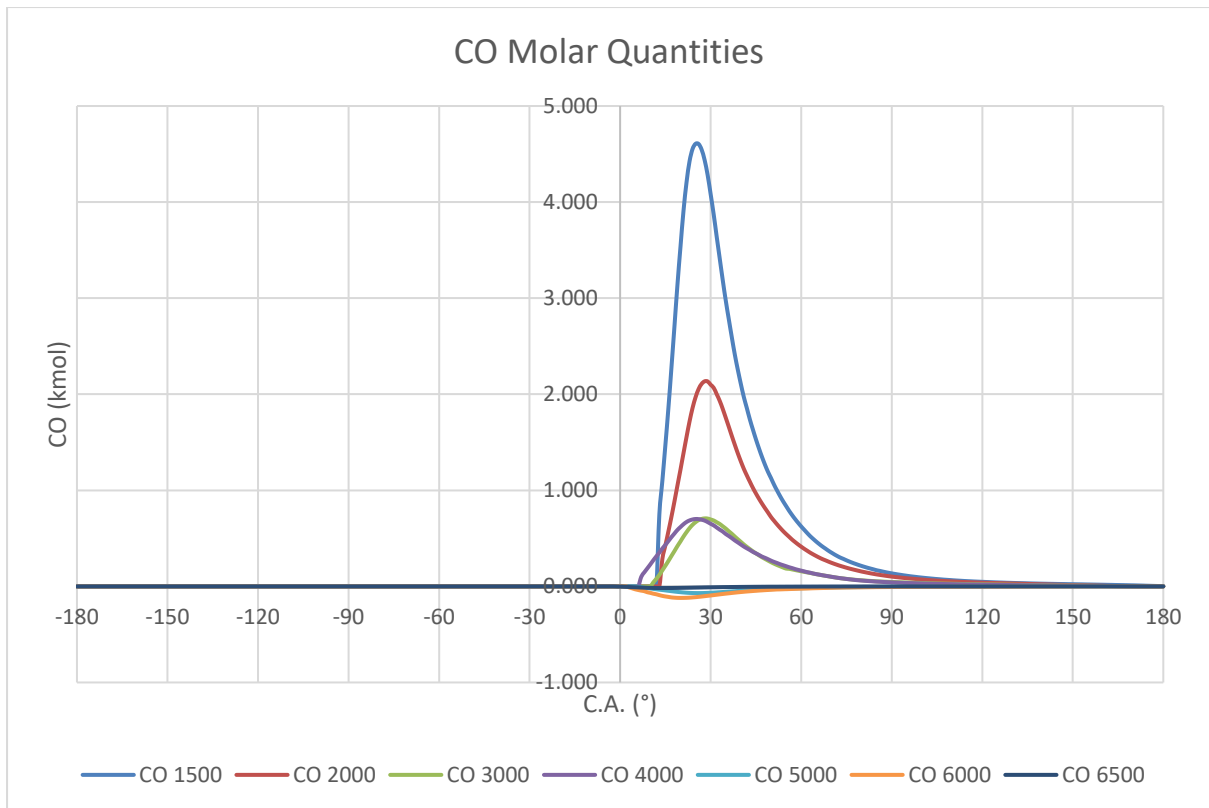


Figure 9-40: CO Molar Quantities

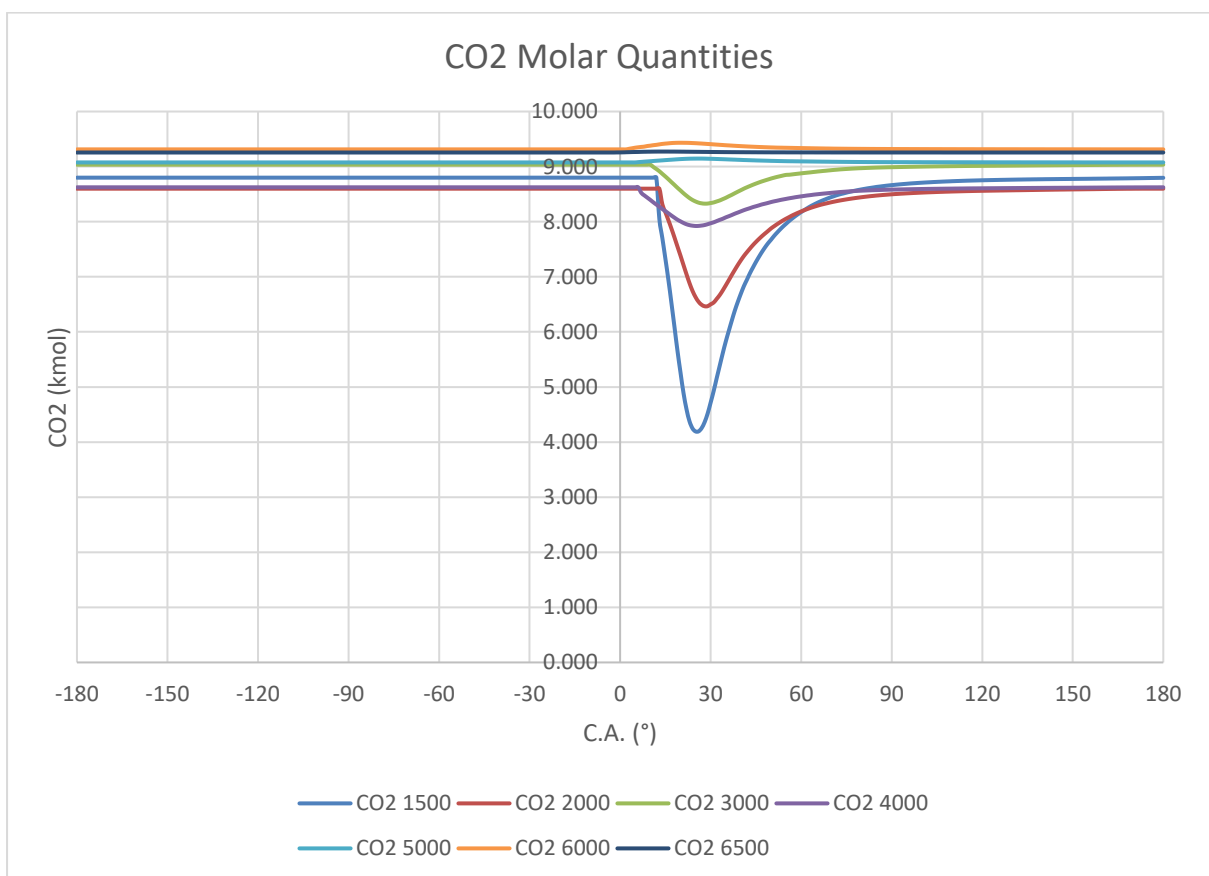


Figure 9-41: CO2 Molar Quantities

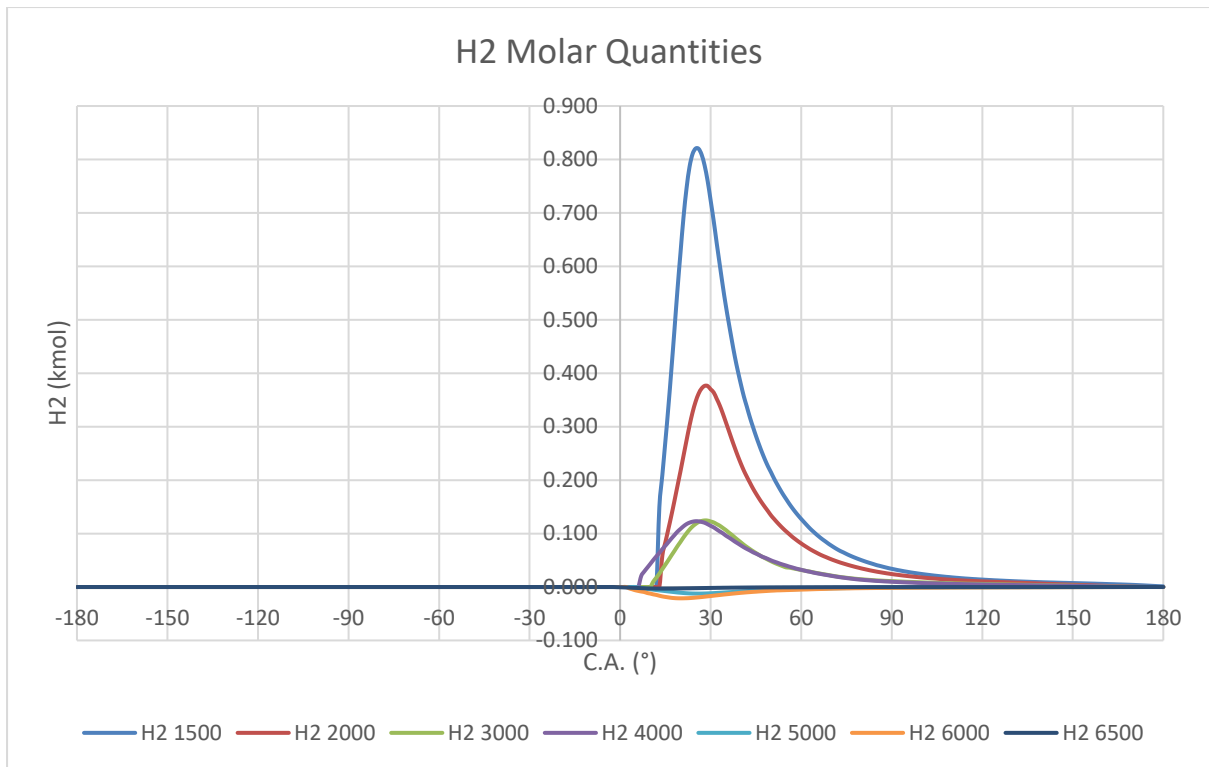


Figure 9-42: H₂ Molar Quantities

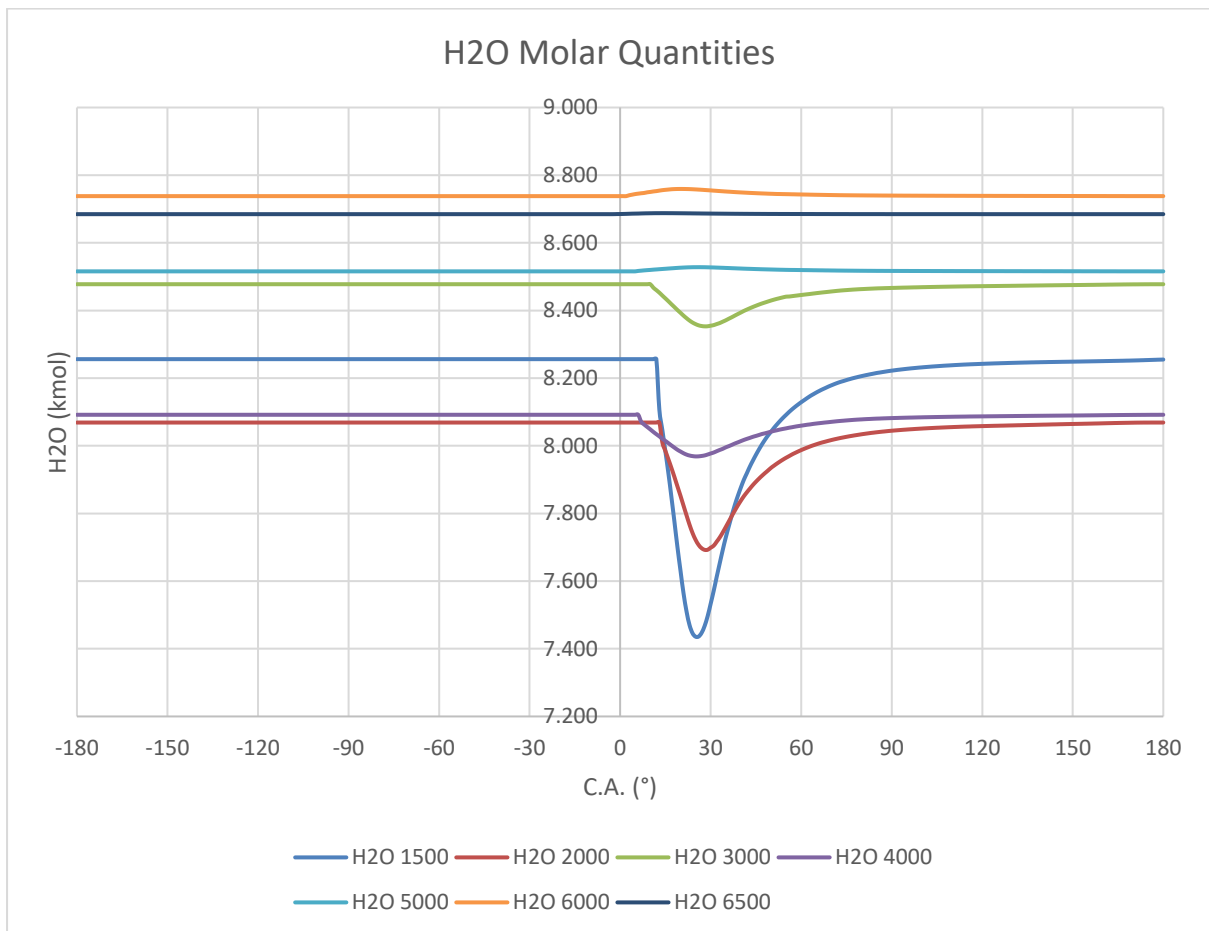


Figure 9-43: H₂O Molar Quantities

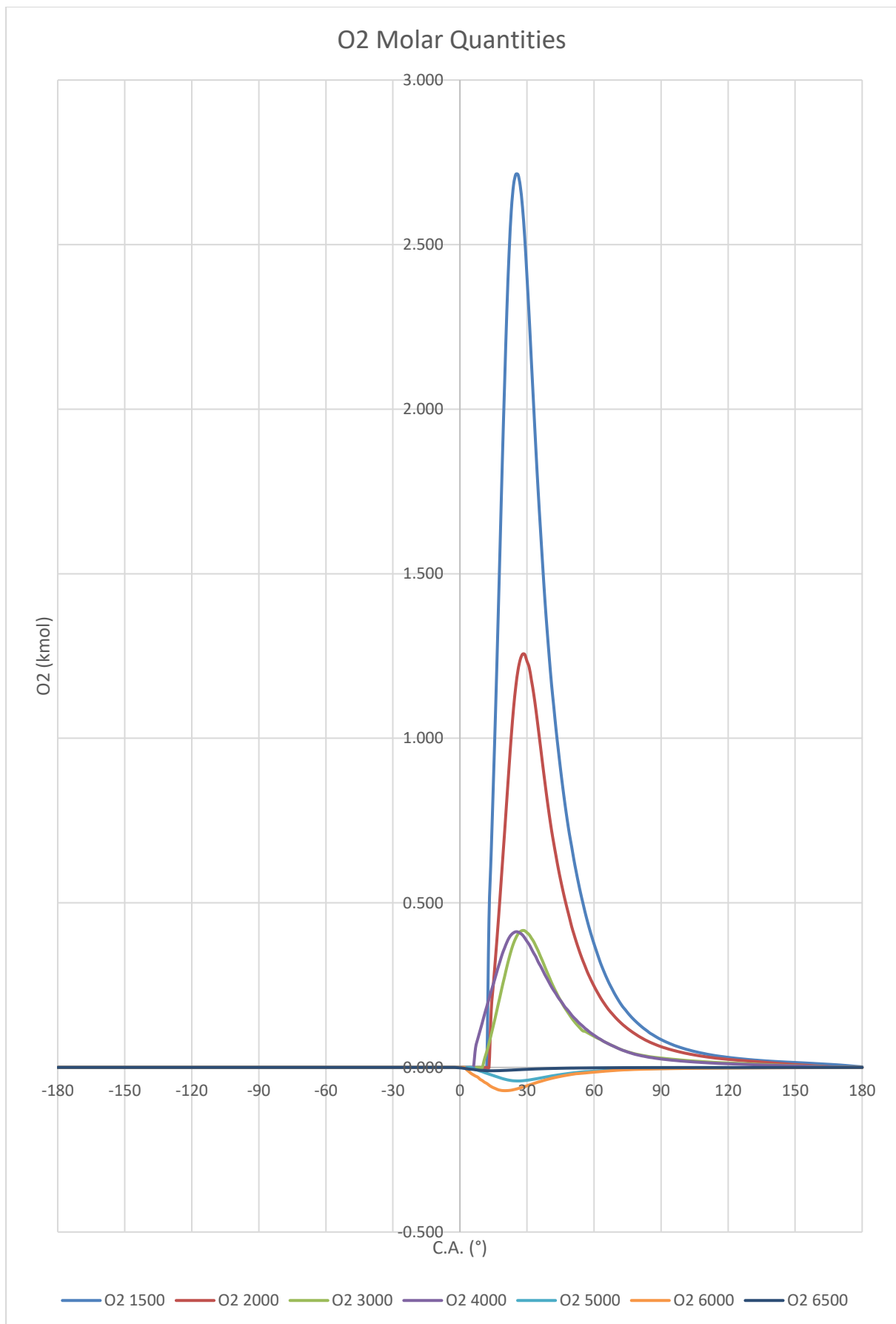


Figure 9-44: O₂ Molar Quantities

9.4 POLYTROPIC INDEX DURING COMBUSTION

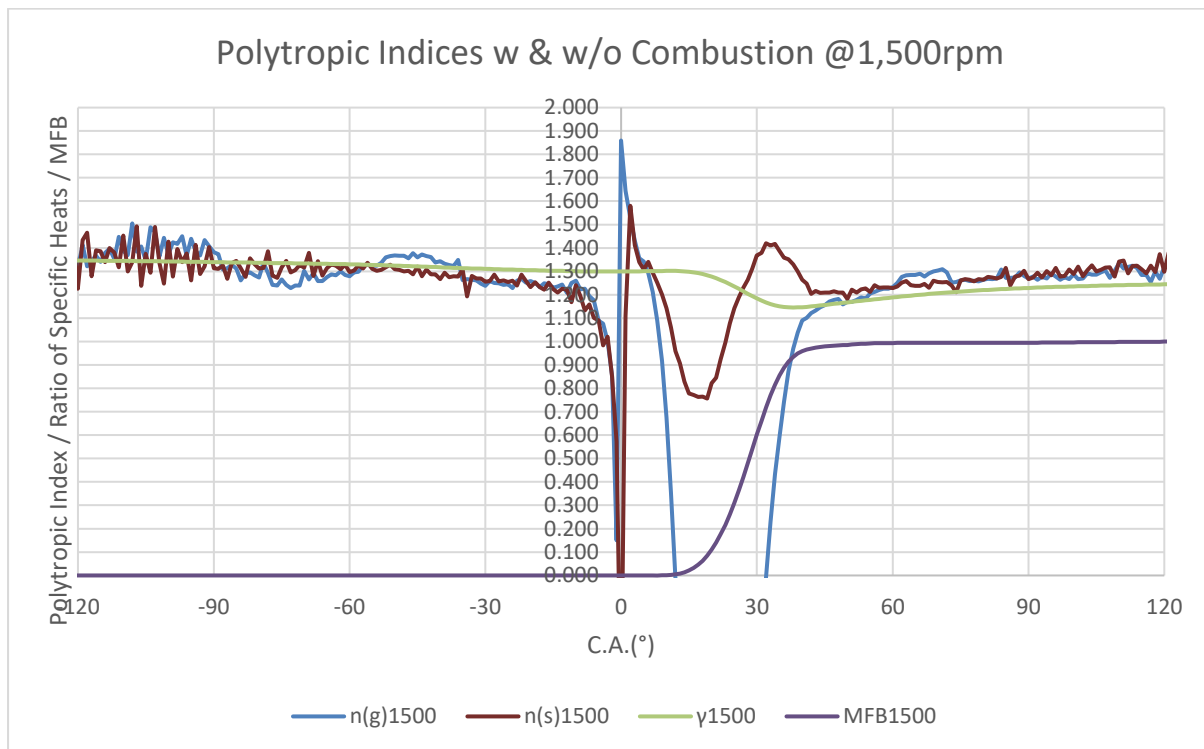


Figure 9-45: Polytropic Indices w & w/o Combustion @1,500rpm

