# HCCI Combustion Using Engine Fuels with and without Oxygenated Compounds

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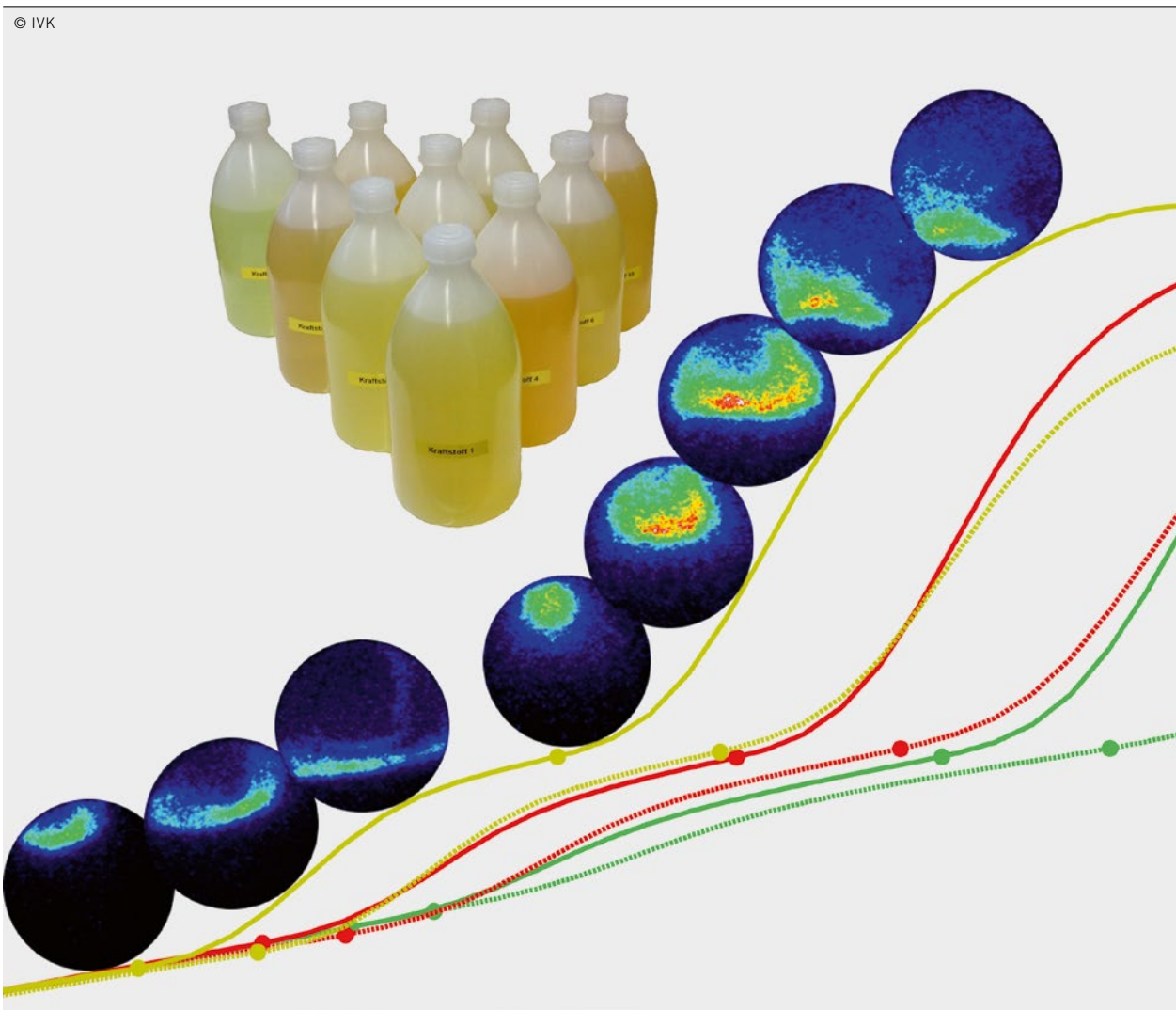
For further development of pre-mixed diesel combustion processes, as well as their model-based numerical calculation, a deep understanding of two-stage ignition of homogeneous diesel fuel air mixtures is indispensable. In the FVV research Project Fuel Indices (Kraftstoffkennzahlen II), 1-D/3-D ignition delay models have been developed for fuels with and without oxygenated compounds with a range of cetane numbers based on measurements from single-cylinder engines and a Rapid Compression Expansion Machine. The transferability of the parameterisations based on the surrogate fuels characterised in the RCEM to the engine data with real fuels is successfully demonstrated.





