Influence of the Temperature Distribution on the Auto-Ignition in the End Gas of Otto engines

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ABSTRACT

Engine knock is an undesired mode of combustion resulting from inhomogeneities in the unburnt endgas of Otto engines. This inhomogeneity is so-called "exothermic centres" or "hot-spots" which possess a higher temperature level compared to their surrounding. This paper reports on detailed numerical simulations of exothermic centres important for the understanding of engine knock. As a model chemical system stoichiometric mixtures of hydrogen/oxygen are investigated. Based on a radical chain mechanism this system exhibits many important features - especially at the high temperatures controlling the flame propagation - but cuts down the computational effort allowing comprehensive parametric studies. Therefore the key results of this study can be transferred to fuels composed of hydrocarbons. For a one-dimensional geometry the Navier-Stokes equations are solved using both a detailed reaction mechanism and a detailed molecular transport model. As an input to the simulations single as well as double hot-spot structures are employed. Pressure, temperature gradients and peak temperatures are varied in order to investigate a wide range of parameters.

INTRODUCTION

Internal combustion engines are expected to keep their significance in powering passenger cars for the next decades. Therefore detailed information on physical as well as chemical processes is required to improve the state of the art of fuel exploitation and a reduction of the emission of pollutants in order to save limited resources.

In Otto engines engine knock limits the maximum compression ratio and therefore the thermodynamic efficiency of the combustion process. Hence this phenomenon attracted the attention of a number of researchers [e.g., 1 - 3] who investigated engine knock from a theoretical as well as an experimental point of view. Although engine knock has been the object of intense research, the detailed processes leading to and occurring during engine knock have (as a fact of their complexity) not been understood very well for a long time. Only during the last years modern diagnostic methods, which allow the time- and space-dependent observation of engine knock together with the availability of numerical simulations of chemically reacting flows have led to an improved understanding of knock processes [4, 5].

Even if the temperature of the compressed endgas is nearly homogeneous in space, non-uniformities in temperature or pressure cause the formation of "hot-spots", that means locations in the mixture, which have an increased temperature with respect to their surrounding [6]. Due to the sensitivity of the ignition delay time with respect to the temperature the hot-spots will ignite much earlier than their surrounding leading to a variety of processes such as the formation of flame fronts, pressure induced ignition or even the formation of detonation waves [7]. The auto-ignition can be divided into three periods [6, 8]: the first period is the induction time, where a radical pool is generated. If a critical concentration of radicals is reached the excitation phase starts (2nd period). Most remarkable for this phase is the strong increase in temperature. If the ignition is "successful" a subsequent self-sustaining flame propagation in its different possible modes occurs. Otherwise the flame extinguishes.

One phenomenon that has not received much attention in the past is the interaction of hot-spots. The pressure wave formed during the ignition of one hot-spot can induce the ignition of another hot-spot located close
to the first one. In this paper we outline a mathematical model which allows to study the interaction of hot-spots. It is based on the numerical solution of the one dimensional conservation equations for mass, species mass, momentum and energy, respectively [9]. Detailed parametric studies are presented for the hydrogen/oxygen-system which is used as a model system that exhibits many features observed in the combustion of higher hydrocarbons but due to its simplicity reduces the computational effort. At the beginning of the auto-ignition mixture composition as well as pressure are considered to be uniform in space. The influence of different initial temperature distributions upon the process of auto-ignition is investigated. The speed of propagation of the reaction wave for single hot-spots is analyzed as well as the interaction between two hot-spots located close to each other.

THEORETICAL BACKGROUND

A detailed description of the mathematical procedure is given in [8]. Here just some fundamental principles are highlighted. The mathematical simulation of the induction and excitation phase of an auto-ignition as well as the propagation or extinction of the flame is performed by solving the coupled conservation equations for total and species mass, momentum and energy together with the state equation, represented by the ideal gas law. A detailed reaction mechanism is used consisting of 37 elementary gas phase reactions and 8 chemical species [10]. Fits from JANAF [11] tables are used to obtain thermodynamic properties. A multispecies transport model based on the Curtiss-Hirschfelder approximation is employed [9]. To simplify matters and to cut down computational effort we restrict here only to one-dimensional geometries (i.e. infinite slab).

The resulting equations are transformed to Lagrangian coordinates in order to eliminate the convective terms which are difficult to handle numerically [12]. The partial differential equation system is discretized in space using standard finite differences on a statically adapted mesh [12]. The ordinary differential and algebraic equations resulting from the spatial discretization are solved using a semi-implicit extrapolation method [13]. Typically computation times on a workstation differ between 30 min for low pressures (2 bar) and a day for high pressures (9 bar).