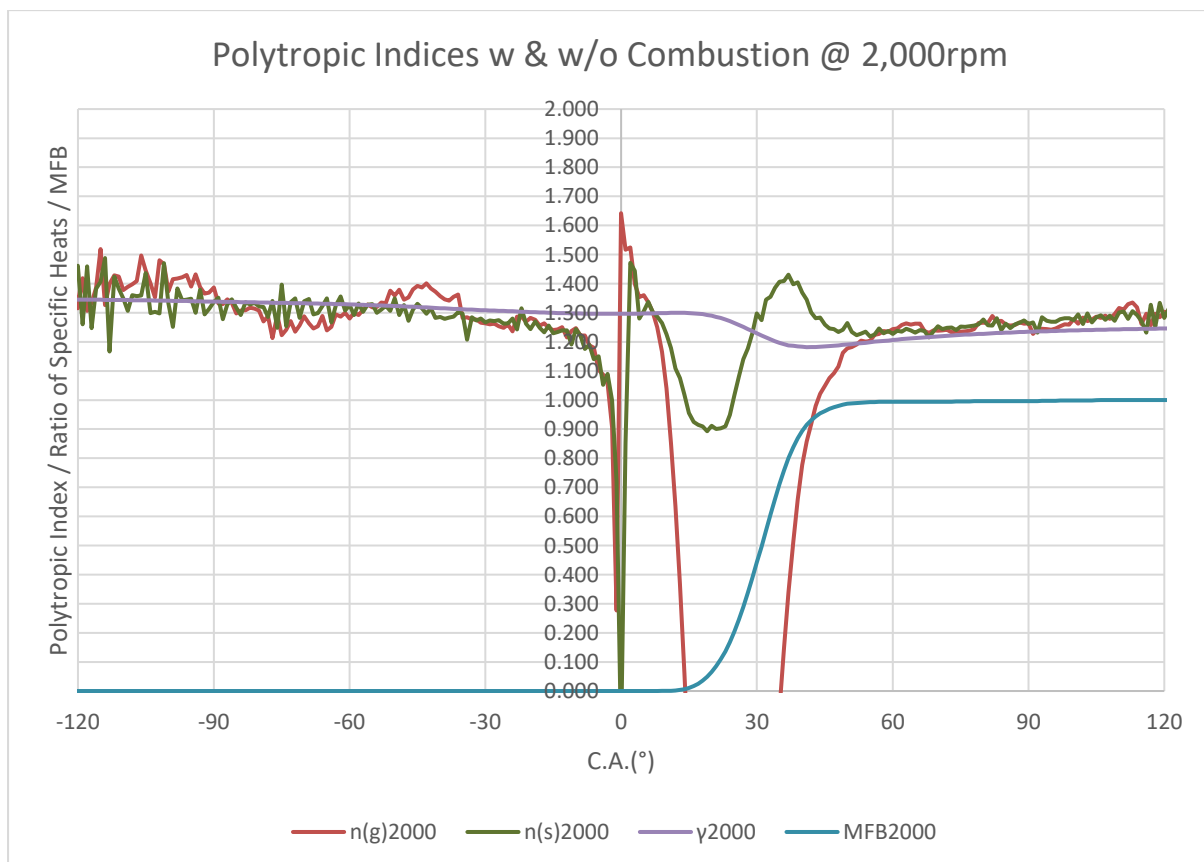


Figure 9-46: Polytropic Indices w & w/o Combustion @ 2,000rpm

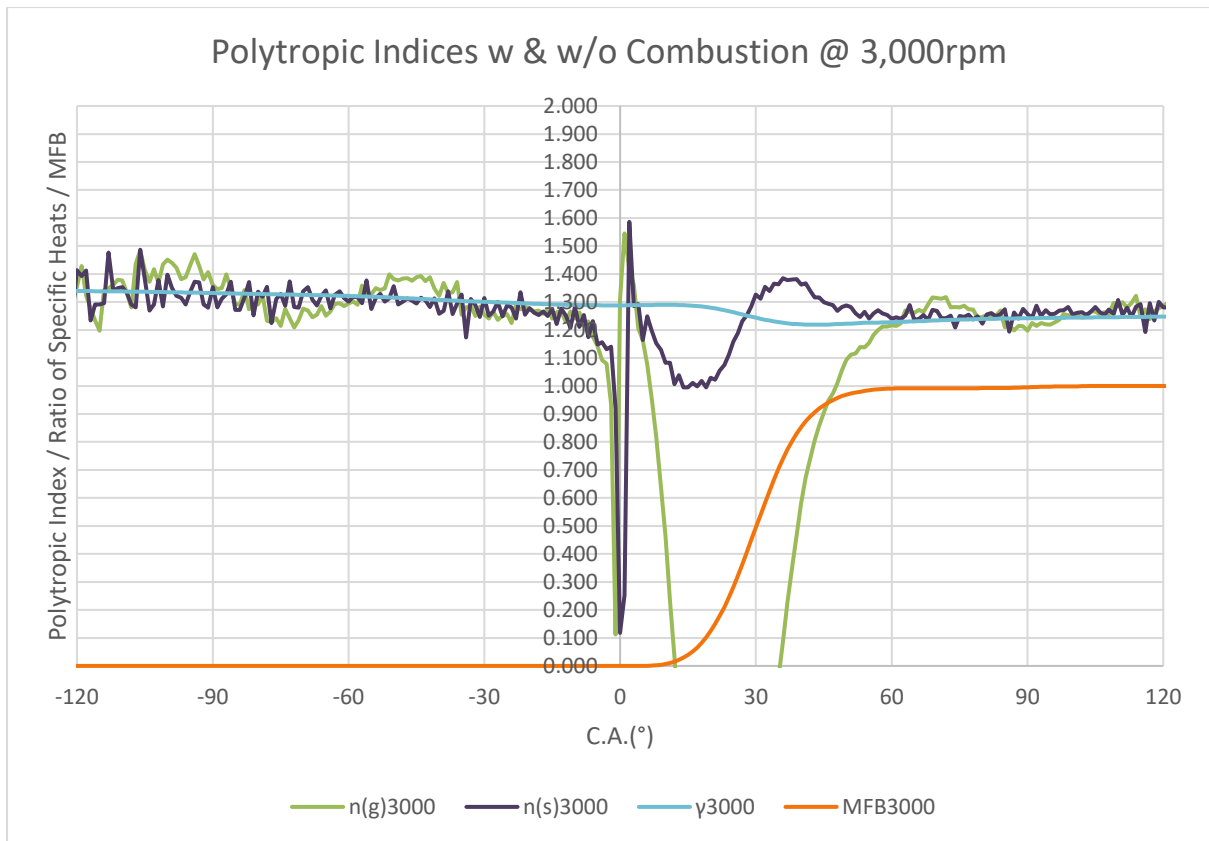


Figure 9-47: Polytropic Indices w & w/o Combustion @ 3,000rpm

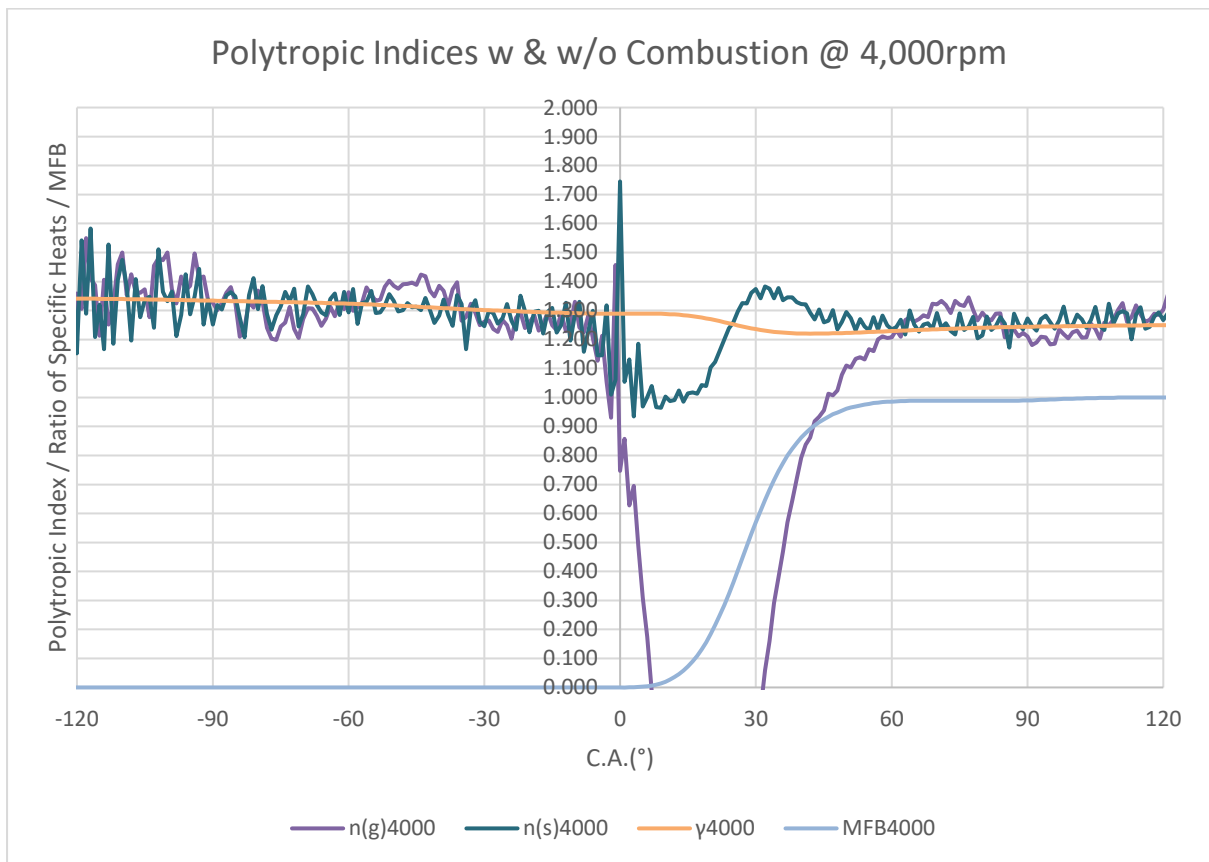


Figure 9-48: Polytropic Indices w & w/o Combustion @ 4,000rpm

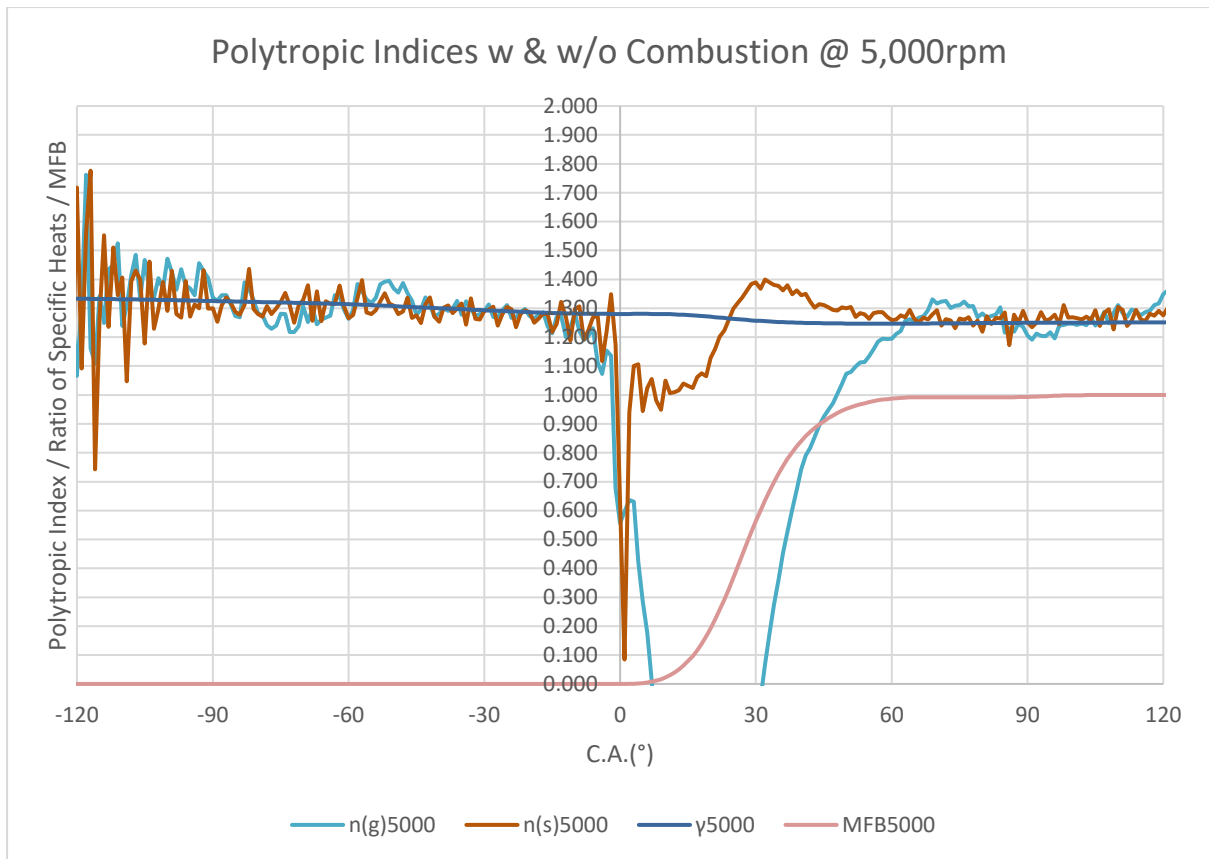


Figure 9-49: Polytropic Indices w & w/o Combustion @ 5,000rpm

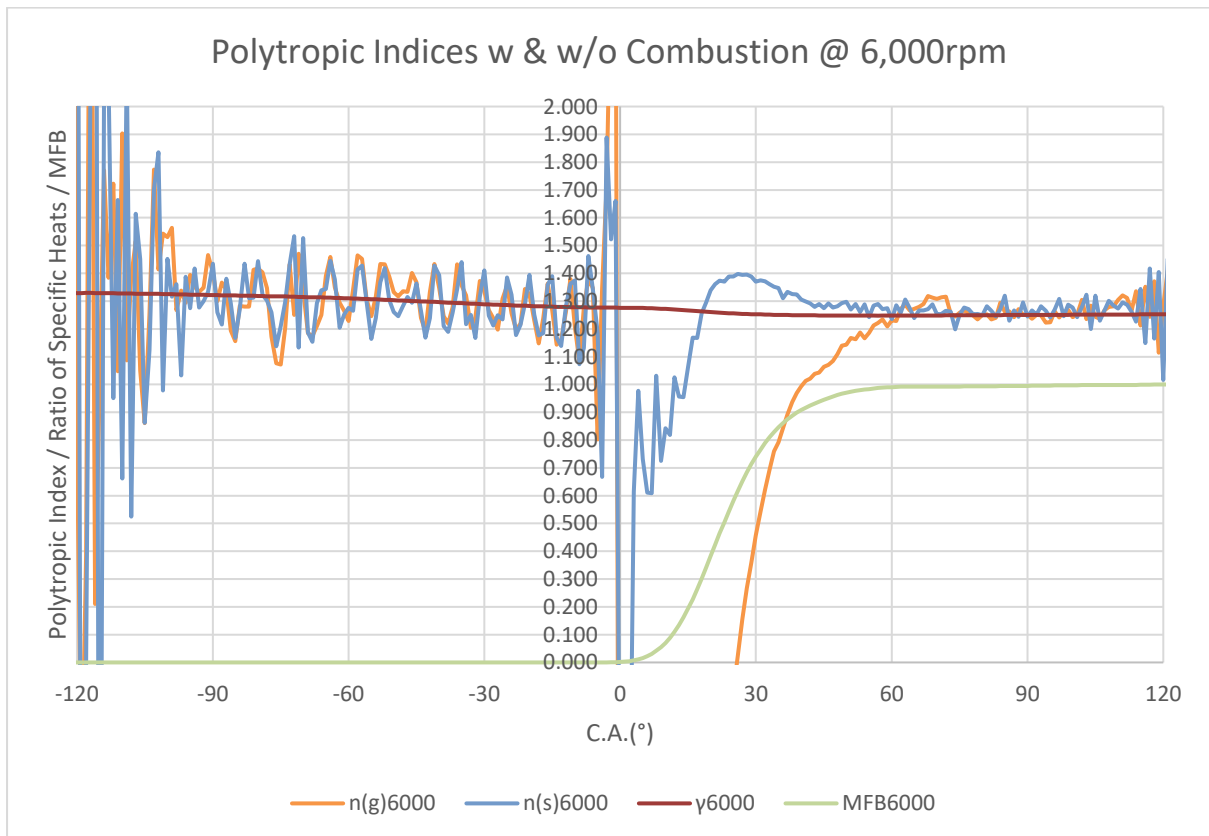


Figure 9-50: Polytropic Indices w & w/o Combustion @ 6,000rpm

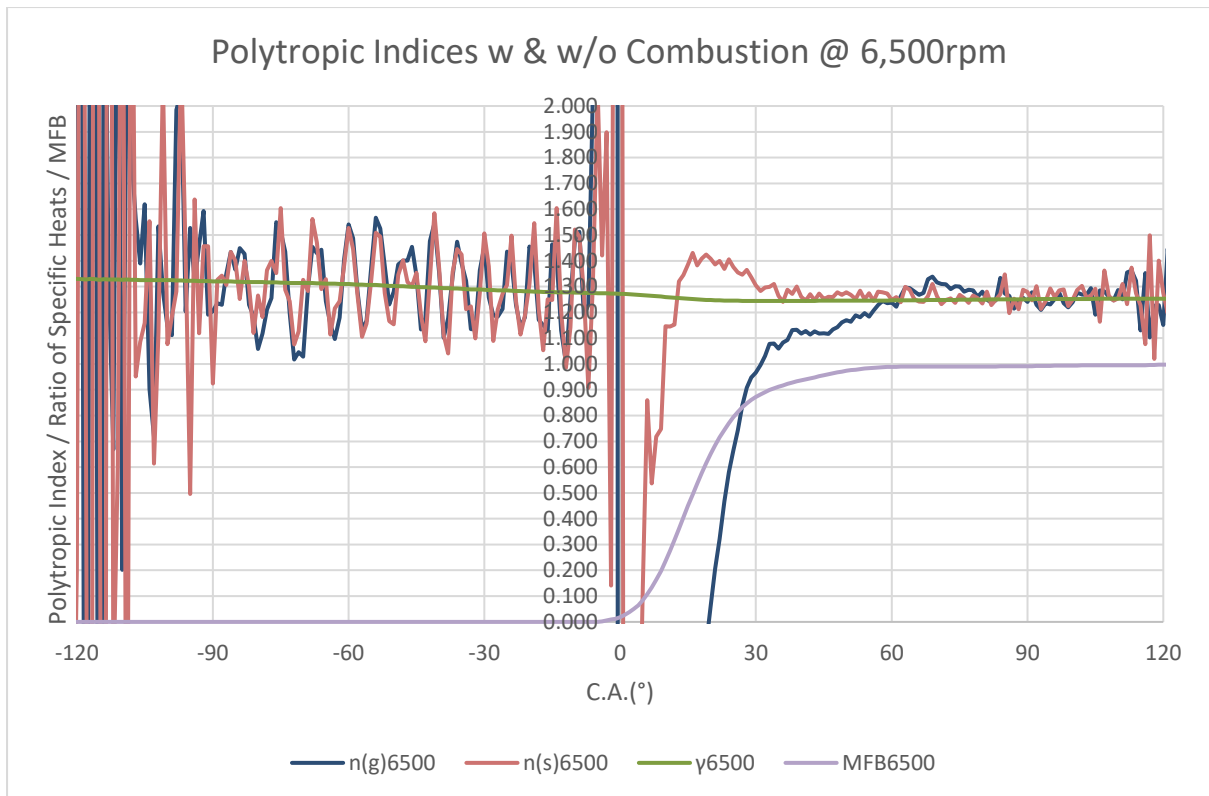


