Schweizerische Eidgenossenschaft
Confédération suisse
Confederazione Svizzera
Confederaziun svizra

Eidgenössisches Departement fürUmwelt, Verkehr, Energie und Kommunikation UVEK

Bundesamt für Energie BFE

Schlussbericht 2010, 04. Juli 2011

Brennstoffe für homogene selbstgezündete Verbrennungsprozesse

---

Auftraggeber:
Bundesamt für Energie BFE
Forschungsprogramm 101514
CH-3003 Bern
www.bfe.admin.ch

Kofinanzierung:
Forschungsvereinigung Verbrennungskraftmaschinen e.V, Postfach 710864, D-60498 Frankfurt, Projekt Nr. 609480

Auftragnehmer:
ETH Zürich
Institut für Energietechnik, Laboratorium für Aerothermochemie und Verbrennungssysteme
Prof. Dr. K. Boulouchos
ETH Zentrum ML J39
Sonneggstrasse 3
CH-8092 Zürich
www.lav.ethz.ch

Autoren:
Annelies Vandersickel, LAV ETH Zürich, vandersickel@lav.mavt.ethz.ch
Dimitrios Mitakos, LAV ETH Zürich, mitakos@lav.mavt.ethz.ch
Bruno Schneider, LAV ETH Zürich, schneider@lav.mavt.ethz.ch
Konstantinos Boulouchos, LAV ETH Zürich, boulouchos@lav.mavt.ethz.ch

BFE-Bereichsleiter: Sandra Hermle
BFE-Programmleiter: Stephan Renz
BFE-Vertrags- und Projektnummer: 151786 / 101514

Abstract

1. Gegenstand dieses Projekts ist die theoretische und experimentelle Untersuchung der Selbstzündungs- und Verbrennungseigenschaften von Brennstoff-Luft-Gemischen, wie sie in Verbrennungsmotoren im selbstgezündeten, homogenen Betriebsbereich (HCCI, Homogeneous Charge Compression Ignition) vorhanden sind. Das Projekt ist eng verknüpft mit dem Forschungsvorhaben „Kraftstoffkennzahlen für homogene Verbrennung“ der Forschungsvereinigung Verbrennungskraftmaschinen (FVV Projekt Nr. 609480 Arbeitspunkte TP2 und TP3). Ziel dieses Forschungsvorhabens ist die Erarbeitung von theoretischen und experimentellen Grundlagen, die es ermöglichen, neue Kraftstoffkennzahlen zu definieren, welche das Verhalten unterschiedlicher Kraftstoffe beim HCCI Brennverfahren gut zu beschreiben vermögen (analog zu der Cetan-Zahl, welche das Zündverhalten von Kraftstoffen unter dieselmotorischen Bedingungen charakterisiert).

2. Am Laboratorium für Aerothermochemie und Verbrennungssysteme der ETH Zürich werden im Rahmen des FVV Teilprojekts TP2 numerische Reaktionsmodelle für die theoretische Beschreibung der Selbstzündung und Verbrennung der Kraftstoff-Luft-Gemische entwickelt. Für die Anwendung im HCCI-Brennverfahren sind dabei insbesondere die Niedertemperaturreaktionen und der Bereich mit negativem Temperaturkoeffizient von grossem Interesse (bei Kraftstoffen, die ein zweistufiges Zündverhalten aufweisen). Da detaillierte Reaktionsmechanismen für komplexe Brennstoffmischungen bisher noch kaum existieren und sie zudem für die Kopplung mit 3D-CFD Simulationen zu komplex (d.h. langsam) sind, werden phänomenologische Modelle eingesetzt.

   Das erste Modell basiert auf einem einfachen Zündintegral erlaubt eine schnelle Abschätzung des Einflusses der Betriebsbedingungen auf die Zündverzugszeiten im HCCI-Betrieb. Das zweite Modell ist ein globales Reaktionsmodell und beschreibt die zweistufige Zündung mittels 7 Reaktionen, an dem 8 Spezies beteiligt sind. Die Parameter dieser beiden Modelle sind für jeden betrachteten Kraftstoff optimiert worden. Die zugrundeliegenden experimentellen Daten stammen aus Messungen in einem Stosswellenrohr (Teilprojekt TP1 des FVV Projekts). Es konnte eine sehr gute Übereinstimmung zwischen den Modellvorhersagen und den experimentellen Daten gefunden werden, im Hinblick auf die Zündverzugszeiten sowohl bei der Hochtemperaturreaktion als auch der Niedrigtemperaturreaktion. Auch die Wärmefreisetzung und Spezies-Evolutionen des globalen Reaktionsmodells zeigen eine gute qualitative Übereinstimmung mit detaillierten Referenzmechanismen.

   Beide Modelle sind bereit für den Einsatz in 3D-CFD Simulationen. Durch die Kopplung der Modelle mit 3D-CFD Simulationen können jetzt die innermotorischen Abläufe in HCCI-Motoren detailliert untersucht werden.

3. Die Arbeiten am Labor im Rahmen des FVV Teilprojekts TP3 befassen sich mit der experimentellen Untersuchung der Brennstoffeigenschaften (Zündverzüge, Wärmefreisetzung) unter HCCI-Bedingungen. Das Einhubtriebwerk des Labors ist ein idealer Versuchsträger für diese Untersuchungen. Es ermöglicht Experimente unter motorischen Bedingungen bei gleichzeitig ausgezeichnetem Zugang zum Brennraum für optische Messverfahren. Wichtige Parameter für die Darstellung unterschiedlicher Motortypen wie das Kompressionsverhältnis und der Gaszustand im Zylinder vor Kompressionsbeginn (Druck, Temperatur, Zusammensetzung) können frei gewählt werden.

   Im Rahmen des Projektes wurde das Einhubtriebwerk weitgehend revidiert. Um auch für die erst bei höheren Temperaturen verdampfenden Brennstoffe gute homogene Bedingungen erreichen zu können, wurden neue beheizte Bauteilen entworfen, gefertigt und angebaut. Zudem wurde die messtechnische Ausrüstung komplettiert und am Versuchsträger aufgebaut. Detaillierte Temperaturmessungen zeigen, dass mit den neuen beheizten Bauteilen genügend hohe Temperaturen für die Verdampfung der schwersiedenden Kraftstoffe erreicht werden können. Das vorliegende Temperaturfeld zeigt zudem, wie erwünscht, eine sehr gute Homogenisierung.

Anhand der ersten Messreihen mit n-Heptan wurden die Einstellungen des Einhubtriebwerks bestimmt, mit denen man eine homogene Vormischverbrennung bei Bedingungen wie sie im Motor vorhanden sind erreicht. Die verschiedenen Messverfahren wurden verglichen und im Hinblick auf eine möglichst eindeutige Bestimmung der Zündverzugszeiten optimiert. Im weiteren Verlauf des Projekts wurde das Zündverhalten aller Kraftstoffe (mit Ausnahme der schwerverdampfenden Diesel) unter HCCI-Bedingungen charakterisiert. Die Ergebnisse zeigen ein ähnliches Verhalten der Kraftstoffe wie sie im Einzylindermotor des IVK beim Betrieb mit der Common-Rail Einspritzausrüstung beobachtet wurden, d.h. das Zündverhalten der Kraftstoffe wird durch die zum Zeitpunkt der Selbstzündung immer noch vorhandenen Inhomogenitäten der Kraftstoff/Luft Mischung stark beeinflusst. Nur bei n-Heptan zeigt sich bei den Messungen im Einhubtriebwerk ein deutlich längerer Zündverzug als bei den anderen Kraftstoffen – obwohl n-Heptan die höchste Cetan Zahl aller untersuchten Kraftstoffe aufweist! Dies dürfte darauf zurückzuführen sein das n-Heptan bei einer konstanten Temperatur von nur 98°C verdampft (der tiefsten Verdampfungstemperatur aller untersuchten Kraftstoffe) – die schnelle und vollständige Verdampfung führt zu einer wesentlich besser homogenisierten Kraftstoff/Luft-Mischung, so dass der Zündverzug nicht durch lokale Zonen mit fetterem Gemisch beeinflusst wird.

Project Context

After the successful completion of the FVV (Forschungsvereinigung Verbrennungskraftmaschinen) cluster project Nr.811 ’Theoretische und experimentelle Untersuchung der homogenen Dieselverbrennung’ in March 2006 (supported by BFE, Project Nr. 40070), at the end of 2007, the follow-on FVV project, Kraftstoffkennzahlen für homogene Verbrennung’ started. Within the frame of the BFE Project reported here, the BFE contributes to the start-up and first phase of this new FVV project.

Background of the project

Homogeneous charge compression ignition combustion is one of the main focuses in combustion research since years. The strong NOx and soot emission reduction achievable with such homogenous processes, however, comes at a certain price. Since the HCCI process relies on auto-ignition to start combustion, the exact ignition timing can no longer be externally controlled via a spark plug or the injection timings, but must be controlled indirectly via the mixture conditions (pressure p, temperature T, fuel-air ratio and exhaust gas recirculation rates) inside the combustion chamber after inlet valve closure. Especially at high loads and low rotation speeds, the homogeneous mixture generally ignites too early, which results in high peak pressures (high noise and thermal stresses) and low thermodynamic efficiencies. A precise control of ignition is in practical engine applications complicated even further, because of instationary operating conditions and cycle to cycle as well as cylinder to cylinder variations.

Present ‘HCCI’ engines are therefore typically operated in hybrid mode and switch to the conventional diesel combustion mode (diffusion) at high loads. Because of place and cost limitations, the same injector must be used for both operation modes. This means that the injector should simultaneously meet the requirements for mixture formation in diffusion mode (injection close to top dead center, wide Spay angle, high injection and back pressure) as well as in homogeneous mode (Injection at the end of the intake or beginning of the compression stroke, narrow spray angle, low injection and back pressures) – a challenge !

Tailored fuels, as potentially possible to synthesize nowadays, offer a new means to control ignition and hence expand the HCCI operation range. To explore the potential of such fuels and match the fuel to the engine process, however, a profound knowledge of its behavior under homogenous operating conditions is needed. For diesel engines for example, the cetane number has proofed to be an adequate number to describe the ignitability of the fuel. A number which characterizes the behavior of a fuel in homogenously operating engines however has not been defined yet. Each fuel must therefore, at the moment, still be tested in an engine experiment, to define whether it is suitable for a newly developed HCCI engine or not.

Aim of the Project

The FVV Project ‘Kraftstoffkennzahlen’ aims at defining a number or ‘fuel index’ to characterize the ignition behaviour of technically relevant fuels under homogeneous charge compression ignition (HCCI) engine operation. Within the framework of this project, the ignition and combustion characteristics of a large set of fuel is therefore being investigated in detail. Starting from perfectly premixed experiments in a shock tube, followed by optical investigations on the single stroke machine at our lab and finally experiments on a car, respectively a heavy duty single cylinder engine, a large process chain of experiments is built up and an extensive set of data is being collected. On the simulation side, phenomenological reaction mechanisms applicable to all of the project fuels are being developed at our lab. In combination with a 3D-CFD code, these models should allow simulating the entire engine cycle.

Table 1 gives on overview of the fuel mixtures investigated within the FVV ‘Kraftstoffkennzahlen’ project. The Cetane Number on the first row describes the fuel’s willingness to ignite under diesel engine conditions (for conventional diesel the CN nowadays typically lies between 50 and 60). Although, as mentioned before, the cetane number is only partially suited to describe the ignition behaviour under homogenous conditions, the large span of CN selected indicates that - with the selected compositions - a wide range of ignition chemistry is covered. This multitude of chemical components considered poses a significant challenge for the development of chemical reaction mechanisms. Also the volatility of the fuels differs significantly: The initial boiling point ranges from 40°C to 224°C, the final boiling point from 165°C up to 333°C.

