

Ignition Delays of Different Homogeneous Fuel-air Mixtures in a Rapid Compression Expansion Machine and Comparison with a 3-Stage-ignition Model Parameterized on Shock Tube Data

Dimitrios Mitakos, Christopher Blomberg, Annelies Vandersickel, Yuri Wright, Bruno Schneider,
and Konstantinos Boulouchos
Swiss Federal Institute of Technology

ABSTRACT

An optically accessible Rapid Compression Expansion Machine (RCEM) has been used to investigate the homogeneous auto-ignition of five candidate fuels for Homogenous Charge Compression Ignition (HCCI) combustion. Two technical fuels (Naphthas) and three primary reference fuels (PRF), (n-heptane, PRF25 and PRF50) were examined. The Cetane Numbers (CN) of the fuels range from 35 to 56. The PRF25 and PRF50 were selected in order to approximately match the CN of the two Naphthas. Variation of the operating parameters has been performed, in regard to initial charge temperature of 383, 408, and 433K, exhaust gas recirculation (EGR) rate of 0%, 25%, and 50%, and equivalence ratio of 0.29, 0.38, 0.4, 0.53, 0.57, and 0.8. Pressure indication measurements, OH-chemiluminescence imaging, and passive spectroscopy were simultaneously implemented.

Experiments with n-heptane have also been examined against homogeneous, variable-volume perfectly stirred reactor (PSR) simulations with various chemical mechanisms. The experimental ignition delay has been compared to the computations of an empirical three-stage, Arrhenius-type ignition delay model. The model has been parameterized on shock tube data for the n-heptane and Naphtha fuels. For the PRF25 and RPF50 the parameterizations of the Naphtha 2 and Naphtha 1 respectively have been used.

Very good agreement has been observed between the 3-Arrhenius empirical model and the experimental ignition delay data, for the fuels that have been parameterized (n-heptane and Naphthas) based on shock-tube data. Fuels that have not been explicitly parameterized, exhibit fairly good agreement as well. The empirical model, utilized through a knock integral, is found to be applicable in the transient environment of the RCEM. The potential of the RCEM as a device for fast evaluation of the homogeneous fuel-air mixtures auto-ignition delay is discussed.

CITATION: Mitakos, D., Blomberg, C., Vandersickel, A., Wright, Y. et al., "Ignition Delays of Different Homogeneous Fuel-air Mixtures in a Rapid Compression Expansion Machine and Comparison with a 3-Stage-ignition Model Parameterized on Shock Tube Data," *SAE Int. J. Engines* 6(4):2013, doi:10.4271/2013-01-2625.

INTRODUCTION

The potential of homogeneous charge compression ignition (HCCI) combustion for the simultaneous, in-cylinder soot and NO_x reduction is rendering it an appealing process for future internal combustion engines. The process is well known and already investigated with gasoline-like fuels in the late 70s [1, 2]. However its wide-spread implementation in internal combustion engines is hindered by difficulties mainly related to its controllability under varying operation conditions. The absence of an explicit ignition-controlling

event, such as spark or liquid fuel injection, leads to ignition timing and heat release rate that depend on chemical kinetics of the charge. The high extent of homogeneity leads to spatially even distribution of ignition. The subsequent volume-reactions result to rapid heat release, which is mainly characterized by the chemical kinetics of the charge [3]. Thus, ignition control relies on the control of engine operating parameters, such as charge inlet temperature and EGR.

Renewal of the interest on the HCCI, especially in regard to Diesel-fuels occurred in the mid-90s. The capability of the process to be run with various fuels [4, 5], in conjunction with the ability to produce synthetic fuels “tailored” to the needs of the HCCI process, renders the fuel itself an important parameter for the development of a controlling strategy. Towards this goal, the detailed knowledge of the auto-ignition behavior of practical and alternative fuels under different operating conditions is necessary [6].