Figure 9-51: Polytropic Indices w & w/o Combustion @ 6,500rpm

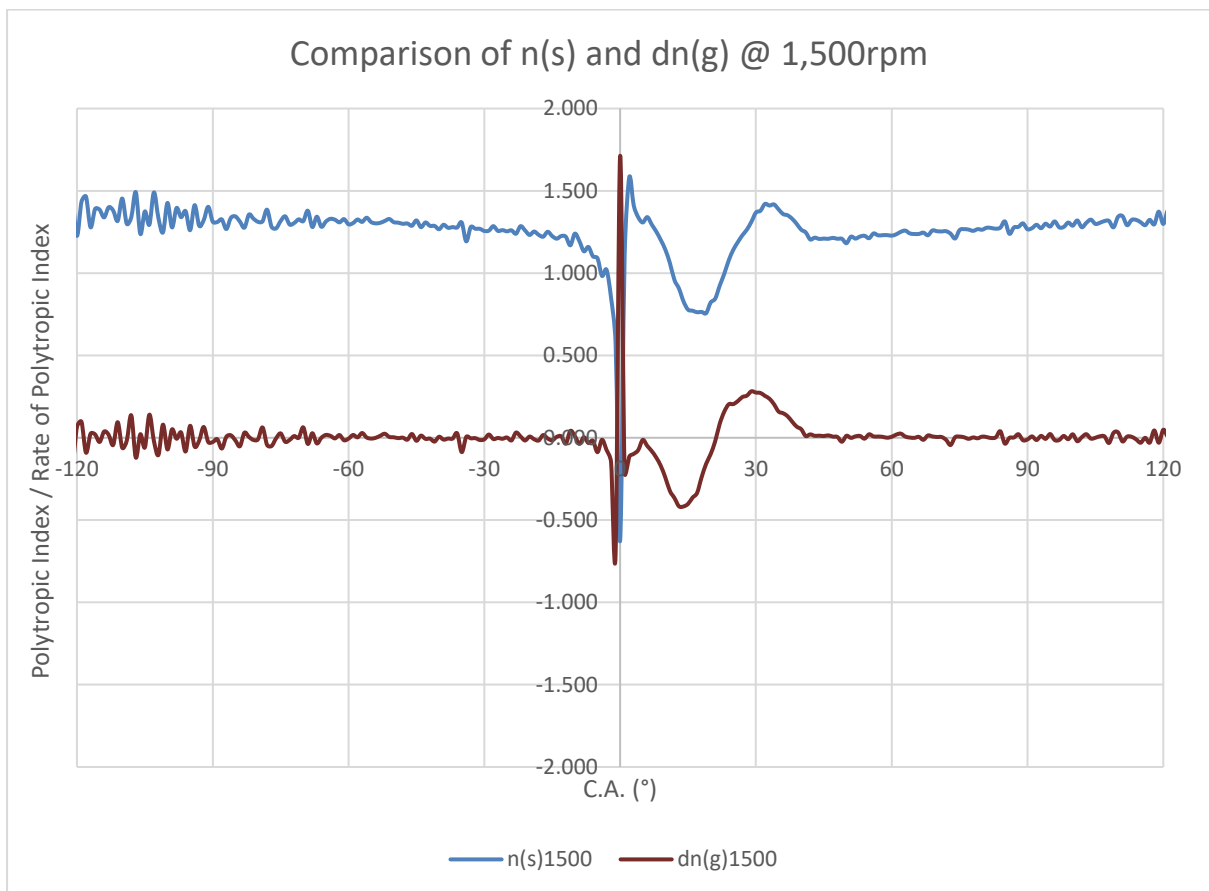


Figure 9-52: Comparison of $n(s)$ and $dn(g)$ @ 1,500rpm

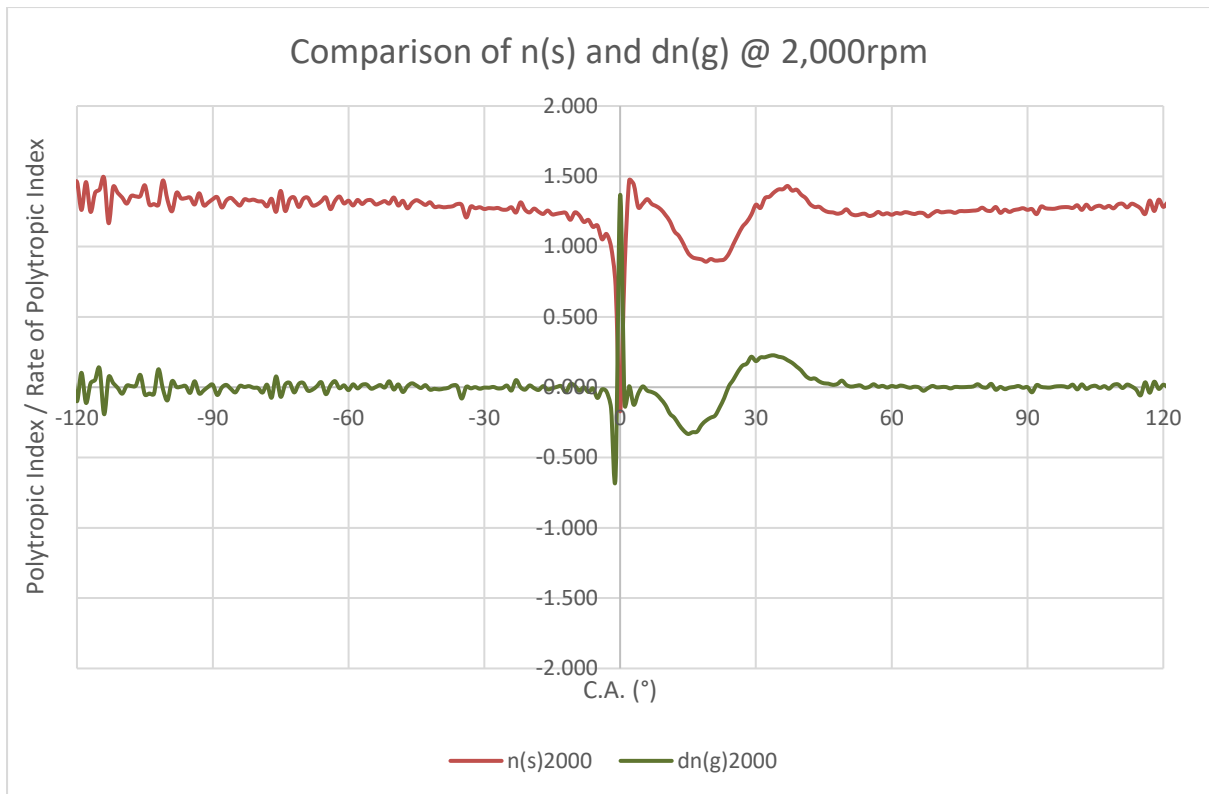


Figure 9-53: Comparison of $n(s)$ and $dn(g)$ @ 2,000rpm

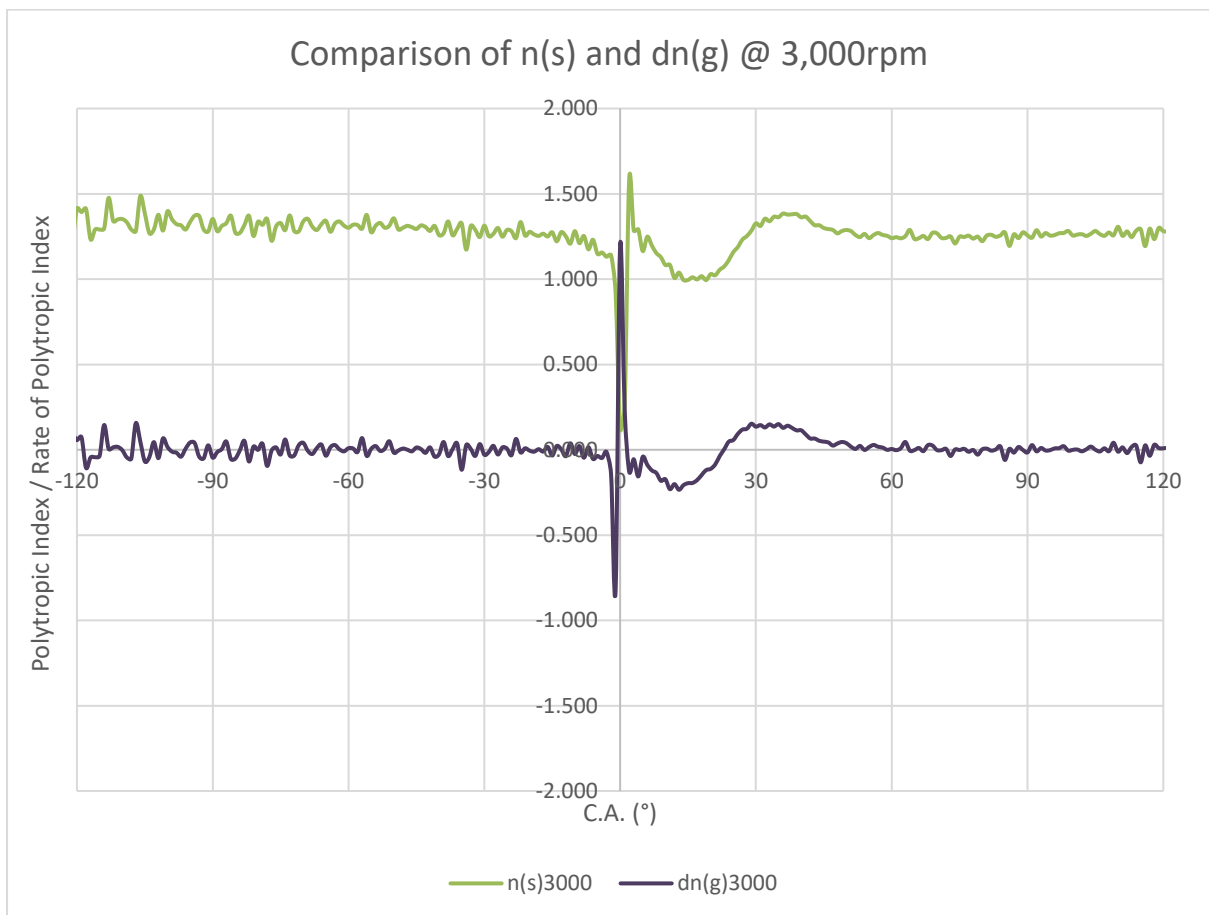


Figure 9-54: Comparison of $n(s)$ and $dn(g)$ @ 3,000rpm

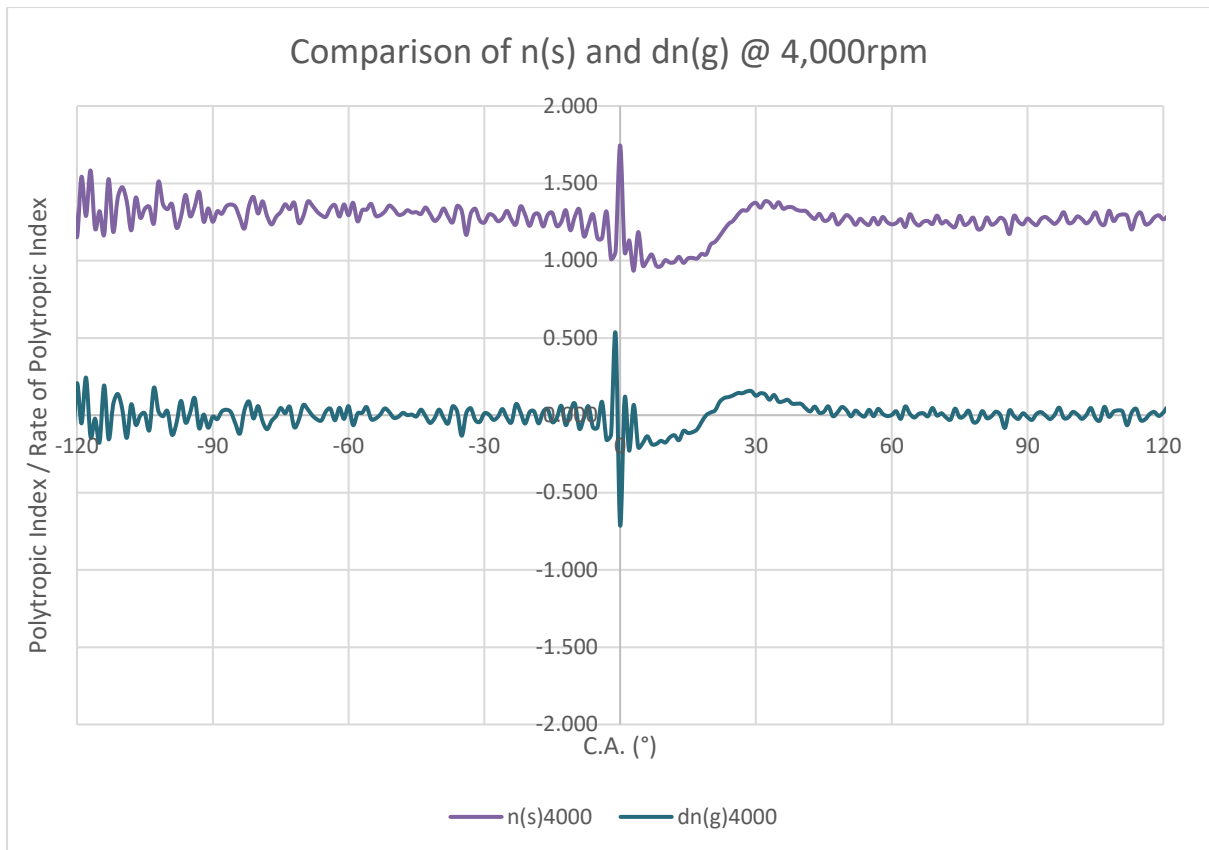


Figure 9-55: Comparison of $n(s)$ and $dn(g)$ @ 4,000rpm

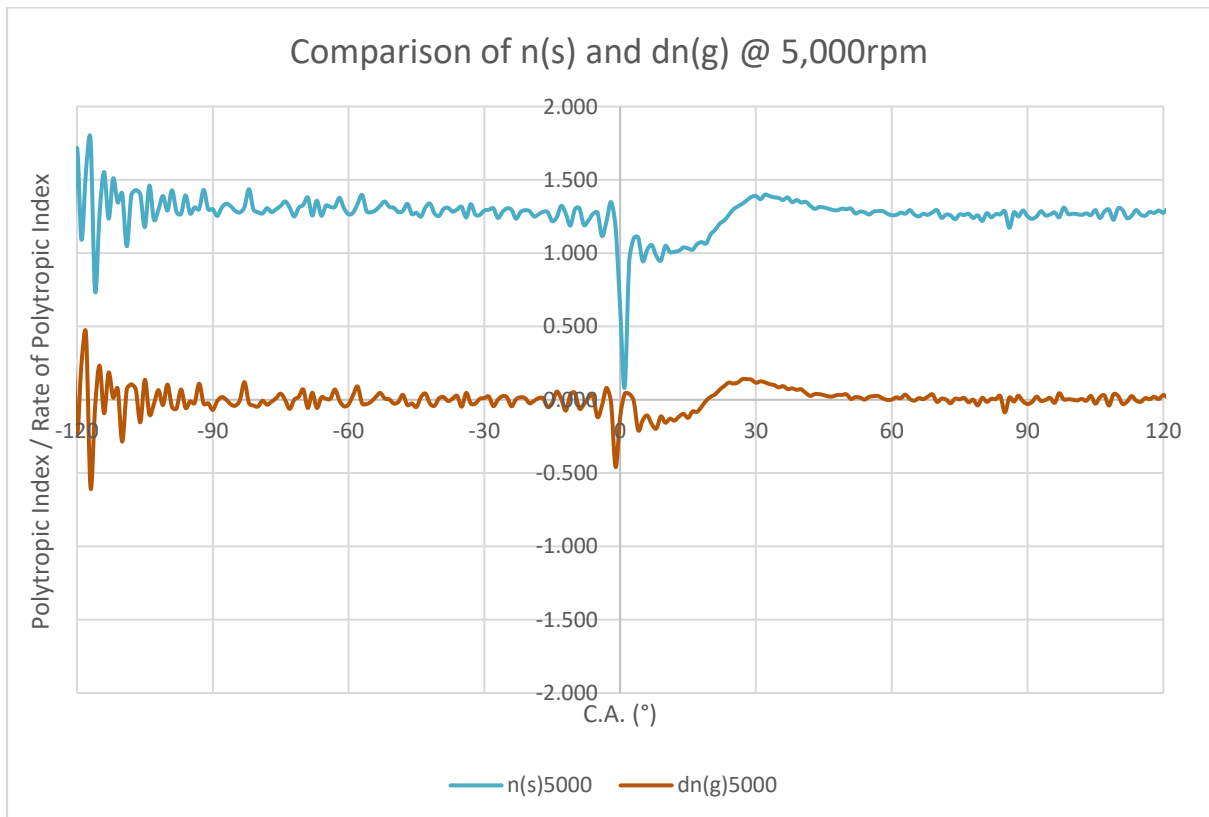


Figure 9-56: Comparison of $n(s)$ and $dn(g)$ @ 5,000rpm

