

Pressure Sensitivity of HCCI Auto-Ignition Temperature for Primary Reference Fuels

Ida Truedsson, Martin Tuner and Bengt Johansson
Lund University

William Cannella
Chevron USA Inc

ABSTRACT

Some fuels with the same research octane number (RON) have different HCCI engine performance. Therefore RON alone cannot be used for determining auto ignition in HCCI combustion. The current research focuses on creating an HCCI fuel index suitable for comparing different fuels for HCCI operation. More thorough studies are needed to map the fuel effects. One way to characterize a fuel is by using the Auto Ignition Temperature (AIT). The AIT and the amount of Low Temperature Heat Release (LTHR) together describe the auto ignition properties of the fuel. Both can be extracted from the pressure trace. The assumption is that the pressure and temperature are known at inlet valve closing (IVC) and that the mass in the cylinder does not change after IVC.

The purpose of this study was to map the AIT of different Primary Reference Fuels (PRF) for HCCI combustion at different cylinder pressures. Different pressure levels were achieved by changing inlet air temperatures in 5 steps from 50°C to 150°C. A Cooperative Fuel Research (CFR) engine with variable compression ratio was used. The compression ratio was varied from 5.5 to 15.5 to keep combustion phasing, defined as 50% of total heat released, constant at $3 \pm 1^\circ$ after TDC. The experiments were carried out in lean operation with a constant equivalence ratio of 0.33 and with a constant engine speed of 600 rpm.

The results showed that the AITs of the PRFs ranged from around 580 K for PRF 0 to up to 800 K for PRF 100. Auto ignition was defined as the point where the rate of heat released had reached 0.2 J/CAD. At the lowest inlet air temperatures all fuels except PRF 100 showed Low Temperature Heat Release (LTHR) from about 3% LTHR/Total Heat Release for PRF 95 with up to 19% for PRF 0. Amount of LTHR was found to decrease linearly with increasing octane rating.

The low octane PRFs ignited at almost the same temperature independent of the cylinder pressure. The high octane number PRFs (PRF 95 - 100) displayed a wide range of auto ignition temperatures resulting from the different inlet air temperatures. PRF 80, PRF 85 and PRF 90 showed an intermediate behavior. A constant auto ignition temperature was seen at the low inlet air temperature but at higher inlet air temperatures the IAT quickly rose when the LTHR disappeared.

CITATION: Truedsson, I., Tuner, M., Johansson, B. and Cannella, W., "Pressure Sensitivity of HCCI Auto-Ignition Temperature for Primary Reference Fuels," *SAE Int. J. Engines* 5(3):2012, doi:10.4271/2012-01-1128.

INTRODUCTION

HCCI is a combustion mode used to reduce emissions to the level of traditional spark ignition engines combined with maintaining efficiency as high as for diesel combustion. The main challenge for HCCI is to control the ignition timing and combustion rate, since they are not controlled by a spark (SI combustion) or by fuel injection (CI combustion) but are controlled by chemical kinetics.

The aim of this work was to map the auto ignition temperatures of different Primary Reference Fuels (PRF) at

different cylinder pressures. This study tries to establish whether it is possible to determine the temperature at Start of Combustion and relate this to the HCCI engine fuel performance. The auto ignition is dependent on temperature, pressure and fuel air ratio, but also on the residence time of the fuel air mixture. Much work has been reported in the literature on auto ignition of PRFs, but only a small amount of it was conducted in combustion engines.

RON and MON are known to be insufficient to explain the fuel behavior in an HCCI engine [1,2,3]. More knowledge of the combustion process is needed to create a useful HCCI



