Experimental determination of PDFs of OH radicals in IC engines using calibrated laser induced fluorescence as a basis for modeling the end-phase of engine combustion

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Abstract

Gaining a deeper insight into the combustion process of IC engines is still a challenging task in view of improving exhaust characteristics as well as of reducing fuel consumption of passenger cars. Although the capabilities of mathematical simulations of technical combustion processes are developing extremely fast, a detailed comparison with experimentally obtained information is still necessary. This is especially true for the improvement and validation of statistical as well as chemical models used to determine the emission of exhaust gases which are limited by strict laws. For this reason experimental methods are required which yield for example information about absolute number densities of key-species determining the course and the emission characteristics of a combustion process.

For this purpose laser based techniques have attracted considerable attention due to their high temporal and spatial resolution as well as to their non-intrusiveness. The measurements of scalars (temperature, species concentration) and vectors (velocity, dissipation rates) is possible by point and multi-dimensional techniques. However, especially the quantification of techniques capable of measuring the concentration of minor species (radicals, intermediates) is still a challenging task.

In this study quantitative measurements of the OH radical in a fired IC engine are used in conjunction with results from an ensemble of precalculated combustion scenarios to obtain an improved estimation of the shape of composition probability density functions (PDFs). In post-processing steps of CFD calculations such PDFs are necessary to calculate exhaust gas species like NO_x [1]. The shape of these PDFs is usually presumed and not validated by experiments. Therefore an improvement of the quality of the prediction of exhaust gases like NO_x by commercial combustion codes can be expected if a more realistic estimation of the shape of the composition PDF is provided.

Experimental Procedure

In comparison to other methods the special merits of laser based techniques are a high temporal as well as spatial resolution. Furthermore these techniques have the advantage to be non-intrusive [2]. From a variety of optical methods laser induced fluorescence (LIF) stands out due to its high sensitivity. Using this technique intermediate species present in combustion processes at a level of a few ppm can be detected even in adverse environments like in the combustion chamber of automotive engines or gas turbines. On the other hand the quantification of LIF signals is rendered difficult because of molecular collisions quenching laser-exited states. This quenching depends sensitively on gas composition, temperature, and pressure. Different approaches to realise a quantification of LIF signals are discussed in the literature [2]. In the approach presented in this paper the transmission of the laser radiation through the combustion chamber is measured simultaneously with OH LIF signals on a single shot base. In this way OH LIF signals can be calibrated if the assumption holds that quenching changes only weakly over the measurement volume [3]. The advantage of this method is that no detailed knowledge about the gas composition responsible for molecular quenching is required. This is especially important for the investigation of turbulent combustion processes where in general no information about the local gas composition is available.

The method of the simultaneous measurement of LIF and transmission through the combustion chamber is applied to a modified two-stroke engine equipped with an excellent optical access. The experimental set-up is shown in figure 1.