Chemical kinetic modeling mechanisms [7, 8, 9, 10, 11, 12, 13, 14] are usually not developed for multi-component fuels and are practically too large to be implemented in CFD calculations, even when reduced. Computationally efficient tools often used to study the auto-ignition of practical fuels are phenomenological ignition delay models. These can be utilized easily in CFD calculations and engine control algorithms. The models rely on Arrhenius-type expression fits on experimental ignition delay data from shock tubes, rapid compression machines (RCM), and HCCI engines or chemical kinetics simulation data with detailed or reduced chemical mechanisms. The simplest are single Arrhenius expression models, where the ignition delay is function of temperature; their parameterization however is independent of temperature [15, 16, 17]. These models do not consider the negative temperature coefficient (NTC) effect of the ignition delay associated with higher hydrocarbons. In order to capture the NTC effect different approaches are followed. A single Arrhenius expression model where the parameters are functions of temperature is able to reproduce the NTC behavior [18]. Another approach is to use three Arrhenius expressions with constant parameterization, each one representing one temperature regime (low, intermediate, high). The expressions are either ‘stitched’ together with a piece-wise approach [19, 20], or coupled mathematically [21, 22, 23]. The availability and extent of experimental data is crucial for the global validity and applicability of these models. An overview of the different models and their performance can be found in [24].

The reported ignition delay models describe the chemical ignition delay at specific steady-state conditions. However in an engine environment the homogenous combustion system undergoes a series of different conditions in a transient manner. The knock integral method [25] is widely used to transfer the steady-state ignition delay to the transient operation of an internal combustion engine.

In the present work, the transferability of auto-ignition delay measurements from a shock tube to the transient engine-like operation is investigated. Shock tube measurement data for technical fuels have been used previously to parameterize a three-stage Arrhenius type model as proposed by Weisser [23] and further extended by Vandersickel [26] to include EGR influence. Utilized through a knock integral approach, the computed ignition delay of the three-stage Arrhenius model, parameterized for n-heptane and two Naphtha type fuels are compared to the ignition delay, as measured in an optically accessible RCEM

operating in homogeneous mode. Two additional PRF (n-heptane/iso-octane mixtures) fuels, matching the cetane numbers of the two synthetic Naphthas were also examined in the RCEM. Complementary to highly time-resolved pressure indication measurements, high-speed OH-chemiluminescence imaging and passive spectroscopy are used to detect the distinct spectral response of HCCI [27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37], in order to assess the highly homogeneous operation of the RCEM. The experimental and modeled n-heptane ignition delays in the RCEM are further compared to perfectly stirred reactor chemical kinetics simulations with various reaction mechanisms.

This paper is structured as follows: First the experimental facility is presented along with the test conditions, processing and analysis techniques. Then, the results are presented consecutively in regard to optical methods, experimentally determined ignition delay in the RCEM and comparison between experimental, simulation and three-Arrhenius modeling data.

EXPERIMENTAL AND COMPUTATIONAL METHODS

Experimental Setup

Rapid compression expansion machine (RCEM)

The RCEM is a free floating piston test rig (Figure 1). It combines excellent optical access with high flexibility in setting operating parameters such as compression ratio, charge initial pressure and temperature. Its modular design allows the custom design of various cylinder heads, which can house different accesses for diagnostic equipment, windows and injectors depending on the needs of the particular experimental campaign. Its transparent piston can be almost flat or bowl. In the current work a virtually flat piston is utilized with a bowl depth of 4mm. A piezoelectric, hollow cone Siemens injector was mounted in an axial direction, centrally on the cylinder head.

The RCEM operates in a single cycle (compression-expansion) mode. Driven by compressed air, a mass balance piston actuates the working piston by hydraulic oil coupling. The two pistons move in opposite directions to minimize vibration during the rapid stroke. First, the driving pressure is set and thus the oil is also pressurized. At this point the pressurized oil cannot act on the working piston rod. The latter is inserted in a sealing cavity, which keeps the high pressure oil away from the rear surface of the piston rod. Second, the loading pressure is set in the combustion chamber. Third, the high pressure oil flows to the back of the piston rod through a bypass throttle valve. The stroke starts at very slow speed. As soon as the working piston rod exits the sealing cavity, the high pressure oil can act on the piston rod unrestricted, commencing the rapid compression. The driving and loading pressures can be freely chosen. More details on the operation principle of the RCEM can be found in [38].