Documents

Document Sharing Hub

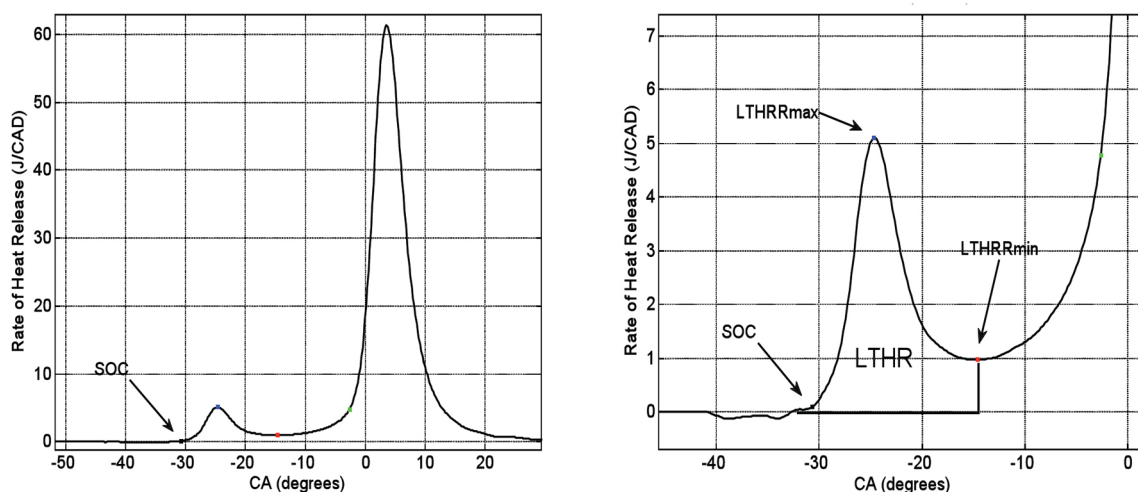


Figure 1. Definition of Heat Release Data.

fuel index, which is why a standardized method for determining the HCCI fuel performance was desired. The idea is that the fuel auto ignition temperature in combination with the amount of Low Temperature Heat Release (LTHR) can be related to the fuel performance in an HCCI engine. It was decided to use a standardized engine for the experiments, which is why the Cooperative Fuel Research (CFR) engine was chosen. This engine is normally used in SI mode to measure RON and MON values for fuels. This engine is suitable because it can be used for many types of fuels since it has a variable compression ratio. It is equipped with a spark plug and can therefore be used for both HCCI and SI combustion.

When burning fuels that contain a significant amount of n-paraffins, such as n-heptane, a characteristic bump is usually seen before the main heat release. This is called the Low Temperature Reactions (LTR) or the Low Temperature Heat Release (LTHR), referring to the exothermic pre-reactions that occur before the main combustion event (see Figure 1). At lower inlet air temperatures, depending on the fuel, there can be extensive LTHR, but this decays with higher temperature because of the higher amount of available energy and therefore earlier main combustion. The amount of LTHR also decreases with higher engine speed because there is less time for reactions [4]. A higher cylinder pressure induced by super- or turbocharging is also known to increase the amount of LTHR [5]. When LTHR is present the auto ignition temperature is substantially lower.

The oxidation mechanism of hydrocarbons is shown in Figure 2. Reactions are initiated by the abstraction of H from a fuel molecule (RH) by O_2 , where an alkyl radical (R) and HO_2 are formed. At low temperatures the alkyl radical then reacts with oxygen to produce RO_2 . This then gives H_2O and an alkyl peroxide ($O=ROOH$). This is a highly exothermic reaction. This continues until the temperature is high enough for the alkyl radical and oxygen to instead form olefins and HO_2 , which terminates the first reaction step. After this the

high temperature reaction starts producing olefins and H_2O_2 . This is the stage between LTHR and HTHR. Here the rate of temperature rise decreases sharply, called the Negative Temperature Coefficient (NTC) zone. After this the temperature slowly rises until the H_2O_2 decomposes leading to a branched thermal explosion. At this stage the $O=ROOH$ and olefin decompose irreversibly to H_2O and CO . Then CO is converted to CO_2 in the reaction $CO+OH=CO_2+H$ [6,7].

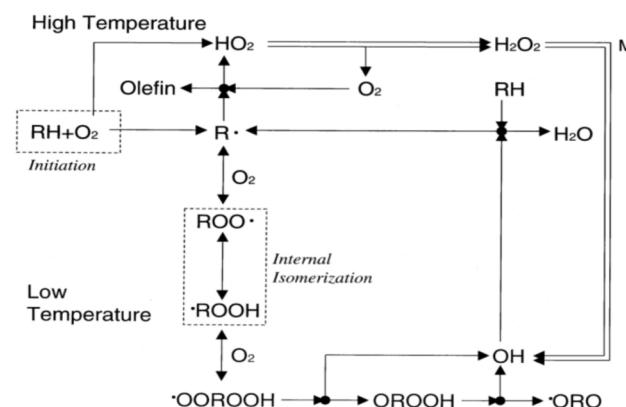


Figure 2. Oxidation scheme for heavy hydrocarbons at low and high temperatures. Reprinted from 6, copyright (2003), with permission from Elsevier.