	1	2	3	4	5	6	7	8	9	10
	CEC-RF	**n-Heptan**	**Naphtha 1**	**Naphtha 2**	**Kero 1**	**Kero 2**	**CCS-Fuel**	**Diesel 1**	**Diesel 2**	**Diesel 3**
Aromat %					25					
Naphten %			23		30	40	60			
Paraffin %		100	77	80	45	50	40	100	100	100
Olefin %				20		10				
Distillation										
IBP °C	210	98	87	40	153	149	159	192	206	230
5%	227		95	81	166	162	166	198	216	243
10%	235		98	90	166	163	167	201	222	247
50%	275		114	120	177	168	177	244	272	275
90%	329		143	150	247	292	195	305	311	309
95%	352		148	156	267	313	210	318	324	322
FBP	365	98	169	180	283	317	212	327	334	327
CN	54	57	35	55	38	52	44	50	57	60

Table 1: Fuels used in the FVV 'Kraftstoffkennzahlen für homogene Verbrennung' Project

From previous experimental work on the single stroke machine at our lab (which has been done within the frame of the preceding project) it is known that both the mixture and temperature inhomogeneities present inside the combustion chamber significantly influence ignition timing and location. Our single stroke engine with its horizontally oriented cylinder and the only partially heated combustion chamber walls could therefore not fulfil the stringent homogeneity requirements of the project in his original configuration. Furthermore, to evaporate the high boiling fuel components, additional heating measures are required and need to be installed.

The aim of the experimental project part was therefore in the first step the redesign of our single stroke engine in order to improve the homogenization of the fuel/air mixture and maximize the evaporated fuel fraction at the time of ignition. Since the properties of the selected fuels (especially the boiling curves) differ substantially, the optimal strategy differs from fuel to fuel. Additionally, a fundamental revision of the test rig is required to ensure its proper operation in the future. Once the functioning of the newly designed set-up is demonstrated, the aim of the experiments is to systematically investigate the ignition properties of the project fuels based on the optical measurement data.

In the revised/redesigned single stroke machine ignition delay measurements under a transient, engine relevant Pressure-Temperature trace are conducted for different fuels. EGR and lambda influence is investigated, while the start of injection is selected towards direction “early” so that it assures operation away from diffusion mode, but nevertheless “late” enough for maximizing the chance of full evaporation of the fuel and formation of a premixed charge. Optical OH-Chemiluminescence high speed recordings are revealing the distribution of ignition locations and reaction zones. With the abovementioned measurements, trends of the ignition delay as a function of Cetane Number, as well as the extent of homogeneity of reaction zones can be assessed.

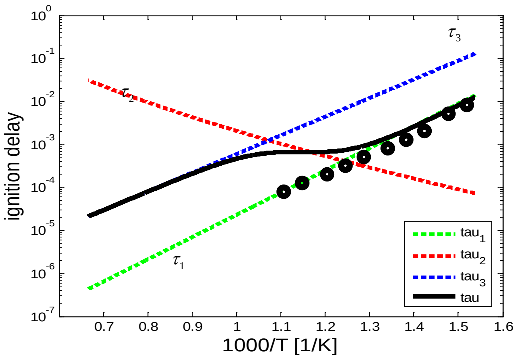
Simulation Part – Development of an ignition/combustion mechanism for practical fuels in HCCI combustion

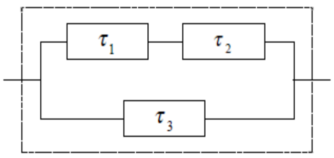
Annelies Vandersickel

Under HCCI conditions, the low temperature and negative temperature dependence of fuels exhibiting two-stage ignition are of particular interest. At present, however, detailed reaction schemes for complex fuel mixtures including aromatics, iso- or cyclo-parrafins are only just appearing or even non-existent. Furthermore, even after reduction, the resulting mechanisms typically remain too large to incorporate into CFD simulations. The main goal of this simulation part was therefore the development of compact and phenomenological ignition/combustion models applicable to each of the project fuels. An extensive set of ignition delay data generated in one of the partner projects at the University of Duisburg provides the basis for this model development.

Ignition Integral based on a 3-Arrhenius ignition delay model

The first model developed, is based on a classical ignition integral and is meant to quickly assess the impact of engine operating conditions on both first stage and main ignition timings. The shock tube delays in the integral expression are described using a 3-Arrhenius model, which in the present work has been extended to account for the presence of EGR in the gas mixture. An overview of the final model and the corresponding model equations is given in Figure 1. First stage ignition delay times (τ1, circles in Figure 1) are described by a single Arrhenius expression, whereas the main ignition delay times τ are described as a combination of three ignition delays τ1, τ2 and τ3 representing respectively the low, medium and high temperature chemistry. More details about the model and its calibration for three of the project fuels are submitted for publication in FUEL [1].





$$\frac{1}{\tau} = \frac{1}{\tau_1 + \tau_2} + \frac{1}{\tau_3}$$

Original: G.A..Weisser, Diss. ETH No. 14465

$$\boxed{\tau_i = A_i \cdot \left(\frac{p}{p_{ref}}\right)^{\beta_i} \cdot T^{b_i} \cdot \exp\left(\frac{T_{Ai}}{T}\right) \cdot \varphi^{\gamma_i} \cdot \left(\frac{[N_2]}{[O_2]}\right)^{d_i} \cdot \exp\left(\frac{[N_2]}{[O_2]} \cdot \frac{e_i}{T}\right)}$$

Figure 1: Overview of the extended 3-Arrhenius shock tube ignition delay model (pressure p [bar], p_{ref} = 1 bar, temperature T [K], equivalence ratio φ [-])

After calibration of the model parameters, an excellent agreement with the shock tube data [1, 2] from the partner project in Duisburg could be achieved. For each of the project fuels, the average error on the ignition delay predictions is as small 0.2 to 0.4 ms, which is of the same order as the experimental uncertainty. The 3-Arrhenius model as such has proven a useful tool to clarify and illustrate trends in the experimental data and has been applied to elucidate the correlation between fuel composition and ignition behaviour. The results of this study as well are included in the paper submitted for FUEL.

The complete ignition model, using the 3-Arrhenius model in conjunction with the ignition integral, has been validated based on engine data obtained from a partner project at the University of Stuttgart [3]. The model successfully captures the influences of changing operating conditions on both the first and main ignition delay times, as illustrated in Figure 2.

Overall, a satisfying agreement of measured and predicted ignition delay values could be obtained. The remaining deviations can be attributed to the incomplete homogenisation during real engine operation. Especially for operating points using later injection timings this effect becomes important. To resolve and understand these inhomogeneity influences reactive 3D-CFD simulations are needed. Before meaningful simulation can be done, however, a reduced reaction mechanism with representative species needed to be developed and adapted to each of the project fuels. This development is addressed in the following paragraphs.

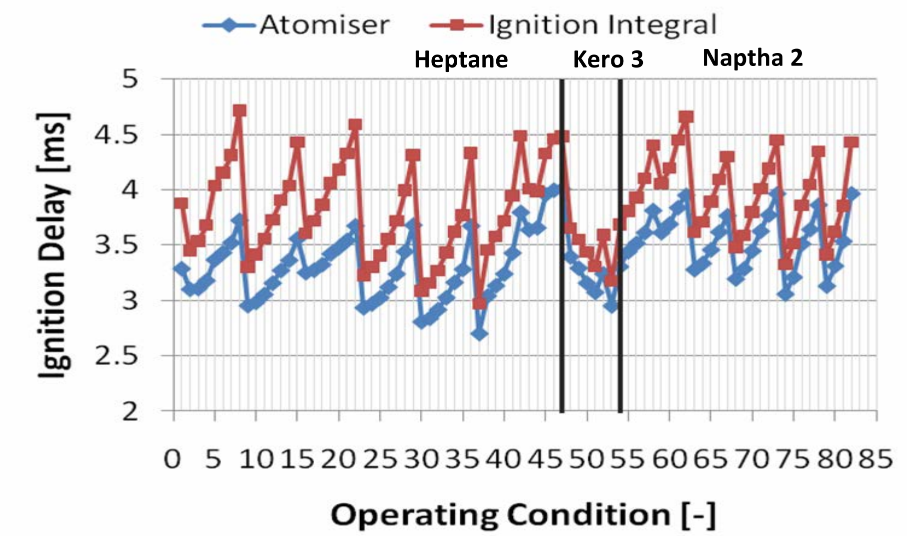


Figure 2: Comparison of measured (blue) and calculated (red) main engine ignition delay times

Lumped or Global Auto-ignition model

The global reaction model developed describes the dynamics of the 2-stage ignition process and aims at accurately predicting global quantities like ignition delay timings as well as pressure, temperature and important tracer species evolutions, using the same overall scheme for each of the fuels considered.

To understand the complex interplay of the vast amount of species involved in the ignition of practical multi-component fuels, several existing detailed, skeletal and reduced mechanisms have been analysed and a comparison with more phenomenological approaches has been carried out. Furthermore, an in-depth literature review on the chemistry of non-alkanic fuel compounds, such as alkenes, cyclo-alkanes and aromatics, has been completed.

Based on the gained knowledge, a 7-step reaction model has been proposed. The model is based on a previous reduced model [4] for which the stoichiometry and thermo-physical properties are adapted to the fuel under consideration. The details of these modifications are presented at the THIESEL 2010 Conference and can be found in the accompanying paper [5]. The reaction rate parameters are adjusted using a genetic algorithm optimization methodology to improve the model predictions and to define a set of parameters for each of the fuels. The optimization is guided by a sensitivity study of the ignition delay predictions with respect to each of the rate parameters, and is performed based on shock tube data [1,2] for a broad range of HCCI relevant conditions as follows:

1. In a first step, the mechanism has been coupled with a *single objective* optimization algorithm and the rate parameters have been optimized based on the main ignition delay times only. [3]
2. In a next step, the parameters have been further adjusted to reproduce the available low temperature ignition delay and overall heat release data in addition to the main ignition delays. To this end, the model has been coupled with a *multi-objective* optimization tool, which aims at minimizing the error between the measured and simulated values for each of the objectives. More detailed information about this optimization step, using two objective functions, has been presented at the IEA Task Leader Meeting in Japan as well as the THIESEL 2010 Conference. [5]
3. To improve the predicted evolution of the main traces species, the number of objectives has in a next step been further increased from two to four. This optimization step has been successfully completed for each of the project fuels. The overall error on the ignition delay predictions is as small as 0.2-0.4ms and both the heat release and main species evolutions show a very good qualitative agreement with detailed reaction mechanisms. The results are briefly illustrated in Figure 3 to Figure 6 and will be published in Combustion and Flame.

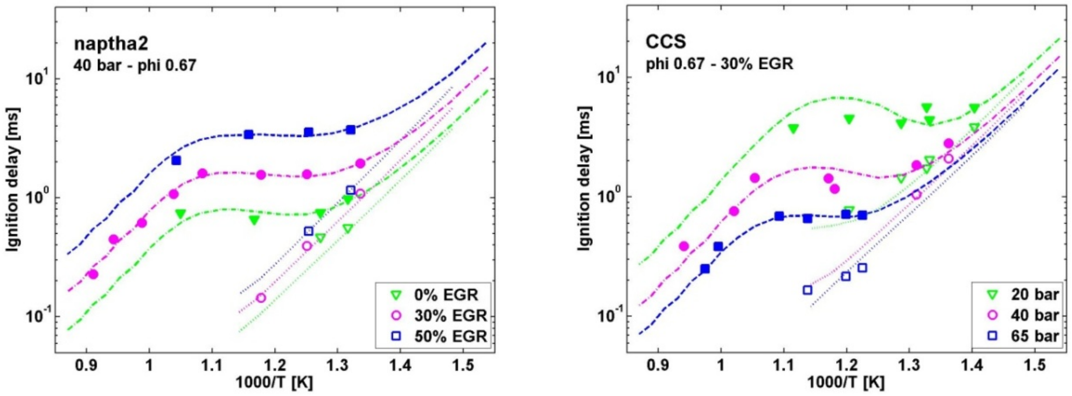


Figure 3: Exemplary comparison of calculated (lines) and experimental (symbols) shock tube ignition delay for two of the tested fuels. The open symbols indicate first stage ignition delays, the closed symbols the main ignition delays.

