Wall Film Evaporation causing Pre-ignition in Turbo-charged Gasoline Engines

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1 Introduction

Turbo-charging of modern gasoline engines may reduce the fuel consumption considerably. A drawback of this technology is the occurrence of stochastic pre-ignition events, which may initiate a randomly localized flame kernel and subsequent turbulent flame propagation. This induces a rise in pressure and thereby a temperature increase of the remaining charge. In the unburnt part of the charge a secondary auto-ignition event may take place, which, under locally unfavorable conditions, may initiate a local detonation. This scenario has been advocated by Rudloff et al. [1] who base their subsequent analysis on the regime diagram for developing detonations by Bradley et al. [2] and Gu et al. [3]. The theory behind this work has been summarized by Bradley and Kalghatgi [4] and Kalghatgi and Bradley [5] and goes back to the theory of Zeldovich [6]. Based on Bradley's regime diagram Peters et al. [7] have designed a prediction procedure which uses input from classical CFD models to calculate the detonation probability.

In the engine community this phenomenon is referred to as abnormal combustion, super-knock or mega-knock. The full sequence of events is often not well understood in the literature and the pre-ignition event is typically not distinguished from the secondary auto-ignition and the detonation. The entire phenomenon leading to mega-knock is then referred to as pre-ignition.

In a comprehensive experimental and theoretical approach Zahdeh et al. [8] have identified several parameters which may have a direct effect on the onset of pre-ignition including liner wetting, injection targeting, mixture stratification, mixture motion and oil formulation. Among these, injection targeting is found to be most crucial. They suggest that oil mixing with the fuel would lower the self-ignition temperature and would hence cause premature combustion. A 3-D model of piston ring dynamics was developed to understand the stochastic nature of oil intrusion into the combustion chamber. Nevertheless, the authors note that the mechanism of oil and fuel accumulation to produce self-ignition is not fully understood.

There is the hypothesis that oil intrusion causes the first pre-ignition event [9,10]. The oil film adhering to the cylinder wall would be diluted by the fuel spray, such that a mixture of hydrocarbons with a cetane number higher than that of gasoline would be released as fuel droplets out from the top land crevice during deceleration of the piston just before TDC. These droplets could deposit on the piston and evaporate from there. Another scenario is that the oil film evaporates directly from the cylinder wall. The higher cetane number of the evaporating mixture would cause a lower ignition delay time compared to gasoline.

The objective of the present paper is to test whether in addition to above-mentioned hypotheses gas dynamic effects could also cause lower pre-ignition delay times. That hypothesis is based on the prediction by Klein and Peters [11] that cumulative pressure waves would shorten the ignition delay

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time considerably if the effective non-dimensional activation energy is large enough. The estimate of that number for the low temperature auto-ignition of n-heptane based on Peters et al. [12] is around 25 which would provide only a 10% reduction in the ignition delay time according to [11]. However, since hydrocarbon ignition kinetics are more complex, it seems important to quantitatively evaluate this hypothesis. For that purpose we choose as in [11], a one-dimensional configuration between the piston and the cylinder head originally filled with a stoichiometric iso-octane air mixture at 40 bar and 774 K. This is the temperature, for which the calculated ignition delay time in the NTC regime at 40 bar is at a minimum. Liquid n-heptane is supposed to have been deposited on the piston wall and has reached its boiling temperature of T_L =560 K, which is equal to the wall temperature T_w. It then evaporates due to heat flux q_w from the hot gaseous mixture. After evaporation is finished, mixing between n-heptane and the stoichiometric iso-octane-air mixture is assumed to occur rapidly such that the resulting mixture is fuel rich and contains in terms of mass fractions 50% n-heptane and 5 % iso-octane mixed with air. Ignition delay times calculated by using a 248 species mechanism for PRF (Primary References Fuel) mixtures by Cai and Pitsch [13] are shown in Fig. 1. It is seen that the ignition delay time in the NTC (Negative Temperature Coefficient) region at 40 bar is for the fuel rich n-heptane-iso-octane-air mixture more than one order of magnitude shorter than for a stoichiometric iso-octane air mixture.