For $t = 0$ pressure and mixture composition are assumed to be homogeneous in space and the mixture is supposed to be in rest. For later times the formation and development of shock waves is taken into consideration. A temperature distribution which mimics the occurrence of exothermic centres is given as an initial condition. In the parameter study presented here, single as well as double hot-spots are considered. Peak temperatures and temperature gradients are varied for the different distributions. A typical temperature distribution is shown in figure 1.

![Figure 1](image.png)

**Figure 1** Initial temperature distribution used for the simulation of double hot-spots, the temperature of the surrounding of the hot-spots is 1150 K. $T_{max}$ represent two peak temperatures and $\Delta T/\Delta r$ the temperature gradient.

RESULTS AND DISCUSSION

The investigations presented here consist of two parts. In part I single hot-spots are considered. Temperature and pressure dependence of the induction time and the duration of the excitation phase of an auto-ignition are analyzed as well as the influence of initial temperature gradients at the boundary of a hot-spot on the velocity of the reaction wave. In part II the interaction of two hot-spots is investigated. Initial pressure, peak temperatures, temperature gradients and the separation of the hot-spots are varied to evaluate possible modes of interaction.

**Part I**

In figure 2 a typical ignition process of an exothermic centre is shown. In this example the initial peak temperature is 1200 K and the temperature gradient at the border of the hot-spot equals 86 K/mm. Here the end of the induction time and the beginning of the excitation phase were defined via the time of the rapid growth of
temperature, while the time when a temperature of 3000K was reached was set as the end of the excitation phase. 

![Graph showing temperature changes over time](image)

**Figure 2** Typical ignition process of an exothermic centre located around r=0 m, the time axis is depicted for t>10 μs, within this temperature scale the initial temperature distribution (first trace) appears nearly flat.

By varying the peak temperatures from 1160 to 1250 K induction times as well as the duration of the excitation phase of the auto-ignition were analyzed. Results for the case of an ambient temperature of 1150K and a pressure of 2 bar are presented in figure 3. As one expects a strong decrease of the induction time is found by increasing the peak temperature but just marginal variations are obtained for the duration of the excitation phase within the range of temperatures studied in this paper.

![Graph showing temperature dependence](image)

**Figure 3** Temperature dependence of the induction time (squares) and duration of the excitation phase (triangles).

This behaviour can be understood by the fact that during the induction phase, where a radical pool develops up to a critical value, the growth of the radical concentration is strongly dependent on the rate of chain branching reactions. These reactions have a large activation energy and thus show an extremely high sensitivity with respect to temperature.

If a critical value of radical concentration is reached the excitation phase starts and a strong increase of temperature is observed. Due to this rise in temperature the initial peak temperature is of minor significance. In the hydrogen/oxygen system the evolution of the excitation phase is mainly dependent on the exothermic elementary reaction

$$H_2 + OH \rightarrow H_2O + H.$$ 

The pressure dependence of this process can be seen from figure 4 where the pressure was varied from 1 to 10 bar for a peak temperature of 1200K.

![Graph showing pressure dependence](image)

**Figure 4** Pressure dependence of the induction time (squares) and duration of the excitation phase (triangles).

It is obvious that for pressures above 5 bar the duration of the excitation phase is increasing due to the influence of three body-collisions annihilating reactive radicals. However, the induction time shows a quite similar pressure dependency reflecting the fact that the most efficient production of radicals is obtained around 5 bar.

The influence of the temperature gradient at the outer layer of the hot-spot upon the speed and the mode of propagation has been studied for an initial peak temperature of 1200 K and a pressure of 2 bar (in [4] it was stated that depending on the steepness of the temperature gradient different modes of engine knock are observed). The temperature gradient has been varied between 14 K/mm and 125 K/mm. The temporal evolution of the flame front - given by the position of the maximum value for heat conduction - has been analyzed. A movement as well as an acceleration of the flame front appears as the excitation phase begins. At short
distances up to a few millimeters ahead of the igniting hot-spot differences for the speed of propagation are observed dependent on the different temperature gradients used as input. For distances around 10 mm these differences vanish and typically velocities of approx. 3000 m/s are obeyed.

This speeds of propagation correspond to velocities typical for detonations. Investigations have been carried out in order to analyze the transition to a detonation. For this analysis the steepest pressure gradient - indicating the location of the shock front - and the peak pressure - indicating the position of the chemical reaction wave - have been projected to the subspace spanned by time and space as shown vicarious in figure 5 for $\Delta T/\Delta t = 14 \text{ K/mm}$.

For this study temperature maxima of the initial temperature distribution (compare figure 1) and the pressure have been varied.