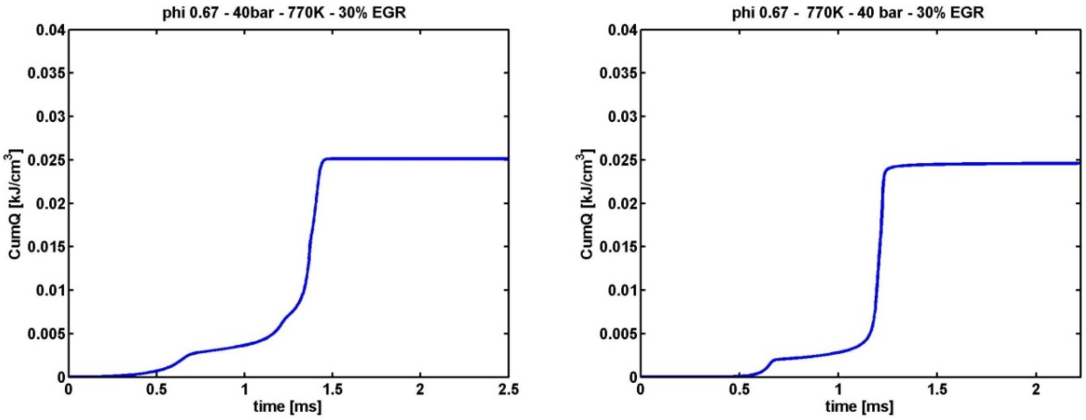


Figure 4: Comparison of the cumulative heat release obtained with the present lumped reaction model (left) and the 'detailed' reaction mechanism of Tsurushima [6] (right). The two stage heat release is seen to be captured very well.

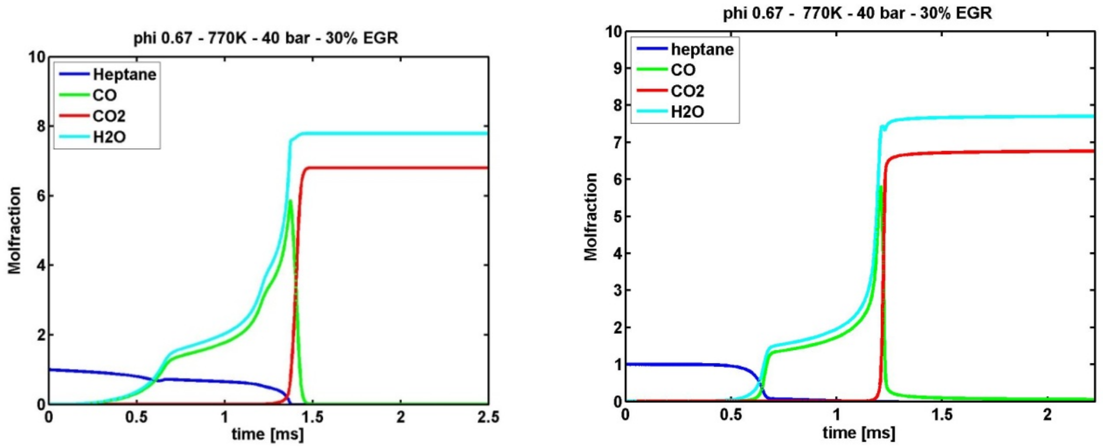


Figure 5: Comparison of major species profiles present during heptanes ignition, obtained with the present lumped mechanism (left) and the 'detailed' reaction mechanism of Tsurushima [6] (right). An excellent agreement, qualitatively as well as quantitatively, between the lumped and detailed model predictions can be observed for CO, CO2 and H2O. The heptane amount between first and second stage of ignition is deviating due to the fact that -in the lumped mechanism- heptane is grouped with other major radicals existing during this stage of ignition.

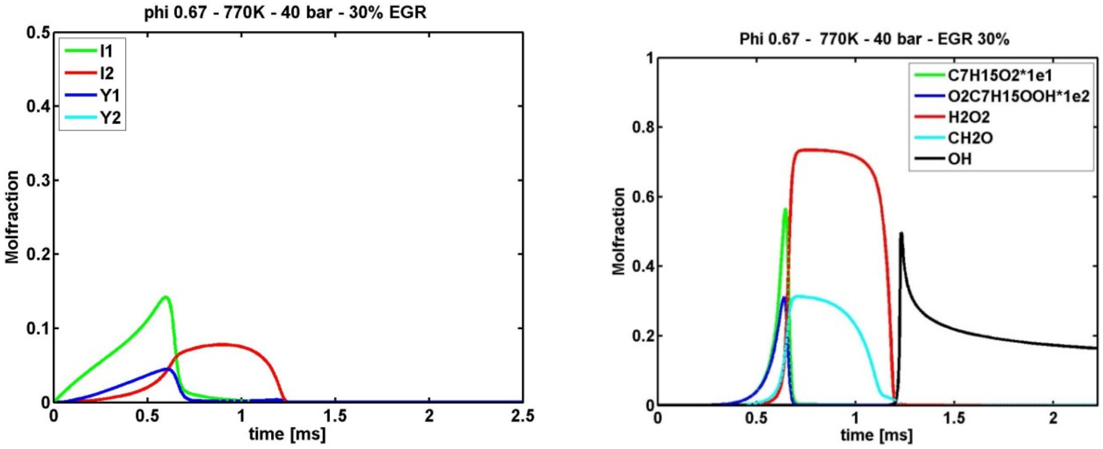


Figure 6: Comparison of important traces species profiles during two stage ignition of n-heptane/air mixtures, obtained with the present lumped reaction model (left) and the 'detailed' reaction model of Tsurushima [6] (right). The species in the lumped reaction model are fictuous species, each representing a group of species with similar behavior of which the most important ones are given here: I1 corresponds to C7H15O2, Y1 to O2C7H15OOH, I2 groups H2O2 and CH2O and Y2 represents mainly OH. As can be seen by comparing both graphs, the profiles of the mentioned intermediates are very well reproduced. This qualitative agreement indicates that the main dynamics of the two-stage ignition process are captured and gives confidence that the model will give reasonable results even outside the validation range. The intermediate species predictions furthermore allow identifying which stage of ignition is taking place at which location inside the combustion chamber when used in 3D-CFD simulations.

To test the optimized model in transient conditions, it has been implemented in a single zone engine model. The resulting engine model shows a good agreement with measured heat release and pressure/temperature data from atomizer engine experiments from a partner project in Stuttgart. Especially the influence of changing operating conditions on the auto-ignition and combustion chemistry is very well captured as shown in Figure 7 and Figure 8 .

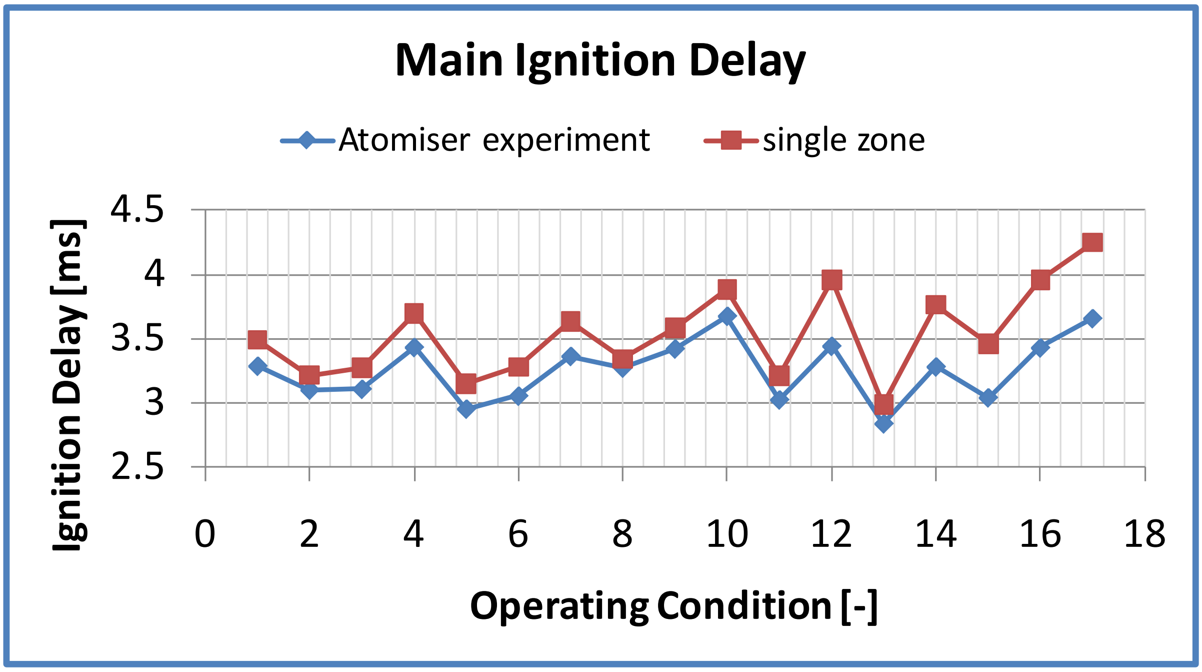


Figure 7: Comparison of measured (blue) and predicted (red) engine ignition delays. The predictions are obtained with the lumped reaction model in combination with the single zone engine model.

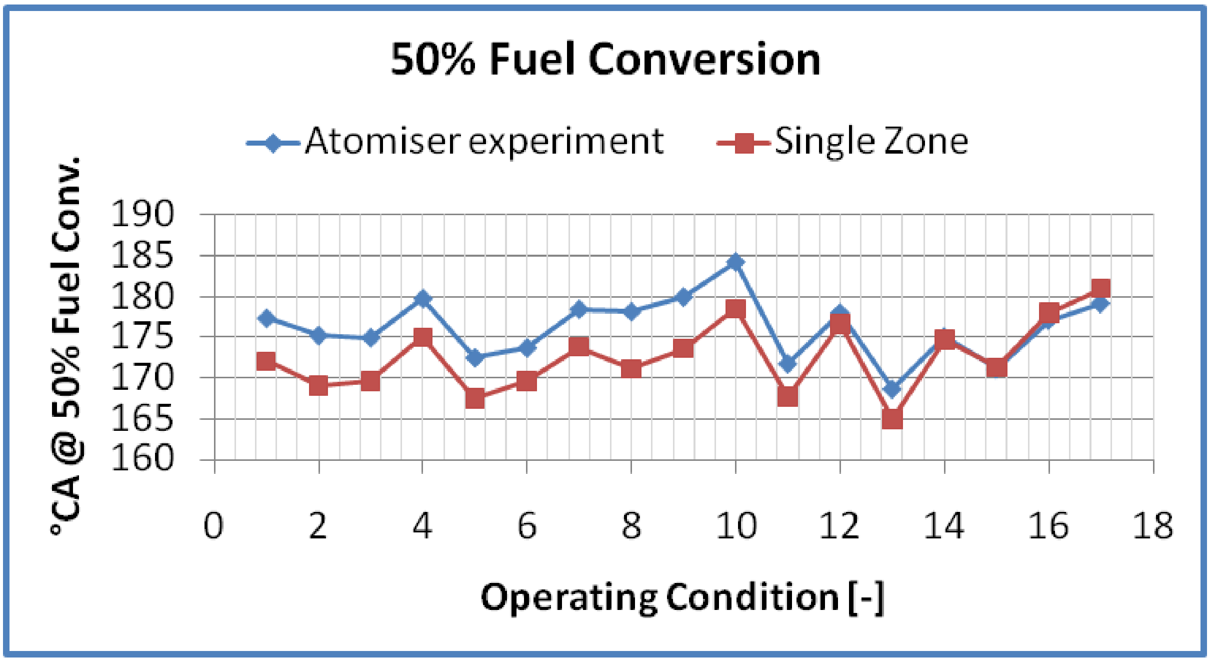


Figure 8: Comparison of measured (blue) and predicted (red) crank angle at which 50% fuel conversion is reached. The predictions are obtained with the lumped reaction model in combination with the single zone engine model.