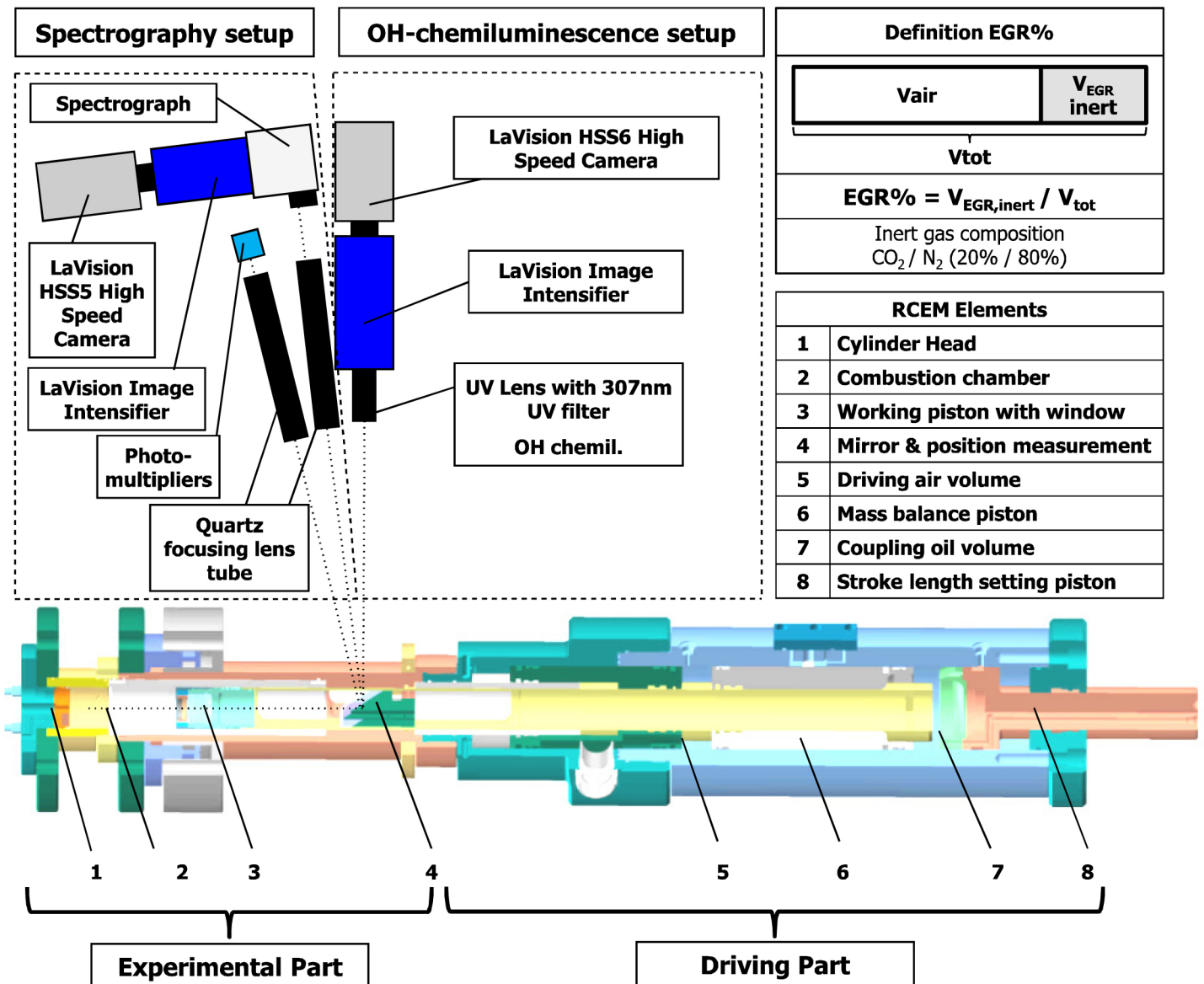


Figure 1. Rapid Compression Expansion Machine and optical setup [39]

The main technical characteristics of the RCEM can be seen in Table 1.