Three different temperature gradients ($\Delta T/\Delta t = 127$, 31 and 16 K/mm) and three different pressures ($p = 2$, 5 and 9 bar) have been investigated. For the temperature gradient $\Delta T/\Delta t = 127 \text{ K/mm}$ the maxima of the two temperature peaks have been chosen to equal 1372 K and 1227 K, for both other cases maxima of 1192 K and 1164 K have been used. For example a typical result is shown in figure 6, viewing the evolution of the temperature distribution in time and space. In this case the following parameters were employed: $\Delta T/\Delta t = 31 \text{ K/mm}$, $p = 2$ bar.

In general three different cases of mutual influence of two hot-spots can be distinguished. First - as shown in figure 6 - a shock front from the first hot-spot reaches the second hot-spot when it is already igniting. By the superposition of the reaction wave of the first hot-spot with the igniting second hot-spot an acceleration of the combined reaction wave can be observed. Consequently the formation of a detonation can be favoured by the second hot-spot. No essential influence of the shock wave on the duration of the excitation phase of the second hot-spot is observed.

In this case for early times up to 13 $\mu$s a shock wave is formed leaving the hot-spot. The shock wave entails a rise in temperature which promotes chemical reactions. A reaction wave is formed running behind the shock front. After approx. 14 $\mu$s the reaction wave combines with the shock front generating a detonation. As a consequence the speed of propagation of the reaction wave is accelerated severely (cf. fig. 5).

**Part II**

As stated by Oppenheim the "coherent" self-ignition of two or more exothermic centres leads to a strong ignition which has been identified with the phenomenon of engine knock [14]. Besides in [5] typically a set of exothermic centres have been observed for knocking cycles in a two-stroke engine. For this reason in the following section the mutual influence on induction times and excitation phases of two hot-spots located close to each other is investigated.

**figure 5** Position of shock front (circles) and reaction wave (crosses) as function of time

**figure 6** Temporal evolution of an initial temperature distribution specified in the text, time is shown for $t > 10 \mu$s, first kind of interaction
In a second scenario the initial shock wave is caught up by the reaction wave of the first hot-spot before the second one is reached (this behaviour of the first hot-spot is similar to that described by figure 5). The second hot-spot is ignited by the reaction wave of hot-spot 1. Again a significant acceleration of the speed of propagation can be observed when the reaction wave of hot-spot 1 combines with the second hot-spot. Because the second hot-spot is "overrun" by the reaction wave from the first, one cannot speak any more of an induction time and excitation phase of the second hot-spot.

In a third case a shock front from hot-spot 1 ignites the second hot-spot. This kind of interaction takes place at relative high pressures (in this study 9 bar) because the induction time of the second hot-spot is quite large under these circumstances (cf. figure 4). A typical result for this type is shown in figure 7 (ΔT/Δr = 31 K/mm, p = 9 bar) where the excitation phase of hot-spot 2 is not fully terminated when it is reached by the reaction wave of the first hot-spot.

"excitation phase" results from the detonation superimposing the ignition process of hot-spot 2

CONCLUSIONS

In this paper a method was presented allowing the mathematical simulation of single as well as a set of exothermic centres responsible for engine knock. It was shown that there is a strong influence of peak temperature and pressure on the induction time and the excitation phase of the auto-ignition. In many cases the appearance of a shock wave results in an acceleration of the reaction wave leading to a detonation with propagation speeds in the order of a few thousand m/s. This shock wave was shown to be able to ignite hot-spots close to the initiating one. Another mode of interaction was shown to be the ignition of a second hot-spot by a reaction wave originating from the first igniting hot-spot. In this case as well as for the third case - where the ignition of a second hot-spot is unaffected by the first one - an acceleration of the initial reaction wave can be observed when it is approaching the adjoining hot-spot. This shows that the mutual influence of hot spots may lead to fast propagation speeds of reaction waves which cause the appearance of engine knock.

Because at high temperatures for fuels composed of hydrocarbons the rate limiting elementary reactions remain the same as those for the hydrogen/oxygen system the findings concerning the kind of propagation can be transferred to auto-ignition processes in engines running with i.e. propane or iso-octane/n-heptane-air mixtures. In addition in the case of a fast propagation (i.e. detonations) differing characteristics for molecular transport processes for different fuels is of minor importance because fluid dynamics dominates this process.

Of course the results obtained in this investigation can directly be applied to concepts pushing ahead passenger cars using hydrogen as fuel.

figure 7 Temporal evolution of an initial temperature distribution specified in the text, time is shown for t>110 μs, third kind of interaction

Here the induction time and excitation phase of the second hot-spot are shortened to 119.3 μs and 0.1 μs corresponding to a decrease of 11 % and 99.9 %. The reduction of the induction time is due to the shock wave increasing the temperature while the extremely short
REFERENCES