Experimental Part – Developments in the experimental facility

Dimitrios Mitakos

During this project various modifications and upgrades have been done to the single stroke engine (EHT) experimental facility to comply with safety regulations, improve its operation and fulfill the requirements of this project in terms of homogeneous conditions, emulating engine HCCI operation. During 2008 [7] all non-stainless components of the pneumatic system have been replaced with stainless parts (piping, air bottle, valves, air compressor). At the same time the EHT laboratory was reorganized in order to separate signal cables from power lines to avoid electrical cross-talk between data acquisition and the control systems. Further on, a new heating system was designed, manufactured and implemented to provide higher air temperature with a homogenous distribution within the combustion chamber.

In the yearly report of 2009 [8] the design of a homogeneously heated EHT combustion chamber with 6 independently controlled heating zones, needed for this project, has been presented. The new heating system has been implemented as designed, installed in the existing EHT facility and brought into operation. In Figure 9 the EHT is depicted with the new heating system installed.

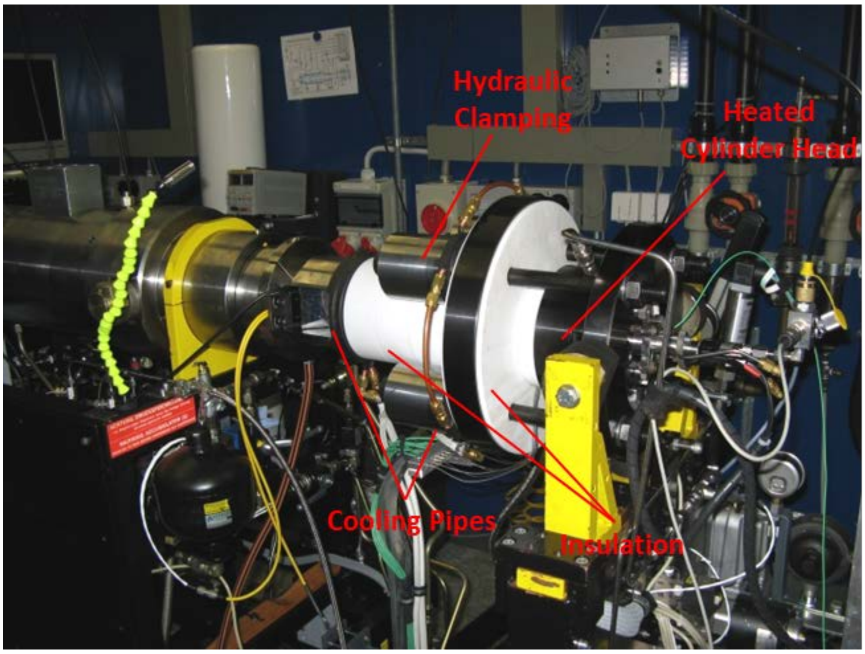


Figure 9: EHT with the new heating system installed

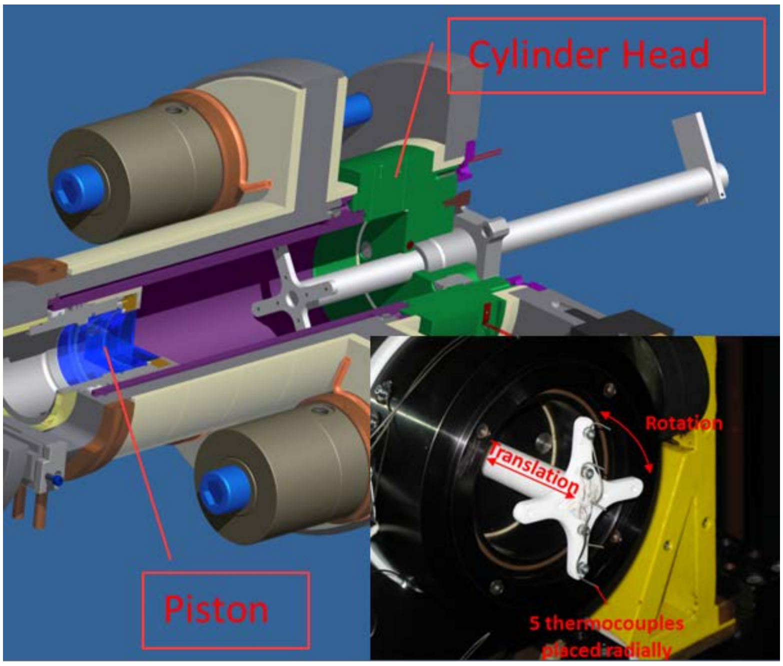


Figure 10: EHT Temperature homogeneity assessment, Temperature Probe

After the installation of the new heating system and the verification of the good and safe operation of its controls the actual temperature distribution within the combustion chamber of the EHT had to be evaluated [9]. For this reason a temperature measuring probe, which can be seen in Figure 10, was built to measure the air temperature distribution in the combustion chamber before compression stroke starts. The temperature probe is made from PTFE which (due to its low thermal capacity) minimizes the influence of the probe on the measured air temperature. It has five K-type thermocouples installed along its diameter and it is inserted in the combustion chamber through the injector opening with the help of an adapter that ensures proper sealing of the pressurized EHT cylinder. It can be moved in a rotational and translational manner along the axis of the combustion chamber so the temperature field of the complete air volume can be acquired.

For the temperature homogeneity measurement two planes of the cylindrical volume (vertical and horizontal cross sections) were measured. First a steady state temperature distribution was acquired, then followed by the transient measurement of the air temperature distribution during the filling process, where the cylinder volume is filled with air until the desired pre-compression pressure is reached.

It has been found that in order to get a homogeneous air temperature distribution in the cylinder after the filling process, the set wall temperatures in the different heating zones must be adjusted individually to compensate for the locally different heat losses from the cylinder to the machine base / environment.

In Figure 11 temperature field measured in the EHT combustion chamber is shown for a vertical plane cut through the combustion chamber. It is shown that with the new heating system for a set temperature of 130°C a mean air temperature of 126°C with a standard deviation of 3.26°C is reached. The temperature stratification in the original EHT configuration with only partially heated walls is no longer observed for the fully heated case, where an almost symmetrical profile is apparent. The air temperature range for the heated case is small, in the order of 15°C, with only limited less well heated regions (around the clamping mechanism) with temperatures lower than 120°C. Conclusively, the EHT's new heating system is operating as designed, providing increased pre-compression air temperature levels and at the same time the necessary homogeneous temperature distribution needed for HCCI experiments.

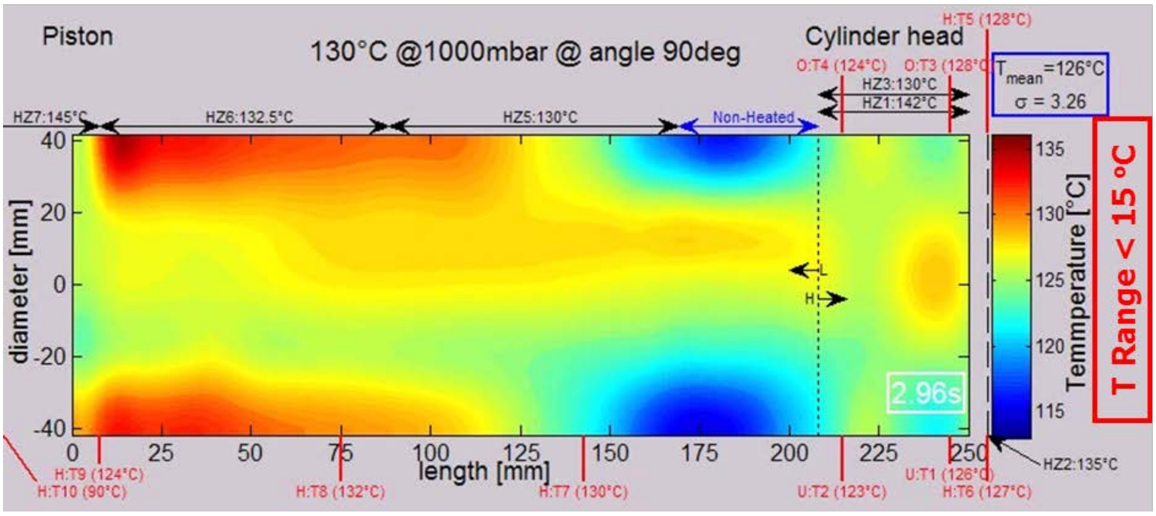


Figure 11: Temperature homogeneity in the EHT combustion chamber with the new heating system

Experimental Part – OH Chemiluminescence of the Homogeneous Combustion Process

Dimitrios Mitakos

In the framework of this project the EHT testing facility has been used to conduct homogeneous self-ignited combustion experiments for a variety of technically relevant fuels (see Table 1). The Diesel fuels were excluded from the test matrix to avoid problem related to their partial evaporation due to low temperatures in the EHT. First, exploratory experiments have been carried out with n-Heptane (Fuel Nr. 2 in the FVV test matrix / Table 1) initially in a non-heated combustion chamber and, after the implementation of the new EHT heating system, in a heated combustion chamber as well. n-Heptane was chosen for initial measurements as it is an easy to evaporate and easy to ignite fuel (boiling point of 98 °C). These measurements allowed the assessment of the overall behavior of the experimental device, the setup and optimization of the measuring techniques and the definition of the test matrix, in terms of lambda and EGR percentage, for the experiments with the rest of the fuels. Further information on the techniques used and a description of the testing facility can be found in [7] and [8]. Subsequently, production measurements with the rest non-Diesel fuels have been carried out.

In Figure 12 the Pressure – Temperature (P-T) compression trace selected for the experiments (black line) is presented. The shape of the curve is a function of the wall temperature and the loading pressure. These two parameters were selected ($T_w = 380K$ & $P_{load} = 1.4bar$) so that the P-T trace lies in-between the higher load (red line) and the lower load (blue line) P-T traces followed by FVV research partner in University of Stuttgart for engine experiments (TP5). Additionally it also lies within the range of Pressure and Temperature used for shock tube experiments in the University of Duisburg. In the same figure the ignition points for engine experiments equipped with an atomizer are shown (green triangles). Star shapes indicate the predicted ignition point in the EHT calculated with the ignition integral method [1] for start of injection (SOI) at $P_{Cylinder} = 15bar$. A set of experiments where SOI is varied is needed to identify the proper SOI in order to have fully evaporated fuel, premixed conditions and ignition Pressure and Temperature relative to shock tube and engine experiments, avoiding at the same time combustion in a diffusion mode. Using also optical information it has been concluded that the start of injection should occur at cylinder pressures between 15 and 20bar for the selected P-T trace. However, the optimal value depends on the composition of the investigated fuel as well.

