Knock Limits in Spark Ignited Direct Injected Engines Using Gasoline/Ethanol Blends

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Submitted to the Department of Mechanical Engineering in Partial Fulfillment of the Requirements for the Degree of

DOCTOR OF PHILOSOPHY IN MECHANICAL ENGINEERING

AT THE

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

SEPTEMBER 2011

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Abstract

Direct Fuel Injection (DI) extends engine knock limits compared to Port Fuel Injection (PFI) by utilizing the in-cylinder charge cooling effect due to fuel evaporation. The use of gasoline/ethanol blends in DI is therefore especially advantageous due to the high heat of vaporization of ethanol. Additionally ethanol blends also display superior chemical resistance to auto-ignition, therefore allowing the further extension of knock limits.

An engine with both DI and port fuel injection (PFI) was used to obtain knock onset limits for five gasoline/ethanol blends and different intake air temperatures. Using PFI as a baseline, the amount the intake air needed to be heated in DI to knock at the same conditions as PFI is the effective charge cooling realized and ranges from ~14°C for gasoline to ~49°C for E85.

The Livengood-Wu auto-ignition integral in conjunction with the Douad-Eyzat time to auto-ignition correlation was used to predict knock onset. The pre-exponential factor in the correlation was varied to fit the experimental data. An “Effective Octane Number-ONES” is thus obtained for every blend ranging from 97 ONES for gasoline to 115 ONES for E85. ONES captures the chemistry effect on knock and shows that there is little antiknock benefit beyond 30-40% ethanol by volume unless the fuel is used in a DI engine.

Using this approach, the anti-knock benefit of charge cooling can also be quantified as an octane number. To achieve that, the ONES calculated for an actual DI operating point including charge cooling effects is compared to the ONES obtained from the auto-ignition integral if the unburned mixture temperature is offset to cancel the charge cooling out. The resulting increase in ONES, which can be viewed as an “Evaporative Octane Number” ranges from 5 ONES for gasoline to 18 ONES for E85.

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This thesis is dedicated to Sofia Theodoridou.
Acknowledgements

The pursuit of a doctoral degree can be a long, often quite lonely journey. Through my personal lonely journey to the doctoral degree, I was fortunate enough to receive support, help and guidance from several remarkable people.

I would like to thank Professor John B. Heywood for his guidance. We have had a great working relationship over the years. I have tried to learn and benefit from his amazing ability to steer research in interesting and useful directions and understand and present results in the most meaningful way.

I would also like to thank the members of my committee Professor William H. Green, Professor Ahmed F. Ghoniem and Professor Wai K. Cheng for their contribution and guidance. Many of the concepts presented in this thesis stemmed from discussions with the committee members.

I appreciate the help of Sloan Automotive Laboratory staff, Thane DeWitt, Raymond Phan, Janet Maslow, Karla Stryker and Leslie Regan from the Graduate Office in getting things done and taking care of day to day operations.

I am grateful to my fellow students in the Sloan Automotive Lab for the fruitful discussions and the help in the test cell. especially the other experimentalists: Jason Dimou, Ralf Hiller, Dongun Lee, Amir Maria, Vikram Mittal, Alex Sappok, R.J. Scaringe, Eric Senzer, Simon Watson. I am especially grateful to Kevin Cedrone and Craig Wildman. Kevin and Craig never seemed to be too tired or busy no matter how long it would take to give me a second point of view on my data or grab a wrench and help me get things up and running in the test cell.

During the course of this project I was lucky enough to work with a talented group of undergraduate students, Justin Negrete, Stefan Jannsen and Bjoern Hoepke who contributed significantly to the project.

This research was made possible through the sponsorship of the Fuel and Engines Consortium. I would like to thank the members Ford Motor Company, Volkswagen AG, Saudi Aramco and especially General Motors for their financial and technical support. I would like to specially thank Mr. Ron Herrin and Mr. Rick Davis for their leadership and support of the project, Mr. Henrik Nordin, Mr. Jason Pieper and Mr. Simon Schmuck-Soldan for their help with engine controls and Dr. Yangbing Zeng for his help with the CFD simulations.

Finally, more than anyone else, I would like to thank my parents, Panayioti and Vasiliki. Anything I ever achieved wouldn’t be possible without you.

This thesis is dedicated to my great love, Sofia Theodoridou for her love, patience, advice and for keeping me sane and going. With you beside me, I feel I can achieve anything._
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Nomenclature-Abbreviations

SI: Spark Ignited- Engines where combustion is initiated by a spark.
End Gas: The still unburned fuel air mixture in an internal combustion engine.
\( \eta_{fu} \): is the fuel indicated efficiency
\( r_c \): Engine compression ratio
\( \gamma \): Ratio of specific heats
MBT spark timing: Maximum Brake Torque spark timing
CAD: Crank angle Degree
BDC: Bottom Dead Center. An “a” or “b” prefix symbolizes before or after
TDC: Top Dead Center
\( f_{m,n,p} \): Combustion Chamber Resonant Frequency
\( \alpha_{m,n,p} \): is the wave number determined from the Bessel Equation
\( L_{m,n,p} \): is the relevant length scale for the resonant frequency formula
\( c \): is the speed of sound.
\([x]\): is the concentration of substance x in moles/m\(^3\),
\( A \): is the pre-exponential factor, \( E_A \) the activation energy of the reaction,
\( R \): the universal gas constant,
\( m, n \): the order of a reaction with reactants A,B with respect to A and B
ON: Octane Number
RON: Research Octane Number
MON: Motor Octane Number
CFR: Cooperative Fuel Research Engine- A standardized engine for ON tests
PFI: Port Fuel Injection
DI: Direct Injection
E"X"-e.g. E20: A gasoline ethanol blend that is “x” % ethanol by volume. E20 is 20% ethanol.
LHV: Lower Heating Value
\( h_{lv} \): Heat of Vaporization
\( A/F_{stoich} \): Stoichiometric Air to Fuel Mass Ratio.
\( m_{fuel} \): Mass of Fuel
\( m_{air} \): Mass of Air
\( c_p \): Constant Pressure heat capacity.
\( T_u \): is the unburned mixture temperature without charge cooling,
\( K \): is the polytropic coefficient
\( m_{air} \): is the airflow rate
\( \rho_{intake} \): the charge density at the intake,
\( V_d \): the engine displacement volume
\( N \): rotational frequency in rev/s.
RPM: Rounds per minute
M: Molecular Weight
IVC: Intake Valve Close
IVO: Intake Valve Open
EVC: Exhaust Valve Close
EVO: Exhaust Valve Open
CFD: Computational Fluid Dynamics
**Base Boost:** Engine Load Conditions when the throttle is wide and the turbocharger waste gate bypassing as much flow as possible-around 1.3-1.4 bar MAP.
MAP: Manifold Air Pressure
ECU: Engine Control Unit
PWM: Pulse Width Modulated
MEP: Mean Effective Pressure
λ: fuel to air ratio over stoichiometric fuel to air ratio
V_u: The volume occupied by the unburned gas
V_b: The volume occupied by the burned gas
x_b: Mass fraction burned
SOC: Start of combustion
EOC: End of combustion
MEP: Net Mean Effective Pressure
COV: Coefficient of variance — standard deviation normalized by mean.
SOI: Start of (fuel) injection
KI: Knock Intensity— the (single-sided) amplitude of the high pass filtered pressure trace.
kf: knocking fraction
KLSA: Knock limited Spark Advance
K : Fuel sensitivity equal to RON-MON
RCM: Rapid Compression Machine
τ: Ignition Delay if referring to an RCM or a Diesel engine, time to auto-ignition for knock in a spark ignited engine
t_c : critical time of auto ignition, upper limit of auto-ignition integral
ONEFF : Effective Octane Number
θ: Position in crank angle degrees
k: The polytropic coefficient obtained from the P-V diagram
ONEVAP: Evaporative Octane Number
ONTOTAL: Total Octane Number
1. Introduction

1.1 Background-Motivation.

1.1.1 Engine Knock.

Engine knock is an abnormal combustion phenomenon that occurs in spark ignited (SI) engines. In an SI engine, after the fuel-air mixture has entered the cylinder during intake, it is compressed during the compression stroke until combustion is initiated by a spark. A flame front subsequently propagates outwards consuming the unburned mixture on the outside of the flame (called "end gas"), releasing heat and increasing the mixture (burned and unburned) pressure. As the end gas pressure and temperature rises due to the compression caused by this process, auto-ignition of the fuel might occur in certain spots. The auto-ignition spots interact with the flame front in a complicated way creating pressure oscillations which could potentially cause significant hardware damage to the engine. The sequence of events leading to engine knock is shown schematically in Figure 1-1 and using images from a high speed in-cylinder video obtained from a knocking engine in Figure 1-2. A good background reference for knock is [1].

![Sequence of Events Leading to Knock](image-url)
Anteignition Region:

Figure 1-2: Images from a high speed video of a knocking engine cycle from [3]. The video recorded the light emission from the high temperature burned gases, and the intensity increases with increasing gas temperature. Auto-ignition occurs in Frame 2.

Because of the potentially damaging pressure oscillations caused by engine knock, it has always been and still is the most important limitation on improving SI engine efficiency. This is the case because avoiding knock for a given fuel quality is usually achieved by compromising one or more of the following engine parameters:

- **Engine Compression Ratio.** Increasing compression ratio, increases engine efficiency as indicated by a simple ideal gas Otto Cycle analysis:

  \[ \eta_{f,i} = 1 - \frac{1}{r_c^{\gamma-1}} \]  

  Where \( \eta_{f,i} \) is the fuel indicated efficiency, \( r_c \) the engine compression ratio and \( \gamma \) is the ratio of specific heats. However, higher compression ratios also increase in-cylinder peak pressures and temperatures causing knock. The compression ratio of SI engines using gasoline is therefore limited to 8-12:1 for modern automotive engines.

- **Spark Timing:** For a given engine and fuel, at every operating point, there is an optimum spark timing which results in Maximum Brake Torque
(hence its name-MBT spark timing) and lowest specific fuel consumption (highest efficiency). Because of engine knock, spark timing often needs to be retarded from optimum. The engine as a result suffers an efficiency penalty. Retarded spark timing alleviates knock because earlier spark results in higher peak pressures and temperature that cause knock.

> **Turbocharging.** Turbocharging combined with downsizing to keep engine power constant is a relatively easy way to improve engine efficiency. This is because throttling losses are reduced and friction losses roughly scale with cylinder surface while power scales with volume. With turbo charging, the engine essentially produces more power out of the same volume, efficiency therefore rises. However, turbo charging also increases peak in-cylinder pressures making the engine more prone to knock. The compression ratio of turbo charged production engines is therefore usually reduced by 1-2 compared to naturally aspirated engines. The fuel efficiency benefit of turbocharging is thus partially offset by the reduced compression ratio.

An example of the potentially catastrophic pressure oscillations caused by knock can be seen in Figure 1-3. An in-cylinder pressure trace is plotted vs. Crank Angle Degree (CAD) after Bottom Dead Center (aBDC). Draper [4] managed to relate these oscillations to the resonant vibration modes of the combustion chamber which he calculated and measured. The frequencies of the resonant modes are given by the solution to the wave differential equation:

\[ f_{m,n,p} = \alpha_{m,n,p} \frac{c}{\pi L_{m,n,p}} \]  

(2)

where \( \alpha_{m,n,p} \) is the wave number determined from the Bessel Equation and \( L_{m,n,p} \) is the relevant length scale, \( c \) is the speed of sound.

The first mode that gets excited is the first circumferential mode which corresponds to \( L_{m,n,p} \) being the cylinder bore. For a typical automotive engine bore size of 80-90 mm, this first resonant frequency is around 6 kHz. This resonant frequency creates the typical “pinging” sound associated with knock. There are several different options for the second resonance that gets excited depending on the shape of the combustion chamber and where the pressure transducer recording the signal is located, but generally it is somewhere between 9-15 kHz.

Engine knock is the result of an auto-ignition process which needs to be completed before the flame consumes the end gas. As a result, the fundamental variables that determine if knock occurs in an engine are:

> **Unburned Mixture Temperature and Pressure.** Auto-ignition is the result of a chemical reaction. This overall reaction can be broken down to
elementary reactions, all of which follow an Arrhenius law. For the single step reaction:

\[ \text{A} + \text{B} \rightarrow \text{C} \]

The reaction rate is:

\[ \frac{d[C]}{dt} = \exp\left(\frac{-E_A}{RT}\right) \text{[A]}^m \text{[B]}^n \] (3)

Where: \([x]\) is the concentration of substance \(x\) in moles/m\(^3\), \(A\) is the pre-exponential factor, \(E_A\) the activation energy of the reaction, \(R\) the universal gas constant, \(m\) and \(n\) the order of the reaction with respect to \(A\) and \(B\) respectively. It is obvious from Eq. 3 that the rate of the auto-ignition reaction depends on the temperature of the end gas. It also depends on the end gas pressure because that affects the concentration terms. In an engine, the pressure and temperature of the end gas are not constant, they increase as the compression first and the combustion process later progresses.

- **Time available for auto-ignition**: In order for knock to occur, auto ignition needs to take place before the flame consumes the end gas. The available time is therefore determined by engine speed, combustion speed and ignition timing.

The quality of a fuel to resist auto-ignition and thus knock is measured by its octane number (ON). The ON is essentially a comparison in terms of anti-knock performance of the fuel to a mixture of n-heptane (poor anti-knock performance) and 2,2,4-trimethylpentane (iso-octane- good anti-knock performance). The test is performed in a standardized engine with variable compression ratio (CFR engine). For example, gasoline with the same knocking characteristics as a mixture of 90% iso-octane and 10% heptane by volume would have an octane rating of 90. There are two standardized versions of the test and thus of the octane ratings: The Research Octane Number (RON) and the Motor Octane...
Number (MON). The two tests are conducted under significantly different engine conditions. RON is found to reflect modern engine knock conditions better [2, 5,6,7,8]

1.1.2 Fuel Direct Injection.
The automotive industry has been moving from traditional port fuel injection (PFI) towards direct fuel injection (DI) in SI engines. The difference between the two is that in PFI the fuel is sprayed in the intake port against the (closed at the time) hot intake valve whereas in DI the fuel is sprayed directly inside the cylinder. An animation of the two fuel injection types is presented in Figure 1-4. Direct Fuel Injection has a couple of advantages over PFI. Namely:

- **Charge Cooling:** The heat of vaporization of the fuel can be extracted in DI engines from the charge instead of the walls, thus cooling it. This effect improves engine breathing/volumetric efficiency and thus power output compared to PFI. More importantly however, this “charge cooling” effect can be used to extend knock onset limits and thus improve efficiency by allowing higher compression ratios, boost pressures and optimized spark timing. Understanding this phenomenon better is one of the main focus points of this thesis.
- **Better mixture preparation:** Spraying the fuel directly in cylinder leads to improved transient response and reduction of over-fueling in cold start.
- **Lean/Stratified Operation:** Direct in cylinder injection can be used to create a close to stoichiometric mixture locally, while the overall mixture is lean without any flammability problems. This strategy is beneficial for efficiency because of the increased gamma due to enleanment and also because of reduced throttling at low loads. The issue with going lean is that three way catalysts can’t work efficiently any more. Although this concept has been applied successfully in other markets, U.S. stricter NOx emission standards would require the use of prohibitively expensive reductive exhaust after treatment systems. For this reason, the focus of this thesis is exclusively homogeneous, stoichiometric DI engine concepts.

The challenge for DI engines is making sure fuel evaporation takes place on time and there is adequate time for mixing so that the fuel doesn’t hit the walls or the piston and the mixture in the end is truly homogeneous. If the fuel hits the walls not only does that cause loss of potential charge cooling but more importantly significantly increased hydrocarbon and particulate matter emissions [9]. Several methods are employed to make sure fuel evaporation and mixing is satisfactory in DI engines. Most importantly, the injection pressures in DI have to be significantly higher than PFI (150 bar compared to ~4 bar). DI engines therefore have a small cost penalty compared to PFI engines due to the more sophisticated fuel system hardware.
1.1.3 Ethanol Gasoline Blends.

In the U.S there has been for a while a strong political will to promote ethanol as an automotive fuel [11]. The argument in favor of this effort is that it can be domestically produced from agricultural crops such as corn. Therefore ethanol use as a fuel has the potential to improve energy security and potentially could also improve well-to-tank carbon dioxide emissions.

Regardless of where it comes from, ethanol as an automotive fuel has several advantages:

- **Reducing Tailpipe Emissions**: Ethanol is an oxygenate fuel. As a result, it could potentially, blended with gasoline, significantly improve hydrocarbon and particulate emissions assuming adequate mixing conditions exist [12, 13].

- **Improving Knock Margins due to fuel chemistry**: Ethanol has excellent anti-knock qualities as indicated by its 109 RON [14]. It can therefore be used to increase compression ratio, boost pressure or optimize spark. This is a benefit related to the combustion/auto-ignition chemistry of ethanol and can, of course, be realized in both PFI and DI engines.

- **Improving Knock Margins due to Fuel Evaporative Cooling in DI**: In addition to the chemical benefit in preventing knock which is realized in both DI and PFI engines, ethanol-gasoline blends have a significant synergy with DI in that ethanol has an especially high heat of vaporization. It can therefore provide a significant charge cooling effect due to fuel evaporation. This effect, in addition to the chemical anti-knock effect can be used in DI engines using ethanol blends to increase compression ratios and boost pressures even further without being limited by knock.
In order to understand the advantages of ethanol blends as a fuel, especially in DI engines some of the most important properties of gasoline-ethanol blends are presented in Table 1. A blend that is X% by volume ethanol is symbolized as "EX", e.g. E20 is 20% ethanol, E50 is 50% ethanol etc.