Originally the RCEM was designed for diffusion spray and combustion experiments [39]. It was redesigned in the Aerothermochemistry and Combustion Systems Laboratory (LAV), in order to have a fully heated combustion chamber and thus providing a high-temperature homogeneous environment that is needed for HCCI experiments, especially with liquid fuels. Its new liner and cylinder head are fitted with electrical heating elements, arranged in six separately controlled zones. Therefore, the heating power can be adapted to the local heat loss conditions optimizing the steady-state pre-compression temperature distribution towards homogeneity. The pre-compression temperature homogeneity has been assessed with dedicated experiments, where the gas temperature distribution in the cylinder has

been measured with a set series of K-type thermocouples. Very good temperature homogeneity has been observed without any indication of stratification. The standard deviation of the gas temperature is in the order of 3K. Moreover, the transient gas temperature evolution was measured during the loading pressure setting process. It was found that the distribution of temperature is barely affected by the gas in-flow. Due to the slow speed and long duration of the process the system marginally deviates from the steady-state temperature distribution [38, 40]. Overall, the RCEM provides a 'clean' homogeneous, engine-like environment, relieved from the complex engine in- and out-flow phenomena.

Data acquisition

Table 1. Technical characteristics of the Rapid Compression Expansion Machine (RCEM)

Bore (B)	84 mm
Stroke length (s)	120 – 249 mm
Compression ratio (ϵ)	5 - 30
Loading Pressure (LP)	1 – 3 bar
Max. cylinder pressure ($P_{\max}$)	200 bar
Piston window diameter (d_{win})	52 mm
Piston bowl depth	4 – 18 mm
Piston window material	Quartz
Cylinder head	Flat, flexible configuration
Pressure measurement	Piezoelectric pressure transducer, Kistler 7061B, range: 0-250bar
Heating system	Cylinder head and cylinder liner. Six separately controlled heating zones. Wall Temperature up to 473K. (Piston is also heated indirectly from the liner)
Injection system	Access through cylinder head, various injectors possible
Cylinder head accesses	Adaptation for different instrumentation possible (i.e. optical probes, 2 nd pressure transducer)
# of experiments	10 – 15 per hour

A series of optical diagnostic systems are installed by the RCEM. Optical access to the combustion chamber is achieved through the Quartz-made piston window. The light emission is redirected vertical to the axis of the RCEM by a mirror which is placed inside the hollow, slotted piston rod. High-speed OH-chemiluminescence imaging has been implemented with an intensified LaVision HSS6 high-speed camera with a dynamic range of 12 bits, set at a sampling rate of 30 kHz at a resolution of 384×384 pixels. For the observable domain, this corresponds to a spatial resolution of 0.22 $\mu\text{m}/\text{pixel}$. Passive spectroscopy measurements were performed with an Acton SpectraPro150 spectrograph (grating: 150 l/mm, Slit width: 150 μm , Blaze wavelength: 500nm) coupled with an intensified LaVision HSS5 high-speed camera also running at 30 kHz. The whole system was

calibrated for differences in wavelength-dependent sensitivity by the use of an integrating sphere. The resolution of the spectroscopy system was 0.66nm/pixel. An array of four Hamamatsu H5784-03 photomultipliers (PHM), spectrally filtered at 310, 365, 430 and 510nm, captured the spatially integrated light emission through the piston window.

The transient pressure, piston position and photomultipliers signals along with control and synchronization signals (i.e. camera triggers) have been recorder at 100 kHz with a PC-based transient measurement recorder.

Test Fuels and operating conditions

Fuels investigated

In total five fuels have been examined under homogeneous conditions in the RCEM. The two technical multi-component fuels (Naphthas) and the mono-component fuel n-heptane have been used previously in the framework of an FVV cluster project [41]. They are composed by typical petroleum derivatives. The exact mixture is selected in order to provide a wide but distinct range of composition, boiling characteristics and cetane number (CN). The characteristics of the fuels set can be seen in Table 2. The two Naphthas have distinctly different CN. As multi-component fuels they exhibit a boiling curve (percentage [vol%] evaporated as a function of temperature), rather than a single boiling point. Their exact boiling behavior is depicted in Figure 2. The n-heptane has the highest CN 56 of all fuels tested, similar to automotive Diesel fuels (typical $\text{CN}_{\text{Diesel}} = 51\text{-}55$). Their much lower boiling point, at 98°C, promotes evaporation and homogenization.