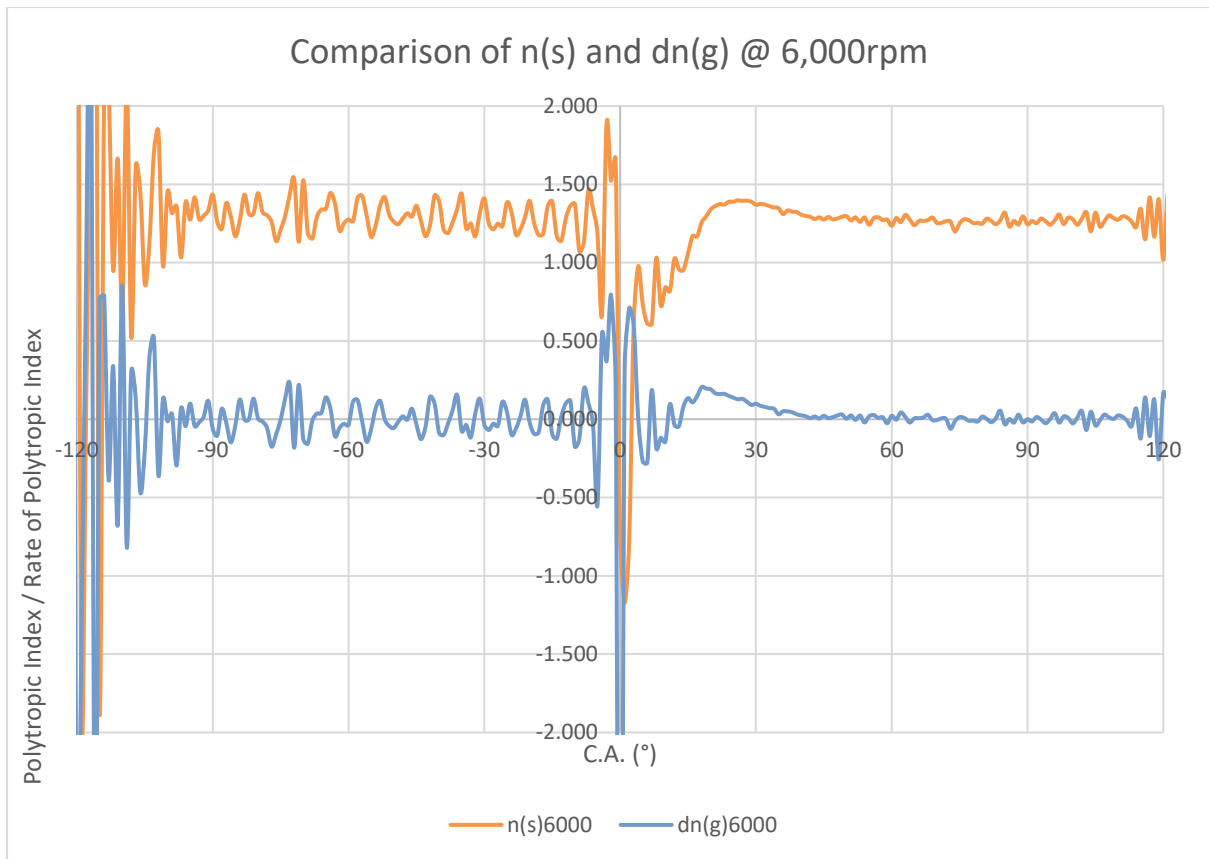


Figure 9-57: Comparison of $n(s)$ and $dn(g)$ @ 6,000rpm

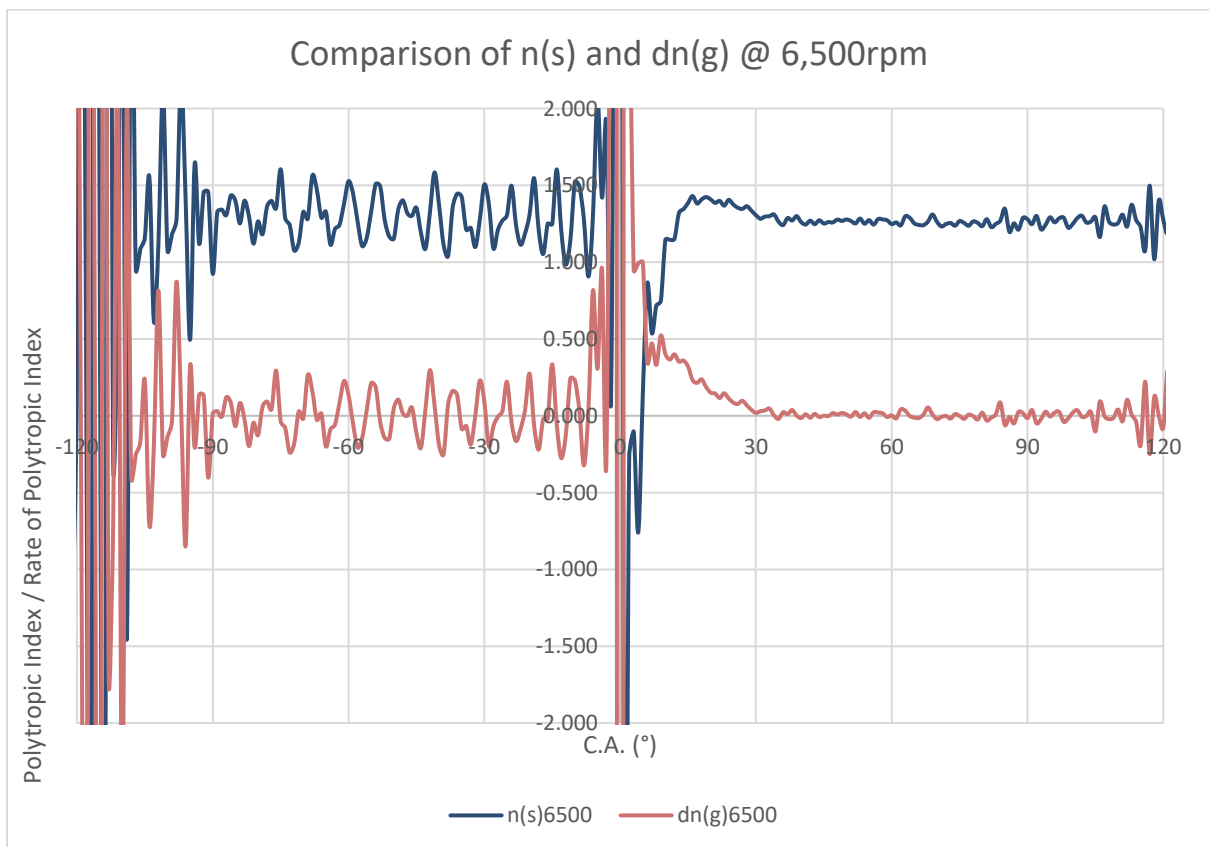


Figure 9-58: Comparison of $n(s)$ and $dn(g)$ @ 6,500rpm

9.5 GEOMETRICAL ACQUISITION

The positive volumes of the intake & exhaust ports as well as combustion chamber were silicone cast as shown in Figure 9-59, this was done since author had access only to a traditional surface optical scanner, as represented in Figure 9-60, which also shows that the surface measurements of