<table>
<thead>
<tr>
<th></th>
<th>Gasoline (E0)</th>
<th>E10</th>
<th>E20</th>
<th>E50</th>
<th>E85</th>
<th>Ethanol (E100)</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>LHV(MJ/kg fuel)</td>
<td>43</td>
<td>41</td>
<td>40</td>
<td>35</td>
<td>29</td>
<td>27</td>
<td>Lower Heating Value</td>
</tr>
<tr>
<td>h_v(kJ/kg)</td>
<td>305</td>
<td>366</td>
<td>426</td>
<td>603</td>
<td>836</td>
<td>885</td>
<td>Heat of Vaporization</td>
</tr>
<tr>
<td>h_v/LHV *1000</td>
<td>7</td>
<td>9</td>
<td>11</td>
<td>17</td>
<td>27</td>
<td>33</td>
<td>Vap. Heat/ Heating Value</td>
</tr>
<tr>
<td>A/F_stoich</td>
<td>14.7</td>
<td>14.1</td>
<td>13.5</td>
<td>11.8</td>
<td>9.8</td>
<td>9.0</td>
<td>Stoichiometric Air/Fuel Ratio</td>
</tr>
<tr>
<td>LHV(MJ/kg mixture)</td>
<td>2.73</td>
<td>2.73</td>
<td>2.73</td>
<td>2.72</td>
<td>2.70</td>
<td>2.69</td>
<td>Based on Equation 4 and isentropic compression</td>
</tr>
<tr>
<td>ΔT air Intake (K)</td>
<td>19</td>
<td>23</td>
<td>28</td>
<td>44</td>
<td>69</td>
<td>81</td>
<td></td>
</tr>
<tr>
<td>ΔT air at Spark-TDC (K)</td>
<td>30-34</td>
<td>37-42</td>
<td>45-52</td>
<td>73-82</td>
<td>112-127</td>
<td>130-149</td>
<td></td>
</tr>
<tr>
<td>Laminar Flame Speed</td>
<td>0.33 m/s</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>0.41 m/s</td>
<td>Stoichiometric (298°K, 1 bar)</td>
</tr>
<tr>
<td>Adiabatic Flame T (K)</td>
<td>2289°K</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>2234°K</td>
<td>Unburned at 298°K</td>
</tr>
<tr>
<td>Research ON</td>
<td>97 (premium)</td>
<td>99</td>
<td>100</td>
<td>-</td>
<td>-</td>
<td>109</td>
<td>Source: [1],[14],</td>
</tr>
</tbody>
</table>

Table 1: Gasoline-Ethanol Blend Properties

The enthalpy of vaporization values used in Table 1 were obtained for 50° C starting liquid fuel temperature. Heat of vaporization depends significantly on starting fuel temperature as seen in Figure 1-5 for ethanol.
It can be seen from Table 1 that ethanol has almost four and a half times higher heat of vaporization per unit LHV. To estimate how much of a temperature difference due to cooling this enthalpy of vaporization \( (h_{lv}) \) can be translated to, let’s assume evaporation during intake and that the initial temperatures of fuel and air are close so that the sensible part can be neglected\(^1\). The charge temperature drop due to fuel evaporative cooling is described by (4):

\[
\Delta T_{\text{intake}} = \frac{m_{\text{fuel}} * h_{lv}}{(m_{\text{fuel}} + m_{\text{air}}) * c_{p,\text{mixture}}} \quad (4)
\]

The compression process amplifies this temperature difference. Assuming a polytropic process:

\(^1\) For a more complete treatment of the topic please refer to [16]
\[
\frac{T'_u}{T'_{IVC}} = \left( \frac{V_{IVC}}{V_2} \right)^{(k-1)} \quad \Leftrightarrow \quad T'_u = T'_{IVC} \left( \frac{V_{IVC}}{V_2} \right)^{(k-1)} \Rightarrow \\
T'_u = T_{IVC} \left( \frac{V_{IVC}}{V_2} \right)^{(k-1)} - \Delta T_{IVC} \left( \frac{V_{IVC}}{V_2} \right)^{(k-1)} \Rightarrow \\
T'_u = T_u - \Delta T_{IVC} \left( \frac{V_{IVC}}{V_2} \right)^{(k-1)}
\] (5)

Equation 5: Where \( T'_u \) is the unburned mixture temperature with charge cooling, \( T_u \) is the unburned mixture temperature without charge cooling, \( k \) is the polytropic coefficient and \( V \) is the volume.

As seen in Table 1 the temperature difference using (4) ranges from 19° K for gasoline to 77° K for ethanol. The compression process amplifies these temperature differences to 30-34° K at spark for gasoline and 130-149° K for ethanol (assuming isentropic compression). The range accounts for variation in spark timing. This causes variation in effective compression ratio from 30 CAD bTDC to TDC. The polytropic coefficient of compression was assumed to be 1.31. A geometric compression ratio of 9.2 was used, same as that of the engine used for the experiments in this thesis. These numbers represent the theoretical upper limit compared to a no charge cooling baseline based on thermodynamics.

In a real engine however, the time available for evaporation heat and mass transfer is limited. A significant fraction of the fuel therefore might end up on the walls or piston, in which case the heat for evaporation comes from the walls instead of cooling the charge. The life time of a droplet calculated based on Spalding's heat and mass transfer theory for droplet evaporation in quiescent air from [16] is presented in Figure 1-1 for isoctane. For a ~10\mu m diameter droplet typical for 120 bar injection pressure, the lifetime is 1-2 ms for 400° K air. This is equivalent to 30-60 CAD at 2000 rpm. Scaling these numbers by 4 to account for the higher heat of vaporization and stoichiometric fuel air ratio of ethanol, results in 120-240 CAD at 2000 rpm. Compared to a quiescent environment, the in-cylinder charge and fuel spray motion in an engine will enhance heat and mass transfer conditions significantly. Additionally, the charge temperature during compression increases significantly improving heat and mass transfer. Still however, as will be seen in Chapter 4, the travel time available for the fuel spray before it impinges on the wall is only about 50 CAD. It is understandable therefore that especially for high ethanol content fuels, without special care, a significant fraction of the fuel in a DI engine might end up evaporating by extracting heat from the walls instead of cooling the charge.
The following is a list of the most important macroscopic engine parameters that affect how much of the thermodynamic charge cooling potential gets realized in an engine:

- **RPM**: Higher rotating speed means there is less time available for the fuel to evaporate. Realizing the full charge cooling benefit thus becomes more challenging.
- **Load**: Higher load generally makes it more difficult to realize all the charge cooling potential. This is because the amount of fuel that needs to be injected is increased. Injection duration is thus increased and the chances of fuel wall impingement are higher.
- **Injection Timing**: Injecting early during the intake stroke increases the chances of fuel wall impingement as the piston is close to the injector. Later injection generally results in higher charge cooling realized. However
if injection is so late that part of the fuel evaporation takes place after Intake Valve Close (IVC), the charge cooling is still realized and helps with avoiding knock but doesn't contribute as much to increasing airflow rate and thus power output.

- **Injection pressure**: Higher pressure leads to better atomization and thus reduces droplet lifetimes. However, it also increases the momentum of the spray and thus decreases its travel time to the walls.
- **VVT**: Valve timing can affect the in-cylinder flow patterns and thus improve or worsen evaporation.

### 1.1.3 Air Flow Rate Change due to Charge Cooling.

For a four-stroke internal combustion engine, the airflow rate can be approximated as:

\[
\dot{m}_{air} = \eta_\text{aw} \cdot \rho_{\text{INAKE}} \cdot V_d \cdot N \tag{6}
\]

Equation 6: Where: \(\dot{m}_{air}\) is the airflow rate, \(\rho_{\text{INAKE}}\) the density at the intake, \(V_d\) the engine displacement volume and \(N\) the rev/s.

If the airflow rate after fuel evaporation is divided by the airflow rate before and assuming \(\eta_v\) remains the same; we get based on Equation 6 and the ideal gas law:

\[
\frac{\dot{m}_{air}'}{\dot{m}_{air}} = \frac{\rho_{\text{INAKE}}'}{\rho_{\text{INAKE}}} = \frac{M'}{M} \cdot \frac{P'}{P} \cdot \frac{T'}{T} \tag{7}
\]

Equation 7: \(M\) is the molecular weight; prime numbers indicate variables after evaporation (mixture) non prime are air (pre-evaporation numbers).

Neglecting humidity and assuming that the pressure in the intake is constant we get using the partial pressures of air and fuel vapor and the ideal gas law:

\[
\frac{P'}{P} = \frac{P_{air}'}{P_{air} + P_{fuel}} = \left(1 + F/A \cdot \frac{M_{air}}{M_{fuel}}\right)^{-1} \tag{8}
\]

Equation 8: \(F/A\) is the fuel air mass ratio.

Substituting (8) into (7), we get:

\[
\frac{\dot{m}_{air}'}{\dot{m}_{air}} = \frac{M'}{M_{air}} \cdot (1 + F/A \cdot \frac{M_{air}}{M_{fuel}})^{-1} \cdot \frac{T}{T - \Delta T_{\text{charge\_cooling}}} \tag{9}
\]

Equation 9: Change in airflow rate due to fuel evaporation
Using Equation 9, it can be seen that for no charge cooling (all heat of vaporization from the walls), the airflow rate is decreased compared to the airflow rate without any fuel evaporation (a motored engine air flow rate if MAP and wall temperatures are the same). This is due to the volume taken up by the fuel vapor and is called the "displacement" effect. However when comparing DI to PFI, the displacement effect is present in both cases. It can therefore be neglected from the calculations.

For the two extreme cases of no charge cooling and maximum charge cooling we get the following results for gasoline and ethanol.

- **Gasoline**: Maximum charge cooling (190 °C) results in 6.5% increase over the no charge cooling case including the displacement effect.

- **Ethanol**: Maximum charge cooling (81 °C) results in a 33% increase over the no charge cooling case including the displacement effect.

### 1.2 Literature Review

Several industry papers have discussed the potential benefits and the practical challenges in designing an engine for ethanol use often combined with engine measurements. Examples include [17,18] for PFI, [19] for PFI and DI and [20,21,22,23,24] focusing exclusively on DI. [25] investigated the potential increase in compression ratio using ethanol blends in naturally aspirated PFI engines and [26,27] in naturally aspirated DI engines. It was shown that even when used in PFI, ethanol blends can deliver significant antiknock benefits. The antiknock benefit is even more pronounced in when the fuel is used in DI [27] also includes an insightful analysis of the secondary efficiency benefits associated with ethanol fuel use other than knock avoidance. These will be discussed further in chapter 3.

One interesting suggestion for using the anti-knock benefit of ethanol more effectively was made in [28]: An engine concept with two fuel systems. The engine normally burns gasoline in port injection but switches to direct injection of ethanol or E85 when it detects knock. Only a small amount of ethanol is thus needed and efficiency is significantly improved. The concept is currently being explored in a prototype engine described in [29, 30, and 31].

In terms of exploring the fundamental science behind ethanol use in DI engines for knock avoidance, the first question is how much charge cooling takes place. [16] described the fundamental thermodynamics behind charge cooling and proposed using the effect of charge cooling on increasing air density and thus airflow to quantify the effect. Using air flow rate as a diagnostic has since been

---

2 This number was calculated for a starting temperature of 50 °C. Starting air temperature does have a significant effect.
the main method used in the literature to quantify charge cooling.[16] measured a
difference of 2% in airflow out of a maximum of 6-7% when comparing DI to PFI
using gasoline.[32] showed that the maximum theoretical charge cooling is not
just limited by thermodynamics but also by mass transfer as the air might
become saturated in fuel vapor during intake, especially at high MAP.[32] also
measured the difference in airflow between PFI and DI for gasoline, E10,
methanol and 10% methanol blends and found it between 50-70% of the
thermodynamic maximum. [33,34] used the difference in volumetric efficiency
between experimentally observed and that predicted by a one dimensional gas
dynamics model to calibrate a fuel wall wetting model.

Other methodologies that have been suggested in the literature include using
MAP as a diagnostic, CFD and optical experiments. [35] proposed throttling the
intake air flow until it is choked and using the change in MAP as a diagnostic of
charge cooling. This method however is only suitable for low intake air flow rates
and not the high load conditions relevant for knock. Several studies such as [36]
have used computational fluid dynamics (CFD) to look at charge cooling. CFD
though valuable as a tool of looking at the details of the flow inside the cylinder,
is not really a diagnostic as it needs to be calibrated against experimental data.
Similarly, several studies such as [37, 38,39] have used optical methods to look
at in cylinder fuel evaporation. Optical methods are very useful in revealing
details of the in-cylinder flows but can't be used to quantify how much charge
cooling took place in terms of a temperature difference. The main method used
therefore so far has been the effect on airflow.

Unfortunately the methodology of using air flow rate as a diagnostic of charge
cooling has several shortcomings:

- First, the method only captures the amount of fuel evaporation that takes
  place during the intake stroke. After the intake valve closes, evaporation
doesn't affect airflow. [16] showed qualitatively that the effect of post IVC
evaporation can be seen on the slope of the polytropic compression in a
pressure-volume diagram. The effects on the slope of the polytropic are
however very difficult to quantify. [40] attempted some sophisticated data
processing to quantify the effect on the polytropic coefficient but the
method is complicated, relies on having an accurate friction model and
could introduce numerical artifacts.

- Secondly, using airflow rate as a diagnostic of charge cooling is not
  suitable for turbocharged engines as will be seen in Chapter 3.

- Finally as seen previously, the maximum theoretical change in airflow for
gasoline is of the order of a few percent. Making airflow measurements
with a couple of percent accuracy is quite challenging, especially
considering the effect of day to day variations due to ambient conditions.

It is obvious from the discussion above that a better method of quantifying the
charge cooling effect is clearly needed.
In terms of quantifying the chemical antiknock benefit of ethanol blending, the simplest approach is to look at the RON. Doing that, it is clear that the RON doesn't increase linearly with volumetric ethanol content [14]. As will be explained in Chapter 5; the addition of ethanol shows diminishing returns in terms of its chemical benefit. [14] suggested that the RON vs. ethanol curve becomes linear when using molar ethanol concentration instead of volumetric. From a fundamental point of view, the chemical effect is captured in ignition delays that could be predicted by chemical kinetics mechanisms. Several recent publications deal with developing a model of gasoline-ethanol ignition delay models based on chemical kinetics such as [41] and [42]

[43,44] attempted to quantify the effect of charge cooling on knock. The full thermodynamic charge cooling potential was assumed and a chemical kinetics code was used to quantify the benefit of charge cooling on knock. [45] looked at the experimental knock limited load of fuels that have the same RON but different heat of vaporization.

In terms of knock limit predictive models for engines that cover ethanol blends, [46] is worth mentioning. A knock limit integral approach was used with the same auto ignition time correlation for both gasoline and ethanol.

1.3 Thesis Objectives-Methodology

1.3.1 Thesis Objectives

The objective of this study was to improve the understanding of the effect of direct fuel injection (DI) of gasoline/ethanol blends on knock limits in boosted engines. In order to simplify the problem, the methodology used, consists of decoupling the thermal (charge cooling) and chemical effects on knock. More specifically, the overall problem was broken down into three partial questions:

1. How much charge cooling takes place due to fuel evaporation in DI?
2. How does the change in air temperature due to charge cooling affect knock?
3. How does fuel chemistry affect knock for higher ethanol content?

Finally the answers to the partial questions above were combined into a knock limit predictive model that covers blends from pure gasoline to E85 (85% ethanol by volume) and direct as well as port fuel injection (PFI).

The details of the individual questions and the plan to answer them are presented below:

1) How much charge cooling actually takes place?
As discussed, in a real engine, the time available for fuel evaporation heat and mass transfer is limited. Fuel wall wetting does occur and some of the heat required to evaporate the fuel might come from the walls instead of the charge.
The strategy for estimating how much charge cooling actually takes place in a DI engine using gasoline/ethanol blends consists of using PFI as a no charge cooling baseline and using knock as a diagnostic of charge cooling. Essentially, the experiment measures how much does the intake air in DI need to be heated to cancel charge cooling out and make DI knock at the same conditions as PFI. To perform this experiment all that is needed is an engine that is equipped with both DI and PFI and has independent control of intake air temperature.

It could be argued that using PFI is not the perfect no charge cooling baseline. The literature seems to agree that there is some (0-30% would be a good estimate) charge cooling taking place in PFI [40, 47, 48, 49, 50, 51, 52]. The method described above doesn’t measure the amount of charge cooling compared to a no charge cooling baseline but the difference in charge cooling realized in DI vs. PFI instead. However, from an engineering point of view it is exactly this difference that is of interest: How does DI compare to the standard technology-PFI.

In addition to the experiments described above, Computational Fluid Dynamics (CFD) modeling was performed. The CFD models helped quantify the effects of different intake air temperature and engine load on evaporation times and amount of charge cooling realized. CFD also provided some idea of the in-cylinder stratification in DI in terms of temperature and composition. Even engines that are designed to be homogeneous like the ones that are the focus of this thesis might end up having significant in-cylinder stratification that affects knock onset. This is especially true when using higher ethanol blends when the longer evaporation times leave less time for mixing.

2) How does charge temperature affect knock?
Once the amount of charge cooling realized has been estimated, separating the thermal effect on knock is simple. For a given fuel blend in PFI the sensitivity of knock limits on intake air temperature answers exactly this question.

3) How does ethanol chemistry affect knock?
The simplest way to answer this is for a given charge temperature, compare the knock limits of two gasoline/ethanol blends in PFI.

4) Develop a Knock Limit Predictive Model that covers all blends from gasoline to E85 in DI and PFI.
The plan here is to use thermodynamics and 1-D gas dynamics to calculate the unburned mixture temperature from the experimental data at knock onset. The pressure and unburned mixture profile can subsequently be used to model the chemical kinetics of auto ignition for every fuel.

The standard method of quantifying a fuel’s anti-knock quantities is using an ON. However ON tests are performed in standardized engines that where
standardized in the 1930's and are not necessarily representative of modern engine antiknock performance. More importantly they do not include the charge cooling antiknock benefit. For these reasons, the knock limit predictive model used, the logic of which will be explained in Chapter 5, was purposely selected to quantify the anti-knock performance of a fuel using a modified version of an ON based on the experimental data. By comparing these modified versions of the ON between two fuel blends with different ethanol content, the chemical antiknock benefit of ethanol can be quantified. Moreover, if the charge cooling antiknock benefit is also translated to an improvement in ON, it can be directly compared to the chemical effect.

1.3.1 Experimental Plan

The main experimental set for this thesis is essentially a series of spark sweeps up to knock. These spark sweeps were performed for 5 different fuel blends (E0-gasoline, E10, E20, E50 and E85) in both DI and PFI for several intake air temperatures. The fuel blends were splash blended using Haltermann premium reference test gasoline and 99.999% ethanol. Rotational Speed was kept at 2000 rpm for these tests. Intake and exhaust geometry was also kept constant, with the throttle wide open and the waste gate (since the tests were performed in a turbocharged engine) also open-bypassing as much flow from the turbine as possible. These engine "geometry" settings result in an intake Manifold Air Pressure (MAP) of around 1.3-1.4 bar and will hence be referred to as "base boost. Stoichiometry was kept at $\lambda=1$ for all tests. The valve timing for these experiments was kept constant (Intake Valve Open-IVO at 22 CAD bTDC, Exhaust Valve Close-EVC at 19 CAD aTDC). Fuel injection timing was also kept constant with start of injection at 60 CAD aTDC for DI and end of injection 20 CAD before IVO for PFI.

The details of the experimental set are summed up in Table 2.
### 1st Exp. Set- Spark Sweeps

<table>
<thead>
<tr>
<th>Variable Parameters</th>
<th>Fixed Parameters</th>
<th>Measurable Quantities</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spark Timing</td>
<td>2000 rpm, ( \lambda=1 ), Wide Open Throttle and waste gate, (~1.4 ) bar MAP (BASE BOOST)</td>
<td>Conditions at Knock: P, flow rate</td>
</tr>
<tr>
<td>Fuel Composition (E0, E10, E20, E50, E85)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Injection Type (DI-PFI)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Intake air T</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 2: 1st Experimental Set

To examine the effects of engine load and speed, additional spark sweeps up to knock were performed. These were performed for both DI and PFI for gasoline (E0) at 30° C intake air, for E50 at 100° C intake air and for E85 at 120° C intake air. 3 different loads were tested at 2000 rpm and 3 rotational speeds at base boost load.

Finally, the effect of injection timing was investigated. Injection timing is important in determining how much charge cooling takes place due to fuel evaporation. Start of injection timing sweeps were performed for all fuels with 20° C intake air and spark timing at MBT or the most advanced point that was not knock limited.
2. Experimental Setup and Modeling Tools

2.1 Experimental Setup

The experimental setup was designed and built from scratch for the purposes of this experiment. It can be seen in Figure 2-1. It consists of a turbocharged engine that was originally DI but was retrofitted with PFI as well and placed on a motoring dynamometer for testing. The intake system was designed to have the ability to vary the intake air temperature independently of engine operating parameters. The setup is fully instrumented.

Figure 2-1: The Experimental Setup.