Table 2. Test fuels properties and composition [26, 40]

Fuel	-	n-heptane	Naphtha 1	Naphtha 2	PRF 25	PRF 50
Density (25 °C)	kg/m ³	683	720.1	734.9	687.3	690.5
Cetane Number	-	56	35.4	48.2	47.5	35
C/H-ratio	-	0.44	0.46	0.47	0.44	0.44
Lower Heating Value	MJ/kg	44.57	44.37	44.23	44.5	44.4
Composition*						
Hexane - C6H14	wt%	-	0.8/0.5	-	-	-
Heptane - C7H16	wt%	100	6.5/12	6.8/3.3	72	47
Oktane - C8H18	wt%	-	2.1/24.7	7.7/7.3	28	53
Nonane - C9H20	wt%	-	1.8/0	20/0	-	-
Decane - C10H22	wt%	-	-	8.2/0	-	-
Cyclo-alkane	wt%	-	29.3	46.7	-	-

* For naphtha 1 and 2 fuels composition linear and branched alkanes are identified separately (n-alkanes/iso-alkanes resp.)

The fuel matrix was complemented by two mixtures of n-heptane/iso-octane (PRF25 and PRF50). Their boiling point is essentially the same as n-heptane (iso-octane has a boiling point of 99°C). Thus, relative to n-heptane the influence of CN alone could be studied. Nevertheless their composition was selected so that their CN match those of the two Naphtha fuels. The CN was calculated from the motor octane number (MON) using the correlation by Wilkes as given in [42] (Eq. (1)). As depicted in Figure 3, the influence of CN and boiling characteristics can be studied independently.

$$CN = 60 - 0.5 * (MON)$$

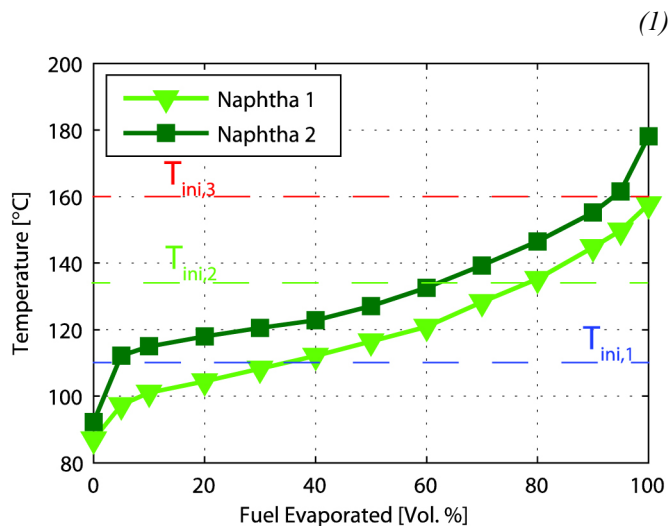


Figure 2. Boiling curves of Naphtha 1 and Naphtha 2 fuels. The boiling temperature of n-heptane is 98 °C and of PRF25 and PRF50 is 98-99 °C. The examined initial charge temperature levels are also depicted.

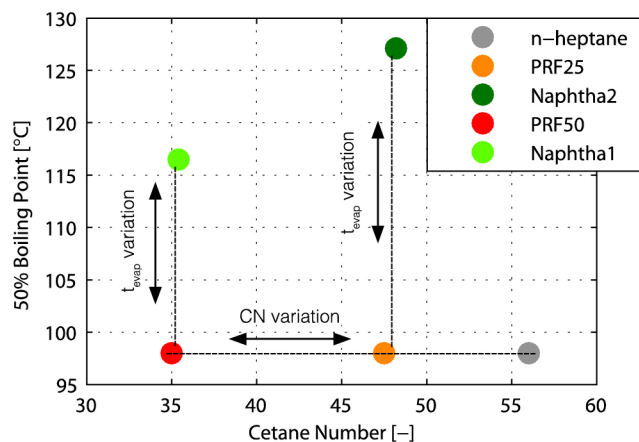


Figure 3. Selection of the fuels based on evaporation characteristics and Cetane Number variation.