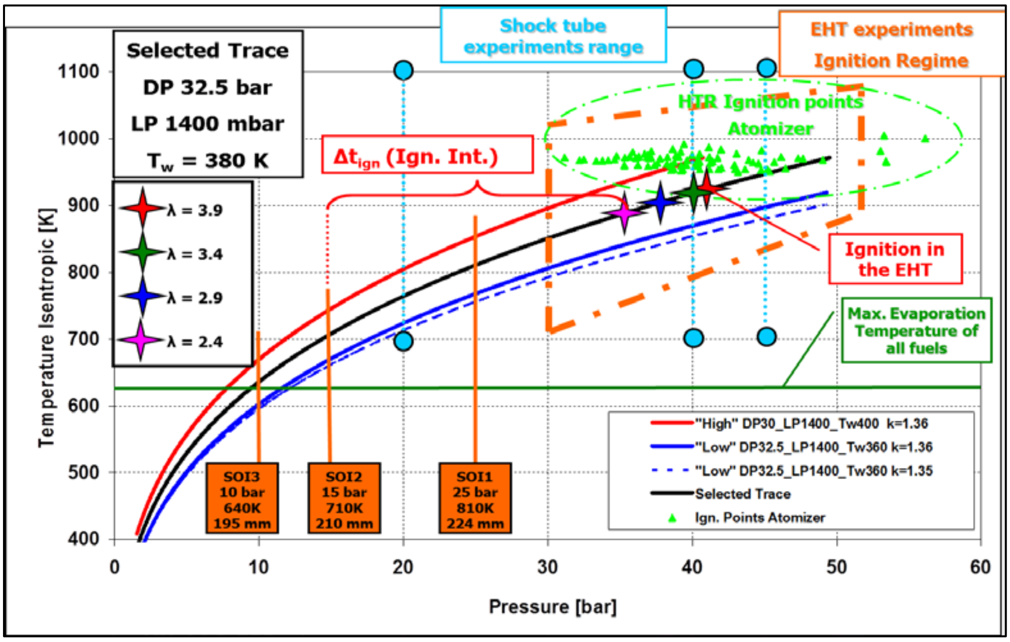


Figure 12: Pressure – Temperature trace selected for experiments in the EHT, in comparison with experimental matrices of FVV project partners

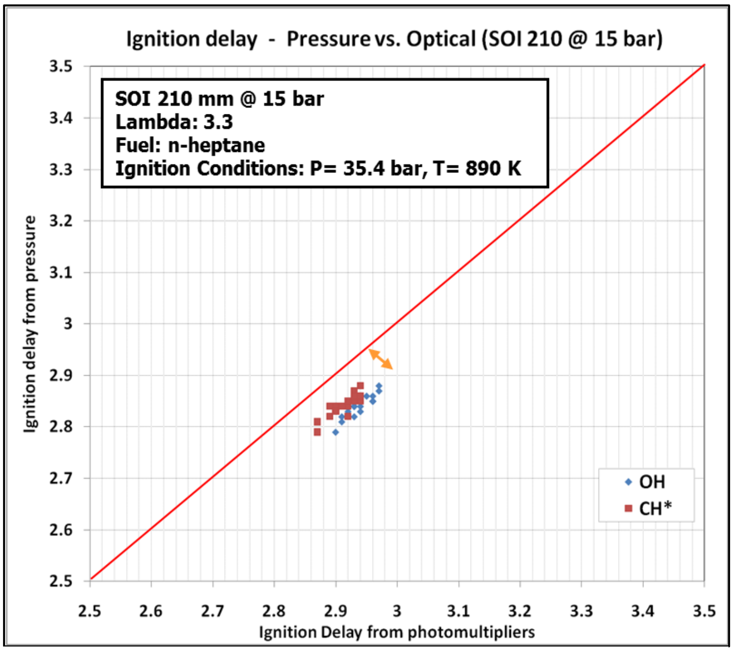


Figure 13: Ignition delay, 3 methods SOI at $P_{cyl@SOI}$=15 bar

Three methods have been used to estimate the experimental ignition delay: The pressure trace, the OH-chemiluminescence signal at 310nm and the CH*-chemiluminescence signal at 430nm were processed to calculate the ignition point. Cylinder pressure is acquired with a fast response Piezoelectric sensor and OH and CH* emission with 2 Photomultipliers equipped with the respective interference filters each. In Figure 13 a small systematic difference (O 0.05ms) between the ignition delays calculated from pressure and optical data can be seen for the $P_{cyl@SOI}$=15bar case. The scattering of the ignition delay is rather low with a standard deviation in the order of σ=0.2ms.

The actual ignition delay in the EHT and the ignition delay calculated from the ignition integral are compared in Figure 14 as a function of equivalence ratio (lambda). The ignition delays calculated with the three methods show good agreement with each other, especially when SOI is moved to an earlier time. The experimental ignition delay shows an independency from lambda, because due to inhomogeneity the local lambda of ignition is the same (lower than the global lambda) at the richer zones where ignition occurs. The ignition integral model assumes full homogeneity of the mixture, thus the calculated ignition delay exhibits strong dependency on lambda.

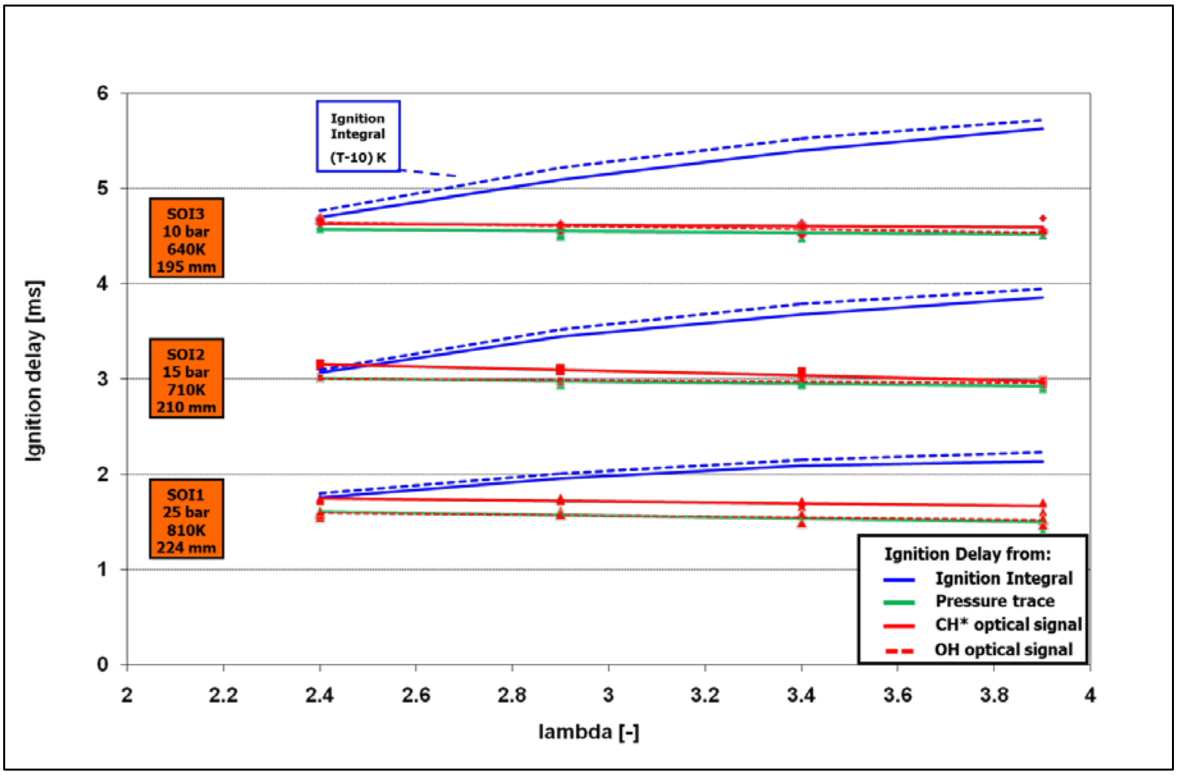


Figure 14: Ignition delay calculated from experimental thermodynamic and optical data compared with ignition delay calculated with ignition integral method

In [8] it has been demonstrated that OH-chemiluminescence is the most appropriate optical method to investigate reaction zones in a homogeneous mixture, since under homogeneous combustion no visible light is emitted. The optical setup is also described in the same report. The ensemble average of flame OH-chemiluminescence over approx. 20 realizations is depicted in Figure 15. The time step from picture to picture is Δt=0.1ms, the fuel is n-heptane the injection pressure P_{inj}=130bar, the cylinder pressure at SOI $P_{cyl@SOI}$=15bar and the injection duration Δt_{inj}=0.85ms.

Ignition occurs at 4.40ms bTDC and for the next 0.2ms there is a relatively even distribution of light Intensity across the combustion chamber. From 4.20ms bTDC onwards, light intensity is higher at the center of the combustion chamber indicating stronger reactivity in this region, probably due to higher temperatures originating from lower heating losses relative to regions closer to the walls. It should be noted though that there are not any regions that show no reactivity at all, indicating that combustion is in the premixed mode, even if not completely homogeneous, resembling the actual engine operation.

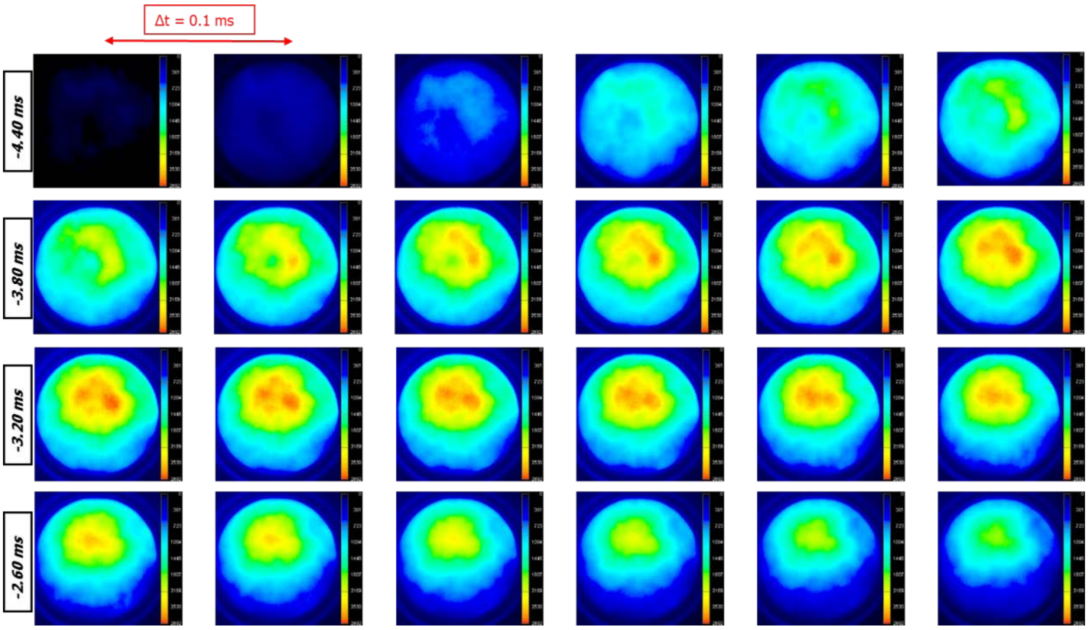


Figure 15: Ensemble Average OH-Chemiluminescence 310nm, SOI 210mm, $P_{cyl@SOI}$=15 bar, λ=3.3, n-heptane.

With the n-heptane tests the repeatability of the measurements was validated. Additionally the consistency of thermodynamic as well as the optical data was verified. After the processing of the data collected for n-heptane and in conjunction with the measurement conditions of the FVV cluster-projects partners, the test matrix (Table 2) for the production measurements with the rest of the fuels is defined.