2.1.1 The base engine

The engine used for the experimental part of this thesis is a modified version of a production General Motors engine, the General Motors LNF from the ECOTEC family. The engine is the first production turbocharged DI engine offered in the U.S. market. Basic engine parameters are listed in Table 3. Although the engine has fully variable valve timing, the valve timing for all experiments presented in this thesis was fixed at the values presented in Table 4.
### Displacement Volume (Vd)

| Cylinders | 1-4 |
| Bore      | 86 mm |
| Stroke    | 86 mm |
| Max Boost | 1 bar |
| Compression Ratio | 9.2:1 |
| Valve Timing | Dual Independent Cam Phasing |

**Table 3**

| IVO | 22 | CAD bTDC Gas Exchange |
| IVC | 28 | CAD aBDC Compression |
| EVO | 21 | CAD bBDC Expansion |
| EVC | 19 | CAD aTDC Gas Exchange |

**Table 4**

### 2.1.2 Intake and Exhaust Systems.

A schematic of the intake and exhaust system of the experimental engine can be seen in Figure 2-2. After a filter, the intake air is directed through a rotary (turbine) flow meter. Subsequently, it passes through a damping tank which is used to dampen out engine flow oscillations. Next in line, is the turbocharger compressor. The compressor is equipped with a bypass valve to avoid surge when there is an abrupt decrease in load. The intercooler follows which was originally air cooled but has been modified to be water cooled. The intercooler can cool the air temperature down from 70-110°C after the compressor to 10-20°C depending on city water temperature. A 10 kW closed loop controlled electric heater downstream of the intercooler can heat the intake air up to at least 170°C. The engine throttle follows upstream of the engine itself with PFI and DI fuel injection. In the exhaust, there is a pneumatically actuated waste gate for controlling the amount of the exhaust gases that pass through the turbine and hereby determines the turbocharger speed of rotation and the boost the compressor creates. Finally, after the turbo, there is a gate valve which can be

---

3 Estimate based on flow rate and heater heat losses recorded. Only up to 130°C tested, the engine throttle servomotor shuts down beyond that.
used to emulate the pressure drop in the catalyst before the exhaust gases end up in the exhaust trench. The gate valve in the exhaust was kept wide open in the experiments described in this thesis.

**Figure 2-2: The Experimental Setup Intake and Exhaust System.**

### 2.1.3 Mechanical Setup

The engine was placed on a motoring dynamometer for the tests. The layout of the facility can be seen in Figure 2-3 It consists of the engine, a 30 kW AC motor used as a starter and to motor the engine and a Digalog AE 150 Eddy Current Dynamometer. The dynamometer is closed loop controlled, absorbing whatever load the engine is generating so that the powertrain remains at constant speed. Compared to the configuration on a vehicle, an engine attached to a dynamometer is directly connected to much bigger rotating inertias (dynamometer and A/C motor). Therefore, a bigger flywheel and a elastic coupling designed by VOITH were added to the engine in order to decrease the system's first resonance rotating speed below 1000 rpm. A Cardan shaft is used to correct any misalignment in the powertrain.
2.1.4 Heating Cooling-Fuel System.

A schematic of the engine cooling system is outlined in Figure 2-4. The coolant temperature is close loop controlled to 80±3 °C through a solenoid valve that controls the city water flow to the coolant/water heat exchanger. An electric heater is also used in the coolant tank to quickly heat the coolant up to the temperature of the experiment. All the experiments presented in this thesis were performed at constant 80° C coolant temperature.

A schematic of the engine fuel system is presented in Figure 2-5. Two tanks were used - one for gasoline and low ethanol blends, another for high ethanol blends. This way, fuel contamination could be minimized and material compatibility issues avoided. A purge system was added to flush the fuel system out when switching fuels. The low pressure pump was set to 60 psi to be able to provide adequate flow rate in PFI operation mode. The pump pressure is set relative to intake MAP to account for load variations. The high pressure pump is a piston pump powered by the camshaft and controlled by the ECU to around 150 bar through a solenoid. When switching from PFI mode to DI, the high pressure pump needs to be removed from the engine block and the hole covered. This is because the high pressure pump relies on the fuel to act as a coolant and lubricant. For the same reason, it is important when switching to PFI to replace the DI injectors with dummies otherwise the combustion chamber heat will damage them without the cooling flow of the fuel.
Figure 2-4: Cooling System.

Figure 2-5: Fuel System.
2.1.5 Control

A Yokogawa variable frequency drive was used to control the rpm of the A/C motor. A Dynesystems Dyn-Loc IV PID controller was used to control the Eddy Current Dynamometer speed by changing the voltage fed to the stator coil. The amount of load absorbed is controlled by the engine.

An ETK ECU (Engine Control Unit) by Bosch along with an ETAS ES591 communication module and INCA software was used to control engine operating parameters. Essentially, the ES 591 acts as a modem allowing a regular personal computer to communicate with the ETK ECU. The ETK ECU is a special ECU with two memory modules. When the engine is running, and the operator changes the value of an operating parameter, e.g. spark timing, the new value is stored first in one of the two memories while the other is used to control the engine. The new value is then internally copied inside the ECU from one memory to the other and used to control the engine. This process allows seamless engine operation and varying engine parameters while the engine is running. The ECU uses programming by Bosch.

Engine parameters can be modified using the ETK ECU: Spark timing, injection timing, injection pressure, lambda, valve timing and output torque. Engine load is controlled by controlling the position of the throttle and the position of the waste gate. At low loads (up to about 0.9 bar Manifold Air Pressure), when the throttle is partially closed, the turbocharger is not generating any boost since the exhaust gas enthalpy is insufficient to spin the turbine fast enough. At intermediate loads (~0.9-1.4 bar MAP), the turbo is generating some boost but the partially closed throttle causes a pressure drop to get the required load. The waste gate in the meantime is open, bypassing as much mass flow as possible. When the throttle is wide open and the waste gate bypassing as much flow as possible the engine conditions are described as base boost. The MAP is around 1.3-1.4 bar at base boost conditions. In order for the engine to go to higher load, the waste gate needs to be actively closed. To understand how waste gate position is controlled, a schematic of the control system is presented in Figure 2-6.

The waste gate actuator is pneumatically actuated. A three way solenoid that is Pulse Width Modulated (PWM) by the ECU can control the pressure on the waste gate actuator to any value, from ambient to the magnitude of the pressure after the compressor. The position of the waste gate is the result of the force balance between the spring trying to close it, the force of the exhaust gases trying to open it and the force from the actuator also trying to open it. At base boost conditions, the duty cycle to the solenoid is 0%, the pressure to the solenoid is the same as after the compressor the waste gate open as much as possible and the system equilibrium is around 0.3-0.4 bar of boost (1.3-1.4 bar MAP). At maximum boost, the duty cycle is 100%, the pressure to the actuator is ambient, the wastegate closes fully and the system equilibrium is at 2 bar MAP. An important characteristic of this system is that it acts essentially as a negative
feedback loop on the turbocharger. Assuming that while the engine is at wide open throttle and x% duty cycle, the enthalpy flow to the turbo increases. This could be caused e.g. by a change in spark timing or valve timing, either because the air flow rate increased or because the exhaust gas temperature increased. The turbocharger will spool up creating increased boost. Because the duty cycle to the solenoid is constant, x% of the new, increased boost pressure will be applied on the waste gate actuator opening the waste gate more. The turbocharger therefore slows down and the new equilibrium is close to the old one. The system is stable.

An Athena PID controller using SCR as actuators was used to control the electric air heater. An Omega on-off controller was used to control the solenoid valve to the city water supply to the coolant heat exchanger and the coolant heater and thus coolant temperature.

2.1.6 Instrumentation

The intake and exhaust systems are instrumented with K type thermocouples and Omega PX 219 series piezo resistive pressure transducers as seen in Figure
Additionally a fast, Kistler 4005B pressure sensor was placed in the intake port close to the intake manifold gasket. This sensor has a natural frequency more than 100kHz and can capture pressure oscillations in the intake port. A thermocouple was also placed in the same position, millimeters away from the intake manifold gasket.

All four cylinders are tapped and equipped with flame arrestors to use pressure transducers. The pressure traces from cylinder 1 and 3 where recorded using Kistler 6125 A pressure transducers. The pressure trace from Cylinder 1 was sampled once every crank angle degree (12 kHz at 2000 rpm) and each measurement is started when the piston in Cylinder 1 is at top dead center. The exact position (±1°CAD) of the piston at each point in the pressure trace is thus known and the P-V integral for work or mean effective pressure (MEP) can be calculated. The start of the measurement of the pressure trace from cylinder 3 is again the point when Cylinder 1 is at TDC (and Cylinder 3 is at BDC), but this transducer is sampled at 100 kHz. The reason is that Cylinder 3 is the cylinder that reaches knock onset first (because it is in the middle and runs hotter). In order to capture knock induced pressure oscillations due to knock adequately, a higher sampling frequency is needed as they contain harmonics from around 6 kHz to around 15 kHz. One hundred engine cycles were recorded for each measurement.

A BEI crankshaft encoder was used in order to synchronize pressure measurements with crank angle position. The same crankshaft encoder provides a pulse every time cylinder 1 is at TDC. This pulse is used to trigger the start of a measurement.

Flow rate is measured using two methods. An IMAC rotary flow meter measures it directly in the intake. Additionally, the air flow rate can be calculated through the fuel flow rate. The fuel flow rate can be calculated from the injection pulse width and injection pressure recorded by the ECU. The engine fuel to air ratio over stoichiometric fuel to air ratio (λ) was also recorded from the engine wide band λ sensor and can be used to calculate the air flow rate.

A National Instruments cDAQ 9172 base data acquisition module was used to collect the measurements. Additional modules were connected to the base module for measuring analog voltage signals, digital signals and thermocouple temperature measurements. Labview 9 software was used to control the data acquisition.

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4 For the definition of MEP see [1]
2.2 Modeling Tools

2.2.1 Computational Fluid Dynamics

Computational Fluid dynamics (CFD) modeling was undertaken in order to model the mixing processes in the engine. A commercial CFD code, STAR-CD by CD-Adapco was used. For background reading on the application of CFD in internal combustion engines and the code used [1, 53] are recommended.

The mesh used was developed by GM to model this engine. It can be seen in Figure 2-7. It consists of 700,000 cells and changes shape and size to account for piston motion.

The model uses an Eulerian approach for the gas flow and a Lagrangian tracker for the spray droplets. Several sub-models are incorporated to simulate the spray and its interaction with its environment:

- A spray breakup model is used to simulate the formation of droplets close to the injector.
- The Lagrangian tracker follows a selected group of droplets and uses correlations for the forces exerted on the droplet (e.g. aerodynamic) as its shape changes due to evaporation. The tracker will also take into account the probability of droplets colliding with each other and coalescing.
- The Bai model [54] was used for predicting what happens to droplets when they collide with the walls or piston. The droplets could stick and form a fuel film, rebound or splash.
- The heat and mass transfer processes of evaporation.

An excellent source of background information on spray modeling is [55]. Many examples of spray model methodologies are provided in the text above. However there isn't a single model that can cover every existing case without being adapted first to the details of the specific physical problem. It turns out that modeling ethanol sprays can be particularly challenging due to two facts:

- Due to the high heat of vaporization, the fuel droplets take long to evaporate.
- If too many droplets accumulate inside a single mesh cell, the code crashes.

It was discovered that none of the spray models included in the STAR-CD software package were able to handle ethanol sprays and resulted in numerical instabilities and the code eventually crashing. It was therefore decided to use a proprietary model developed by GM and CD-Adapco especially for handling DI sprays in SI engines and designed to handle ethanol as well. The model was validated using optical experiments from GM laboratories. The details of setting up the boundary conditions of the simulations to gain additional insight into the experimental results will be described in more detail in chapter 4.
2.2.2 1-D Gas Dynamics and Engine Thermodynamics

GT-Power by Gamma Technologies was the software used to simulate the time dependent one dimensional gas dynamics and thermodynamics of the engine. The software discretizes the intake and exhaust system geometry. The pressure drop across the valves is modeled through measured flow coefficients and the turbocharger through a look up table. The software models the gas dynamics generated by piston motion. In terms of in-cylinder processes; combustion characteristics are not simulated but rather externally specified through a user-entered burn profile. Heat transfer is based on a Woschni-type correlation [1]. A sub-model for engine friction is also included. More information on the theory of gas dynamics simulations can be found in [1] and specifically for GT Power in [47]

The model used to simulate the test engine was based on a model developed by GM for this engine. The original model was modified to account for the differences in the intake and exhaust systems between the production engine and the experimental setup and the added PFI. The model can be seen in Figure
The process of matching the model to the experimental results will be explained in detail in chapter 5.

Figure 2-8: Engine Layout for the One Dimensional Gas Dynamics Simulations.

2.2.3. Rassweiler-Withrow Burn Rate Analysis

In order to obtain a burn profile for use in the GT Power simulations, heat release analysis was carried out based on the first law technique developed by Rassweiler and Withrow [56]. This approach uses the measured in-cylinder pressure trace to calculate the heat release during combustion and assumes a polytropic change of state during compression and expansion:

\[ PV^n = \text{const.} \]  

(10)

The volume occupied by the unburned gas, \( V_u \), can be calculated from the reference state at spark timing (index 0) assuming a polytropic compression due to the advancing flame front:

\[ V_u = V_{u,0} \left( \frac{P_0}{P} \right)^{1/n} \]  

(11)

Similarly, the actual burned gas volume behind the flame front, \( V_b \), can be backtracked in reference to the burned gas state at the end of combustion (index f):

\[ V_b = V_{b,f} \left( \frac{P_f}{P} \right)^{1/n} \]  

(12)
At all times, the total cylinder volume \( V \) is composed of burned and unburned gases:

\[
V = V_u + V_b \tag{13}
\]

The mass fraction burned can be expressed for both zones as follows:

\[
x_b = 1 - \left( \frac{V_{u,0}}{V_u} \right)^{\frac{1}{n}} \wedge x_b = \left( \frac{V_{b,f}}{V_b} \right)^{\frac{1}{n}} \tag{14}
\]

Where \( V_0 \) and \( V_f \) are the total cylinder volumes at time of spark and at the end of combustion, respectively. Substituting (11) and (12) into (13) and replacing \( V_{u,0} \) and \( V_{b,f} \) using (14) leads to the resulting relation for the mass fraction burned:

\[
x_b = \frac{p^{\frac{1}{n}}V - p_0^{\frac{1}{n}}V_0}{\left( \frac{p^{\frac{1}{n}}}{p_0^{\frac{1}{n}}} \right)^{\frac{1}{n}}V_f - p_0^{\frac{1}{n}}V_0} \tag{15}
\]

The polytropic exponents are obtained from the experimental data as slopes of the compression and expansion line in the \( \log(p)-\log(v) \)-diagram. In the code used for post-processing the data in this thesis, two anchor points for each line have been defined. The points have a fixed distance from (start of combustion) SOC and (end of combustion) EOC of -10 and -50 °CAD, respectively. The choice of SOC and EOC defines the polytropic coefficients used in (15). SOC and EOC therefore have to be chosen carefully. SOC is usually assumed to occur at spark timing, EOC was chosen to be 30 °CA before exhaust valve opening. Although the resulting shape of the mass fraction burned profile does depend on the choice of EOC, the characteristic parameters of 10%, 50% and 90% burned mass are essentially independent of the choice of EOC.

The Rassweiler-Withrow method is illustrated in Figure 2-9. In the logarithmic \( p-V \) diagram, 0% and 100% mass burned lines can be constructed by extrapolating the 0% and 100% burn lines (compression and expansion). Plotting the results vs. CAD, the mass fraction burned can be interpreted as ratio of the differences between the measured pressure trace and the 0% and 100% burned line, respectively.
Several approximations are used in the Rassweiler-Withrow analysis [1]:

- Heat transfer effects are only included to the extent that the polytropic coefficients used differ from the true ratio of specific heats.
- The pressure rise due to combustion is proportional to the amount of fuel chemical energy released rather than the mass of mixture burned.
- The polytropic coefficient $n'$ is not constant throughout the combustion event due to heat transfer and changing gas composition.
3. Results - Engine Thermodynamics - Knock Limits

3.1 Engine Thermodynamics

3.1.1 Spark Timing Sweep results

As explained in Chapter 1, the main experimental set for this project was a series of spark sweeps up to knock for DI and PFI, different fuel blends and intake air temperatures. These tests were conducted at 2000 rpm and base boost conditions\(^5\). The results of these spark sweeps for constant 20° C intake air temperature are plotted in Figure 3-1 as Net Indicated Mean Effective Pressure (NIMEP)\(^6\) vs. spark timing for all fuels in both DI and PFI. The limit for the spark sweeps on the advanced side was borderline knock, unless the engine was not knocking at all under those conditions. Borderline knock will be defined more rigorously later. On the retarded side, the limitation was engine instability as indicated by a coefficient of variance of NIMEP (COV NIMEP) more than 3%.

Several trends are clear from Figure 3-1. First, at these conditions, (~1.35 bar MAP, 20° C intake air) only gasoline (E0) in DI and PFI and E10 in PFI are knock limited in that knock occurs before they reach their Maximum Brake Torque (MBT) spark timing. E10 in DI and E20, knock but for spark timing more advanced than MBT. E50 and E85 don't knock at all under these intake conditions. This is because the engine used was designed with a compression ratio of 9.2:1 intended for gasoline. MBT spark for all fuels is between 15 and 20 degrees before Top Dead Center (TDC). For the same fuel, the NIMEP in DI is greater than the NIMEP in PFI. DI gasoline NIMEP is ~ 4% higher than PFI. DI E85 NIMEP is about 10% higher than PFI. This is mostly due to the air flow rate in DI being higher due to charge cooling. Additionally, engine brake fuel efficiency is slightly higher in DI as will be seen. For DI, higher fuel ethanol content leads to higher NIMEP because of increased air flow rate due to higher charge cooling. DI E85 NIMEP is about 5% higher than that of gasoline. In PFI, the differences in NIMEP are smaller and there is no clear trend in terms of the fuels. Bear in mind that there is a ±3% uncertainty in IMEP due to day to day variations because of ambient condition variations (temperature, humidity).

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\(^5\) As explained in Chapter 2, base boost is the condition where the throttle is wide open and the waste gate is bypassing as much flow from the turbine as possible.

\(^6\) Mean Effective Pressure is the engine output torque normalized by volume. “Net Indicated” means engine friction is not included but pumping losses are [1].
Figure 3-1: Net IMEP for all blends in DI and PFI for 20 C Intake Air.

An example of spark sweeps for different intake air temperatures is presented in Figure 3-2. The fuel was E20 in DI, the engine speed was 2000 rpm and load was at base boost (~1.35 bar MAP). As intake temperature rises, NIMEP drops. This is because the air flow rate decreases with air temperature since the density in the intake decreases. This can clearly be seen from the volumetric efficiency equation in Chapter 1 (Eq. 9). Also it is clear that the spark timing where the engine knocks is more and more retarded as intake air temperature increases.
Manifold Air Pressure (MAP) is plotted vs. spark timing for gasoline (E0) and E85 in DI and PFI in Figure 3-3 for 20°C intake air. As can be seen in the figure, MAP is essentially independent of fuel and injection type although these parameters do have an effect on airflow rate due to differences in charge cooling as will be seen. This is because of the negative feedback loop of the turbocharger control system described in Chapter 2 that damps out changes. There is however a modest effect from changing spark timing. Later (more retarded) spark timing means that exhaust gas temperature goes up. The enthalpy flow to the turbine thus increases and it spools up creating slightly higher boost. Due to the negative feedback loop in the waste gate controls however, this increase in boost is still quite modest- 0.015 bar out of 1.345 or a 1.1% increase.
Figure 3-3: Manifold Air Pressure for gasoline (E 0) and E 85 in PFI and DI vs. Spark Timing, 20° C Intake Air, 2000 RPM, Base Boost.