The LTHR of the n-paraffins can be explained by the possibility for n-heptane to form a transitional ring with low ring strain for internal H atom transfer, the so called internal isomerization (Figure 2). This reaction has a much higher energy barrier for a more compact molecule as for example iso-octane [12].

Studies of auto ignition properties of different fuels have been done before, for example by Shibata and Kalghatgi [2,3,6]. Shibata et al. [2] studied surrogate fuels and created an HCCI index calculated by using the fuel RON and amounts of the different fuel components. Kalghatgi [6]

developed the Octane Index using the RON and MON for the fuel in combination with an engine specific parameter K. Studies on auto ignition temperatures in engines divided into pre-reactions and main reactions for HCCI combustion were made by Christenssen [8]. Modeling of LTHR for PRFs was made by Silke et al. [9] and for similar fuel surrogates by Mehl et al. [10].

Machrafi and Cavadiasa [7] also studied the combustion of PRFs in a CFR engine. They did an experimental and modeling study. They varied inlet air temperature, equivalence ratio and compression ratio, and looked at the ignition delay for PRF 0 and 40. The effect of different amounts of residuals were also discussed.

EXPERIMENTAL

A Waukesha Variable Compression Ratio CFR engine was used for the experiments. The setup included an air heater mounted after the port injection. A scale was used for measuring the fuel flow. A Kistler pressure transducer was mounted in the cylinder. An intake air conditioner is included in the setup to ensure constant air humidity throughout the experiments. The engine specifications are listed in Table 1.

Table 1. Engine Specifications.

Displacement volume	612 cm ³
Number of cylinders	1
Bore	83 mm
Stroke	114 mm
CR	Variable (4:1 to 18:1)
Number of valves	2
Length of connecting rod	254 mm
Intake valve opens	10°ATDC±2.5°
Intake valve closes	146°BTDC±2.5°
Exhaust valve opens	140°ATDC±2.5°
Exhaust valve closes	15°ATDC±2.5°
Valve lifts	6.25 mm
Valve diameters	9.53 mm
Engine speed	600 rpm
Fuel supply	Port injection

FUELS

The test fuels were 9 different blends of n-heptane and iso-octane. The mixing accuracy is ±1vol%. The fuels used were PRF 0, 20, 40, 60, 80, 85, 90, 95 and 100. PRF 0 is pure n-heptane, PRF 100 is pure iso-octane and the other fuels are a mix of the two, where the number indicates not only the amount of iso-octane but also the octane rating.

METHOD

A fuel matrix consisting of the nine different Primary Reference Fuels (PRFs) were run. All fuels were run with a change in inlet air temperature from 50° to 150°C. For each temperature a combustion phasing with CA50 at 3±1° after TDC was achieved by varying the compression ratio. Motored pressure traces were extracted for all data points for

validation. The engine was run naturally aspirated at 1 bar inlet air pressure. The fuel amount was adjusted for each case to achieve an equivalence ratio of 0.33. All experiments were run at 600 rpm. No EGR was used.

HEAT RELEASE CALCULATION

The heat release calculations were made for each individual cycle of the pressure trace and all figures were based on the mean value of 300 cycles. The heat release calculation is according to Heywood [11]. Equation 1 gives the rate of heat release as a function of CAD, θ . Crevice flow was assumed negligible.

$$\frac{\partial Q}{\partial \theta} = \frac{\gamma}{\gamma-1} P \frac{\partial V}{\partial \theta} + \frac{\gamma}{\gamma-1} V \frac{\partial P}{\partial \theta} + \frac{\partial Q_{HT}}{\partial \theta} + \frac{\partial Q_{crevice}}{\partial \theta} \quad (1)$$

A single zone heat release model was used, assuming that the temperature and the gas composition are the same in the whole bulk. This is quite a good assumption for HCCI combustion. Gamma is approximated by Equation 2 and is temperature dependent. The heat transfer model was tuned by changing the γ_0 and k with respect to the shape of the heat release curves. The heat release was tuned for the motored pressure trace to be as close to zero as possible and that the burned pressure trace at the same time fit fuel measurement data. The same parameters were used for all fuels and cases.