## 1 MOTIVATION

Further improvement of engine efficiency while simultaneously lowering emissions are the main objectives of current internal combustion engine combustion research. Premixed Charge Compression Ignition (PCCI) is seen as a promising concept for part load operation in view of controllability, emission reduction and efficiency [1]. Compared to conventional diesel combustion with short ignition delay (ID) and largely mixing controlled energy conversion, chemical kinetics play an increasingly dominant role for PCCI [2, 3]. Towards PCCI combustion, within the FVV project Fuel indices II HCCI combustion systems are characterised towards improved understanding of chemical kinetic effects for a wide range of engine relevant fuels with and without oxygenated compounds at the limit of perfectly homogeneous conditions. Measurements were carried out using two research engines with Atomizers installed in the intake as well as on a Rapid Compression Expansion Machine (RCEM) to determine ignition delay and heat release rates towards establishing correlations with the fuel Cetane Number (CN).

Empirical 1-D/3-D ignition delay models were further developed based on 1-/3-Arrhenius concepts. A cool flame heat release model was developed to model the heat released by low-temperature reactions typical of long-chain hydrocarbon fuels exhibiting two-stage ignition. The combination of the 3-Arrhenius and cool flame models together with two ignition integrals provides a fully predictive model for both stages of ignition. Research during the project was jointly performed at IVK, University of Stuttgart (with emphasis on the engine measurements) and LAV of ETH Zurich (emphasis 1-D/3-D model development and optical diagnostics).

## 2 MEASUREMENTS

At IVK a BASF official CN test engine [4] as well as a single-cylinder research engine derived from an OM642 diesel engine were used. To ensure transferability between the two, measurements in the OM642 employed a bowl-in piston (representing the series engine) as well as a pancake geometry (corresponding to the BASF). The inclusion of the BASF engine in the campaign enabled assessment of the CN (determined using the official test method) as a suitable index for HCCI combustion. The BASF test motor was extended to fully homogeneous operation by means of an Atomizer and complemented with state-of-the art pressure diagnostics and ID determination methods for HCCI combustion. Likewise, the OM642 was equipped with an Atomizer [5, 6] to ensure the highest possible degree of mixture homogeneity.

Eight fuels with three CN ranges, **FIGURE 1** (left), were studied in the engines to investigate the impact of oxygenated compounds on ignition delay. Aside the specified official test conditions of [4], sweeps in intake air temperature, Exhaust Gas Recirculation (EGR) rate, engine speed and load were performed. At LAV, an optically accessible RCEM was employed to characterise surrogates corresponding to the original fuels, **FIGURE 1** (right). These surrogates were chosen to closely represent the original fuels and subject to the availability of detailed reaction kinetics, which were later employed for model development.

| | Original fuels | | | Surrogate fuels | | |
|---|---|---|---|---|---|---|
| | CN ~ 38 | CN ~ 55 | CN ~ 78 | CN ~ 38 | CN ~ 55 | CN ~ 78 |
| **Non Oxygenated** | CN = 39.6<br>57.5 $\%_{Vol}$ DK B0 +<br>42.5 $\%_{Vol}$ Eurosuper | CN = 55.6<br>DK B0-1 | CN = 78.6<br>HVO | CN = 39.6<br>41 $\%_{Vol}$ Iso-Octane +<br>59 $\%_{Vol}$ n-Heptane | CN = 55.3<br>n-Heptane | CN = 76<br>n-Decane |
| | – | CN 55.8<br>DK B0-2 +<br>Ethylhexyl nitrate | – | – | CN = 51.4<br>92.7 $\%_{Vol}$ n-Heptane +<br>7.3 $\%_{Vol}$ Toluene | – |
| **Oxygenated** | CN = 36.5<br>66.5 $\%_{Vol}$ DK B0 +<br>33.5 $\%_{Vol}$ ETBE<br>(4.4 $\%_{Vol}$ $O_2$-content) | CN = 55.2<br>64 $\%_{Vol}$ DK B0 +<br>36 $\%_{Vol}$ RME<br>(4.2 $\%_{Vol}$ $O_2$-content) | – | CN = 37.8<br>68.2 $\%_{Vol}$ n-Heptane +<br>31.8 $\%_{Vol}$ n-Butanol<br>(7.7 $\%_{Vol}$ $O_2$-content) | CN = 50.1<br>90.9 $\%_{Vol}$ n-Heptane +<br>9.1 $\%_{Vol}$ n-Butanol<br>(2.29 $\%_{Vol}$ $O_2$-content) | – |