MAP vs. spark timing and intake air temperature is plotted in Figure 3-4 for DI E20 at 2000 rpm and base boost conditions. As intake temperature increases, air flow rate decreases due to the reduced density of the air. As a result, the exhaust air flow rate through the turbine also decreases with intake air temperature. The turbocharger therefore slows down and produces less boost. The effect however is quite modest. From the lowest MAP point (most advanced spark, 105° C air) to the highest (most retarded spark, 20° C air) the difference is only 0.04 bar out of 1.34 bar or 3%. For comparison, the intake air temperature (in K) changes by 21% which assuming constant pressure is also the change in intake air density. This is because of the negative feedback loop in the waste gate control. As explained in Chapter 2, when MAP drops, the waste gate will tend to close to compensate. As a result, for all of the operating points measured at base boost conditions and 2000 rpm, the minimum MAP recorded was 1.33 bar and the maximum 1.39 bar. So MAP was roughly held constant for all the base boost experiments within 5% (± 2.5%).
The air flow rate as a function of intake air temperature for all fuels and injection types is plotted in Figure 3-5 for gasoline (E0), E10 and E20 and in Figure 3-6 for E50 and E85. For the same injection type and fuel, as intake air temperature increases, air flow rate decreases because the air density decreases. For every fuel at the same intake temperature, the DI flow rate is higher than the PFI. The difference in air flow rate between DI and PFI is plotted vs. ethanol content in Figure 3-7. Although significant time effort was invested in narrowing the error bars down, there are still error bars of ±2% due to day to day variation and differences between the two measurements used (rotary flow meter and fuel injection pulse width). Even with the error bars however, it is clear that DI has a ~2% (for E0, E10, E20) to ~4% (E50 and E85) higher air flow rate compared to PFI. Additionally an increase due to higher charge cooling, 1.5-4% in air flow rate is observed when comparing DI E0 to DI E50 or DI E85 for the same intake air temperature. These findings are similar to what has been reported in the literature [27].

In Chapter 1 it was seen that the increase in volumetric efficiency for E85 due to charge cooling was expected to be significantly higher (~33%) based on a simple mixing calculation\(^7\). The difference between DI and PFI for E85 therefore seems small in comparison. The observed difference in air flow rate between DI E85

\(^7\) It is reminded that the equivalent number for E0 is 5% volumetric efficiency benefit compared to motored flow and 7% compared to all vaporization heat from the walls (including displacement effect due to fuel vapor volume.)
and DI E0 also seems small based on these ideal numbers. There are two reasons that explain these observations:

➢ The feed back loop on waste gate control that reduces differences in flow rate and boost.

➢ The fact that evaporation and charge cooling in DI takes place with a finite rate inside the cylinder which communicates with the intake only through a flow restriction (valves). This is a significantly different situation in terms of flow physics from instantaneous mixing under constant pressure or volume. The gas dynamics are important. To investigate this effect a gas dynamics model (GT Power) was used. The model was tuned to match an experimental DI E85 operating point in air flow rate, MAP and pressure trace using a finite evaporation profile obtained from CFD analysis. The fuel evaporation time subsequently was switched to instantaneous. The air flow rate in the instantaneous case increased by 10% compared to the realistic, finite evaporation rate case.

The 2-4% increase in air flow rate between DI and PFI isn’t enough to justify all the difference in NIMEP; an increase in efficiency in DI is implied. Indeed, when the indicated efficiency is plotted vs. ethanol content for DI and PFI in Figure 3-8, DI clearly exhibits an efficiency improvement of 1-2 % over PFI. When these numbers are combined with the increase in air flow rate, the increase in NIMEP can be explained. For example, for E85 there is a 4% increase in air flow rate comparing DI to PFI. 104% multiplied by the ratio of DI over PFI indicated efficiencies (36%/34%) gives 110% which is the same as the ratio of DI over PFI NIMEP. There also seems to be a small efficiency benefit as ethanol content goes up. This benefit has also been documented elsewhere [27].
Figure 3-5: Air Flow Rate vs. Intake Air Temperature, 2000 rpm, Base Boost, E0 (gasoline), E10, E20, DI and PFI

Figure 3-6: Air Flow Rate vs. Intake Air Temperature, 2000 rpm, Base Boost, E50, E85, DI and PFI
Several phenomena contribute to the increase in efficiency in DI, and the generally increasing trend with fuel ethanol content:

- **DI Burn Duration**: The location of 50% mass fraction burned and the 10-90% burn duration is plotted in Figure 3-9 and Figure 3-10 vs. spark for all fuels in DI and PFI. Although fuel type doesn't seem to play a significant role, the DI points seem to have ~10% shorter combustion duration than PFI. This could be due to the in-cylinder stratification in DI. Additionally, as will be seen, emissions and engine simulations (GT Power) seem to indicate that although the overall λ was kept at 1, the trapped in-cylinder λ might be a bit rich (~0.97) for DI and slightly lean (1.03) for PFI. This could also be a possible explanation of the difference in burn duration between DI and PFI. Based on engine simulations the difference in burn duration can be translated to about +1% in indicated efficiency.

- **Effective Gamma Effect**: Because of charge cooling, the mixture is colder; therefore its ratio of specific heats (γ) is lower. This can be translated to about +0.5% in efficiency for higher ethanol content. Furthermore, although E85 or E50-air mixtures have about the same expansion γ (after combustion) as gasoline-air mixtures, their compression γ is lower. This effect decreases compression work and improves efficiency [27].

- **Heat Transfer Effect**: Due to charge cooling, peak temperatures are lower in DI for the same intake air temperature. This effect reduces heat losses. Based on GT Power simulations, this can be translated to ~+0.5-1% in efficiency.

- **Combustion Efficiency**: Combustion Efficiency is slightly lower in DI as indicated by higher exhaust carbon monoxide and hydrocarbon emissions. This is probably the result of in-cylinder stratification. Its effect on efficiency is estimated to be about a drop of about 0.5% for DI compared to PFI.

- **Compression-Expansion Work**: If any fuel evaporation takes place after intake valve close (IVC), the polytropic coefficient of the compression process is reduced, therefore improving efficiency. Essentially, this can be thought of as the evaporation making the compression process closer to isothermal. This effect was however small for the experiments presented.

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8 This effect is due to the scavenging effect in a turbocharged engine. During valve overlap, the pressure in the intake is higher than the pressure in the exhaust. Some charge therefore goes straight to the exhaust. In DI where start of fuel injection is after Exhaust Valve Close (EVC), this means that some air doesn't participate in combustion, leading to a richer in-cylinder λ. In PFI, some fuel might be short circuited, going from the intake straight to the exhaust leading to a leaner in-cylinder λ.
in this thesis as even for E85, the biggest part of the evaporation process as will be seen is finished before IVC.

Location of 50% mass fraction burned, 2000 rpm, Base Boost, 20° C Int. Air

Figure 3-9: Location of 50% Mass Fraction burned for all Fuels DI & PFI, 20° C Intake Air, 2000 rpm, Base Boost.

Burn Duration, 10-90% MFB, 2000 rpm, Base Boost, 20° C Intake Air

Figure 3-10: Combustion Duration; 10-90% Mass Fraction Burned for all Fuels DI & PFI, 20° C Intake Air, 2000 rpm, Base Boost.
3.1.2 Fuel Injection Timing Sweep Results

Fuel injection timing can be quite significant in determining performance and emissions characteristics in a DI engine. For the main experimental results presented in this thesis, spark sweeps up to knock, start of fuel injection (SOI) was kept constant and equal to the engine calibration point of 60° CAD aTDC intake. This injection timing, as will be seen, is also close to optimum. For completeness, an injection timing sweep was also performed for all fuels. Spark timing during the injection timing sweeps was held constant at MBT or if MBT was knock limited, at the most advanced point possible. Injection timing effects were also tested for PFI. The NIMEP vs. SOI results for both DI and PFI are plotted in Figure 3-11.

From Figure 3-11, it is clear that there is an optimum fuel injection timing for DI in terms of NIMEP and it is around 60° CAD aTDC SOI. The location of this optimum is the result of the shape of the airflow rate vs. SOI curve presented in Figure 3-12 and the efficiency vs. SOI curve presented in Figure 3-13. PFI NIMEP is generally less sensitive to injection timing. There is however a significant drop in PFI NIMEP for late, essentially open valve fuel injection (Intake Valve opens at ~17 CAD bTDC). This is probably due to some fuel short circuiting-going straight from intake to exhaust during open valve PFI injection.

![NIMEP vs. Start Of Injection for DI&PFI](image)

*Figure 3-11: NIMEP vs. Start of Injection Timing for DI&PFI 20 C Intake Air*
The air flow rate vs. injection timing curve presented in Figure 3-12 is the result of two competing effects: For early injection timing during the intake stroke, the piston is close to the fuel spray which results in a lot of fuel wall wetting and thus lost charge cooling and lower air flow rate. For even earlier injection timing, (e.g. SOI at TDC) there is also fuel being lost to the exhaust as the Exhaust Valve Closes (EVC) at around 20 CAD aTDC. For later injection timing, some of the evaporation might take place after IVC and thus not contribute to increasing airflow. The injection duration ranges from about 37 CAD for gasoline to about 57 CAD for E85.

The efficiency curve presented in Figure 3-13 starts very low for early injection because of fuel escaping directly to the exhaust. Engine operation for injection so early was harsh with high COV of NIMEP values. For fuel injection after IVC, efficiency rises to reach a maximum around an SOI of 60° CAD aTDC. Looking at the 10-90% burn duration in Figure 3-14 it seems to be strongly inversely correlated with efficiency. The maximum efficiency is where the minimum combustion duration is. It is therefore likely that injection timing affects the in cylinder stratification which in turn changes burn duration and efficiency.

![Air Flow Rate vs. Start of Injection](image_url)

Figure 3-12: Air Flow Rate vs. Start of Injection Timing.
Figure 3-13: Indicated Efficiency vs. Start of Injection Timing.
Figure 3-14: 10-90% Mass Fraction Burned Combustion Duration vs. SOI. Data from Two different measurements presented for DI.

The exhaust carbon monoxide (CO) emissions vs. injection timing are presented in Figure 3-15 for DI and PFI. The CO levels are generally low for both DI and PFI indicating good mixing. The PFI levels are so low that they seem to indicate not only good mixing but also slightly lean in-cylinder lambda ($\lambda \approx 1.03$) consistent with the scavenging explanation provided earlier. CO emissions actually drop in PFI for Open Valve injection which further supports the explanation. DI CO emissions indicate in-cylinder stratification which is affected by wall wetting and time available to mix. Notice how most of the DI curves peak close to peak flow rate injection timing (100-150 CAD aTDC SOI) but are low close to minimum burn duration and maximum efficiency (~60 CAD aTDC SOI). It is likely that more homogeneous mixtures burn faster increasing efficiency. Finally, it should be noted that higher fuel ethanol content decreases CO emissions for both DI and PFI.
3.2 Engine Knock Onset Limits

3.2.1 Defining Knock Onset

A methodology needed to be developed to define knock onset. As spark timing is advanced, the following sequence of events is observed:

1. Starting from retarded enough spark timing, no sign of knock is observed.
2. As spark is advanced, the Engine Electronic Control Unit (ECU) detects knock from two knock sensors on the engine block\(^9\) and starts automatically retarding spark. No sign of pressure oscillations visible in the fast sampled in-cylinder pressure trace in Cylinder 3.
3. Automatic spark retard is disabled and spark advanced further. Pressure oscillations begin to be visible. Typical average and worst knocking cycle are plotted in Figure 3-16. A few cycles are knocking lightly. The worst one has a knock intensity of 1.5 bar (KI\(_{max}\))\(^10\). The cycles that knock are the ones where combustion is more advanced than the average and

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\(^9\) The ECU knock sensors are essentially accelerometers detecting block vibrations.

\(^{10}\) Knock intensity (KI) is the peak (single sided) amplitude of the high pass filtered pressure trace.
maximum pressure higher. It also can be seen that the pressure oscillations associated with knock begin about 5 CAD after maximum pressure. 16% is the fraction of cycles with a KI greater than 1 bar – this fraction will hence be called knocking fraction denoted by $k_f$. The mean KI value is based on 100 cycles.

4. Advancing spark further produces pressure traces like the ones presented in Figure 3-17. The oscillations start earlier, closer to maximum pressure. This means that there is more unburned gas available to participate in auto-ignition. Knock intensity therefore has higher amplitudes with a peak ($K_{I_{\text{max}}}$) between 2-4 bar. Furthermore, the knocking fraction, $k_f$ increases. Knock begins to be audible here. This is what would typically be considered knock onset.

5. Advancing knock further starts producing heavy knocking cycles like the one seen in Figure 3-18.

The criterion used to define an operating point as being at knock onset was that the maximum knock intensity ($K_{I_{\text{max}}}$) was more than 2 bar but less than 4 bar. Additionally, it was required that the fraction of knocking cycles (more than 1 bar KI) was more than 10%. As a knocking cycle was defined any cycle with knock intensity more than 1 bar.
To calculate the knock intensity, the pressure trace had to be filtered. A power spectrum obtained from a fast discrete Fourier transform for a knocking and a non-knocking pressure trace is displayed in Figure 3-19. It is clear that the knocking spectrum differs mainly around two peaks: 6.2 KHz and 10.3 KHz which are equal to the first and second cylinder modes calculated based on Draper's formula (Eq. 2) in Chapter 1. The filter consists of a fast discrete Fourier
transform, setting the coefficients of harmonics lower than 2 kHz equal to zero\textsuperscript{11} and performing the inverse Fourier transform. It is essentially therefore, a high pass filter with a response that is 0 below the cut-off frequency and 1 above. The advantage of this method compared to using a transfer function filter is that minimum phase lag is introduced. An example of the original signal, a low pass and a high pass filtered version of it, can be seen in Figure 3-20. It is clear that the filter works well without any visible phase lag.

\[ \text{Power Spectrum} \]

\[ \text{(bar}^2) / \text{kHz} \]

\[ \text{Frequency (kHz)} \]

Figure 3-19: Knocking and Non-Knocking Pressure Trace Power Spectrum.

\textsuperscript{11} The rotational speed is 2000 rpm or 33 Hz; 2 kHz was therefore chosen as a limit beyond which any harmonics are either associated with knock or noise.
3.2.2 Knock Onset Operating Points-2000 rpm and Base Boost Conditions

The knock limited spark advance (KLSA) based on the knock onset criteria presented previously is plotted vs. intake air temperature in Figure 3-21. The y-axis is the difference of the knock limited spark timing from optimum (MBT). It can be seen that with increasing air temperature, the knock limited spark advance is retarded—becomes more limited as expected. Furthermore, DI operating points are generally less knock limited than PFI operating points using the same fuel. This is a result of charge cooling.

Under these conditions in the engine, the only fuels that are knock limited before they reach MBT spark timing for realistic intake air temperatures (up to 50° C) are gasoline in both DI and PFI, and E10 in PFI. For higher ethanol content, spark timing needs to be advanced past MBT to make the engine knock. Engine operation is therefore not limited in terms of efficiency by knock for anything except gasoline and E10. This is because the engine used is a production engine designed for gasoline with a compression ratio of 9.2:1. If the engine were to use higher ethanol content, the compression ratio would naturally be increased to utilize the fuel antiknock qualities. Finally, due to the significant physical (charge cooling) and chemical resistance to knock of E85 in DI, only a single knocking point was obtained without running into the pressure and temperature limits of the hardware.
Although widely used in the automotive industry, KLSA alone is insufficient to describe the phenomena that lead to knock in the context of this thesis. This is due to the significant difference in antiknock properties of the fuels used and the different engine conditions in DI and PFI. This becomes clearer when examining two examples of operating points at knock onset presented in Figure 3-22. The two operational points were obtained for the same fuel—gasoline, at the same rpm and load, at the same intake air temperature—20°C and happen to knock at exactly the same spark timing, 14.25° bTDC. However, as seen in Figure 3-22, the maximum pressure of both the knocking cycle and the average cycle of the DI operating point is significantly higher than that of the PFI operating point. This is due to:

- Evaporative charge cooling increasing air flow rate. More mass is therefore compressed increasing maximum pressure.
- Evaporative charge cooling reducing the peak unburned mixture temperature for the same intake air temperature. The same fuel therefore knocks at higher pressures because the temperatures in the end gas are lower.
Figure 3-22: Average and Knocking Cycles at knock onset for gasoline in DI and PFI. Same intake air Temperature (20° C) and spark (14.25° bTDC).

The main conclusion from Figure 3-22 is that knock limited spark advance is not adequate to describe conditions at knock when different fuels and injection types are involved. As described in Chapter 1, knock depends on the following variables:

- **Pressure history.** As will be seen later it depends much more on the short history before auto ignition which is close to maximum pressure. Maximum pressure is therefore a good proxy for the effect of the whole pressure history.
- **Unburned Mixture Temperature History.** Again, the values shortly before knock around maximum pressure are much more important for knock than the early part of the history. Unlike pressure however, which is directly measured, unburned mixture temperature needs to be calculated from other measurements.
- **Time available for auto ignition:** This depends on engine speed, ignition timing and burn duration. Essentially, it is the time the end gas is subjected to compression before the flame consumes it.

Based on this analysis, it was selected to use maximum pressure to examine knock as it is a much more fundamental parameter than KLSA. As the controlled variable in the experiments was intake air temperature, maximum pressure at
knock onset will first be examined as a function of intake air temperature. Unburned mixture temperature is the result of a calculation, not measured directly and will be introduced later. Time available for auto ignition will be ignored for now. Later, it will be shown that the time available for auto ignition was similar for points that are going to be compared. Available time is also taken into consideration in the knock limit predictive model presented in Chapter 5.

Maximum pressure at knock onset vs. intake air temperature is presented for all the fuels in PFI in Figure 3-23. The maximum pressure values in this plot are the average of all the cycles recorded at an operating point (100 each time) after they had been low pass filtered, regardless if they were knocking or not. For the same fuel, as intake air temperature rises, the engine knocks at lower maximum pressures as expected. Regression fitted lines are also presented in Figure 3-23. Since the points were obtained at knock onset-light knock, each of these lines defines the knock borderline for a fuel blend. This is illustrated in Figure 3-24 for E20. At these speed and load conditions, the engine will be knocking for any intake air-maximum pressure point above the line but not below it. Comparing different fuel lines, it is clear that the addition of ethanol in the fuel blend pushes the knock borderline to higher pressures and temperatures. This effect is primarily due to ethanol chemistry, since little or no charge cooling takes place in PFI. The addition of ethanol however, does show signs of diminishing returns in terms of its chemical anti-knock benefit. Going from pure gasoline to 20% ethanol has a significant impact on pushing the knock boundary. The same is true for going from E20 to E50. Going to E85 from E50 doesn't seem to further improve the knock boundary significantly.