Lambda	EGR [%]	$P_{cyl\ @\ SOI}$ [bar]
1.5	50	15
2.5	30	15
3	10	15
4.5	10	15
3.5	0	15

Table 2: Test matrix definition for the measurement of the FVV fuels

The fuels investigated are limited to non-Diesel fuels in order to avoid problems observed in the shock tube (TP1) and engine experiments with an atomizer (TP5), related to the higher evaporation temperature range and the heavier components of the Diesel fuels. The ignition delay was measured in the EHT along with optical information from high-speed OH-Chemiluminescence recordings. The measured ignition delay is compared against the one measured in the IVK engine test facility.

In Figure 16 the main ignition delay measured for different conditions in the EHT is depicted normalized with the respective n-Heptane ignition delay. The general trend observed is that the ignition delay decreases with increasing Cetane Number as expected. For fuels with intermediate Cetane Number (44.2 to 50.3) this trend is not followed in every case. Depending on the operating conditions of each measurement point the reversal of the generic trend has been also observed in the IVK engine experiments (TP5) with conventional common rail injection system and the shock tube experiments (TP1). n-Heptane (CN 57) ignition delay expected to be the lowest; however it lies in the same order of magnitude as the Kerosene 1 (#5) fuel. Due to being a single component fuel with the lowest and constant evaporation temperature (98^{o}C), n-Heptane is probably forming a much more homogenous (although not completely homogenous) mixture than the rest of the fuels, leading to a less rich fuel/air mixture and therefore a higher ignition delay time.

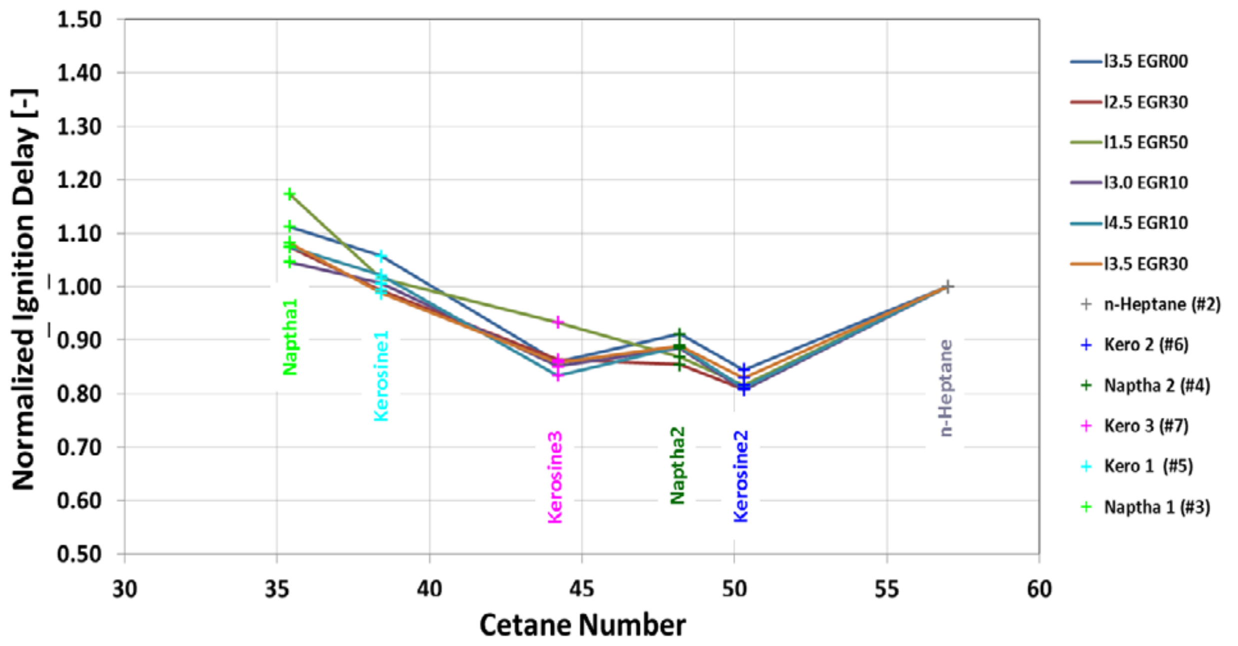


Figure 16: Normalized Ignition Delay (relative to n-Heptane Ignition Delay) versus Cetane Number: Comparison of the six measured fuels in the EHT for different EGR-lambda operating points

In the IVK engine the EGR percentage is defined as the ratio of the recirculated exhaust gas mass to the total gas mass in the cylinder. In the EHT the EGR percentage is estimated directly from the O_2 concentration in the cylinder. So each EGR percentage following the EHT definition might correspond to different EGR percentages in the IVK engine due to varying composition of the exhaust gases relative to the operating point.

Thus, in order to be able to compare results from the EHT with results from the IVK engine, a correlation has been developed for the EGR-lambda conditions between the two experimental setups. In Figure 17 the correlation of EGR in the EHT and the IVK engine is shown.

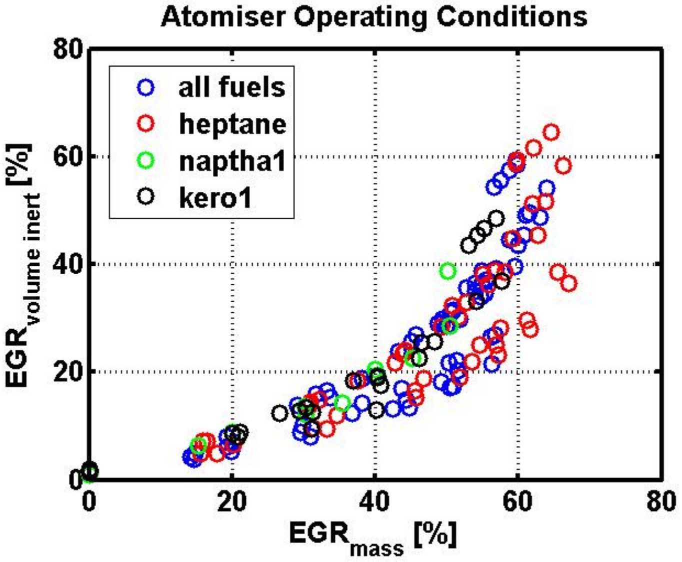
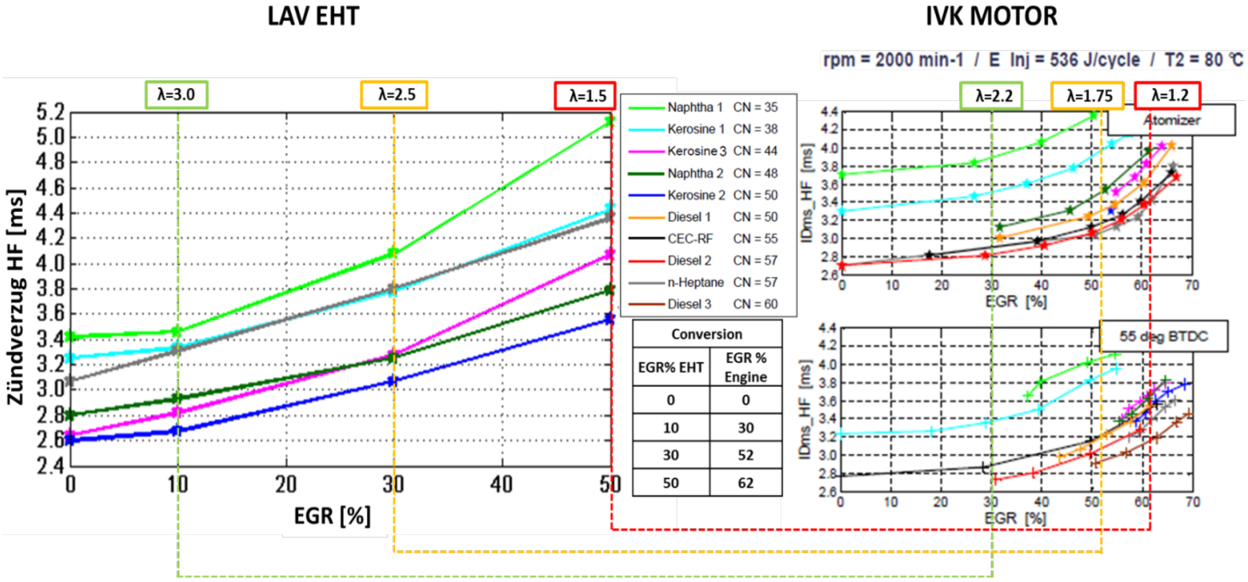


Figure 17: EGR Correlation between EHT and IVK-Engine, A. Vandersickel, LAV.

In Figure 18 the ignition delay measured in the EHT is compared with the ignition delay measured in the IVK engine for a load point of P_{mep}= 4bar. It should be noted that EGR and lambda should be not compared one to one among the two experimental setups due to different definition. The conversion table should be used to “connect” relevant EGR values. It can be seen that generally the trends observed in the EHT are in agreement with these observed in the IVK engine operating with a conventional common rail injection system under partially homogenous conditions.

EHT conditions have been selected so that it follows the same Pressure-Temperature trace as the IVK engine. However the IVK engine runs approximately twice as fast as the EHT through it, having set at the same time earlier SOI timing (at lower cylinder Pressure and Temperature). This results coincidently in the same range of ignition delay values in the two setups.



Conversion	
EGR% EHT	EGR % Engine
0	0
10	30
30	52
50	62

Figure 18: Comparison between the measured ignition delay in the EHT (left) and in the IVK-Engine (Operation point: 2000-4-80, right) in operation with the Atomizer (top) resp. with the Common-Rail injection (SOI 55bTDC, bottom)

OH-chemiluminescence high speed recordings provide information about the distribution of ignition centers and reaction zones. Thus, the degree of homogeneity in terms of combustion evolution can be assessed.

In Figure 19 and Figure 20 the ensemble averaged OH-Chemiluminescence intensity of the EGR 0% – λ = 3.5 measurement point for all fuels measured is shown. It can be seen that for the majority of the fuels ignition happens at multiple positions, if not almost evenly distributed, in the case of n-Heptane. Experiment-to-experiment standard deviation over mean value is low in every case indicating low cyclic variation. At ignition time the standard deviation/mean appears to be higher due to the very low signal intensity levels