Operating conditions

The fuel was delivered in the combustion chamber of the RCEM through a Siemens hollow cone piezo-injector with a cone angle of 90°. Its fuel delivery rate has been previously

measured with an IAV injection rate analyzer. For given fuel and cylinder pressure the fuel mass is defined a priori by setting the injection duration. The injection occurred well before the compression start, during the cylinder gas loading process. The gas loading process lasts around 40 sec, a period which is much longer than the timescale of evaporation. Thus, the fuel has enough time for evaporation and mixing.

Long hydrocarbons are prone to thermal decomposition when mixed in heated bulk external vessels with residence times in the order of hours [43]. Especially for non-volatile fuels elevated temperatures are needed, increasing the risk of thermal decomposition. Similar to this work, direct fuel injection methods have been utilized by other researchers through either an injector [44] or a syringe [45]. It has been shown [44] that even for less volatile fuels than in this work, full fuel evaporation and good homogeneity can be achieved, avoiding simultaneously the thermal decomposition of the fuel. The fuels examined here are composed by light molecules with relatively low evaporation temperatures. Thus, for the temperature range examined the likelihood for thermal decomposition of the fuel is very limited.

Prerequisite for the evaporation of the fuels is that the cylinder temperature, both walls and gas, is higher than the evaporation temperature of the fuel (or its highest evaporating component). Due to high residence times during the gas loading process of the RCEM, the set wall temperature defines the initial charge temperature. The evolution of pressure and temperature during a compression stroke is a function of initial volume, initial pressure (loading pressure) and initial charge temperature. For this work the initial volume and initial pressure have been selected to be constant for all experiments (V_0 corresponding to full stroke length of 249mm and $P_{ini}=1.34$ bar). Driving pressure which defines the piston speed and consequently the rate at which the system goes through the pressure-temperature trace has also been kept constant ($DP=30$ bar), in order to be able to compare ignition timings.

The initial charge temperature is used to influence the evolution of temperature relative to the pressure through the stroke. Hence by modifying the initial temperature the auto-ignition chemical kinetics can be studied at different conditions. Three initial charge temperatures were investigated, 110°C, 135°C and 160°C. They were selected so that n-heptane, PRF25 and PRF50 fuels fully evaporate. For the Naphthas no experiments were performed at 110°C. Very limited evaporation of these fuels at this temperature leads to extreme wall wetting and very poor homogeneity. At 135°C 60% of the Naphtha 2 and 80% of Naphtha 1 is evaporated. The rest of the fuel evaporates fully or partially during the stroke. Partial homogeneity can be expected for this case. Finally at 160°C Naphtha 1 evaporates fully, while Naphtha 2 evaporates up to 95%. Hence high homogeneity can be achieved. The tests performed relative to temperature setting can be seen in Table 3.

Table 3. Initial charge temperatures investigated for each fuel (grey boxes) in the RCEM. $P_{initial}=1.34$ bar, $DP=30$ bar

RCEM Wall / Initial Charge Temperature [°C]	110	135	160
n-heptane			
Naphtha 1			
Naphtha 2			
PRF 25			
PRF 50			

The influence of EGR and equivalence ratio was also studied. Additionally to pure air (0% EGR), two EGR levels have been investigated, 25% and 50%. As illustrated in Figure 4, experiments were performed for two different thermal loads, each one representing a distinct mass of fuel brought into the RCEM. For each load, an EGR sweep has been done. By diluting the mixture with increasing inert gas (EGR), the effective (relative to O_2) equivalence ratio increases. However, the energy brought into the system stays constant for a given thermal load. Eventually for each EGR setting two equivalence ratios were examined.

