Detailed Numerical Simulation of Droplet Combustion

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Abstract

Auto-ignition and combustion of single fuel droplets of methanol, n-heptane and iso-octane are studied. The numerical simulations are based on a detailed vaporization model, a detailed transport model and detailed chemical kinetics. The governing equations of the two phases are solved in a fully coupled way. The influence of different physical parameters like droplet temperature, gas phase temperature, ambient gas pressure and droplet velocity on the ignition process is investigated and the results are compared. It turns out that the ambient gas temperature highly influences the ignition delay time similar to the case of the auto-ignition of a homogeneous gas mixture. The ignition delay time decreases with increasing pressure, which can also be observed in homogeneous gas mixtures. This decrease can be described by a rational law. The influence of the droplet temperature is negligible. In addition the ignition delay time is almost independent of the droplet velocity, provided that the flow is not too strong, so that the flame is ”blown out”.

Introduction

In many technical systems sprays of small fuel droplets are burnt in the presence of air. The liquid fuel is injected into the combustion chamber and the combustion arises as the droplets vaporize and fuel vapor mixes with air. A reliable description and simulation of spray combustion requires a detailed understanding of droplet ignition and combustion. The simplest model of the fuel spray ignition process is the ignition of an ensemble of single fuel droplets. If microgravity droplet combustion is regarded, i.e. no gravitation, no relative motion of droplet and gas phase, the considered system can be assumed to have a spherical symmetry. Hence only a system of one-dimensional conservation equations has to be solved. This regime is appropriate to investigate the basic physical and chemical processes, like vaporization, molecular transport and chemical kinetics and their interaction. Particularly for describing transient processes like the ignition of the droplet the understanding of this interaction is necessary. To account for a gas flow around the droplet or the ignition process of an array of droplets at least two-dimensional geometries have to be simulated. The combustion of a single liquid droplet in a quiescent atmosphere has been studied extensively both experimentally and numerically. Most of the experimental researches deal with the fuel methanol [1, 2, 3, 4, 5] and n-heptane [6, 7, 8, 2, 9]. Numerical simulations have been presented for methanol droplets [10] and n-heptane droplets [11, 12, 13, 14]. Only a little number of studies do not assume spherical symmetry and nevertheless consider the physics of the droplets and the chemical processes in detail [15, 16, 3, 5]. Because the d^2-law yields relatively good estimates of the vaporization rate K of the droplet this vaporization rate is presented in most of the researches. Therefore the vaporization rates of methanol, n-heptane and iso-octane droplets obtained from our numerical simulations are stated and compared with former results found in literature. With regard to technical applications, like in gas turbines or combustion engines, the influence of ambient physical properties on the ignition process are of major interest. Thus parametric studies are performed to construct libraries of droplet combustion which can be used, e.g. in flamelet-like calculations of turbulent spray combustion. Parameters like the droplet temperature, gas temperature, pressure as well as the boundary conditions are varied. Studies of the ignition and combustion of methanol, n-heptane and iso-octane droplets in air are presented.

Specific Objectives

To construct libraries of droplet combustion, which can be used e.g. in flamelet-like calculations of turbulent spray combustion, the influence of different physical properties on the ignition and the combustion process has to be investigated in

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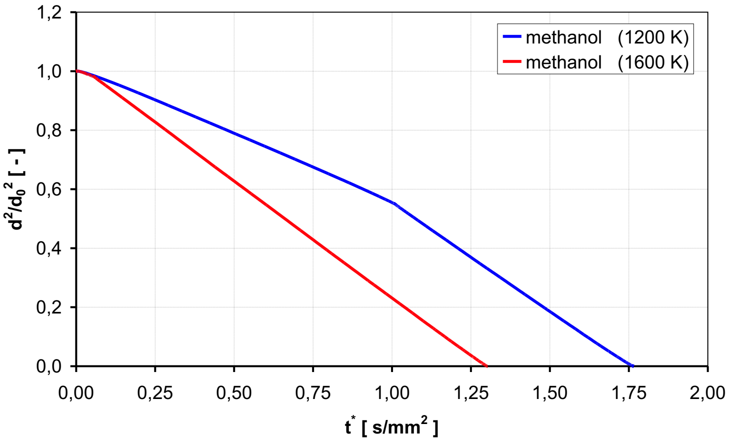

Figure 1: d^2-law of a methanol droplet in air ($p = 1$bar, $r_D = 100\mu$m)

detail. Parametric studies of the dependence of the ignition delay time on the droplet temperature, ambient gas temperature, ambient gas pressure and the gas flow are performed and the results are presented.