$$\gamma = \gamma_0 - \frac{T_{cyl} - 300}{1000} \cdot k$$

	γ_0	k
Motored	1.40	0.07
Combustion	1.37	0.05

(2)

The heat loss term is calculated in Equation 3 according to Woschni with constants recalculated to fit the SI-unit system.

$$h = 131 \cdot B^{-0.2} \cdot p^{0.8} \cdot T^{-0.55} \cdot w^{0.8} \quad (3)$$

Where:

$$w = 2.28 \cdot S_p + 3.24 \cdot 10^{-3} \cdot \left(\frac{V_d}{V_{IVC}} \right) \left(\frac{p_f - p_m}{p_{IVC}} \right) \cdot T_{IVC} \quad (4)$$

To calculate the temperature in the cylinder when the Inlet Valve Closes (IVC), the heat transfer between the fuel air mixture and the walls in the intake was calculated. The Woschni heat transfer model was used with the same parameters as in the cylinder, and with an assumed wall temperature of 100°C. Equation 5 gives an effect of ±5°C.

The effect of heat transfer to the fuel mass was assumed to be negligible.

$$\Delta T_{inlet} = \frac{hc_{inlet} \cdot A_{inlet} \cdot (T_{wall,inlet} - T_{in})}{m_{air} \cdot c_{p,air}} \quad (5)$$

The amount of residuals was used to calculate the temperature in the cylinder when the inlet valve closed. The amounts of residuals in the cylinder were approximated using Equation 6 [11]. The cylinder pressure 10 CAD before exhaust valve opens was used as p_4 and the measured pressure in the exhaust was used for p_e . This gives about 3% residuals at high compression ratios (CR=15.5) and up to 10% at lower compression ratios (CR=5.5). This gives a heating effect of +5° to +35°.

$$x_r = \frac{\left(\frac{p_e}{p_4}\right)^{1/\gamma}}{r_c} \quad (6)$$

T_{IVC} is then calculated with Equation 7. The residuals were assumed to have the same temperature as the measured exhaust gas temperature.

$$T_{IVC} = T_{air,cyl} \cdot (1 - x_{res}) + T_{exhaust} \cdot x_{res} + \Delta T_{inlet} \quad (7)$$

RESULTS AND ANALYSIS

CALCULATED T_{IVC}

The temperature in the inlet was held constant at five different temperatures from 50°C to 150°C. Due to heat transfer in the inlet and mixing of air and residual gas, the temperature changes before the inlet valve closes. The temperature change, ΔT , calculated from the models (See section above on Heat Release Calculations) is shown in Figure 3. The higher ΔT for the low octane number PRFs is a result of the lower compression ratios needed which leads to a higher amount of hot residual gas.

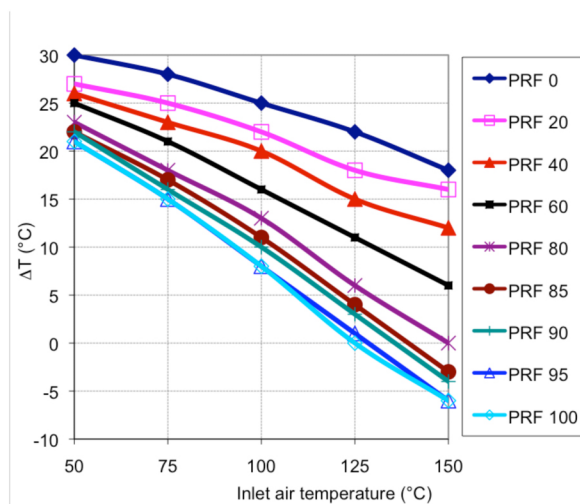


Figure 3. Calculated T_{IVC} for the different fuels and inlet air temperatures.

CA 50 PRESSURE SENSITIVITY

Since the CA50 is kept constant by changing the compression ratio, a high compression ratio corresponds to a higher ignition resistance. Figure 4 shows the different compression ratios required for a constant CA50 at $3 \pm 1^\circ$ after TDC for the PRFs as a function of inlet air temperature.