the piston crown were acquired with the same method. Due to the optical nature of the scanner, a thin layer of dull-grey primer was applied to all surfaces, due to the opaque and reflective characteristics of the silicone casting and piston respectively. This however, which introduced a relatively small inaccuracy.



Figure 9-59: Single Piece Positive Volume Cast of Ports and Combustion Chamber of the Ford Fox GDI Engine



Figure 9-60: Piston Crown of the Ford Fox GTDI Engine in the Process of Surface Scanning

Author then used Geomagic For Solidworks software package to repair the resultant point cloud and turn it into surface meshes, from which solid CAD models were created. Author estimates this method's total tolerance to be in the ballpark of $\sim \pm 200\mu\text{m}$, although many variables such as primer layer thickness or the casting deformation due to gravity, are challenging to account for. Author believes the estimated tolerance to be accurate enough for its intended purpose.

Other components which had non-organic geometry (e.g. poppet valves and spark plug), were measured via vernier callipers and micrometres were appropriate. The measurements were then directly used to create CAD models using 'traditional' CAD drawing techniques, in Solidworks software package. However, due to the scale of the fuel injector nozzles shown in Figure 9-63, author had to use microscope in Figure 9-62, in order to take a picture shown in Figure 9-61. Due to the lack of equipment able to measure the injector nozzle diameter, author has resulted to utilising solid gauge shown on the left-hand side of Figure 9-63, in order