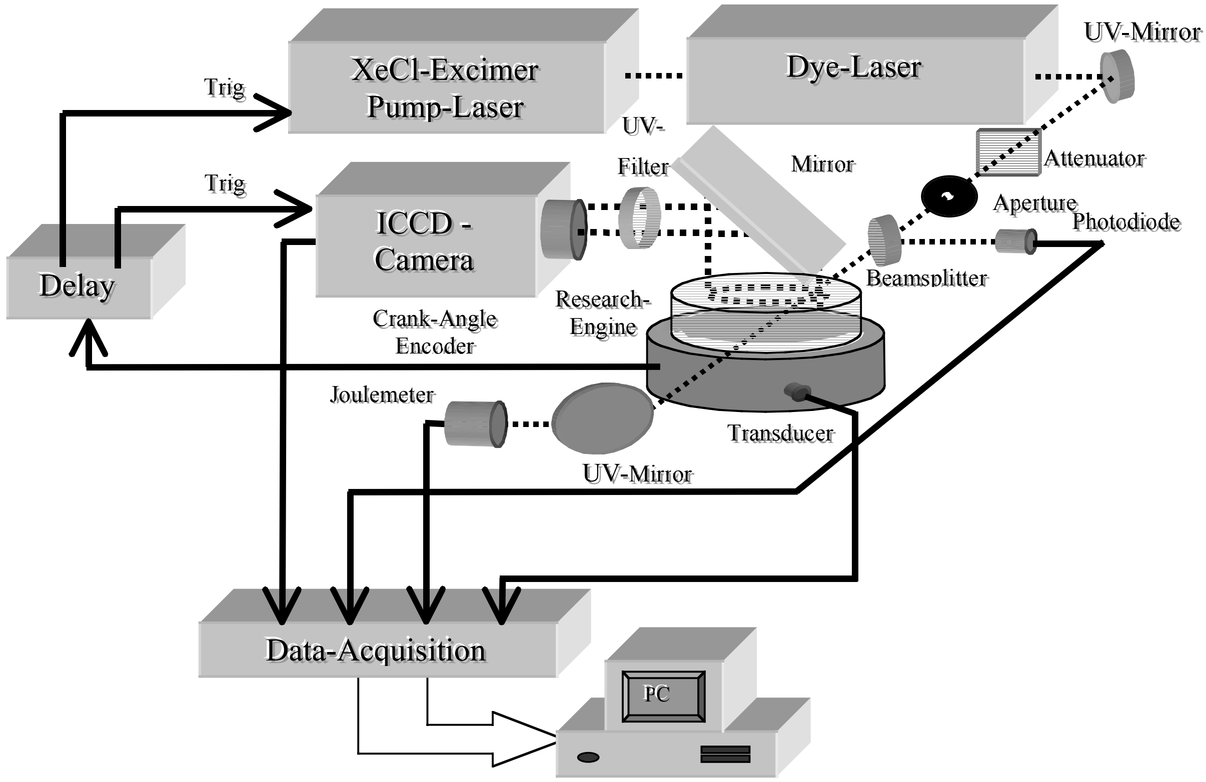

Figure1 *Experimental set-up of quantitative OH measurements in the combustion chamber of a two stroke engine*

Number densities of OH radicals are measured for different pressures during the expanding stroke along a line intersecting the combustion chamber. In this way the spatial distribution of the absolute OH radical number density in the burnt gas is measured on a single shot base. By binning for distinct ranges of pressures these measurements allow to deduce probability density functions (PDFs) of OH concentrations in the burnt gases in dependence of the pressure. In order to eliminate the effect of cooling by the wall and the complex processes within the turbulent flame front, the analysis focuses on the domain of the burnt gas which is sufficiently far away from the flame front as well as from the cylinder wall. Measurements are performed every 5 degree crank angle between 25 degree ATDC and 60 degree ATDC (where the whole load is burnt) corresponding to a range of pressures between 26 and 10 bar, respectively. By repeating the experiment 128 times for each crank angle statistic information about cycle-to-cycle and spatial variations of the OH concentration is obtained.

Precalculated combustion scenarios

Mathematical simulations are performed on the base of an ensemble of strained laminar flamelet calculations (to describe the composition of the burnt gas) and homogeneous reactor calculations (to describe the end-phase of the combustion process) using a validated, detailed chemical reaction mechanism [3] which describes the oxidation of the fuel iso-octane used for engine operation. Validation of the reaction mechanism relies on ignition delay times. Initial and boundary conditions are chosen in accordance with experimental values. A stoichiometric mixture of iso-octane and air is employed and a temperature of the load prior to compression of

340 K is assumed. Calculations are performed for different pressures which correspond to different degrees crank angles of the engine measurements.
Based on an analysis of the results of these calculations information on correlations between the OH concentration and other scalars like the temperature or the O-atom concentration important for the NO_x production is obtained.

Results

As a result of the experiments spatial variations of the OH concentration and cycle-to-cycle variations are obtained. These results yield time or pressure dependent PDFs, respectively, for the OH number density in the burnt gases of the engine. As an example figure 2 shows a PDF of OH radicals obtained from measurements which are performed within a pressure range between 17 and 19 bar. For this graph approx. 65 single shots are used. From each single shot 301 data points are extracted. One data point corresponds to a voxel of 0.4 mm^3. Local OH number densities are binned into 25 subsections. For this pressure range the observed maximal OH number densities are below 10^{23} m^{-3}. It is obvious that the shape of the PDF is asymmetric and can not be represented by a simple Gaussian.

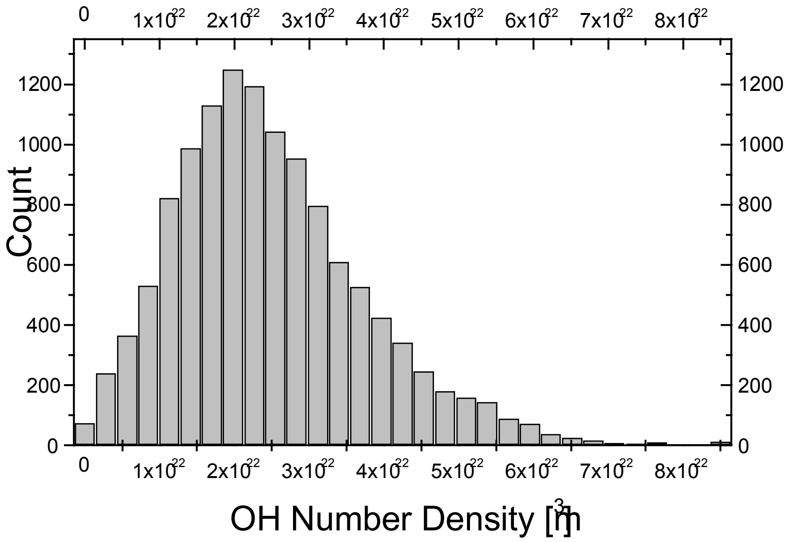

Figure 2 *Probability density function (PDF) of the OH number density in the burnt gases of an operating IC engine. 20000 data points were used for this graph which all were recorded during the expansion stroke at pressures between 17 and 19 bar.*