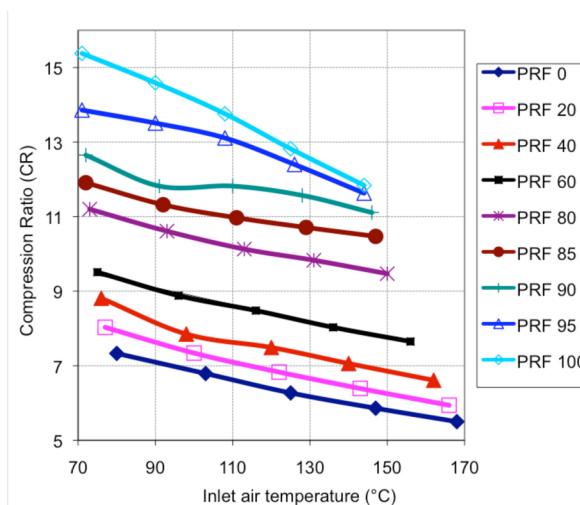


Figure 4. Compression ratios - pressure sensitivity for the different fuels.

Linear fit approximations were made for all fuels and these are presented in Table 2. The largest pressure difference is for PRF 95 and PRF 100, the fuels with little or no LTHR. A much smaller change in compression ratio is needed for the low octane number PRFs.

Table 2. Correlation between Inlet Air Temperature(x) and Compression Ratio(y)

Fuel	Equation	R ²
PRF 0	$y = -0.0209x + 8.95$	0.995
PRF 20	$y = -0.023x + 9.73$	0.992
PRF 40	$y = -0.024x + 10.46$	0.964
PRF 60	$y = -0.023x + 11.13$	0.993
PRF 80	$y = -0.022x + 12.73$	0.987
PRF 85	$y = -0.019x + 13.14$	0.969
PRF 90	$y = -0.018x + 13.77$	0.888
PRF 95	$y = -0.031x + 16.20$	0.966
PRF 100	$y = -0.049x + 18.94$	0.997

LOW TEMPERATURE HEAT RELEASE

The LTHR and start of combustion for the PRFs are shown in Figure 5, Figure 6, Figure 7, Figure 8, Figure 9, Figure 10, Figure 11, Figure 12, Figure 13, Figure 14. The five curves for each PRF represent the 5 different inlet air temperatures, with more extensive LTHR at the lower inlet air temperatures. One possible explanation for the higher amount of LTHR at the lower inlet air temperatures is the higher compression ratio used to achieve a constant CA50, since high pressure is known to increase LTHR. The black dots mark the start of combustion, defined as 0.2 J/CAD (See section below on Start of Combustion for further discussion). For PRF 0-80 LTHR is seen for all inlet air temperatures.

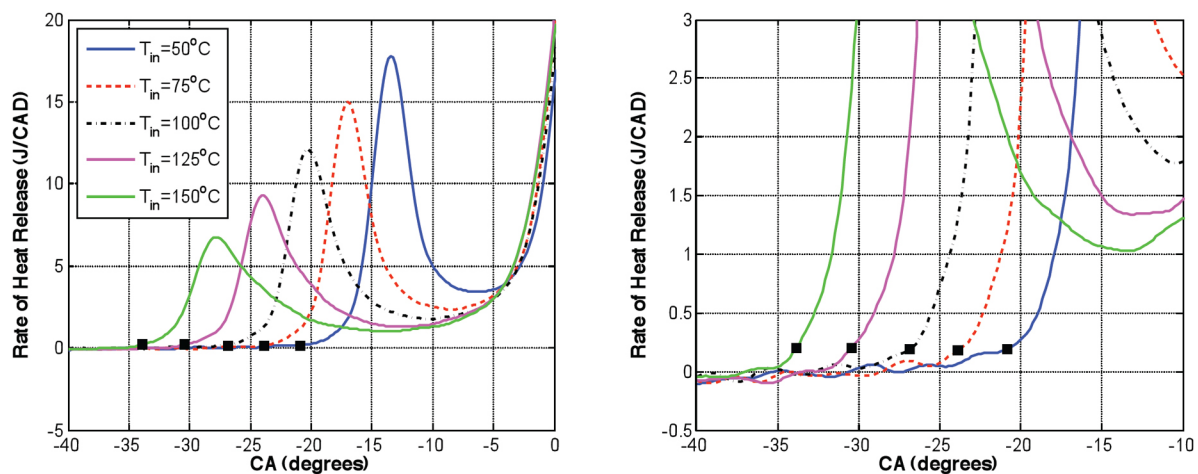


Figure 5. Low Temperature Heat Release and Auto Ignition for PRF 0. The dots mark start of combustion defined as 0.2 J/CAD. The picture to the right is a zoom of the picture to the left.