**FIGURE 1** Original fuels used in BASF and OM642 (left) and corresponding surrogates used in RCEM (© IVK)

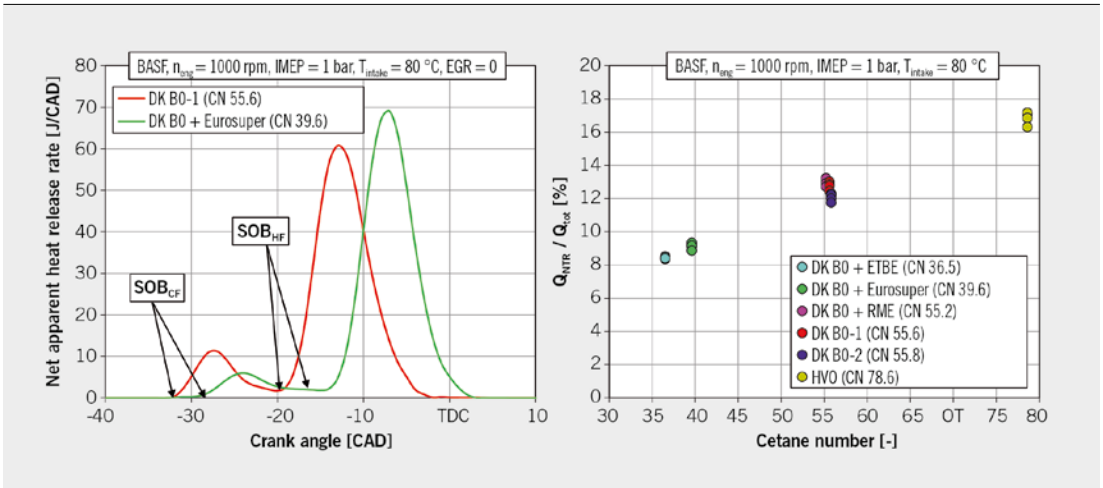



**FIGURE 2** Comparison of heat release rates for HCCI combustion of two different CN fuels in the BASF engine (left) and arrows indicate start of burn of cool-flame and high temperature ignition; ratio of cool-flame to total heat release as a function of CN for all fuels (right) (© IVK)

## 2.1 EXPERIMENTAL RESULTS

Calibration was initially performed on the BASF engine to ensure reproducibility of the official testing procedure [4]. In-cylinder pressure measurement and heat release analysis showed significant levels of low temperature reactions (LTR) – also known as cool flame (CF) – heat release ($Q_{LTR}$), in particular for fuels with high CN [6]. The CN determined by the standard test procedure in [4] provides an integrated value which includes $Q_{LTR}$, leading to the observed correlation between CN and $Q_{LTR}$ in HCCI combustion, which is supported by similar findings documented in the literature (for example [7]) concerning CN versus ID and $Q_{LTR}$.

The dependence of $Q_{LTR}$ on CN is illustrated schematically in **FIGURE 2** (left) for two fuels with intermediate and low CN. The correlation between CN and $Q_{LTR}$ is further independent of fuel composition as can be observed in **FIGURE 2** (right). Concerning the onset time of cool flame reactions ($SOB_{CF}$), the higher CN fuel shows earlier start of burning ($SOB_{CF}$), **FIGURE 2** (left), which can be attributed to the longer-chain alkane molecule promoting ignition. As a consequence, $SOB_{CF}$ starts at lower temperatures for high CN fuels, while stable compounds more resistant to ignition require higher temperatures (corresponding to later crank angles due to compression work) before cool flame reactions commence, as discussed also in [8].