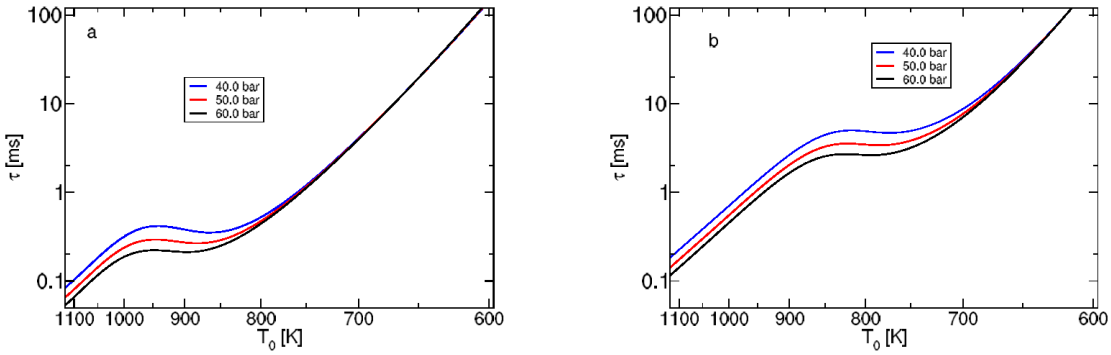

Figure 1. Ignition delay times a) for a fuel rich n-heptane-iso-octane-air mixture; b) for a stoichiometric iso-octane air mixture at three different pressures.

2 Numerical set-up

At the wall the heat flux balances the convective flux q_w due to evaporation is

$$q_w = \kappa \frac{\partial \overline{T}}{\partial y} = \rho v_w h_L \qquad (1)$$

Here κ is the temperature conductivity, T is the temperature, y the distance from the wall, ρ is the density v_w ist the evaporation velocity and h_L is the heat of evaporation. Using the boundary layer assumption with the boundary conditions

$$y = 0 : u = 0, T = T_w, y \to \infty : u = u_\infty, T = T_\infty$$

Reynolds' analogy between heat and momentum transport over the boundary layer leads to

$$\frac{q_w}{\tau_w} = c_p \frac{(T_\infty - T_w)}{u_\infty} \quad (2)$$

Here τ_w is the wall shear stress and u_∞ the convective velocity at the outer edge of the boundary layer The wall shear stress can be calculated by considering the momentum balance in the viscous sub-layer and the log layer close to the wall

$$\tau_w = \mu \frac{\partial \overline{u}}{\partial y} - \rho \overline{u'v'} \quad (3)$$

which, further away from the wall, where the viscous transport terms vanishes, becomes

$$\tau_w = -\rho \overline{u'v'} \sim \rho k \quad (4)$$

Here $-\rho \overline{u'v'}$ is the turbulent shear stress and k is the turbulent kinetic energy. Solving eq. (1) for v_w leads to

$$v_w = \frac{q_w}{(\rho h_L)} = \tau_w \cdot c_p \frac{(T_\infty - T_w)}{(u_\infty \cdot \rho h_L)} \simeq k \cdot c_p \frac{(T_\infty - T_w)}{(u_\infty \cdot h_L)} \quad (5)$$

Estimating the turbulence level $k^{½}/ u_\infty$ as 50% one obtains with T_∞ = 774 K, T_w = 560 K and h_L/c_p = 160 K an evaporation velocity which is one third of the velocity u_∞ at the edge of the boundary layer. We have chosen two cases:
Case A with u_∞ = 6 m/s leading to v_w = 2 m/s and case B with u_∞ = 12 m/s which leads to v_w = 4 m/s. These velocities were imposed at the lower boundary of the domain during an estimated evaporation time of 0.02 ms for case A and 0.01 ms for case B. The domain between piston and cylinder head was fixed and set as 10 mm.

We have used the Kurganov and Tadmor [14] MUSCL (Monotone Upstream-centered Scheme for Conservation Laws) scheme to solve the one-dimensional equations for continuity, momentum, energy and species equations. For the chemistry the 248 species mechanism by Cai and Pitsch [13] was used. The numerical method can be viewed as a modification to the Lax-Friedrich scheme. It uses central differences with comparable performance to Riemann type solvers. We have used reflective and non-reflective boundary conditions at the outer edges of the domain of integration and opted finally for the reflecting boundary conditions in order to test whether sound waves would accelerate the auto-ignition.