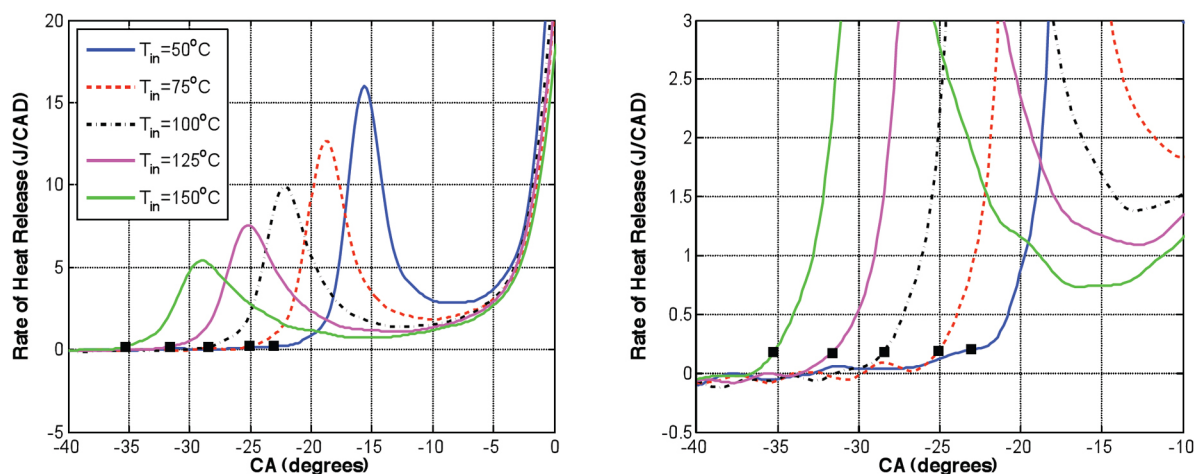


Figure 6. Low Temperature Heat Release and Auto Ignition for PRF 20. The dots mark start of combustion defined as 0.2 J/CAD.

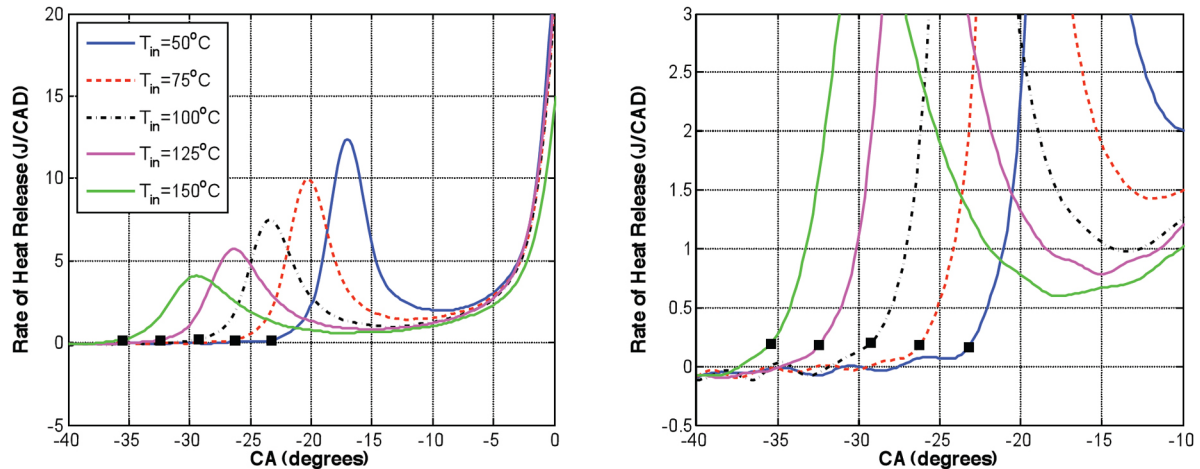


Figure 7. Low Temperature Heat Release and Auto Ignition for PRF 40. The dots mark start of combustion defined as 0.2 J/CAD.