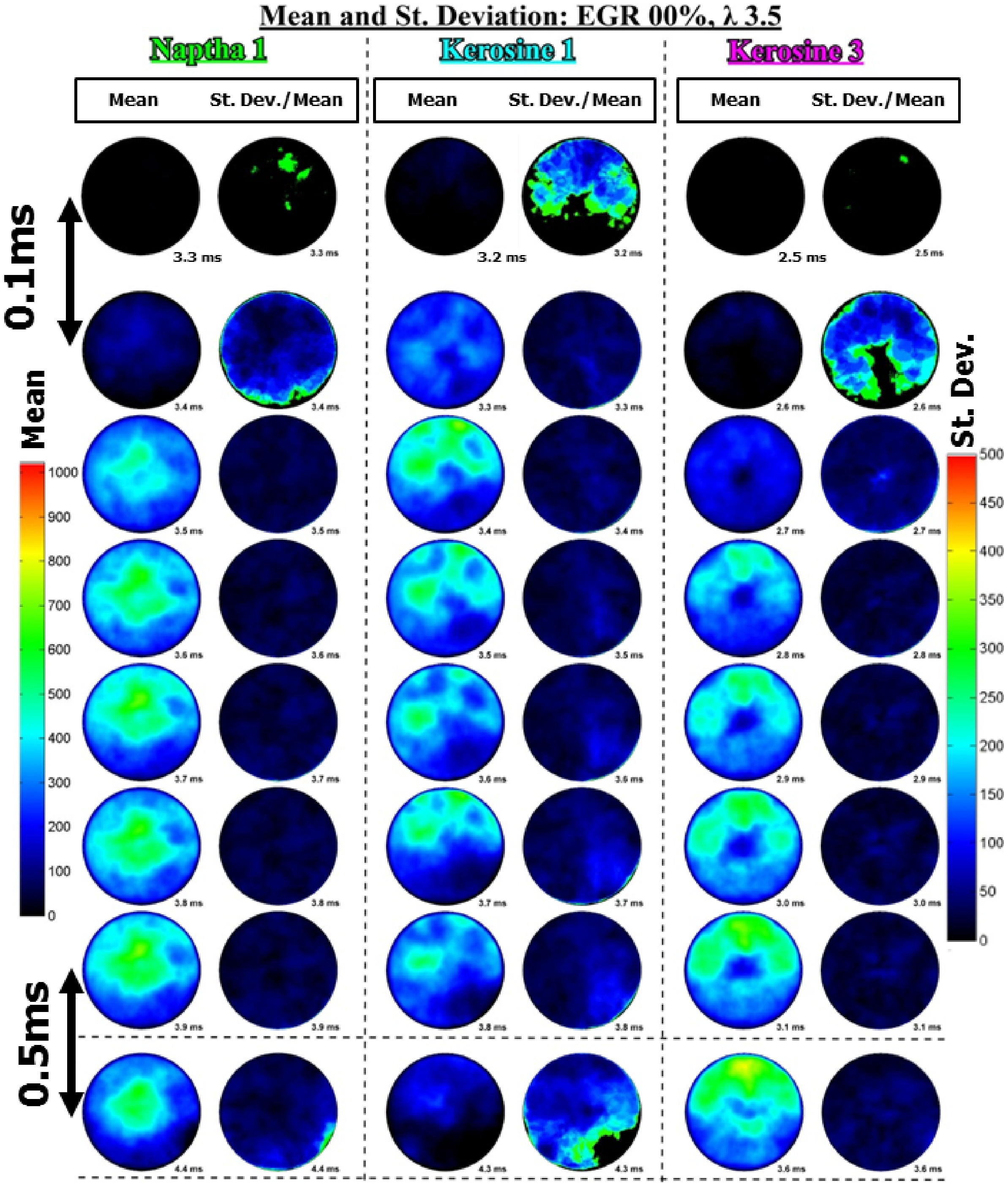


Figure 19: OH-Chemiluminescence recordings. Naptha1, Kero1, Kero3, EGR 0%, λ = 3.5

The hollow cone injector is positioned in the center of the cylinder head, spraying the fuel in a conical sheet both radially and towards the piston. Through interaction between the injected fuel and the surrounding air, vortices are created that transport the vaporized fuel towards the center of the cylinder [10]. For fuels with low evaporation temperature (n-Heptane) and/or low Cetane Number (Naphta1, Kerosine1) more time is available for evaporation and mixing before ignition (faster evaporation, lower Cetane Number). Thus, these fuels show more evenly distributed reaction zones with a single intensity peak. A low intensity region in the middle of the cylinder is observable for the rest of the fuels (Kerosine3, Naphta2, and Kerosine2) because the fuel is not completely evaporated and/or distributed towards the center before ignition occurs.

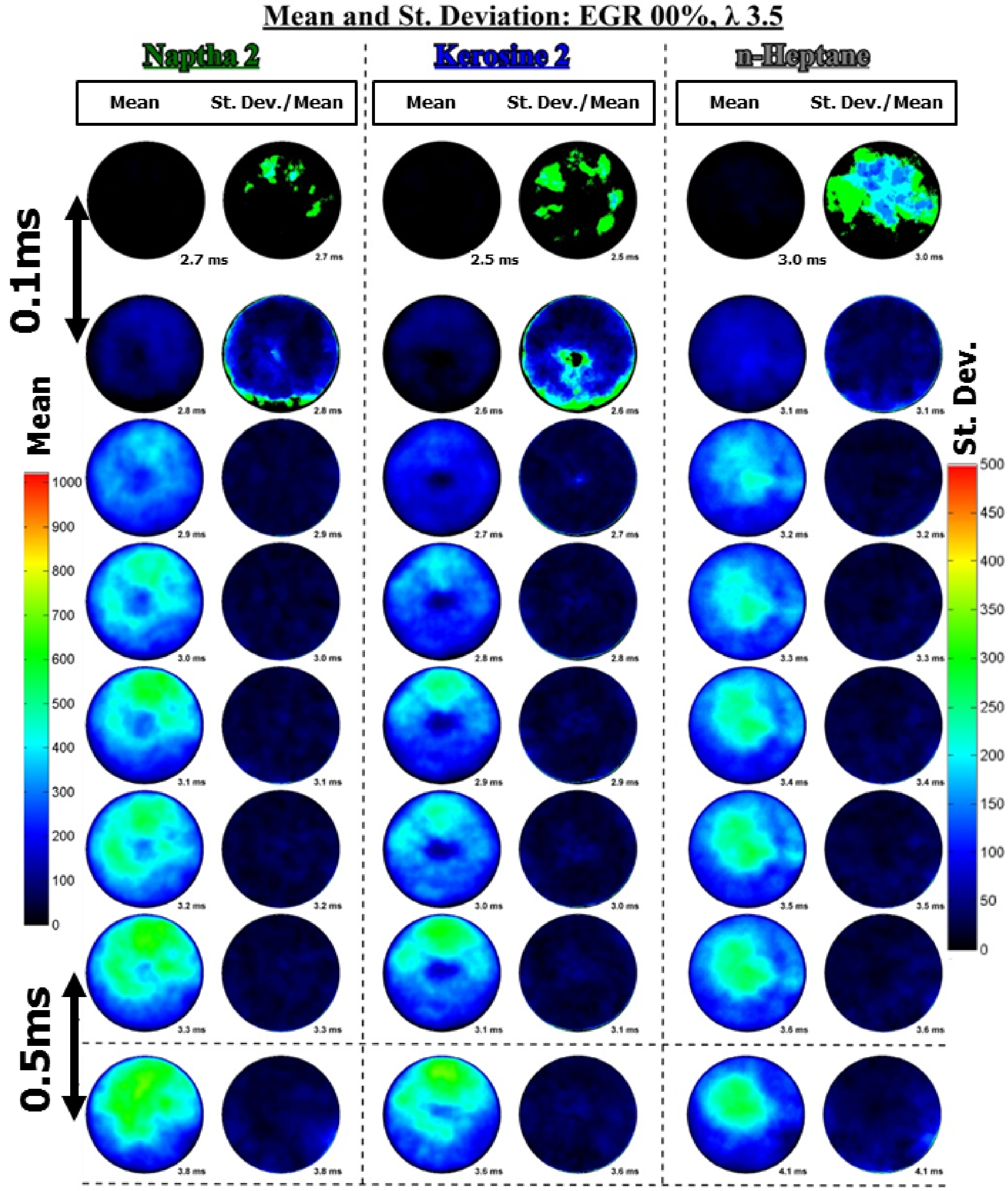


Figure 20: OH-Chemiluminescence recordings. Naptha2, Kero2, n-Heptane, EGR 0%, λ = 3.5

In Figure 21 and Figure 22 the spatial distribution of the ensemble average start of burning (equal to ignition delay) and its corresponding standard deviation is depicted for all measurement points and fuels. It can be seen that for the EGR 0%, 10% and 30% cases for all fuels, ignition spreads to the whole visible area within a single time step (sampling time step = 100µs), indicating a rapid growth of the reaction zones. Standard deviation is generally low and it is even lower at the points where ignition occurs at first, showing that combustion starts at the same location in each cycle. There is a full coverage of the observation window for these cases suggesting that some amount of fuel is distributed everywhere and reaction has taken place.

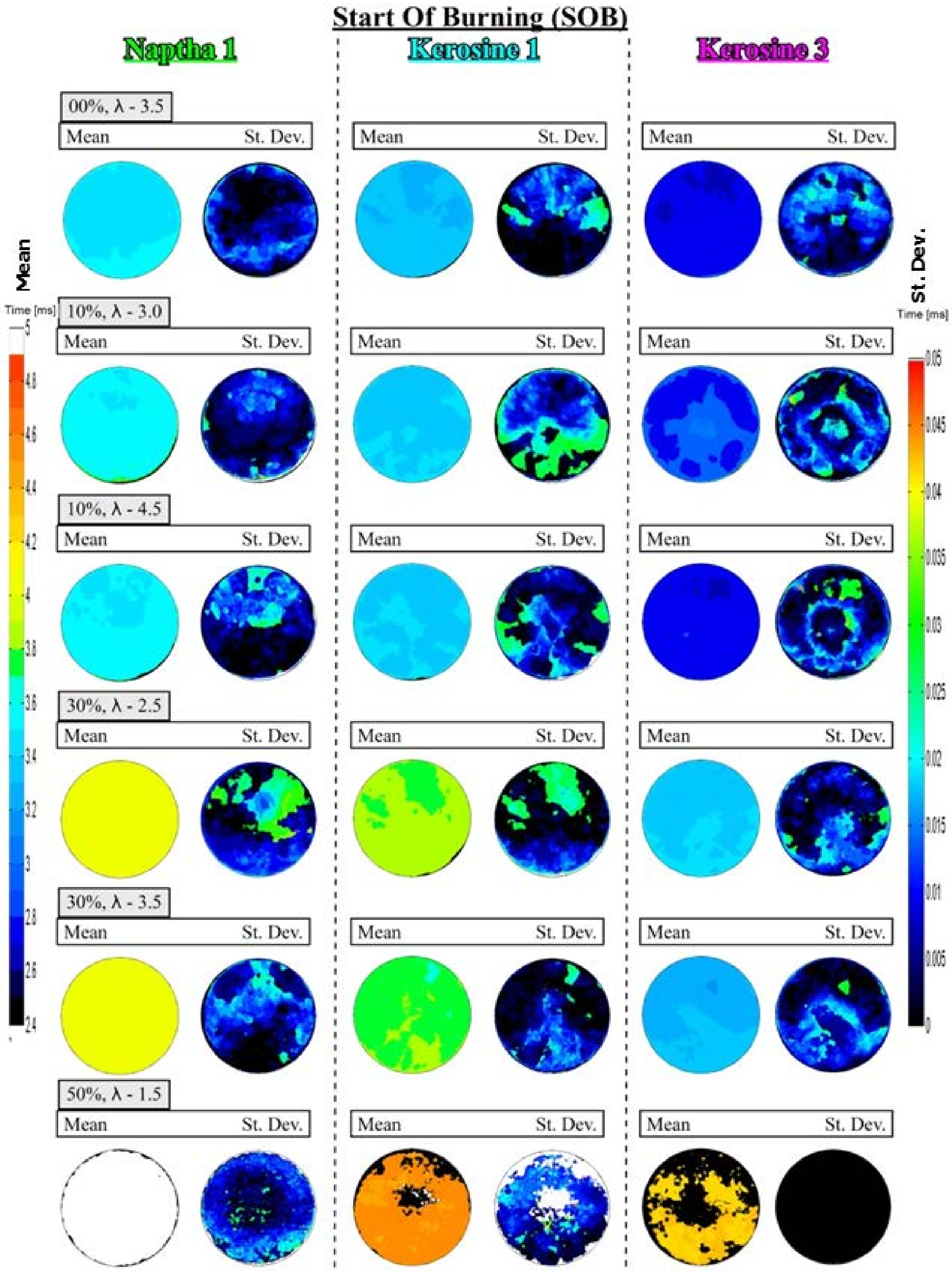


Figure 21: Spatial distribution of ignition delay. Naptha1, Kero1, Kero3

For the EGR 50% – λ = 1.5 case there are fuels such as Naptha2, Kerosine1 and Kerosine3 where zones that do not exhibit ignition and combustion are observed. Low intensity combined with the high standard deviation of these cases, indicates high cyclic variation and possible difficulties to ignite and burn these fuels with EGR 50%.