In Fig. 2 we have plotted the development of species profiles for case B for several time steps between 0.5 and 1.0 ms. Until 0.5 ms there is practically no change in the species mass fraction profiles at x = 0. As time evolves from 0.5 ms to 0.83 ms, the mass fraction of n-heptane shown in Fig. 2a decreases rapidly to 10% of its original value in the region from x = 0 to x = 0.1 mm, while iso-octane shown in Fig. 2b decreases approximately by a factor of two. The temperature shown in Fig. 3a rises at first slowly during first stage ignition, then passes the threshold of 1000 K at 0.75 ms to second stage ignition. The profile of HO_2 shown in Fig. 2c, which is advocated by Shao and Rutland [14] as a suitable chemical indicator in simulations of engine knock problems, first increases until 0.72 ms, then decreases slightly when the threshold of 1000 K is reached and increases again during second stage ignition thereafter. The mass fractions of the sum of all keto-hydroperoxide isomers of n-heptane shown in Fig. 2d first increase during first stage ignition but are depleted after 0.91 ms.

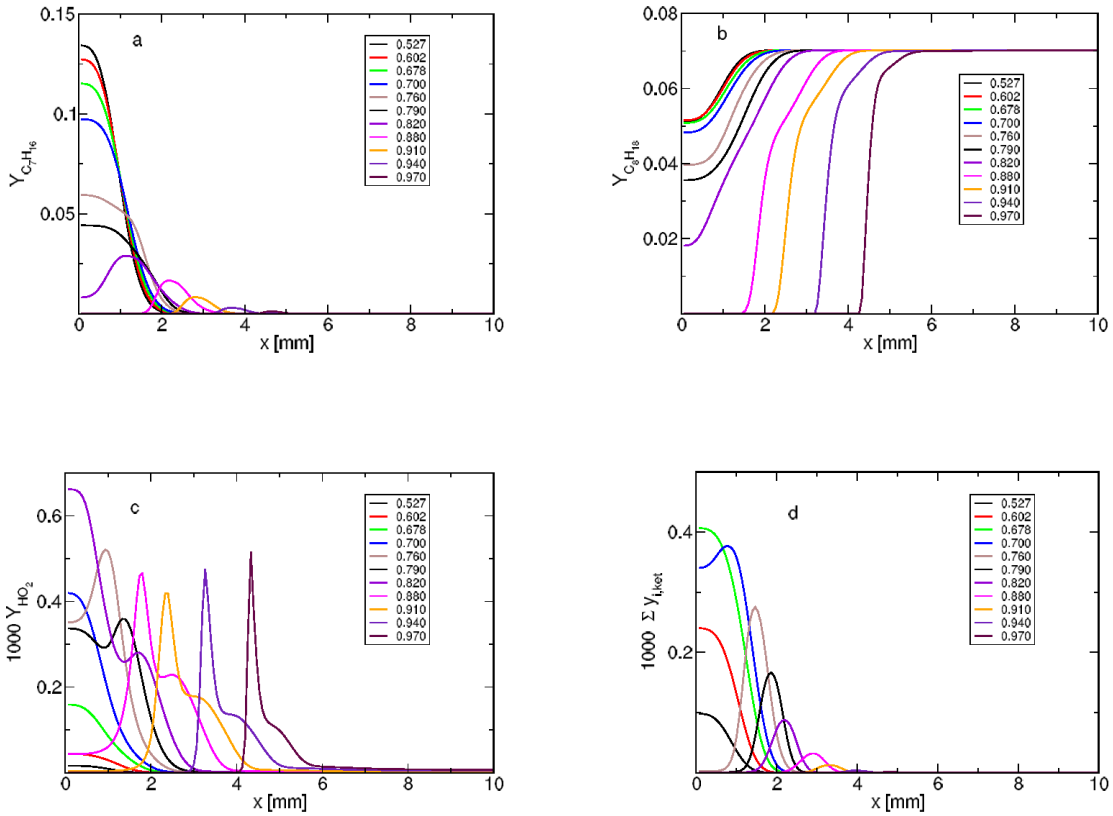

Figure 2. Development of species mass fraction profiles from 0.5 to 1 ms. a) n-heptane, b) iso-octane, c) hydrogen-peroxide radical, d) sum of all keto-hydroperoxide isomers of n-heptane. The inserts indicate the time in milliseconds.