An alternative way of presenting the experimental data is using the average maximum of only the knocking cycles after filtering out the pressure oscillation. Data from the same operating points presented in Figure 3-23 are re-plotted in Figure 3-25 in terms of the average maximum pressure of only the knocking cycles. The average maximum pressure of only the knocking cycles for the same fuel at the same intake temperature is higher compared to the average maximum pressure of all cycles. This is to be expected since it is the cycles where combustion is slightly faster than average and thus reaches higher maximum pressures that knock. In terms of which version of the plot is more representative; both sides could be argued for. Using just the knocking cycles is more representative in terms of the physical phenomenon since knock did not occur in the other cycles. However, because only a fraction of the cycles is knocking and that fraction can be as low as 10%, statistically the average of all cycles is a more robust measurement since only 100 cycles were recorded each time.
Figure 3-23: Average Maximum Pressure at Knock Onset vs. Intake Air Temperature- All Fuels in PFI-All Cycles Used for Average.

Figure 3-24: Knock Border Line Definition.
Maximum pressure at knock onset as a function of intake air temperature is plotted for all fuels in DI in Figure 3-26 using the average of all cycles and in Figure 3-27 using the average of just the knocking cycles. The maximum pressure values are higher than those for port injection of the same fuel due to the additional anti-knock effect of charge cooling. Otherwise, the trends are similar to those in PFI. Higher intake air temperature leads to lower maximum pressures at knock onset for the same fuel and higher ethanol content increases the knock boundary limit to higher pressures and temperatures.

Looking at Figure 3-26, it becomes clearer why there is only a single knocking operating point for DI E85. The engine used has been designed for gasoline. The head gasket therefore isn’t able to handle pressures higher than 100 bar for long. For safety reasons therefore, the maximum pressure in the experiments was limited to 100 bar. An engine that is intended to use ethanol should be designed to handle high pressures to be able to realize the efficiency advantage of the fuel. In terms of going to higher intake air temperatures instead, it was found that the servomechanism of the throttle isn’t able to handle temperatures more than about 125° C. In conclusion, hardware limitations prohibit getting more DI E85 knocking operating points at these speed and load conditions.
Figure 3-26: Average Maximum Pressure at Knock Onset vs. Intake Air Temperature- All Fuels in DI-All Cycles Used for Average.

Figure 3-27: Average Maximum Pressure at Knock Onset vs. Intake Air Temperature- All Fuels in DI-Only Knocking Cycles Used for Average.
The sensitivity of knock onset to intake air temperature can be obtained for each fuel when examining the slope of its knock border line in PFI. The slope of these lines for DI and PFI is presented in Figure 3-28. It is clear that the slope increases with ethanol content until about E50 and remains roughly constant after that. This indicates that the sensitivity of knock to intake air temperature increases with ethanol content. This is a well known fact in the fuel industry. One measure of the knock sensitivity of a fuel to intake air temperature is the fuel sensitivity, K, calculated as the difference between the Research and Motor octane tests. This is because the tests are conducted at very different intake air temperatures. K increases significantly with ethanol content indicating an increasing sensitivity to intake air temperature [57].

Finally it should be mentioned that knock is a semi-stochastic phenomenon. Furthermore, it is influenced by ambient conditions, especially humidity. Given the above, the experiments presented here had good repeatability as indicated by the point tested the most-DI gasoline 20°C intake air. This test was repeated 6 times on different dates. As seen in Figure 3-26 and Figure 3-27, the maximum pressure only varies by ±2 bar when the average of all cycles is used. The variation decreases when the average of only the knocking cycles is used.

![Figure 3-28: Slope of the Knock Boundary Lines-Sensitivity of Knock to Temperature.](image)
3.2.3 Knock Onset Operating Points-Different Speed and Load Conditions

For completeness, spark sweeps up to knock were also performed at different rpm and loads. These tests were performed for three fuel blends in PFI and DI:

- E0 using 30°C intake air
- E50 using 100°C intake air
- E85 using 120°C intake air

Two different load levels were tested:

- With the throttle wide open, setting the pulse width duty cycle to the waste gate actuator to 50% to actively close it. This resulted in increasing manifold air pressure (MAP) and NIMEP by 10-15% compared to base boost conditions (0% duty cycle).
- Closing the throttle down to 35%. This produces MAP slightly below atmospheric. Only gasoline knock data were obtained at these conditions as spark advance for getting E85 to knock was already significantly over advanced at base boost conditions.

The MAP and NIMEP at knock onset for the different load conditions are presented in Figure 3-29. The knock limited spark advance in Figure 3-30 and the maximum pressure at knock in Figure 3-31.

![NIMEP at Knock vs. MAP](image)

Figure 3-29: NIMEP vs. MAP at Knock Onset
It is clear from Figure 3-30 that knock limited spark advance becomes more retarded at higher load. This is because pressures and temperatures increase with load as air flow rate increases and more mixture mass is compressed. The maximum pressure at knock displayed in Figure 3-31 increases with load. One way to explain this is that because spark timing is more retarded at higher loads, pressure (and temperature) needs to be higher for the end gas to auto-ignite as there is less time available before the flame consumes it.

**Figure 3-30: Knock Limited Spark Advance vs. Manifold Air Pressure.**
The maximum pressure at knock onset is presented in Figure 3-32 vs. rotating speed. It can be seen that the minimum required maximum pressure to get the engine to knock is at the lowest speed tested-1750 rpm. Lowering rpm has two effects on knock: First, time available for the end gas to auto-ignite before it is consumed by the flame increases. This increases the chances of knock occurrence. Second, heat transfer per cycle increases at lower rpm, cooling the end gas and decreasing the chances of knock [1]. The worst rotating speed in terms of likelihood of knock occurrence is anywhere from 1500 rpm to 2500 rpm in modern engines. For the speeds tested, the worst was 1750 rpm.
Figure 3-32: Maximum Pressure at knock vs. RPM
4. Results- How Much Charge Cooling Takes Place?

4.1 Experimental-Using Knock as a Diagnostic.

4.1.1 How much does the air need to be heated to cancel out charge cooling due to fuel evaporation?

As explained in Chapter 1, the main method used to experimentally measure how much charge cooling takes place due to fuel evaporation is using knock as a diagnostic. Essentially, the method consists of trying to answer the question: “How much does the intake air need to be heated when the engine is in DI mode to make it knock at the same conditions as PFI?” With this in mind, let’s combine Figure 3-23 with Figure 3-26 and Figure 3-25 with Figure 3-27 to compare maximum pressure at borderline knock versus intake air temperature for DI and PFI. Figure 4-1 is thus obtained when using just the knocking engine cycles and Figure 4-2 when using all recorded engine cycles at knock.

Using these combined plots, the difference in intake air temperature at the same maximum pressure for the same fuel can be obtained as indicated by the arrows in Figure 4-2. This difference essentially answers the question: “How much did the engine need to be heated in DI to cancel out the charge cooling effect and make the engine knock at the same conditions as in PFI mode?” In other words, this is how much charge cooling took place due to fuel evaporation in DI. The DI and PFI lines are generally parallel so it doesn’t matter too much which maximum pressure (which PFI base air temperature) is used to compare DI to PFI. The only exception is E20 where a large range of intake air temperature data (from 20°C to 100°C) was obtained without running into hardware limitations (peak pressure) or extremely retarded spark. The PFI and DI lines for E20 seem to diverge a bit at higher intake air temperatures. The divergence of the lines means that the realized charge cooling increases with air temperature. This is to be expected to some extent, as hotter intake air makes evaporation easier and thus reduces the chances of fuel wall wetting. The difference in intake air temperature at the same maximum pressure at knock vs. ethanol content is plotted in Figure 4-3. This is the amount of charge cooling realized due to fuel evaporation in DI for each of the five blends. The comparison was performed at the mid point of the lines. The error bars indicate the spread when different maximum pressures (different PFI intake air temperatures) were used for the comparison.
Figure 4-1: Max Pressure at borderline knock vs. intake air temperature for five blends in DI and PFI. Only knocking engine cycles used.

Figure 4-2: Max Pressure at borderline knock vs. intake air temperature for five gasoline/ethanol blends in DI and PFI. All recorded engine cycles used.
Figure 4-3 shows the estimate of the charge cooling realized in the engine as a function of ethanol content in the fuel. Two estimates are presented: One obtained using the average maximum pressure of all cycles and one using just the knocking cycles. The estimates do not vary significantly. The numbers based on the knocking cycles alone will be used for the rest of the thesis and can be seen in Figure 4-4. Since the test is based on using knock as a diagnostic, using the average of just the knocking cycles is probably more representative. As expected, the amount of charge cooling realized generally increases with ethanol content as the fuel heat of vaporization increases as well.

\[
(T_{\text{intake,DI}} - T_{\text{intake,PFI}}) \text{ at Knock}
\]
\[
(\text{Same } P_{\text{max}})
\]

Figure 4-3: Difference in Intake Air Temperature to make DI knock at the same Maximum Pressure as PFI-Cancel Charge Cooling.
Figure 4-4: Difference in Intake Air Temperature to make DI knock at the same Maximum Pressure as PFI-Cancel Charge Cooling.-Only knocking cycles used.

The only exception to the rule that the ΔT realized due to charge cooling goes up with ethanol content, appears to be E20. The ΔT realized for E20 seems to be lower than that of E10. This is the case when the comparison of DI to PFI is performed at the midpoint of the lines in Figure 4-1 (at 52°C intake air for PFI E10-70°C for DI E10 and 60°C PFI E20 -76°C DI E20). When the comparison of DI to PFI is performed at higher intake air temperatures, the ΔT for E20 as expected is more than E10. The minimum ΔT due to charge cooling for E20 is 13°C for PFI intake air temperature of 30°C. For 100°C intake air temperature the ΔT increases to 20°C. It should be noted that as ethanol content increases on one hand there is more heat to be extracted. On the other, heat and mass transfer limitations to make that happen are increasing, so charge cooling lost to fuel wall wetting is more likely. With all of the above in mind, the experimental results in Figure 4-4 are quite reasonable.

Dividing the ΔT due to charge cooling numbers in Figure 4-4 by the thermodynamic maximum for each fuel presented in Table 1, Chapter 1, the charge cooling realized is presented as a fraction of the maximum theoretical for each blend in Figure 4-5. Looking at Figure 4-5, the charge cooling realized for all fuels seems to be between 70 and 80% for all blends except E20. For E20 we can see the effects of a wide intake air temperature range where the comparison was performed in Figure 4-1. For the higher intake air temperatures (the upper
end of the error bar); the fraction of charge cooling realized for E20 is also around 73%.

It is counterintuitive that the fractions of charge cooling realized for E50 and E85 are at about the same level as lower ethanol blends. At higher ethanol content it would be expected that the fraction of charge cooling realized decreases significantly and heat and mass transfer become more limiting. On the other hand, looking back at Figure 4-1, the knock results for E85 and E50 were obtained at significantly higher intake air temperatures compared to the other blends. The hotter air used for higher ethanol content makes fuel evaporation easier and might have affected the charge cooling results. This phenomenon however is due to the hardware limitations of the particular test engine used. In an engine built to be able to withstand the higher pressures required to make E85 knock at lower temperatures, this secondary phenomenon would be significantly reduced. The fraction of the charge cooling realized for higher ethanol content would probably then decrease significantly. CFD is used later in the thesis to quantify how significant is the effect of intake air temperature.

![Fraction Thermodynamic Max](image)

Figure 4-5: Fraction of the Thermodynamic Maximum Charge Cooling Due to Fuel Evaporation Realized in the Test Engine.

It was shown how by comparing DI vs. PFI intake air temperature for the same maximum pressure, the "effective" difference in air temperature due to fuel evaporation charge cooling between DI and PFI can be measured. However, it should be noted that what this method measures is not exactly the same as the
amount of charge cooling due to fuel evaporation that took place in DI mode. The method measures the difference between DI and PFI: In fact, PFI might not be at 0% charge cooling. The literature seems to suggest that there might be 0-30% charge cooling compared to the thermodynamic limits (Table 1, Chapter 1). However, from an engineering standpoint, what is of interest is the difference between DI and PFI-how much improvement was feasible from PFI due to DI, not the comparison to theoretical limits.

Finally, it should be discussed why in using knock as a diagnostic; DI was compared to PFI only by equilibrating maximum pressure. As explained in Chapter 1, the conditions that affect knock are:

1. The history of temperature versus time of the end gas.
2. The history of pressure versus time of the end gas.
3. The time needed for the flame front to consume the end gas. This depends on spark timing and flame speed.

As will be seen in Chapter 5, the last crank angle degrees before knock are much more important than the early part of the end gas pressure and temperature history in terms of causing auto ignition. Additionally, it will be seen that even more important are the conditions at maximum pressure and temperature. Therefore, using the maximum pressure to represent all of the compression history of the end gas is a sensible approach. In terms of the unburned mixture temperature, it will be proven in chapter 5 that for the same fuel, the maximum pressure is a good proxy for the maximum unburned mixture temperature too, independent of fuel injection type. In conclusion, it can be said, that for the same fuel in the same engine, when the maximum pressure of the end gas is the same in DI and PFI, it was subjected to similar compression histories in terms of pressure and temperature. Therefore, it is reasonable to look only at the same maximum pressure to use knock as a diagnostic.

This leaves only one more parameter to worry about: Time. Spark timing was not explicitly held constant during this experiment, therefore it should be examined whether auto ignition had the same amount of time available to develop in DI and PFI. To address this question, the crank angle degree at which maximum pressure occurs is plotted in Figure 4-6 against maximum pressure for the operating points of 1. Since all the points were obtained at the same speed, 2000 rpm, crank angle degree translates directly to time. It is clear from these figures that for the same fuel and the same maximum pressure, the crank angle of maximum pressure is at most less than 2 crank angle degrees apart. To illustrate this fact with an example, the average pressure trace of all knocking cycles for E0 in PFI using 20°C intake air and in DI using 34°C intake air are compared at knock onset in Figure 4-6. These two operating points have almost the same maximum pressure. It is clear from Figure 4-6 that when the maximum pressure at knock is the same for the same fuel in DI and PFI, the position of the maximum and the shape of the pressure traces is going to be about the
same. This validates looking at just the maximum pressure to use knock as a diagnostic.

**Pmax Position (θ) at Knock**

![Graph showing Pmax Position (θ) at Knock](image)

Figure 4-6: Maximum Pressure Crank Angle Degree after TDC vs. Maximum Pressure

**DI and PFI Pressure Traces [Knocking Cycle Average] at same Pmax**

![Graph showing DI and PFI Pressure vs. CAD at the same Pmax](image)

Figure 4-7: DI and PFI Pressure vs. CAD at the same $P_{\text{max}}$. 
4.2 Using Computational Fluid Dynamics to Calculate Charge Cooling.

4.2.1 Motored Flow Case

Initially, a simplified test case was run without any fuel being injected. The boundary conditions used for this case were an experimental manifold air pressure vs. crank angle profile with a mean of 1.36 bar and a constant temperature of 200°C. The rotational speed was 2000 rpm. The wall temperatures were set to 400K for the piston crown and cylinder walls and 450 for the cylinder head walls. Figure 4-8 shows the resulting flow field at 120 crank angle degrees before TDC. Figure 4-9 shows the in-cylinder temperature distribution at 20 degrees before TDC.

![Figure 4-8: CFD Results for "Motored" Case: Velocity Field 120 CAD bTDC](image)

Figure 4-8: CFD Results for "Motored" Case: Velocity Field 120 CAD bTDC
It is clear from Figure 4-8, that this engine has been designed with significant tumble. In fact, the strategy used to minimize wall wetting and ensure longer times for the fuel and air to mix is to spray the fuel in the direction of the tumbling vortex. This will become clearer after looking at the results with fuel injection. Also, looking at Figure 4-9, it is clear that without any fuel injection, the in-cylinder temperature is uniform with thin boundary layers around the time of spark. Most of the charge temperature is between 652 K and 679 K except for the thermal boundary layers that were between 625 K and 652 K.

4.2.2 High Load Mixing Calculation, Ethanol and Isooctane.

To establish a worst case scenario in terms of fuel evaporation and mixing, two CFD cases were run with fuel injection at 1.8 bar MAP and 2000 rpm. This is because as explained in Chapter 1, higher engine load makes fuel evaporation and mixing more challenging. These simulations included fuel injection and mixing but not combustion. In the first CFD case, isooctane (C8H18) was injected as a proxy for gasoline. In the second, pure ethanol was injected. The amount of fuel injected in each case was the amount required to keep the mixture at stoichiometric overall. The start of injection is 55 CAD after TDC intake in both cases. Fuel pressure was 10 MPa, Injection duration was 70° CAD for 82 mg of C8H18 injected and 120° CA for 136 mg of C2H5OH. These conditions are representative of actual engine injection strategies.

The fuel spray droplets for the isooctane case are shown at three time instances: 60 CAD after TDC intake, 120 CAD after TDC and BDC in Figure 4-10, Figure 4-11 and Figure 4-12. For the ethanol case, spray images at the same CAD can be seen in Figure 4-13, Figure 4-14 and Figure 4-15. The droplet size has been
scaled up for viewing purposes. The color of the droplets shows their temperature.

Figure 4-10: CFD Results: Fuel Spray Imaging at 60 CAD a TDC Intake-C8H18 Direct Injection, 1.8 bar MAP, 2000 rpm. Start of Injection was 55 CAD aTDC.

Figure 4-11: CFD Results: Fuel Spray Imaging at 120 CAD a TDC Intake-C8H18 Direct Injection, 1.8 bar MAP, 2000 rpm.
Figure 4-12: CFD Results: Fuel Spray Imaging at 180 CAD a TDC Intake (BDC)-C8H18 Direct Injection, 1.8 bar MAP, 2000 rpm.

Figure 4-13: CFD Results: Fuel Spray Imaging at 60 CAD a TDC Intake-C2H5OH Direct Injection, 1.8 bar MAP, 2000 rpm. SOI was 55 CAD a TDC.
Figure 4-14: CFD Results: Fuel Spray Imaging at 120 CAD a TDC Intake-C2H5OH Direct Injection, 1.8 bar MAP, 2000 rpm. SOI was 55 CAD a TDC.

Figure 4-15: CFD Results: Fuel Spray Imaging at 180 CAD a TDC Intake-C2H5OH Direct Injection, 1.8 bar MAP, 2000 rpm. SOI was 55 CAD a TDC.

The first main thing that is clear from the spray images, that the design concept in this engine for improving fuel air mixing and avoiding wall wetting is spraying the fuel in the direction of the tumbling vortex. The fuel droplets are thus carried
along by the airflow vortex instead of colliding into the cylinder wall. As a result, the fuel has more time to evaporate and mix. Without the tumbling vortex, the droplets would only have about 50-60 CAD to evaporate before they reach the wall in a straight trajectory. The second thing that is evident from the spray images is that in the case of ethanol injection, there is a lot more fuel present at the same time instant. This is of course due to the fact that more fuel was injected, but also because evaporation heat and mass transfer is more challenging in the case of ethanol. This becomes clearer in Figure 4-16 where the injected, evaporated and liquid film masses are shown as a function of CAD.

As seen from Figure 4-16, wall wetting is significant in the case of ethanol but negligible in the case of isooctane as indicated by the fuel mass in liquid films on the walls. This fact has a significant effect on the amount of charge cooling realized due to fuel evaporation as will be seen. Most of the liquid film on the wall forms on the cylinder wall on the exhaust side from droplets that did not get carried along by the tumbling vortex and continued their course to hit the wall. This is evident in Figure 4-17 where the film mass distribution on the wall can be seen. The two areas of high concentration are due to droplets from two out of the six holes of the injector.