A detailed analysis of the mean temperatures present in the cylinder at onset of cool flame and high temperature ignition for all fuels at a given operating condition in the BASF engine for a sweep in EGR rate is shown in **FIGURE 3**. It is evident, that the temperature at $SOB_{CF}$ is negatively correlated with the CN and shows only a weak dependence on EGR rate. High temperature ignition however occurs at almost the same temperature for all fuels studied, largely independent of CN and EGR rate, which is marked by the onset of $H_2O_2$ reactions [9]. The earlier onset of high temperature combustion ($SOB_{HF}$) for higher CN is hence due to the combined effect of earlier onset of $SOB_{CF}$ and increased $Q_{LTR}$ observed for the high CN fuels [6], **FIGURE 2**, (right). Identical findings are reported for the corresponding surrogates characterised in the RCEM in [6].

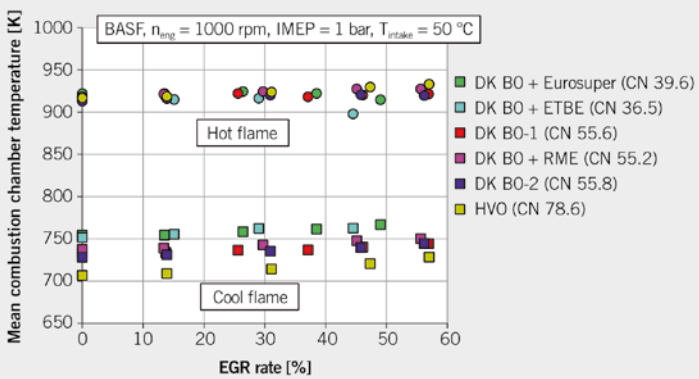



**FIGURE 3** Average combustion chamber temperature at start of cool-flame and high temperature ignition for a variation in EGR rate at one operating condition in the BASF engine (© IVK)

## 3 NUMERICAL MODELLING

Phenomenological HCCI ID-models based on Arrhenius-type expressions were developed both at IVK, University of Stuttgart, and at LAV, ETH Zurich. The model of IVK was a single-Arrhenius expression [5], with activation energy defined as a fuel-dependent variable. Parameterisation and validated by means of the Livengood Wu ignition integral [10] was done with extensive engine data from the BASF and OM642. As discussed in depth in [6] this activation energy can serve as a fuel index to characterise HCCI combustion.

The 3-Arrhenius model [11, 12] was further developed at LAV. It is shown schematically in **FIGURE 4**, together with the three regions of the two-stage ignition of long chain hydrocarbons, that is to say low temperature ignition, the so-called Negative Temperature Coefficient (NTC) range as well as high temperature ignition. In a first step, an initial guess of the model's parameters was made by using IDs computed for perfectly stirred reactors (PSR, using the Senkin package [13] from Chemkin [14]) with detailed reac-

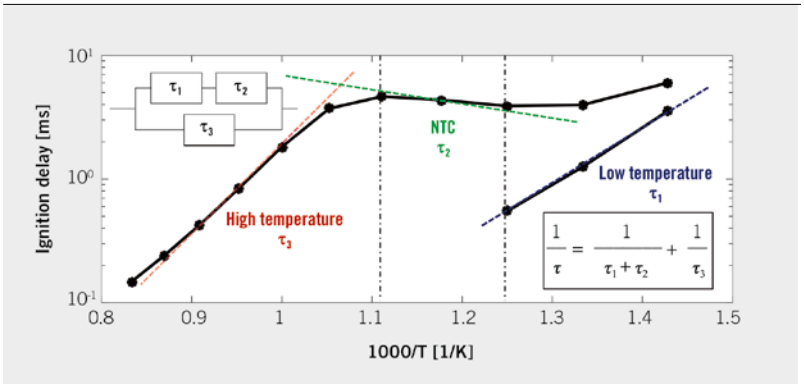



**FIGURE 4** Ignition delays times for fuels exhibiting two-stage ignition behaviour with characteristic low-, intermediate (NTC) and high-temperature regimes and corresponding 3-Arrhenius model (© LAV)

tion kinetics for all surrogates over a wide range of engine-relevant pressures, temperatures, equivalence ratios and exhaust gas recirculation rates.