To investigate the influence of different physical properties on the transient ignition process, the physical and chemical processes have to be simulated in detail. The chemical kinetics of the investigated fuels are governed by a large number of chemical species and elementary reactions. In the case of the methanol combustion the detailed high-temperature reaction mechanism of Chevalier and Warnatz [17] contains 23 chemical species and 166 elementary reactions. In the case of n-heptane and iso-octane detailed chemistry is provided by two reaction mechanisms of Golovitchev [18] including 62 chemical species and 572 elementary reactions (n-heptane) and 84 chemical species and 824 elementary reactions (iso-octane). The transport processes are also modeled in detail. Merely the Dufour effect and diffusion by pressure gradients are not taken into account, because they are negligible compared to the mass diffusion. Fouriers law is used to determine the heat fluxes. For the determination of the diffusion coefficients the approximation of Curtis and Hirschfelder [19] is used. The liquid phase properties are calculated by the data correlations taken from Reid et al. [20]. The detailed vaporization model governs the interface equations, which are based on a local phase equilibrium.

The conservation equations of the gas phase and the liquid phase are solved in a fully coupled way [21]. Efficient numerical methods for the solution of the underlying partial differential equation systems are devised. The governing equations are discretized using finite difference techniques. The resulting differential-algebraic equation system is solved by the linearly implicit extrapolation method LIMEX [22].

Results and Discussion

Simulations are performed for isobaric conditions with ambient pressures of 1bar and 7bar. At first the vaporization rates of the droplets are studied. In the cases of all fuels the temporal evolution of the droplet diameter follows the d^2-law

$$d^2 = d_0^2 - K \cdot t \quad . \tag{1}$$

To evaluate the performed simulations the vaporization rates K of methanol and n-heptane are compared with values taken from literature. To allow comparisons with former experimental and numerical results these simulations are performed with an ambient pressure of 1bar. The vaporization rates K of the three different fuels are determined for initial ambient gas temperatures of 1200K and 1600K.

In figure 1 one can see the time evolution of the diameter of a methanol droplet in air. The sharp bends of the lines clearly identify the ignition points. After ignition the vaporization rates are increased. The vaporization rates after ignition are determined to 0.74mm^2/s and 0.79mm^2/s. These vaporization rates show good agreement with the experimental results of 0.56mm^2/s of Cho et al. [10], of 0.71mm^2/s of Vieille et al. [2] and the numerical results of 0.61mm^2/s of Cho et al. [10], of 0.8mm^2/s of Marchese et al. [1] and of 0.75mm^2/s of Chauveau et al. [4]. A closer comparison of the results is not possible because of the different ambient conditions of the studies.

In the case of n-heptane (figure 2) the vaporiza-

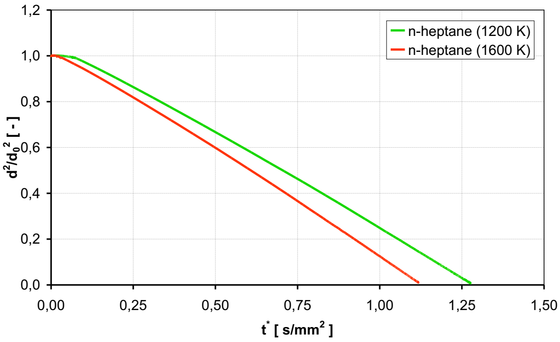

Figure 2: d^2-law of a n-heptane droplet in air ($p = 1$bar, $r_D = 100\mu$m)

tion rates of 0.80mm^2/s and 0.90mm^2/s also comply with the experimental results of 0.85mm^2/s of Vieille et al. [2], of 0.758mm^2/s of Jackson and Avedisian [8] and 0.75mm^2/s of Hara and Kumagai [7] and the numerical result of 0.8mm^2/s of Cho and Dryer [11]. The ambient conditions of the studies also differ from each other as in the case of methanol. For example the ambient gas temperature is much higher in our case because the auto-ignition of fuel droplets in a hot gas phase is investigated. In the studies [2, 8, 7, 11] the droplet is ignited by an ignition source. Therefore a closer comparison of the vaporization rates is not possible.