At 0.86 ms both n-heptane and iso-octane are fully consumed in the region between x = 0 and x = 0.15 mm. The temperature has reached nearly the adiabatic value corresponding to the rich mixture in this region. Only a small amount of n-heptane remains which will be fully consumed in the next 0.1 ms. At 0.9 ms a maximum appears in the temperature profile in the region beyond x > 2 mm where originally

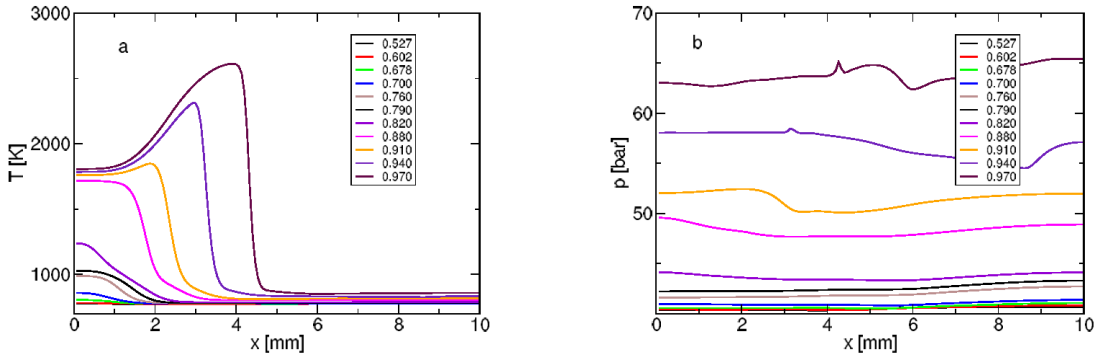

Figure 1. Development of temperature and pressure profiles from 0.5 ms to 1 ms. The inserts indicate the time in milliseconds.

only the iso-octane-air mixture was present. This indicates that a flame starts to propagate into this region. At 0.98 ms the flame front has proceeded to x = 0.55 mm and behind the front the adiabatic flame temperature of the iso-octane air mixture is established between x = 3 mm and x = 5 mm. During the period from 0.5 to 0.98 ms the pressure has continuously risen in the combustion chamber with pressure waves travelling forwards and backwards as shown in Fig. 3b. These waves cause oscillations of the temperature but they seem to have little effect on the evolution of the auto-ignition in the region into which n-heptane has evaporated, nor do they seem to influence the flame propagation in the iso-octane- air mixture. The small isolated pressure peaks occurring at later times seen in Fig. 3b originate from gas expansion effects at the flame front.
The evolution of the temperature over time, taken at two monitor points, at x= 0.5 mm which is in the region into which n-heptane has evaporated and at x = 5.0 mm in the iso-octane-air mixture, is plotted in Fig. 3. This is compared with the temperature evolution of a homogeneous iso-octane air mixture on a homogeneous reactor with the same initial conditions of 774 K and 40 bar. The insert in this figure shows the temperature evolution at the monitor point at 0.5 mm. It is seen that ignition in the region into which n-heptane has evaporated starts at 0.5 ms and is completed at approximately 0.8 ms. Flame propagation has reached the monitor point located in the middle of the gap at approximated 1 ms, while ignition in the homogeneous reactor takes 4.5 ms. The pressure oscillations which manifest themselves as temperature oscillations of approximately 2 K, as seen in the insert, seem to have little effect on the auto-ignition process. Calculations for Case A have produced nearly the same ignition delay times as shown in Fig. 3.

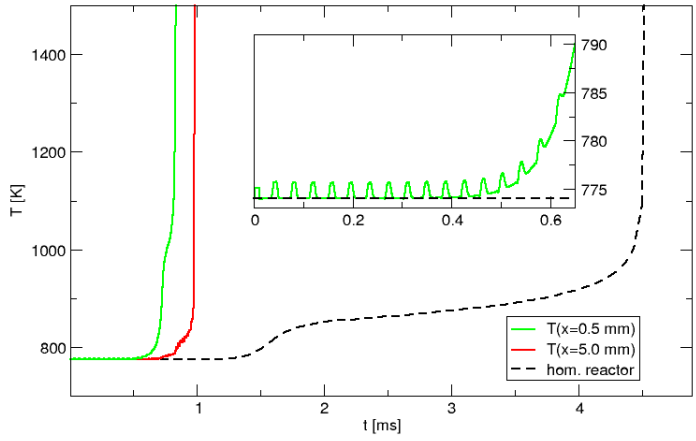

Figure 3. Development of the temperature over time taken at two monitor points, compared with the temperature development in a homogeneous reactor containing a stoichiometric iso-octane-air mixture.

Conclusions

If a liquid like n-heptane which has a higher cetane number than gasoline and therefore auto-ignites more easily evaporates from a wall layer, a shorter overall auto-ignition time results. This is in line with hypotheses which attribute pre-ignition to low cetane number components of the oil, deposited by droplets on the piston or evaporating directly from the cylinder walls. Our calculations show that the cumulative effect of weak pressure waves does not lead to a significant reduction of the ignition delay time.

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