![Figure 4-16: Evaporation History and liquid fuel films as a result of wall wetting for ethanol and isooctane in the 1.8 bar MAP, 2000 rpm case](image_url)
A significant difference in evaporation time between ethanol and isooctane can be seen in Figure 4-16. This is of course due both to the higher amount of fuel in the ethanol case, but also to the more challenging heat and mass transfer. In the case of isooctane it takes 80 CAD from start of injection to evaporate 90% of the fuel. Evaporation is completed long before intake valve close (IVC). In the case of ethanol, it takes 180 CAD to 90% evaporated, which happens after IVC. Even in the ethanol case however, 78% of the evaporation takes place during intake, before IVC.

To establish an upper limit on how much charge cooling due to fuel evaporation can take place, a modified version of the ethanol injection model was run. In this case, labeled “films off” in the plots, the fuel spray-wall interaction model was modified so that all the fuel droplets impinging on the wall have to bounce back into the flow. The amount of heat transfer from the walls is thus minimized and charge cooling maximized. However, as can be seen from Figure 4-16, the resulting evaporation time is significantly longer. It is in fact so long that the fuel doesn’t all evaporate even at TDC compression. About 22% of the fuel remains in the liquid phase at TDC. This result should be taken into consideration when examining the differences in in-cylinder average charge temperature that can be seen as function of CAD in Figure 4-18 for the three cases: C8H18 films on, E100 films on and films off.
From Figure 4-18 it can be seen that compared to the isooctane case which has little charge cooling lost due to wall wetting, the peak charge temperature in the realistic (films on) ethanol case, is 52° colder. Assuming that the full charge cooling potential was realized for isooctane (i.e. 34° at TDC based on Eq. 4, Chapter 1), and adding that to the difference in max temperature between isooctane and realistic ethanol (52° K), we get 86° at TDC compared to a no charge cooling baseline. Assuming polytropic compression (with a y of 1.31) this temperature difference translates to 47 degrees during intake. Since for both cases, most of the evaporation finished before IVC as seen in Figure 4-16, using the polytropic was a reasonable assumption. The end conclusion is that ethanol at 1.8 bar MAP, ambient temperature air case realized the equivalent of 47° K of charge cooling during intake.

The maximum temperature for the isooctane case compared to the ideal ethanol case is 98° higher at TDC. However, as already explained, not all of the fuel was evaporated at TDC for the ideal ethanol case. Dividing this temperature difference by the fraction of fuel that evaporated over the total fuel injected (78%) gives 125 °K. Adding to that the difference of the isooctane from the no charge cooling baseline (34°) results in 159°. This is the temperature difference of the ideal ethanol case from a no charge cooling baseline at TDC. This result is close to the theoretically calculated 149° K difference for ethanol from a no charge
cooling baseline at TDC (Eq. 4, Chapter 1) at TDC. This confirms that the CFD results are physically reasonable.

The in-cylinder temperature distribution for the isooctane case at 20 CAD bTDC (around spark) can be seen in Figure 4-19. It is clear from the figure that the mixture is fairly homogeneous in the isooctane case as most of the charge is between 612 and 636 K with a small part of the gas being between 590 and 611 K. The composition distribution for isooctane was also very homogeneous.

The temperature distribution for the ethanol case at 20 degrees bTDC (around spark) can be seen in Figure 4-20 and the mass fraction distribution in Figure 4-21. Compared to the isooctane case, the mixture for ethanol is significantly more stratified. In terms of temperature, the hottest parcel is ~60K hotter than the coldest. In terms of composition; the overall mixture average is equal to the stoichiometric mass fraction of 0.1. The richest parcel (0.18) has almost double the fuel mass fraction than the leanest (0.092). The composition and temperature distributions are inversely correlated. The richest fluid parcel is the coldest. This seems to indicate that the temperature stratification is mostly due to fuel evaporation.

Figure 4-19: In cylinder Temperature distribution, isooctane, DI 1.8 bar MAP, 2000 rpm, 20 CAD bTDC.
Figure 4-20: In cylinder Temperature distribution, Ethanol, DI 1.8 bar MAP, 2000 rpm, 20 CAD bTDC.

Figure 4-21: In cylinder Fuel Mass Fraction distribution, Ethanol, DI 1.8 bar MAP, 2000 rpm, 20 CAD bTDC.
4.2.3 Base Boost Mixing Calculation, Ethanol and Isooctane.

In order to examine the mixing processes at conditions more relevant to the bulk of the experimental results, two new CFD cases were run for ethanol and isoctane. Same as in the 1.8 bar MAP case, these simulations included fuel injection and mixing but not combustion. The conditions were:

- 1.36 bar Manifold Air Pressure (base boost conditions)
- 2000 rpm
- Intake air temperature: 20° C for the first case (isoctane and ethanol), 120° C for the second (just ethanol)
- Start of Injection: 56 a TDC intake for both
- Pulse duration: 38 CAD at 2000rpm for isoctane, 65 CAD for Ethanol.
- Injection pressure was 11.9 MPa for both
- Total fuel mass injected was 52 and 76mg/cycle for isoctane and ethanol at 20° C and 102mg for ethanol at 120° C

These conditions were picked to be closer to the bulk of the “knock as a diagnostic” experimental results which were performed at ~1.36 bar MAP. Isooctane is used as a proxy for gasoline and ethanol as a proxy for E85. Because in the experiments heating the intake air up to 120° C was used to make E85 knock, both 120° C and 20° C intake air was used in the CFD to estimate the differences in mixing and charge cooling due to evaporation between the conditions of the experiment (120° C air) and more realistic intake air temperatures (20° C air).

From Figure 4-22, it can clearly be seen that load and air temperature have a significant effect on total fuel wall wetting. Going from 1.8 bar MAP to 1.36 bar MAP reduces the amount of wall wetting significantly. This is mainly due to the injection time being shorter, which causes fewer droplets to hit the wall since injection timing was held the same. In a real engine, optimum injection for higher load would probably have to be earlier. Increasing the intake air temperature from 20° C to 120° C also decreases the amount of wall wetting significantly for ethanol as evaporation is much easier. For isoctane, wall wetting is small even for the high load (1.8 bar MAP) case but becomes even smaller when the load decreases.
The evaporation history for ethanol at 1.36 bar MAP for 20°C and 120°C air is depicted in Figure 4-23. In the 1.36 bar 20°C air case, evaporation starts faster compared to the 1.8 bar 20°C air case. This is because there is less fuel around in the lower load case. Subsequently however, the evaporation process slows down in the 1.36 bar MAP case compared to the 1.8 bar MAP case. This is because of the reduced wall wetting compared to the higher load case and also because the air temperatures in the higher load case are higher due to more mass being compressed. Conduction heat transfer from the walls to the liquid fuel film is generally faster than convection from the air to the droplets. Compared to the 20°C cases, in the 120°C air case, evaporation starts much faster because the air is much hotter. The process however slows down a lot towards the end, since wall wetting is minimal compared to the other cases. In all cases, around 80% of the fuel has evaporated by intake valve close.
Figure 4-23: Evaporation history for Ethanol for 20°C and 120°C air-1.8 bar and 1.36 bar MAP. 

The average charge temperature vs. crank angle degree is presented in Figure 4-24 for 120°C and 20°C intake air for ethanol injection at 1.36 bar MAP. In order to get a good baseline for no or little charge cooling due to fuel evaporation, the two cases were also run with the wall impingement model artificially making all impinging fuel droplets stick to the walls. The results for 20°C and 120°C intake air are also displayed in Figure 4-24 labeled as “stick”. As a result of the absence of charge cooling, the “stick case” is 100 K hotter at TDC than the realistic case (labeled ‘film model’ in the figure) when the intake air starts at 20°C and 145 K hotter when the intake air starts at 120°C. Assuming polytropic compression, these numbers can be translated to equivalent numbers before compression (intake numbers). For the cold intake air case, this results in 55 K of temperature difference due to charge cooling before compression. For the hot intake air case, the result is 79 K of charge cooling before compression. Clearly, the higher amount of wall wetting due to slower initial evaporation in the 20°C case resulted in less charge cooling.
Figure 4-24: Average Charge Temperature for Ethanol Injection with 20°C and 120°C Intake air.
The results, in terms of charge cooling for the three cases are summarized in Table 5 and Figure 4-25. It is clear that for the high intake temperature (120 °C) air, base boost (1.35 bar) conditions, almost the full charge cooling potential is realized for DI ethanol (79 °K ΔT). Going to 20 °C intake air, temperature reduces the ΔT realized to 55°K -67% of the thermodynamic upper limit. Increasing the load to 1.8 bar MAP, decreases the ΔT achieved due to charge cooling to 45 K-58% of the thermodynamic upper limit. For isoctane as a proxy for gasoline, it was already shown that fuel wall wetting was minimal and the full charge cooling potential is realized.

Table 5: CFD Results for Charge Cooling at TDC and intake vs. No Charge Cooling Baseline.

<table>
<thead>
<tr>
<th></th>
<th>Upper Limit E100</th>
<th>1.35 bar E100 120 C air</th>
<th>1.35 bar E100 20 C air</th>
<th>1.8 bar E100 20 C air</th>
</tr>
</thead>
<tbody>
<tr>
<td>at TDC [K]</td>
<td>149</td>
<td>145</td>
<td>100</td>
<td>86</td>
</tr>
<tr>
<td>at intake [K]</td>
<td>81</td>
<td>79</td>
<td>54</td>
<td>47</td>
</tr>
<tr>
<td>% of Upper Limit</td>
<td>---</td>
<td>97%</td>
<td>67%</td>
<td>58%</td>
</tr>
</tbody>
</table>
The CFD results can be used to estimate the effect of using hot intake air in the experiments to make E85 knock as well as the effect of different engine loads. The former seems to be more important than the latter. The CFD results however are not directly comparable with the experiment as the experiment measures the difference in charge cooling from PFI, not from a no charge cooling baseline. The closest CFD test case to the E85 experiment is at 1.35 bar MAP intake, 120 °C intake air. The CFD concluded that almost all of the theoretical charge cooling was realized in this case. The experimental result was 71% (compared to PFI, not the theoretical limit) (Figure 4-5). This implies that 29% charge cooling took place in PFI.
4.3 How much charge cooling takes place-Conclusions.

The conclusions from the experiments and CFD simulations looking at how much charge cooling takes place can be summed up as follows:

1. Using knock as a diagnostic, the difference in charge cooling between DI and PFI can be measured.
2. Looking at the difference in intake air temperature needed to make DI knock at the same maximum pressure as PFI for the same fuel is a sufficient way to do that. This is the case because equilibrating the maximum pressure at knock for the same fuel means that to a good approximation the end gas in DI and PFI was subjected to similar pressure and temperature histories.
3. The charge cooling realized increases as a function of ethanol content.
4. The charge cooling realized as a fraction of the thermodynamic maximum, generally stays about constant with ethanol content.
5. Because due to hardware limitations, high intake air temperatures were used to make higher ethanol blends knock, the measured charge cooling for E50 and E85 is probably optimistic compared to real world engine conditions. This is because hot intake air promotes faster evaporation.
6. Using CFD, the effect of intake air temperature on charge cooling realized can be quantified. For injection of ethanol into 120° C air, the charge cooling realized is equal to the thermodynamic upper limit. For 20° C air, it drops to 67% of that limit.
7. It is therefore expected that if the hardware were able to test (make ethanol knock) at ambient intake temperatures, the charge cooling realized as a fraction of the thermodynamic maximum, would decrease with ethanol content.
8. Using CFD, the effect of higher load can be quantified. Going from 1.35 bar MAP to 1.8 bar decreases the charge cooling realized from 67% of the upper limit to 58%.
9. Using CFD it can be seen that in cylinder stratification is modest for gasoline but significant for ethanol.
5. Analysis: Knock Limit Predictive Model

The first step in developing a knock limit predictive model is estimating what the unburned mixture temperature $T_u$ was as a function of crank angle. The unburned mixture temperature along with the experimentally measured pressure trace can then be used to examine the chemical kinetics of auto-ignition that causes knock. However, unburned mixture temperature is very difficult to measure. A 1-D gas dynamics and thermodynamics engine simulation code (GT-Power) was employed therefore to calculate $T_u$.

5.1 GT-Power Modeling Methodology and Results.

5.1.1 GT-Power Modeling Methodology

The following process was used to tune the GT-Power model to the experimental engine results for each operating condition:

1. The fuel properties were varied and it was ensured that the proper amount was injected to keep the mixture at stoichiometric.

2. Using the experimentally acquired pressure trace and the Rassweiler-Withrow heat release rate analysis, the mass fraction burned vs. CAD curve was extracted for Cylinders 1 and 3. These profiles were used in the GT Power code. Cylinder 2 was assumed to have the same burn profile as Cylinder 3. Similarly, Cylinder 4 was assumed to be the same as Cylinder 1, as their heat transfer characteristics are the same. Since the model results would be used to predict knock in Cylinder 3, the pressure trace used to extract the burn profile of Cylinder 3 is the average of just the knocking cycles.

3. With the throttle set to wide open, the waste gate position was adjusted until the resulting flow rate and MAP are within $\pm 3\%$ of the experimentally measured.

4. Charge cooling is set to match the experimental results from Chapter 4. Since the experiments described in Chapter 4 measured the difference in charge cooling between DI and PFI, PFI charge cooling was set to 10% in all cases and DI adjusted to match the results of chapter 4.

5. The heat input from the heater in the model is adjusted so that the intake air temperature matches the experimentally measured at the intake port. Waste gate readjusted if needed.

6. The combustion efficiency and heat transfer are adjusted to match the experimental pressure traces with a maximum error $+1.5$ bar (usually at
maximum pressure). Combustion efficiency was adjusted between 93-97%. Heat transfer based on a Woschni correlation tuned for this engine by GM for gasoline, was adjusted ±5%.

In the end, every simulation needs to match the following experimentally measured variables:

- Airflow rate ±5%
- MAP ±2.5%
- Temperature at the intake port ±2°C
- NIMEP ±2.5%
- Pressure trace: maximum error: 1.5 bar

A typical example of experimentally measured (only knocking cycle average) and the results of the GT Power simulation are presented in Figure 5-1. It is clear that the GT Power simulation results match the experimental pressure trace very well.

![Figure 5-1: Comparison of Experimental Data and GT Power Simulation Results.](image)

**5.1.2 Selecting Operating Points to Model.**

From the operating points at borderline knock at 2000 rpm and base boost conditions presented in chapter 4, at least 3 different intake air temperature points were picked for every blend and injection type (DI-PFI). These points were modeled in GT Power and used in the knock limit model. The only exception was of course DI E85 where only one borderline knock point existed at base boost and 2000 rpm. Additionally, all the different rpm and load points presented in
Chapter 4 were also used. The total number of operating points used for the GT Power simulation and knock limit model was 42.

5.1.3 GT-Power Model Results.

The maximum pressure at knock is plotted in Figure 5-2 against the maximum unburned mixture temperature for the base boost, 2000 rpm operating points. For the same fuel, higher maximum temperatures lead to lower pressures. This is reasonable as both higher pressure and temperature promote fuel auto-ignition and thus knock. Increasing one would mean therefore that the other needs to be decreased to remain at borderline knock conditions.

The most important conclusion from Figure 5-2 is that borderline knock maximum pressure and unburned mixture temperature conditions seem to depend on fuel blend alone and not injection type. In fact, if the DI and PFI points for the same fuel are grouped together in Figure 5-3, regression lines can be fitted with high \( R^2 \) values Figure 5-2. This implies that for the same fuel DI and PFI knock onset limits follow the same relationship. The explanation for this phenomenon is the following:

- Because the operating points were all obtained for the same engine speed and the location of maximum pressure at knock doesn’t depend on injection type as seen in Chapter 4, the time available for the flame front to consume the end gas is the same for DI and PFI for the same fuel. This is the \textit{time available} for auto-ignition to occur and cause knock. The \textit{available time} for DI and PFI is therefore the same at the same \( P_{\text{max}} \).

- The time to auto-ignition of the end gas as will be seen depends on the pressure and temperature near the maximum much more than the early part of the end gas compression history. The \textit{induction time, the time it takes to auto-ignite} as defined in [58] therefore, mostly depends on pressure and unburned mixture temperature conditions close to maximum.

- \( P_{\text{max}} \) and \( T_{u,\text{max}} \) pairs consequently define borderline knock conditions that are unique for each fuel and don’t depend on injection type. It doesn’t matter what was the initial air temperature, air flow rate or how much charge cooling took place. If the \( P,T \) conditions close to maximum are the same and on the borderline knock boundary, the engine will be knocking.

- This result verifies using just the same constant maximum pressure at knock to compare DI to PFI (in order to measure charge cooling).

Furthermore, it can be observed from Figure 5-2 that E 50 and E 85 have the same \( P_{\text{max}}-T_{u,\text{max}} \) knock borderline. This can clearly be seen by the high \( R^2 \) value of the linear fit through the grouped E50 and E85 data in Figure 5-3. This implies that the antiknock performance of the two blends is the same.
However care should be taking when interpreting the antiknock performance of a fuel and an injection type from the borderline knock $P_{\text{max}}-T_{\text{u,max}}$ boundary. The fact that DI and PFI knock at the same end gas maximum $P,T$ doesn't mean that they will perform equally well in terms of preventing engine knock. The $P_{\text{max}}-T_{\text{u,max}}$ boundary shows under which end conditions a fuel blend auto-ignites for a given rpm (available time). It is therefore a chemical property of a fuel blend and there is no reason why it should be different between DI and PFI. The $P_{\text{max}}-T_{\text{u,max}}$ boundary however does not include the effect of charge cooling. It doesn’t say anything about how the end gas got to these conditions. Indeed from Figure 4-2 it was seen that in DI the engine started from higher intake air temperature to end at the same maximum pressure due to charge cooling. Conversely, it was shown in the same figure that for the same intake air temperature and MAP, the engine in DI achieved higher maximum pressure at knock. DI does have an advantage in preventing knock. This effect is not captured by the $P_{\text{max}}-T_{\text{u,max}}$ results. Similarly, although they seem equivalent in the terms of chemical antiknock performance, E85 does have an advantage in preventing knock compared to E50 if used in a DI engine so that the charge cooling benefit is realized. A methodology to quantify and separate the thermal (charge cooling) effect from the purely chemical is clearly needed.

\[ \text{Pmax at knock vs. Tu max, 2000 RPM, Baseboost} \]

![Graph showing Pmax vs. Tu_max for different fuel blends at 2000 RPM](image)

Figure 5-2: Maximum Pressure at Borderline Knock vs. Maximum Unburned Mixture Temperature.-Base boost Conditions 2000 rpm

\[ ^{12} \text{Unless there was a lot of mixture non-uniformity in DI or if flame speeds were significantly different, neither of which seems to be the case.} \]
Figure 5-3: Maximum Pressure at Borderline Knock vs. Maximum Unburned Mixture Temperature—Regression Fitted Lines.

The air flow rate at knock is plotted as a function of maximum pressure in Figure 5-4. For the same maximum pressure at knock, air flow rate doesn’t seem to depend significantly on injection type (DI-PFI). This becomes even clearer in Figure 5-5, where the DI and PFI have been grouped together. Although the DI and PFI points for similar maximum pressures were obtained at very different intake air temperatures, the difference intake air temperature was offset by charge cooling. This further validates the methodology used to measure charge cooling in Chapter 5.
Figure 5-4: Air flow rate vs. Max Pressure at Borderline Knock, 2000 rpm, Base Boost

Figure 5-5: Air flow rate vs. Max Pressure at Borderline Knock, 2000 rpm, Base Boost, DI and PFI grouped together.
The maximum unburned mixture end gas temperature is plotted as a function of intake air temperature in Figure 5-6. It is evident from Figure 5-6 that higher intake temperatures result in higher maximum unburned temperatures as expected. However, as intake temperature increases, knock limited spark advance is retarded as seen in Figure 3-2. The end gas is thus compressed to lower maximum pressures for higher intake air $T$. As a result, for the same fuel and injection type, the difference in maximum unburned mixture temperature between two points at borderline knock is less than their difference in intake air temperature.