Further parameter validation was done by means of the Livengood-Wu ignition integral and RCEM ignition measurements [15]. To this end, two Livengood Wu ignition integrals, one for low and high temperature ignition, are separately integrated along the pressure and temperature trajectory of the compression stroke, **FIGURE 5** (lower left). In order to account for the rise in pressure and temperature as a result of the heat release by low-temperature reactions, the duration and amount of heat released must be predicted. To this end a "cool flame heat release" model was developed [16], based on a Wiebe assumption, **FIGURE 5** (upper left). This was successfully validated for all fuels for wide ranges of conditions, as shown in the cumulative low temperature heat release correlation plot in **FIGURE 5** (upper right). High CN fuels (such as n decane, khaki) release significantly more heat than those with low (for example yellow, n butanol/n heptane). As a result, substantially shorter high temperature IDs are predicted for the former, in good agreement with measurements from the RCEM and in analogy to engine data, **FIGURE 2**. This approach enables fully predictive simulations of high temperature ignition for which

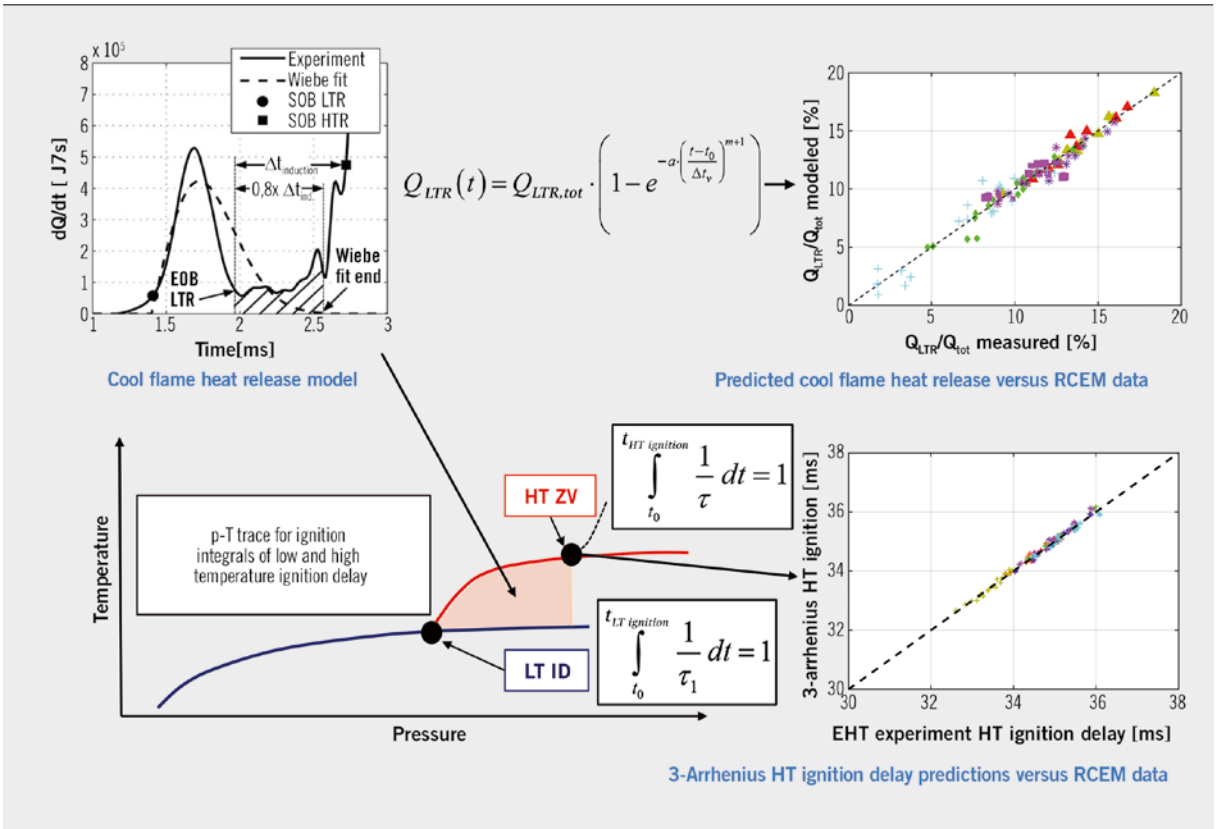



**FIGURE 5** Combination of 3-Arrhenius model and the developed model for cool-flame heat release (upper row) with two Livengood-Wu ignition integrals for low- and high-temperature ignition; integration along the pressure/temperature evolution during the compression stroke (lower left) allows for excellent prediction of main ignition onset (lower right) (colours correspond to fuels in **FIGURE 1**) (© LAV)

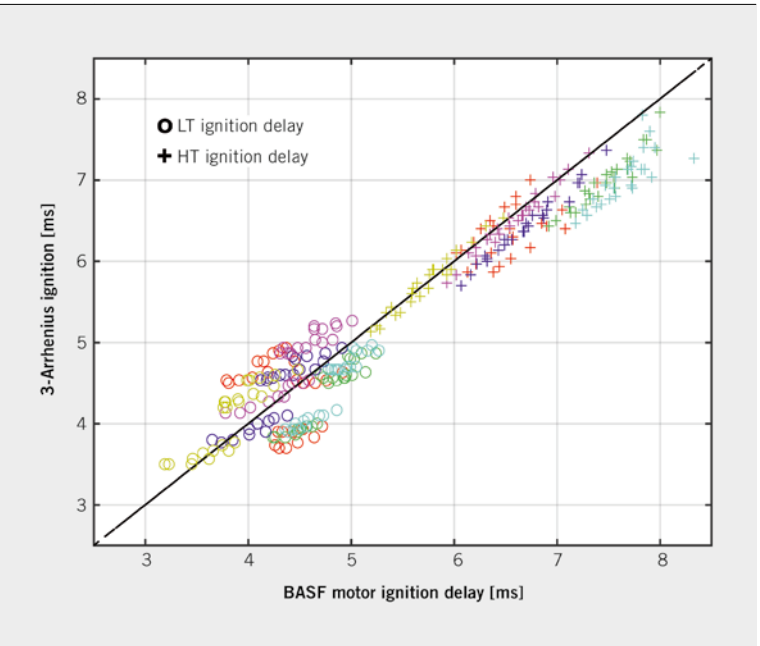