It is now interesting to know whether the PDF information of the OH concentration can be used to extract information on the PDF of temperature or other scalars. In the burnt gases far from the flame front the chemical system is close to chemical equilibrium. For this regions it can be assumed that the dynamics of the chemical system is governed – to a first approximation – by one reaction progress variable only [4]. This means that the OH concentration is directly correlated with the temperature. This can be seen from figure 3, which shows the correlation between the mass fraction of OH radicals and the temperature for a pressure of 18 bar (similar figures have been obtained for other engine relevant pressures between 10 and 26 bar). In this figure an unstreched flame and a flame close to the quench limit (here 10^6 Pa/m^2) are shown to assign the range of possible scenarios of the turbulent combustion process inside the engine. Data points obtained in front of the flame front are shown as circles, data points from the region of burnt gases are shown as squares. A nearly unambiguous correlation between OH radicals and the temperature is given if one devides into unburned and burnt regions. Because in the experiments it is definite that measurements are performed in the region of the post flame gases distinct far from the flame front, the experimentally obtained PDF for OH radicals can be used to estimate the shape of the PDF of the temperature in the region of burnt gases.

As a conclusion one can state that an experimentally obtained PDF of one scalar in connection with the correlation analysis based on the precalculated ensemble of stretched laminar flames allows an improved estimation of the composition PDF of others scalars. This is true for a system which is relaxed to a point where only one progression variable is sufficient to describe the succeeding temporal development of the system. This procedure yields information especially on the end-phase of the combustion process in IC engines where the condition mentioned above is fulfilled satisfying. However, the end-phase of the combustion process is of special importance for the formation of NO_x. For this reason a better estimation of the shape of scalar PDFs may help to better simulate NO_x emissions.

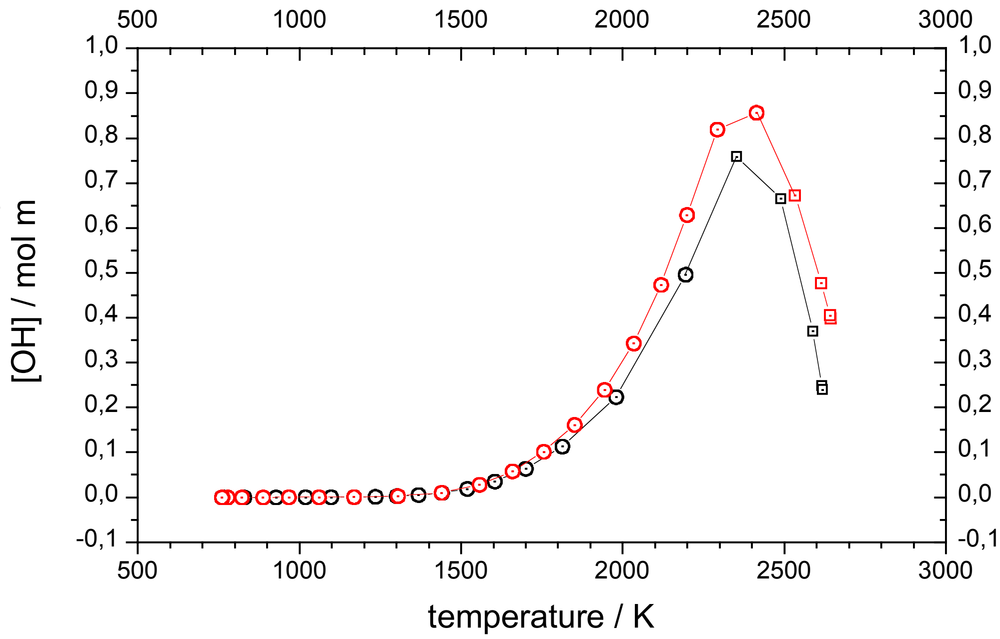

Figure 3 *Correlation between the mass fraction of OH radicals and temperature. This analysis is based on an ensemble of stretched flames calculated for a pressure of 18 bar. Circles mark data obtained in front of the flame front, squares indicate data taken from the post flame region.*

References

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