Moreover, it is clear from Figure 5-6 that for the same fuel and same intake air temperature the maximum unburned mixture temperature in PFI is higher than that in DI. This is due to charge cooling in DI. The difference in maximum unburned mixture temperature between DI and PFI is smaller than the effective charge cooling numbers for each fuel blend presented in Chapter 4. This is because as evident in Figure 4-2, for the same intake air temperature, the maximum pressure at knock is greater in DI than PFI. The end gas is, as a result, compressed to higher pressures which reduces the difference in maximum unburned mixture temperature.

**Tu max at knock vs. Intake $T$**

Figure 5-6: Maximum Unburned Mixture Temperature vs. Intake Air Temperature, 2000 rpm, Base boost Conditions
Moving away from the constant load (base boost) experiments, the variable load knock onset points presented in Figure 3-31 will be examined next. The maximum unburned temperature at borderline knock for these points is plotted in Figure 5-7 vs. intake manifold air pressure (MAP). For the same fuel, the intake air temperature was kept constant. As explained in chapter 3, increasing load/MAP results in higher in-cylinder pressures and thus more retarded knock limited spark advance. Retarding spark also results in lower maximum unburned mixture temperatures as seen in Figure 5-7.

![Tu,max at Knock vs. MAP](image)

Figure 5-7: Maximum Unburned Mixture Temperature at Knock vs. MAP

The maximum unburned mixture temperature as a function of speed is presented in Figure 5-8. Changing rpm has two opposite effects on engine knock: Increasing rpm leaves less time available for the end-gas to auto ignite. On the other hand, increasing rpm decreases the amount of heat transfer per engine cycle, and thus the temperatures in the end gas. Reduced heat transfer at increased rpm tends therefore to increase propensity for knock. The trade off between these two effects usually results in the worst engine speed in terms of knock being somewhere between 1200 and 2500 rpm. For this engine, from the three speeds tested, the worst was 1750 rpm. As seen in Figure 3-32 and Figure 5-8, knock at 1750 rpm occurs at both lower maximum pressures and lower maximum unburned mixture temperatures.

Even at different loads and rpm however, the operating points still follow the general rule that higher maximum pressures will lead to lower maximum unburned mixture temperatures. This is evident in Figure 5-9, where maximum
pressure is plotted against maximum unburned mixture temperature for all points (base boost 2000 rpm and different load and rpm). Regression fitted lines are also presented. Table 6 shows the $R^2$ values of the fitted lines. Including different loads, doesn’t make the linear fit worse, at the same rpm, for the same blend, the borderline knock boundary is about the same. When including different rpm however, because the time available for auto ignition and the heat transfer characteristics change, the points diverge from the 2000 rpm line.

Figure 5-8: Maximum Unburned Mixture Temperature at Borderline Knock vs. RPM
Figure 5-9: $P_{\text{max}}$ at Borderline Knock vs. $T_{u,\text{max}}$, all speeds and loads

<table>
<thead>
<tr>
<th>Load</th>
<th>RPM</th>
<th>$E_0$</th>
<th>$E_{50}$ and $E_{85}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base Boost</td>
<td>2000</td>
<td>0.83</td>
<td>0.9</td>
</tr>
<tr>
<td>All Loads</td>
<td>2000</td>
<td>0.95</td>
<td>0.88</td>
</tr>
<tr>
<td>All Loads</td>
<td>All RPM</td>
<td>0.91</td>
<td>0.75</td>
</tr>
</tbody>
</table>

Table 6: $R^2$ Values for the linear regression fits in Figure 5-9.
5.2 Auto-ignition Model-Background

5.2.1 Background

Assuming a single step chemical kinetic mechanism for the auto-ignition reaction, a single step Arrhenius equation can be used for the reaction rate. The equation relates the concentration of an auto ignition product \([x]\) to its rate of change [59].

\[
\frac{d[x]}{dt} = C' \cdot [x] \cdot P^n \cdot \exp\left(-\frac{B}{T}\right)
\]

Where:
- \([x]\): Concentration
- \(t\): time
- \(P\): Pressure,
- \(T\): Temperature
- \(C', n, B\): Constants

Equation 16: Rate of Reaction of an Auto Ignition Product as a Function of Pressure and Concentration assuming Single Step Chemical Kinetics.

Integrating Equation 16 to a critical concentration of \([x]\) that defines auto ignition for a constant pressure and temperature results in Equation 17 that defines the ignition delay for a fuel under constant pressure and temperature conditions:

\[
\tau = C \cdot P^{-n} \cdot \exp\left(\frac{B}{T}\right)
\]

Where:
- \(\tau\): Ignition Delay
- \(C\): Constant

Equation 17: Ignition Delay for Constant Temperature and Pressure Conditions.

Equation 17 is suitable to describe ignition delay data obtained for example from a rapid compression machine (RCM). The fuel and oxidizer in an RCM are suddenly subjected to a pressure and temperature that remains roughly constant until combustion. However, for the end gas in a spark ignited engine, pressure and temperature conditions are not constant. In a spark ignited engine, it doesn’t even make sense to speak about an "ignition delay" as ignition starts with the spark. The term "time to auto-ignition" will therefore be used.

In order to deal with the varying conditions in the end gas in a spark ignited engine, Livengood and Wu [58] proposed to assume that the underlying auto ignition chemistry for knock is cumulative. The reaction rate (inverse of the time to auto-ignition) due to the time the end gas spent at each pressure and temperature can therefore be stepwise integrated until the critical time, \(t_c\) of auto ignition when the integral value reaches one:
$$1 = \int_{0}^{\tau} \frac{dt}{\tau} = \int_{0}^{\tau} \frac{dt}{C \cdot P^{-n} \cdot \exp\left(\frac{B}{T}\right)}$$

Equation 18: Livengood-Wu Auto-ignition Integral

The constants in Equation 18 can be regression fitted using experimental knock data from spark ignited engines. Correlations for the time to auto-ignition $\tau$, can thus be obtained to be used with the Livengood-Wu Integral. The best known such correlation is the one proposed by Douad and Eyzat\textsuperscript{13} [58]:

$$\tau = 17.68 \left(\frac{\text{ON}}{100}\right)^{3.402} P^{-1.7} \exp\left(\frac{3800}{T}\right)$$

Equation 19: Douad and Eyzat Correlation for Time to auto-ignition [58]

The ON in the correlation is the octane number of the fuel. The correlation was developed for Primary Reference fuels but has been used extensively for gasoline [2, 60].

A modified version of the Douad-Eyzat correlation in conjunction with the Livengood Wu Integral was the approach used to predict knock limits for gasoline-ethanol blends in both DI and PFI in this thesis. For every blend and injection type, the ON in the Douad-Eyzat correlation was varied until using the experimental pressure trace and the unburned mixture history from GT-Power in the auto ignition correlation, the integral reaches one at the experimentally observed "knock onset". The resulting ON is called "Effective Octane Number-ON\textsubscript{EFF}.”. Essentially, varying the ON in the correlation is equivalent to varying the pre-exponential term of the single step chemical kinetics equation. The temperature and pressure exponents were left unchanged compared to the original Douad-Eyzat correlation.

The complete methodology used for developing the knock limit predictive model can therefore be summarized as follows:

1. The unburned mixture temperature for an operating point is obtained from the experimental pressure trace and air flow rate from GT Power.
2. The unburned mixture temperature and pressure are used in the Livengood Wu Integral with the Douad-Eyzat $\tau$ correlation.
3. The ON in the correlation is varied until the integral reaches one at the experimentally determined knock onset position.

\textsuperscript{13} It is important for this method to use experimental data at knock onset (not heavy knock)
4. The Resulting ON that validates the correlation (makes the integral equal 1 at knock onset) will hence be called the "Effective Octane Number" \( \text{ON}_{\text{EFF}} \).

5. For each fuel blend and injection type, the process is repeated for at least 3 intake air temperatures at 2000 rpm and base boost conditions (except DI E85 where there was only one temperature), 3 different loads and rpm for E0, 2 different loads and rpm for E50 and E85.

6. If the method is valid, for the same fuel and injection type, the resulting \( \text{ON}_{\text{EFF}} \) should be the same.

The process is outlined in Figure 5-10.

One issue that remains is the choice of limits for the auto-ignition integral. The start of the integration is usually the point of Intake Valve Close (IVC) since that is where the compression process begins that will eventually lead to knock. As will be seen from the results, the choice of the start of the integral doesn't matter much. Far more important is the definition of the upper limit of the auto ignition integral. In other words, where is the position of knock onset where the integral should equal one? This is important because the value of the integral as will be seen is mostly dependent on the last few crank angle degrees before knock. As a result, the resulting \( \text{ON}_{\text{EFF}} \) from the integral has a sensitivity on the choice of upper limit of 3-4.5 ON/CAD. It is therefore important to define a methodology for determining the upper limit of the integral.

An example of a knocking cycle pressure trace (scaled) and its high pass filtered version that includes the knock induced oscillation are depicted in Figure 5-11. Different methodologies have been proposed in the literature to define knock onset-upper limit of the Livengood-Wu integral. Examples include [2,61]:

- Using the crank angle degree of maximum knock intensity amplitude (Point 1 in Figure 5-11)
- Using the crank angle degree of maximum negative knock intensity amplitude (Point 2 in Figure 5-11)
- Using the maximum of the filtered pressure trace (Point 2 in Figure 5-11)

As can be seen from Figure 11, there are signs of an oscillation even before maximum pressure. However, the oscillation really takes off shortly after the point of maximum pressure (of the low pass filtered signal). First comes the point of maximum negative amplitude and then the point of maximum amplitude.

All three of the above criteria were tested for use with the knock limit predictive model. The results were significantly more consistent (less error in \( \text{ON}_{\text{EFF}} \) for the same fuel) when using the maximum pressure point (of only the knocking cycles). The maximum pressure point also coincides with the maximum unburned mixture temperature point. The reasons why using the maximum pressure
worked better can be related to the physics of the phenomenon and the details of the measurement and signal processing.

The physics behind the observed oscillation in the pressure trace are complicated but can generally be thought off as individual spots in the end gas auto igniting first when the pressure and temperature are high enough. Then, they become big enough that they cause an acoustic oscillation that causes further auto ignition till all the end gas is consumed [1,3]. In that sense, auto ignition happens before the maximum amplitude is observed. The choice of maximum pressure and temperature or max negative amplitude therefore makes more physical sense.

Additionally, using the maximum pressure produces better results because it gets rid of the uncertainties in measuring and interpreting the oscillations in the pressure trace. The measured oscillation in the pressure trace depends on the details of the in cylinder acoustics and as a result on the location of the pressure transducer [2]. Since the location of auto-ignition is not always the same from cycle to cycle [62] this introduces some uncertainty in the location of the maximum. Furthermore the details of the signal processing matter in determining the maximum. On the other hand, determining the point of maximum pressure is a straightforward process which produces more consistent results.

**Knock Limit Model-Outline**

![Knock Limit Model-Outline](image)

Figure 5-10: Outline of the Process of Developing a Knock Limit Model.
### 5.2.2 Further Discussion of the Knock Model Used

Even for primary reference fuels using single step kinetics to describe the auto-ignition process is of course an approximation. Real kinetic mechanisms can have thousand of reactions, so single step approximations are usually valid only in a limited temperature and pressure regime. An example of ignition delay results from a somewhat simplified model is seen for iso-octane in Figure 5-12 vs. temperature and pressure. Three different regions are clearly visible in the figure—Cool Flame, Negative Temperature Coefficient and High Temperature Regions. This is typical of many hydrocarbon fuels. The dependence of ignition delay on temperature is different in each region as a result of significantly different chemical kinetic mechanisms/pathways. Furthermore, real world gasoline is a mixture of many substances which makes using even somewhat reduced chemical kinetic mechanisms practically difficult.

As an alternative to using kinetic mechanisms, ignition delays can be measured experimentally e.g. in a Rapid Compression Machine (RCM). However, even in a rapid compression machine, it can difficult to measure ignition delays for all relevant conditions and fuels. Ethanol blend ignition delays can be difficult to
measure [63]. In any case, a good set of gasoline ethanol blends ignition delays was not available for this thesis.

![Diagram of Ignition Delay for Iso-Octane vs. Pressure and Temperature](image)

**Figure 5-12: Ignition Delay for Iso-Octane vs. Pressure and Temperature.**
Source: [60]

Compared to detailed chemical kinetic models and getting a complete set of experimental ignition delay data, ignition delay correlations such as the one by Douad and Eyzat provide a far simpler alternative. Because they assume one single step mechanism they can do a good job of approximating the fuels ignition delay relationship to pressure and temperature in one of the regions of Figure 5-12 as essentially it represents a line in a logarithmic plot. If the fuel also has a negative temperature coefficient region, the correlation must approximate the two in some "average" way. However as seen from Figure 5-14, ethanol, unlike most hydrocarbon fuels doesn't have a negative temperature coefficient region. Therefore gasoline-ethanol blends are more suitable for using a Douad-Eyzat type correlation than gasoline or PRF's for which it was developed and used successfully for 30 years!
The choice made in this thesis to vary only the pre-exponential factor and leave the pressure and temperature coefficients the same as the original Douad Eyzat correlation implies that the slope of the ignition delay correlation is the same for gasoline H/C components and ethanol-H/C blends. Changing the pre exponential factor essentially translates to changing the offset of the lines in Figure 5-14. The slope of the H/C fuels and ethanol in the high temperature region is not very different as seen e.g. in Figure 5-14 which reinforces the choice of varying only the pre-exponential factor.

Additionally, the choice of using the Douad-Eyzat correlation and vary only the pre-exponential factor was imposed by two practical considerations:

- The Douad-Eyzat offers a well established platform for quantifying antiknock performance as an ON number. This is useful as it boils down the effects in a single, well understood number.
- Regression fitted correlations based on engine data inadvertently include secondary, engine specific physical effects except for the ignition delay of a fuel as a function of pressure and temperature. For example, the end gas is not completely homogeneous; there are heat transfer effects, the flame geometry will be affected by combustion chamber geometry etc. All these details will affect the mathematical fit to Equation 18. For these reasons, a really significant volume of experimental data from more than one engine would be needed to come up with a meaningful correlation that involves changes in all parameters in Equation 18.
All ignition delay data corrected to a pressure of 30 bar

10000
1000
100
10
1
0.1
0.01

Ign. Delay (ms)

1000K/T

0.7 0.8 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7

Figure 5-13: Ignition Delay for six fuels vs. Temperature. Source: [60]
5.3 Knock Model Results

An example of the time to auto-ignition calculated from the Douad-Eyzat correlation is displayed in Figure 5-14 vs. crank-angle degree for an example case-PFI Gasoline 2000 rpm, base boost load 55° C intake air. The spark for this case at borderline knock was 12.75° degrees before TDC. These time-to-auto-ignition values were obtained from the Douad-Eyzat correlation for an Octane Number of 99 which is the octane number that makes the integral go to one at knock onset. The same curve is again plotted in Figure 5-15 zoomed in around the crank angle of maximum pressure and temperature (20 CAD aTDC). The time to auto-ignition during the compression stroke spark is orders of magnitude higher than after spark and more specifically around maximum pressure. For comparison, at 2000 rpm, 1 msec corresponds to 12 CAD. The minimum time to auto-ignition is at the maximum pressure and temperature point. Generally, it can be seen that the end gas pressure and temperature history shortly before the maximum must contribute significantly more to auto ignition than the early part.

**Figure 5-14: Time to auto-ignition vs. Crank Angle Degree Based on the Douad-Eyzat Correlation (ON=99) for PFI E0.**
Figure 5-15: Time to auto-ignition vs. Crank Angle Degree Based on the Douad-Eyzat Correlation (ON=99) for PFI E0-Zoomed In near Max P,T.

The value of the auto-ignition integral as a function of crank angle degree is depicted in Figure 5-16 and in Figure 5-17 zoomed in around maximum pressure and temperature (20 CAD aTDC). Three different ON were used in the Douad-Eyzat correlation. It is clear from Figure 5-17, that the $\text{ON}_{\text{EFF}}$ for this operating point is 99 since this is the value that makes the integral equal one at maximum pressure. Eventually all the versions of the integral even with ON less than 99 will reach one but later than knock onset (defined here as max pressure). From a physical point of view this can be thought of as auto-ignition occurring when not much end gas is left to burn and thus causing no significant pressure oscillations.

It is also evident from Figure 5-16 and Figure 5-17 how much more important are the last few crank angle degrees before maximum pressure, compared to the earlier part of the history. The integral value is 0.05 at ignition (13 CAD bTDC) ~0.3 ten CAD before maximum (10 CAD a TDC) and ~0.56 five CAD before the maximum (15 CAD aTDC). The last five CAD before the maximum are essentially what determines knock and there is practically no contribution before ignition.
Livengood-Wu Integral PFI Gasoline 55 C Intake Air Base Boost 2000 RPM

Figure 5-16: Livengood –Wu Integral Example (PFI E0 2000 rpm base boost, 55 C intake air) - Different ON in Douad-Eyzat \( \tau \) Correlation.

Livengood-Wu Integral PFI Gasoline 55 C Intake Air Base Boost 2000 RPM

Figure 5-17: Livengood –Wu Integral Example (PFI E0 2000 rpm base boost, 55 C intake air) - Different ON in Douad-Eyzat \( \tau \) Correlation-Zoomed In Near Maximum P,T.
5.4 Results-Quantifying the Effect of Ethanol Chemistry

The effective octane results ($\text{ONEFF.}$) are plotted vs. volumetric ethanol content in Figure 5-18. The Research Octane Number (RON) of the premium gasoline used for the experiments (97 ON) and that of pure ethanol (109) are also displayed in Figure 5-18. Research octave numbers are generated from standardized tests in a standardized (CFR) engine. Although correlated, the RON are not directly comparable to the $\text{ONEFF.}$ presented here as they are the result of a different test in a different engine. They are presented for comparison only.

The conclusions that can be extracted from Figure 5-18 are:

- **The method seems valid:** For each of the fuel blends and for both DI and PFI, the ON that validates the Livengood Wu integral with the Douad-Eyzat correlation ($\text{ONEFF.}$) was the same for all the operating points tested. The biggest spread in the results was ±3 $\text{ONEFF.}$ for E50. This translates to a relative error of 2.6%. This is quite remarkable considering that because ON is raised to the power of 3.4 in the Douad-Eyzat correlation a 2.6% error in $\text{ONEFF.}$ is only an error of $3.94 \times 10^{-6}$ in the pre-exponential factor. The method therefore seems to be valid.