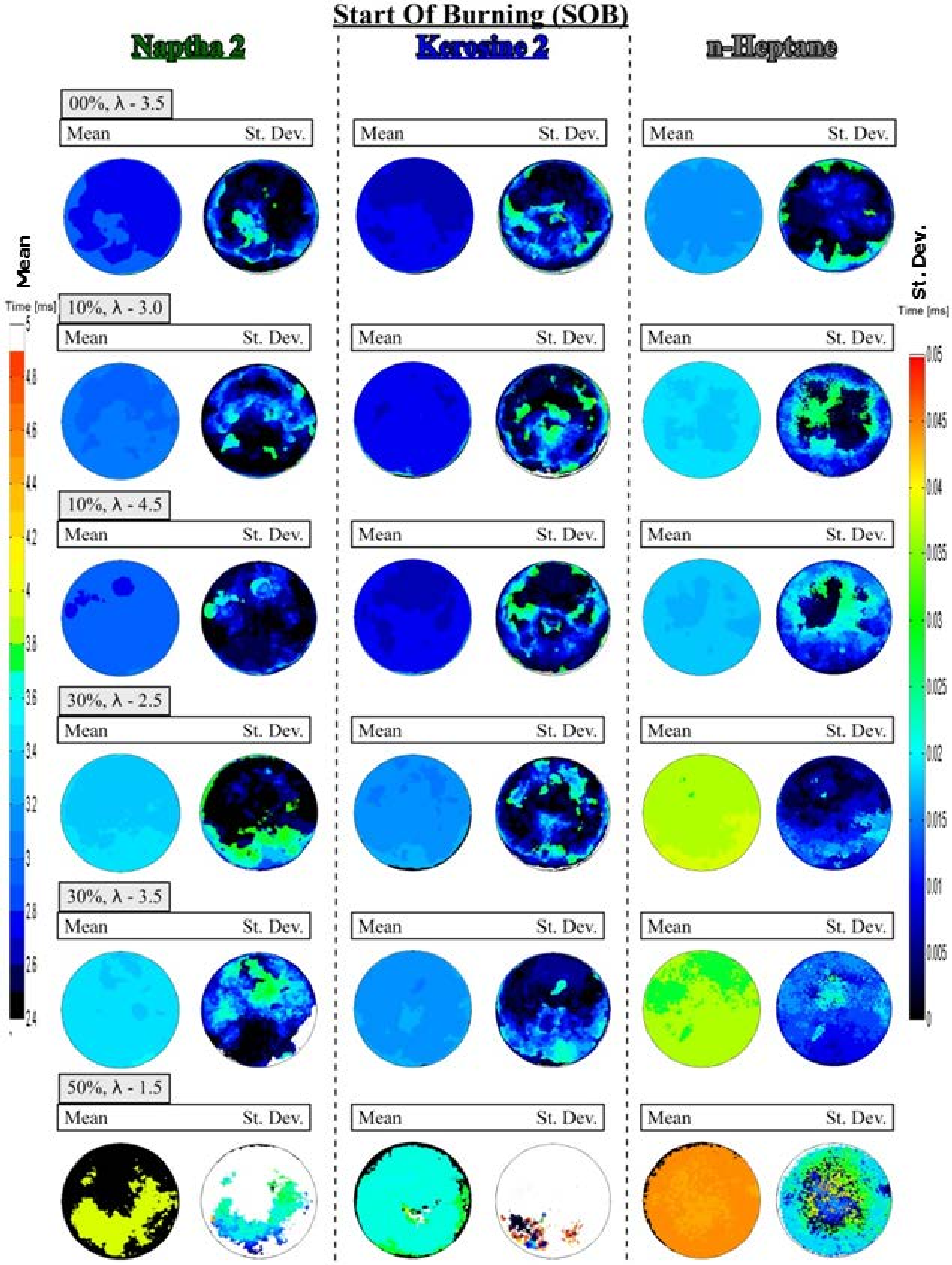


Figure 22: Spatial distribution of ignition delay. Naptha2, Kero2, n-Heptane

Conclusions

On the simulation side, two compact phenomenological ignition/combustion models have been developed and adapted to each of the project fuels. The first model is based on an ignition delay calculation and is meant to quickly assess the impact of engine operating conditions on both first stage and main ignition timings. The second model is more elaborate, using 8 species and 7 reactions to describe the dynamics of the two stage ignition typical for hydrocarbon fuels. It is therefore able to predict the evolution of heat release, pressure, temperature and important species in addition to both ignition delay times.

Both models have been developed based on shock tube data from a partner project in Duisburg and show an excellent agreement with this data set over the entire range of HCCI conditions considered. For each of the project fuels, the average error on the ignition delay predictions is as small 0.2 to 0.4ms. A first validation based on engine data from our partners at the University of Stuttgart shows that especially the effect of changing operating conditions on the auto-ignition is very well captured. The heat release and species evolutions obtained with the global reaction model furthermore show a very good qualitative agreement with detailed reaction mechanisms for n-heptane. As model development is never completed, some further refinements of the global reaction model in order to improve the φ-dependence of the ignition delay times and the heat release rate prior to ignition will be undertaken. The predictive quality of the model is nevertheless at present already equally good or even better as present models of this kind available.

Both models are now ready for application in 3D-CFD simulations and make it possible to assess the additional influence of temperature/mixture inhomogeneities and physical fuel properties on the HCCI ignition and combustion event, even for the complex multi-component fuels produced in refineries nowadays.

In the experimental project part, the single stroke engine has been revised and a new heating system has been installed. The temperature measurements presented in this report demonstrate that the new heating system is functioning well and sufficiently homogenous temperature fields can be obtained (at 126°C air temperature, temperature standard deviation is only 3.6° C). With the new system, the pre-compression air temperature can furthermore be raised higher as before, which allows investigating heavier fuels as well.

Based on a first series of heptane measurements, three different methods to determine ignition delay form the experimental data have been implemented and assessed. The consistency of optical and thermodynamic data has been verified and also the repeatability of the measurements has been validated. Based on further heptane measurements, the engine settings required to obtain the same pressure and temperature ignition conditions as in the other partner projects have been identified. The corresponding OH-chemiluminescence images furthermore demonstrate that - with these settings - the mixture burns in a partially homogenous ‘premixed’ mode, resembling the actual engine operation with a standard Common Rail injection system. The single stroke engine is therefore an adequate instrument/machine/device to investigate and visualise the processes going inside the combustion chamber of an HCCI engine.

After the initial tests with n-Heptane the ignition characteristics, both globally as well as locally, have been investigated in the EHT for six synthetic fuels with distinct Cetane numbers and thermophysical properties. Ignition delay measurements show that there is general trend of decreasing ignition delay with increasing Cetane Number. Reversal of this trend for fuels with intermediate Cetane Number (44 - 50) depending on the operating conditions has been observed in the EHT, which is in accordance with observations in the shock tube (TP1) and in the engine (TP5) experiments. Especially when comparing with the IVK measurements, EHT ignition delay show trends similar to the ones observed in the IVK engine operating with a conventional common rail injection system. Comparison of the measured ignition delay in the EHT with the calculated ignition delay from ignition integral method suggests that lambda of ignition is lower that the global lambda, indicating non-perfect homogenization of the mixture, which is also the case in an engine with a conventional common rail injection system.

High speed OH-Chemiluminescence recordings demonstrate, in general and for the selected conditions and injection system, that the EHT operates away from the diffusion combustion mode in a premixed, partially homogenized regime. Fuels with lower evaporation temperature tend to create a more (although not fully) homogenous mixture as expected.

Conclusively, it has been seen that the Cetane Number captures the general trend of ignition characteristics, but it is not sufficient to describe it in a global non-ambiguous way.

International Cooperation

Apart from the ETH Zürich (LAV, Teilprojekte 2, 3), the Universities of Duisburg (IVG, Teilprojekt 1), Stuttgart (IVK, Teilprojekte 4, 5, 7) and the Technische Hochschule Aachen (Teilprojekt 6) also participate in the FVV Projekt 'Kraftstoffkennzahlen für homogene Verbrennung'.

Assessment of the Project

Simulation Part

Within the framework of this project, two pragmatic, phenomenological models have been developed to describe the ignition/combustion behavior of each of the project fuels. Both models successfully describe ignition delays under homogenous conditions. The lumped reaction mechanism is furthermore able to predict the evolution of heat release and several representative species reasonable well. With these two models, the main objective of the simulation project has been achieved. In view of a PhD thesis, the models will now be further refined and applied in a 3D-CFD simulation to assess the entire combustion process.

Experimental Part

The experimental part was marked by the necessary, but time consuming modifications of the single stroke engine. The new set-up now successfully achieves the necessary requirements with respect to temperature and mixture homogeneity and can reach sufficiently high temperatures to investigate the higher boiling fuels as well. Despite the revision, which inhibited the experiments for a long time, the behaviors of all fuels (except the Diesels) have been characterized. The trends in the ignition delay in respect to the Cetane Number have been identified experimentally and compared with the measurements in the rest of the experiments of the cluster-project. Optical data showed qualitatively the spatial distribution of ignition and reaction zones, as well as the extent of possible inhomogeneity of the fuel/air mixture. Furthermore, in the framework of a PhD thesis, the processing of the optical data will allow the quantitative assessment of reaction zones distribution. Thus, the goals of the project have been therefore met to a large extend.

References

[1] A. Vandersickel, M. Hartmann et al.: ***The autoignition of practical fuels at HCCI conditions: High-pressure shock tube experiments and phenomenological modeling***, *submitted for FUEL*

[2] M. Hartmann, R. Starke: **Abschlussbericht Vorhaben 947: Kraftstoffkennzahlen – TP1 Stosswellenrohr**, FVV Heft 904, 2010.

[3] M. Hartmann, A. Vandersickel, D. Mitakos, S. Beck, V. Rajamani, **Zwischenbericht über die FVV Vorhaben Nr. 943, 944, 945, 946, 947, 948.**, Informationstagung Motoren, Herbst 2009, Dresden

[4] Zheng et al. **SAE technical paper 2004-01-2950**, 2004

[5] Vandersickel et al. : **Global Reaction Model for Practical Fuels in HCCI Applications,** Conference Proceedings THIESEL 2010, Valencia

[6] Tsurushima, **A new skeletal PRF kinetic model for HCCI combustion**, Proceedings of the Combustion Institute 32 (2009) 2835–2841

[7] B. Schneider et al.: **Jahresbericht: Brennstoffe für homogene selbstgezündete Verbrennungsprozesse**, BfE Projekt Nr. 101514, 30. Dezember 2008.

[8] B. Schneider et al.: **Jahresbericht: Brennstoffe für homogene selbstgezündete Verbrennungsprozesse**, BfE Projekt Nr. 101514, 11. Dezember 2009.

[9] R. Rodriguez: **Experimental Investigation of Temperature Homogeneity in the Single Stroke Machine**, Bachelor Thesis LAV, Spring 2010

[10] Schmid, A.; Schneider, B.; Boulouchos, K.; Mojtabi, M.; Wigley, G.: **Experimental investigation on the spray behavior for a hollow cone piezo injector with a multiple injections strategy**, 23rd Annual Conference on Liquid Atomization and Spray Systems, September 2010

Publications

1. Vandersickel et al. : ***Global Reaction Model for Practical Fuels in HCCI Applications***, Conference Proceedings THIESEL 2010, Valencia
2. A. Vandersickel, M. Hartmann et al.: ***The autoignition of practical fuels at HCCI contions: High-pressure shock tube experiments and phenomenological modeling***, *submitted for FUEL*