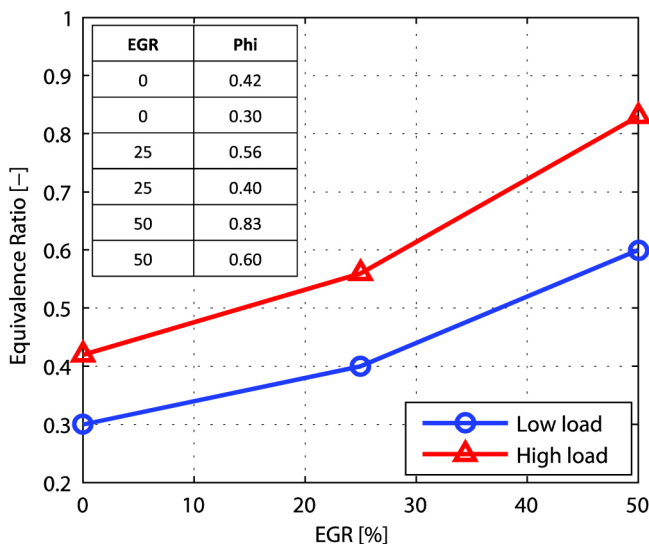


Figure 4. Operating conditions investigated. Constant mass of fuel on each load setting.

It should be noted that even in the high load case (exemplarily EGR 0% - $\Phi=0.42$) the mixture is quite lean. Due to the free floating design of the RCEM's piston, there is no mechanical restriction of its movement. Thus there is a maximum load limitation, in order to avoid collision of the piston rod to the back of the machine at the end of the expansion stroke. Therefore, higher loads cannot be investigated. However higher equivalence ratios can be investigated, but only with simultaneous EGR increase.

Repeatability assessment of the RCEM

Prior to the main experimental campaign, the thermodynamic repeatability of the RCEM was examined. Multiple compressions strokes ('motored') without fuel were performed for all three initial temperatures and analyzed statistically. The deviation of bulk gas temperature, as calculated from the Eq. of state versus the measured pressure, is taken as a criterion since these are the main sizes that influence the chemical kinetics. In Figure 5 the bulk temperature versus the cylinder pressure can be seen for the three different initial temperature levels that have been examined. Close to the top dead center (TDC) (inlay figure) the standard deviation of the bulk temperature is found to be very low, at 3.5K in all cases. Statistical errors are attributed to the repeatability/accuracy of the physical setting of the operating parameters (pressures and temperatures) and mainly to the reproducibility of the hydro/mechanical friction forces acting on the components of the RCEM. In the same figure, the effect of different initial temperature on the evolution of the pressure-temperature trace can also be seen.

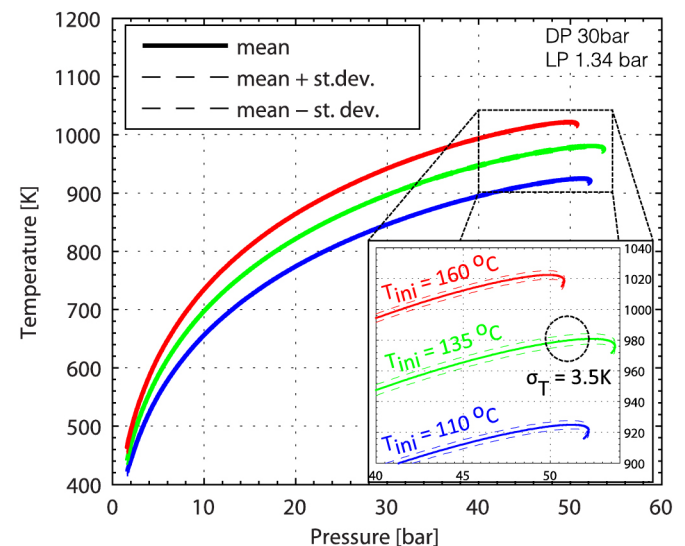


Figure 5. Repeatability of the RCEM - average of 10 Pressure - Temperature compression traces for 0% EGR and three initial charge temperatures. $\sigma_{Temperature} \approx 3.5K$

The reproducibility of the RCEM, as well as of the ignition detection methods have been evaluated for combustion ('fired') strokes. Two methods of ignition delay detection were utilized. Similar to HCCI all-metal engines, the start of burning (SOB) can be detected from the rise of heat release rate (HRR). Alternatively, as usually done in shock tubes, the SOB can be detected by the rise of the CH^* chemiluminescence intensity signal at 431nm as well. Since 431nm lies well within the formaldehyde bands (250-550nm) [27], which are characteristic of low temperature reactions (LTR or cool-flame), the same signal can be used for the detection of the LTR ignition. However the low intensity of