- **DI $\text{ONEFF.}$ is essentially the same as PFI for the same fuel- $\text{ONEFF.}$ shows only chemical benefit:** As seen from the figure, the effective ON numbers for DI are almost the same as those for PFI-only slightly lower. This is because auto-ignition for a given engine geometry depends exclusively on the fuel used, not the injection type. The input to the auto-ignition integral is a pressure and a temperature history. Those may be different for DI and PFI, in that lower temperature due to charge cooling is traded for higher pressure for example. However, the pressure and temperature limits where auto-ignition occurs are determined by the fuel. In other words, because essentially only the part of the pressure temperature history after ignition contributes significantly to auto-ignition, it doesn't matter how the end gas got to the pressure and temperature conditions after combustion. Charge cooling in terms of auto-ignition is equivalent to heat transfer. Charge cooling is embedded in the unburned mixture temperature but doesn't affect the effective octane at knock. The slightly higher $\text{ONEFF.}$ of PFI could perhaps be attributed to mixing inhomogeneities in DI. **The final conclusion is that the $\text{ONEFF.}$ only shows the fuel chemical characteristics in preventing knock.**

- **$\text{ONEFF.}$ (chemical) benefit from blending ethanol is non-linear. No benefit beyond ~30-40% ethanol by volume.** As seen from the figure, the $\text{ONEFF.}$ of the gasoline-ethanol blend is initially significantly improved with increasing ethanol content up until around 30-40% by volume. Increasing ethanol content further does not improve $\text{ONEFF.}$ any
more. What this result is implying is that Ethanol blending provides no antiknock benefit beyond 30-40% by volume, unless it is used in an engine that can realize the charge cooling potential of the fuel.

This non linearity in the chemical antiknock benefit when blending ethanol with gasoline is well known to the oil industry. A number of publications have documented the fact [14,57]. RON from [57] are plotted for four gasoline/ethanol blends vs. ethanol content in Figure 5-19. It is clear that for premium base gasoline with a high RON, the improvement by blending ethanol is non-linear and the ON doesn’t improve further beyond ~25% ethanol. The improvement is more pronounced and more linear for worse base gasoline. These published RON results validate the $\text{ON}_{\text{EFF}}$ results presented in this thesis for a premium (97 ON) gasoline as they show the same trends in terms of the chemical antiknock benefit vs. ethanol content. However, there is still a need to quantify the charge cooling antiknock benefit.

It should be noted that it is generally difficult to find ethanol blend RON data for ethanol concentration above 30%. Also because low RON base gasoline is used, market E85 and E50 have a RON of ~101.6 [16]
5.5 Results—Quantifying the Charge Cooling Anti-Knock Benefit.

The effective ON (ON\textsubscript{EFF}) presented above depends on fuel chemistry alone and therefore doesn't show the effects of charge cooling. DI and PFI ON\textsubscript{EFF} were the same. Yet, it was clear from Figure 4-2 that evaporative charge cooling does improve resistance to knock. The difference is that ON\textsubscript{EFF} reflects the end gas conditions late in the compression stroke, after ignition and those are determined at the knock boundary by the fuel. The evaporative cooling determines for which starting conditions (MAP and intake temperature), the mixture end up at conditions that cause auto-ignition.

In order to quantify the evaporative antiknock benefit, we need to imagine what would happen to a parcel of mixture if evaporative charge cooling didn’t take place. Of course, in a real engine, if we turned off charge cooling somehow (e.g. switch to PFI or inject pre-vaporized fuel) keeping intake conditions the same, air flow rate would drop. The maximum unburned mixture temperature would increase but the pressure of the mixture would decrease so that the ON\textsubscript{EFF} would end up being the same. In order to overcome this hurdle, let's consider a single particle of mixture in a DI engine that is operating at borderline knock, so it is
subjected to the same pressure profile but postulate what would happen to it if there were no charge cooling. The process is the following:

For a parcel of gas in DI (known \( P, T_u, \text{ON}_\text{EFF} \)):

- Keeping the pressure trace the same and equal to the experimentally measured for knocking cycles.
- Using the original unburned mixture temperature history calculated in GT Power, the new unburned mixture temperature is calculated as:

\[
T'_u(\theta) = T_u(\theta) + \Delta T_{\text{charge cooling}}(\theta)
\]
\( \theta \) is position in crank angle degrees

(Equation 20)

- Use the Douad-Eyzat correlation in the auto ignition integral with the new temperature profile and the same pressure, the new \( \text{ON}_\text{EFF} \) is calculated.
- The increase in the required \( \text{ON} \) when cancelling out charge cooling in the temperature profile is the \( \text{ON}_\text{EFF} \) benefit due to fuel evaporation. This difference will be called “Evaporative Octane Number” – \( \text{ON}_{\text{EVAP}} \) hence.

The next question that needs to be addressed is how the unburned mixture temperature should be offset to cancel charge cooling. The effective difference in charge cooling between DI and PFI was calculated using knock as a diagnostic in Figure 4-2. However, these are temperature differences measured in terms of intake air. As the mixture undergoes compression, the temperature is amplified. This is the logic used to calculate the charge cooling \( \Delta T \) as a function of piston position from the charge cooling numbers at IVC that were obtained from using knock as a diagnostic:

- During The Polytropic Compression (before spark):

\[
\frac{T'_u}{T'_{\text{IVC}}} = \left( \frac{V_{\text{IVC}}}{V_2} \right)^{(k-1)} \iff T'_u = T'_{\text{IVC}} \cdot \left( \frac{V_{\text{IVC}}}{V_2} \right)^{(k-1)} \Rightarrow
\]

\[
T'_u = T'_{\text{IVC}} \cdot \left( \frac{V_{\text{IVC}}}{V_2} \right)^{(k-1)} + \Delta T_{\text{IVC}} \cdot \left( \frac{V_{\text{IVC}}}{V_2} \right)^{(k-1)} \Rightarrow
\]

\[
T'_u = T_u + \Delta T_{\text{IVC}} \cdot \left( \frac{V_{\text{IVC}}}{V_2} \right)^{(k-1)}
\]

Equation 21: Where \( T'_u \) is the new unburned mixture temperature, \( T_u \) is the old-from GT-Power, \( k \) is the polytropic coefficient obtained from the P-V diagram and \( V \) is the volume.

- During Combustion:
Equation (22): Where $T'_{SPARK}$ is the new temperature at spark from the previous (compression) step. $P$ is the experimentally measured pressure—the average of the knocking cycles was used.

An example of the original unburned mixture temperature and the offset version used for the calculation of $\text{ON EVAP}$ is presented in Figure 5-20. The $\Delta T_{\text{charge cooling}}$ used to offset the original $T_u$ can be seen as a function of CAD in Figure 5-21. It starts at 49° C at IVC which is the value calculated in Figure 4-4. Then it gets amplified through the polytropic compression up to a maximum of 135 degrees.

Figure 5-20: Example of Original Unburned Mixture Temperature and New, Offset to Cancel Charge Cooling for the $\text{ON EVAP}$ Calculation.
The ratio of the maximum value of the ΔT charge cooling to the value at IVC, called the “ΔT Amplification Factor” is plotted in Figure 5-22. The ratio grows slightly with higher ethanol content because generally spark timing at borderline knock was earlier for higher ethanol content. Earlier spark leads to higher maximum pressures and thus to greater amplification factors.

Figure 5-21: ΔT Charge Cooling as a function of CAD.

Figure 5-22: ΔT Charge Cooling Amplification Factor
The process of offsetting the charge cooling and calculating the increase in ON\textsubscript{EFF} needed to validate the auto-ignition integral was repeated for all fuel blends in DI. The resulting evaporative ON (ON\textsubscript{EVAP}) is plotted in Figure 5-23 vs. ethanol content. The evaporative ON increases with ethanol content roughly reflecting the shape of the \(\Delta T\)_{charge cooling} vs. ethanol curve of Figure 4-4. The end result is a boost of 5 ON\textsubscript{EFF} due to charge cooling in DI for gasoline that rises to 18 ON\textsubscript{EFF} for E85.

The error bars in Figure 5-22 reflect the variability of \(\Delta T\)_{charge cooling} depending which starting intake air temperature is used as explained in Chapter 4. Due to the wide range of intake air temperatures used to calculate \(\Delta T\)_{charge cooling}, the biggest uncertainty was for E20 (±3.5° K) which causes a ±1.6 ON\textsubscript{EFF} uncertainty in ON\textsubscript{EVAP}.

The calculation can also be performed starting from a PFI operating point. The only difference in that case is that the \(\Delta T\)_{charge cooling} has to be subtracted from instead of added to the original unburned mixture temperature. The ON\textsubscript{EVAP} in this case is the decrease in the required ON for the auto-ignition integral to validate the experimental knock onset data. The resulting ON\textsubscript{EVAP} values were almost the same as the ones from the equivalent DI points within 1 ON.

\[
\Delta(ON)_{\text{EFF}} \text{ due to Charge Cooling-ON}_{\text{EVAP}}
\]

![Graph](image)

**Figure 5-23: Evaporative Octane Number (ON\textsubscript{EVAP}) vs. Ethanol Content.**

In order to compare the chemical to the evaporative effect, the ON\textsubscript{EFF} and the sum of ON\textsubscript{EFF} and ON\textsubscript{EVAP} named “Total ON” are plotted vs. ethanol content in
Figure 5-24. The plot shows how the improvement due to evaporative cooling is of the same order of magnitude as the $O_{NEFF}$ improvement due to the effects of chemistry. For higher ethanol blends there is only improvement due to higher evaporative cooling no benefit due to chemistry. Both the improvement due to ethanol chemistry alone ($O_{NEFF}$) and the compounded effect including evaporative chemistry as well (Total $O_{N-ONTOTAL}$) are plotted. When including the evaporative charge cooling effect, it is clear that unlike the chemical benefit alone, the total antiknock benefit increases monotonically with ethanol content. In other words, although in a PFI engine there doesn’t seem to be a point in going to more than 30-40% ethanol, in a DI engine, higher ethanol content will always improve antiknock performance.

**TOTAL ON ($O_{NEFF}$+$O_{NEVAP}$)**

![Graph](image)

Figure 5-24: $O_{NEFF}$ (Chemical Antiknock Effect) and Total ($O_{NEFF}$+$O_{NEVAP}$) – (Chemical+ Evaporative Charge Cooling Effect) vs. Ethanol Content.
5.6 Knock Model Conclusions

A knock limit model was developed by using the Livengood Wu auto-ignition integral and adapting the Douad-Eyzat correlation for auto-ignition. An effective Octane Number can thus be obtained by fitting the pre-exponential term of the correlation to experimental data. This “effective octane number-ON_{EFF}” reflects the chemical antiknock performance of the fuel at the test engine operating conditions examined. Plotting ON_{EFF} vs. ethanol content reveals that ethanol blending shows diminishing returns. The calculated ON_{EFF} starts around 97 for gasoline (same as the RON of the gasoline used) and increases quickly to about 113 ON_{EFF} for E20 and 115 for E50. There seems to be no considerable improvement in antiknock fuel performance beyond about 40% ethanol content, unless it is used in a DI engine that can utilize the charge cooling effect.

The ON_{EFF} doesn’t contain any information about the charge cooling effect in preventing knock. DI and PFI ON_{EFF} for the same fuel are therefore practically equal. This is because the ON_{EFF} reflects primarily the temperature and pressure conditions shortly before knock onset and not how the mixture got there. In order to quantify the charge cooling effect in preventing knock, we postulate what would happen to a fluid particle in a DI engine if the evaporative cooling was turned off. A new ON_{EFF} is thus calculated for that fluid particle keeping pressure the same as what experimentally measured but offsetting the unburned mixture temperature to cancel out charge cooling. The increase in the required ON_{EFF} called “Evaporative Octane Number-ON_{EVAP}” is in effect the antiknock benefit due to fuel evaporative charge cooling. The calculated ON_{EVAP} is around 5 ON_{EFF} for gasoline and 18 ON_{EFF} for E 85. Adding the ON_{EVAP} to the ON_{EFF}, a “Total ON-ON_{TOTAL}” is obtained that includes evaporative and chemical effects. Plotting the ON_{TOTAL} vs. ethanol content, shows that in an engine that can make use of the fuel’s charge cooling effect (DI engine) the antiknock benefit increases monotonically with ethanol content.
6. Conclusions & Future Work

6.1 Conclusions

Measuring Charge Cooling

1. An experimental methodology was developed to measure how much more charge cooling takes place in a DI engine compared to a PFI engine. The methodology uses knock as a diagnostic by essentially asking the question: "How much does the intake air need to be heated in DI in order to make the engine reach knock onset at the same conditions as PFI?"

2. Using the same maximum pressure at knock onset at the same engine speed proves to be adequate to make this comparison between DI and PFI. This is because to a good approximation, when maximum pressures at knock onset are the same, the maximum temperatures will also be similar. It is mostly the last part of the pressure and temperature rise to these maximum values that matters for knock and it is the fuel chemical characteristics that determines what these conditions are at knock onset, not the injection type.

3. The charge cooling realized generally increases as a function of ethanol content.

4. Intake air temperature does play a role in influencing how much charge cooling takes place. For E20, which was tested over a wide range of intake air temperatures, going from 20° C intake air to 100 °C changes the amount of additional (compared to PFI) charge cooling realized from about 50% of the theoretical maximum to about 75% of the theoretical maximum. Similarly, using CFD, it was found that for pure ethanol, going from 120 °C intake air to 20 °C, the amount of charge cooling realized decreases by around 35% of the theoretical maximum.

5. Due to hardware limitations on maximum pressure, high intake air temperatures were used to make higher ethanol blends knock instead. The measured charge cooling for E50 and E85 is as a consequence probably optimistic compared to real world engine conditions since the hot air promotes faster evaporation. This is not a limitation of the methodology used, just the experimental apparatus.
Modeling Knock For Gasoline/Ethanol Blends—Separating Chemical and Charge Cooling Effects

1. A knock limit model was developed by using the Livengood-Wu auto-ignition integral and adapting the Douad-Eyzat correlation for auto-ignition. To adapt the correlation for use with higher ethanol content fuel blends, the pre-exponential term of the correlation is varied to fit the experimental data.

2. An effective Octane Number-ON\textsubscript{EFF} can thus be obtained for every blend. ON\textsubscript{EFF} reflects the antiknock performance of the fuel only due to chemistry.

3. DI and PFI ON\textsubscript{EFF} for the same fuel are therefore practically equal. This is because the ON\textsubscript{EFF} reflects primarily the temperature and pressure conditions in the end gas shortly before knock onset and not how the mixture reached these conditions. Therefore it does not describe the antiknock benefit due to charge cooling.

4. Plotting ON\textsubscript{EFF} vs. ethanol content reveals that ethanol blending shows diminishing returns in terms of chemical antiknock benefit. The calculated ON\textsubscript{EFF} starts around 97 for gasoline and increases quickly to about 107 for E10, 113 for E20 and 115-116 for E50 and E85. There seems to be no significant improvement in antiknock fuel performance beyond about 40% ethanol content, unless it is used in a DI engine that can utilize the charge cooling effect.

5. In order to quantify the charge cooling effect in preventing knock, the unburned mixture temperature for a DI operating point was offset by the amount of charge cooling that took place and the ON\textsubscript{EFF} recalculated for the same pressure profile.

6. The increase in ON\textsubscript{EFF} to "counteract" the increase in temperature when charge cooling is cancelled out is in effect the antiknock benefit due to charge cooling expressed as an octane number. It is named "Evaporative Octane Number-ON\textsubscript{EVAP}”.

7. ON\textsubscript{EVAP} is 5 ON\textsubscript{EFF} for gasoline and increases to 18 ON\textsubscript{EFF} for E85. The charge cooling benefit is generally comparable in magnitude to the chemical benefit.

8. By adding the ON\textsubscript{EVAP} to the ON\textsubscript{EFF}, a "Total ON- ON\textsubscript{TOTAL}" is obtained that includes both evaporative and chemical effects. Plotting the ON\textsubscript{TOTAL} vs. ethanol content, shows that in an engine that can make use of the fuel’s charge cooling effect (DI engine) the antiknock benefit increases monotonically with ethanol content.
6.2 Contribution and Practical applications of this Work

A methodology was developed to accurately quantify how much more charge cooling due to fuel evaporation takes place. The only method existing in the literature to address this issue used the change in air flow rate. Using the effect of charge cooling on air flow rate is sufficient to provide some qualitative trends but difficult to extract quantitative information especially in a turbocharged engine. Using knock as a diagnostic instead directly produces temperature drop numbers due to charge cooling.

The Knock Limit Predictive Model using the Livengood-Wu integral and the Douad-Eyzat correlation was expanded to be used for use with ethanol/gasoline blends. Varying the pre-exponential term proved to be sufficient to model the experimental results. This type of model could be used in the design of engine concepts that use ethanol blends. The model covers DI as well as PFI engine knock. When used along with an engine thermodynamics code like GT Power, it can be used to answer questions like: “How much of an increase in compression ratio or boost can be achieved by using E85 in PFI vs. E50 in DI?”.

One of the main contributions of this thesis is that the antiknock benefit due to chemistry and that due to fuel evaporative charge cooling were quantified using a single, easy to understand number: an effective octane number-ON\textsubscript{EFF}. Using this number and its increase due to charge cooling (ON\textsubscript{EVAP}), a complete framework is provided to assess a fuel on the basis of its anti knock performance including the evaporative effect which is not explicitly taken into account in the standardized RON and MON tests. This framework is not limited to ethanol/gasoline blends and can be used to assess any fuel with a significant heat of vaporization, e.g. methanol blends.

It was seen that using ethanol blends with a volume concentration more than 40-50% provides no benefit unless it is used in a DI engine. This conclusion has significant implications in making optimal choices on how to use ethanol blends most efficiently. This is particularly important given the current desire for increasing ethanol use as a fuel and the limited amounts of ethanol available.
6.3 Suggestions for further study

1. **Modify hardware to test at lower intake air temperatures and higher pressures.** It was explained how due to hardware limitations, the intake air temperature had to be increased substantially to make higher ethanol blends knock to use knock onset as a diagnostic of charge cooling. Using the same methodology, it would be valuable to be able to test at more realistic intake air temperatures (no more than 40-50°C) and pressures higher than 100 bar. Such conditions would be more relevant for practical use. The effect of intake air temperature on charge cooling realized could thus be assessed. Also the validity of the knock model should be tested under these conditions. However, this investigation would require significant hardware changes such as changing engine head bolts, head gaskets and possibly pistons and connecting rods.

2. **Test with higher compression ratios and boost pressures.** The motivation for using higher ethanol blends to counter knock is using higher compression ratios and boost pressures. It is therefore important to experimentally validate the methodologies and conclusions presented in this thesis under higher compression ratio and boost.

3. **Test other fuels: lower grade gasoline blended with ethanol and methanol.** The gasoline used in this thesis was premium test gasoline (97 RON). Even with premium gasoline, the engine is significantly knock limited. Testing lower octane gasoline blends is interesting for two reasons: First, in the fuels industry, the base gasoline blended with ethanol for commercial use is usually low grade, the ethanol acts as the octane booster to bring the ON up. It is therefore more applicable to the real world to investigate the effect ethanol blending would have on lower grade gasoline. Second, lower grade gasoline/ethanol blends will be easier to knock. They can therefore be tested at lower intake air temperatures without the need for prohibitively high pressures. Also examining methanol blends would be interesting as methanol has an even higher heat of vaporization than ethanol.

4. **Use a more sophisticated autoignition model.** If enough experimental knock data become available, preferably from more than one engine, all of the parameters in the time to auto-ignition formula (pre-exponential, pressure and temperature exponents) can be fitted to the experiments for gasoline ethanol blends. Alternatively, if a reliable set of ignition delay data from a rapid compression machine become available for gasoline/ethanol blends, these could be used in the form of a lookup table directly in the Livengood-Wu integral.
References


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