**FIGURE 6** Comparison between predicted and measured low and high temperature ignition delays when applying the surrogate fuel parameterisation from the RCEM to the OM642 engine running on the original fuels (colours correspond to fuels in **FIGURE 1**) (© IVK and LAV)

excellent agreement is shown for all fuels over a wide range of operating conditions in the RCEM, **FIGURE 5** (lower right). The transferability of the surrogate parameterisation to the engine running on the original fuels was examined in a last step, where very good agreement could be successfully demonstrated for wide ranges of operating conditions as shown in **FIGURE 6**.

## 4 SUMMARY

In the framework of the FVV project Fuel indices II, measurements were carried out using two research engines equipped with Atomizers and an optically accessible rapid compression expansion machine to characterise engine relevant fuels with and without oxygenated compounds for HCCI operation towards establishing "fuel indices" for engine combustion of fully homogenous mixtures. The findings provide insight concerning the correlation between CN and HCCI combustion and support the use of the CN as a suitable index.

1- and 3-Arrhenius ID models were further developed; the former parametrised using engine measurements with the original fuels, the latter with corresponding surrogates characterised in the RCEM. The 3-Arrhenius ID model was optimised using genetic algorithms, starting from an initial parameter estimate based on ignition delays calculated with detailed kinetics for a wide range of conditions. The implementation of the 3-Arrhenius model – in conjunction with a newly developed model for the cool flame heat release – in the context of two Livengood-Wu ignition integrals enables fully predictive calculation of low and high temperature ignition delays. Extensive validation of the model was carried out using data from the RCEM and the transferability of the surrogate parameterisation to the OM642 engine running on the original fuels has been successfully demonstrated.

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