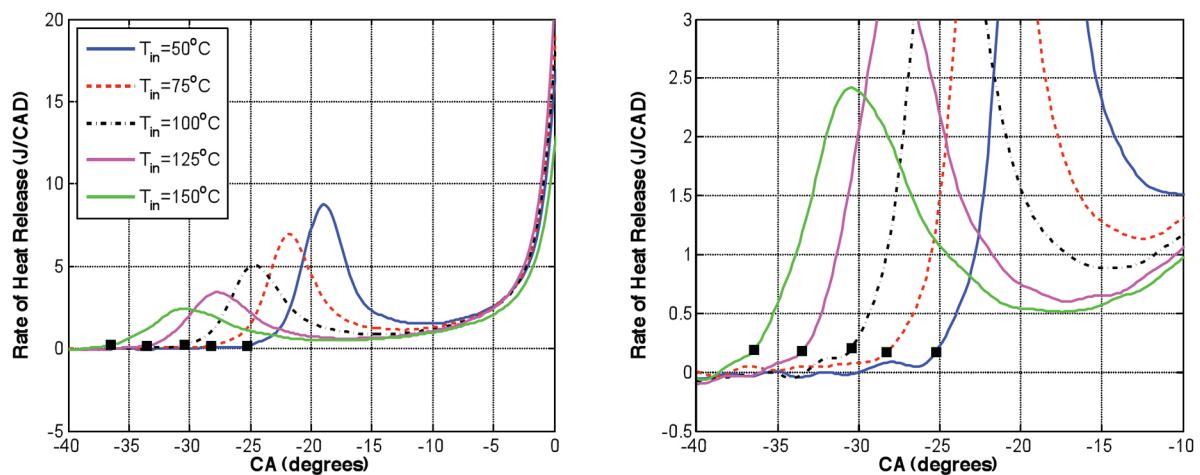


Figure 8. Low Temperature Heat Release and Auto Ignition for PRF 60. The dots mark start of combustion defined as 0.2 J/CAD.

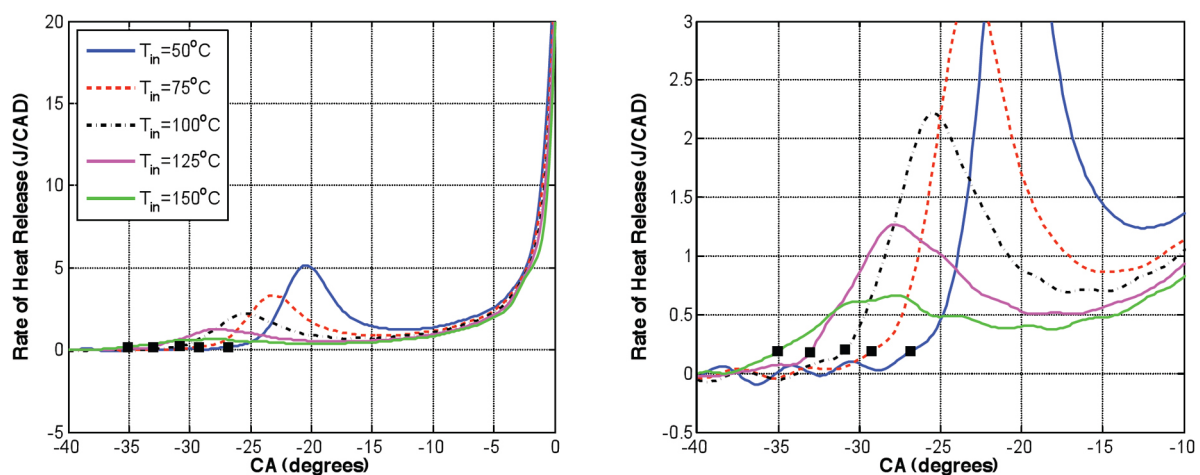


Figure 9. Low Temperature Heat Release and Auto Ignition for PRF 80. The dots mark start of combustion defined as 0.2 J/CAD.