to measure the nozzle chamber diameter to author's best ability. That measurement was then used in Figure 9-61 to interpolate the nozzle diameter. Author believes this method to be inaccurate, however, it was the best method available to the author.



Figure 9-63: Scale of the BOSCH Direct Fuel Injector Tip from Ford Fox GTDI Engine

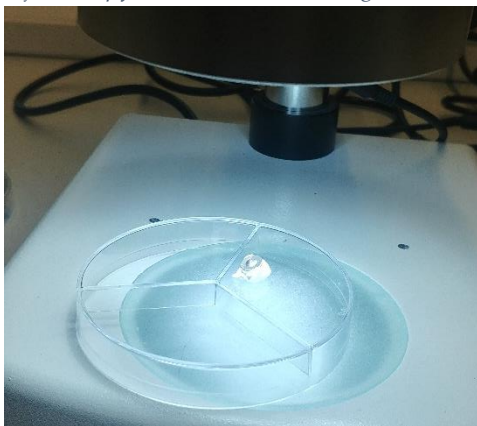


Figure 9-62: BOSCH Direct Fuel Injector Tip under Microscope

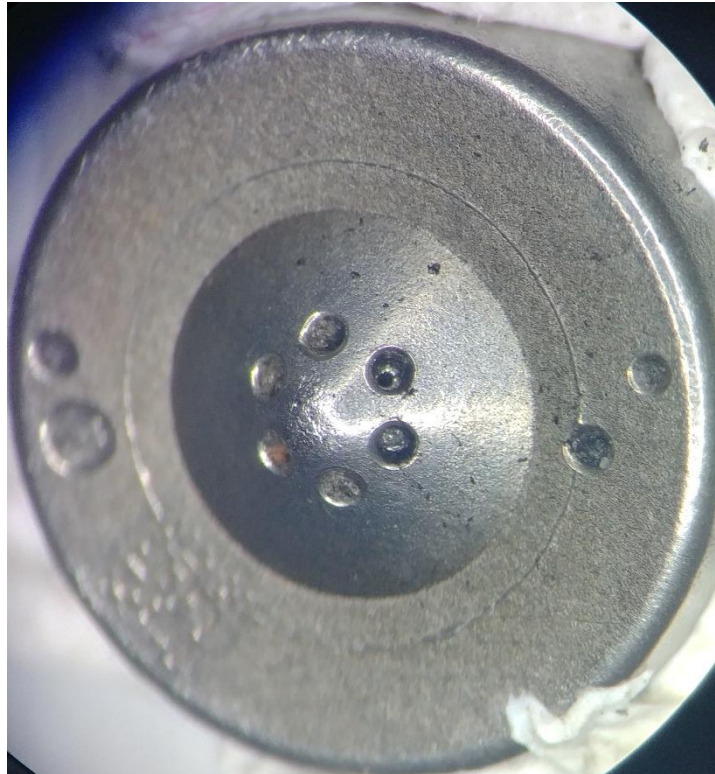


Figure 9-61: Microscope Picture of BOSCH Direct Fuel Injector Tip