To the best of our knowledge vaporization rates of burning iso-octane droplets cannot be found in literature. Figure 3 shows vaporization rates of 0.75mm^2/s for the initial ambient gas temperature of 1600K. It can be summarized, that the vaporization rates of the droplets of the fuels methanol and n-heptane show good agreement with results taken from literature. In the case of iso-octane a vaporization rate of 0.75mm^2/s is determined.

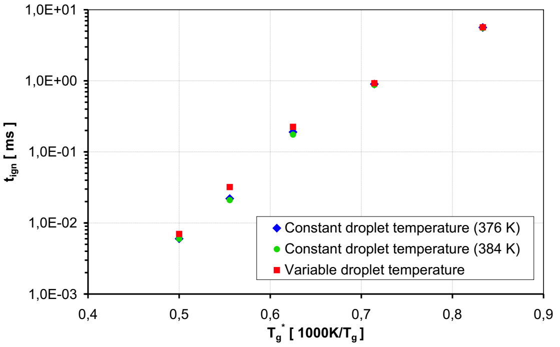

Figure 4: Arrhenius plot of the ignition delay time for different droplet temperatures in the case of methanol droplets ($p = 7$bar, $r_D = 100\mu$m)

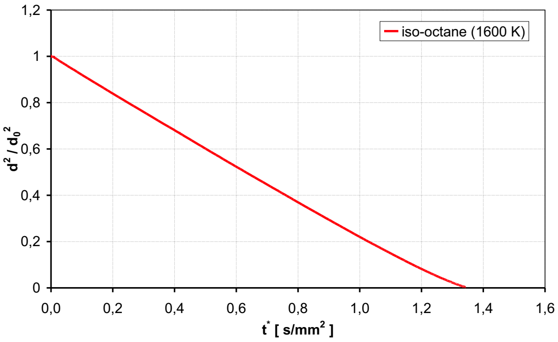

Figure 3: d^2-law of a iso-octane droplet in air ($p = 1$bar, $r_D = 100\mu$m)

In the following the dependence of the ignition delay time of single fuel droplets on several physical properties will be investigated. In figure 4 and 5 the ignition delay times for simulations with fixed and variable droplet temperatures are presented. In the case of a variable droplet temperature the temperature of the liquid phase depends both on time and space. At an ambient pressure of 7bar the boiling temperature of methanol is 396K. Thus to investigate the influence of the droplet temperature a temperature of 384K, close to the boiling temperature, and a lower temperature of 376K are chosen. In the case of n-heptane the boiling temperature at an ambient pressure of 7bar is 454K. Analogous to the case of methanol a temperature close to the boiling temperature and a lower temperature are chosen. So the fixed droplet temperatures are set to 450K and 379K.

Figure 4 and figure 5 show a minor dependence of the ignition delay time on the droplet temperature. If the fixed droplet temperature is high enough, it does not influence the ignition delay time. Thus to reduce the computing time and

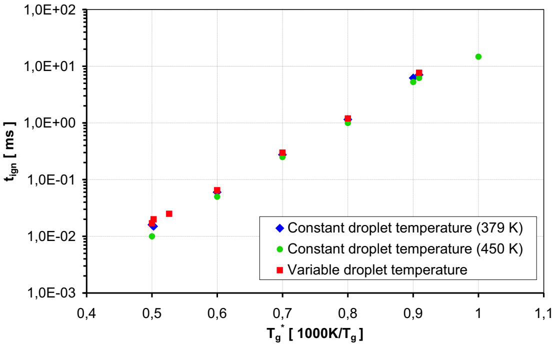

Figure 5: Arrhenius plot of the ignition delay time for different droplet temperatures in the case of n-heptane droplets ($p = 7$bar, $r_D = 100\mu$m)

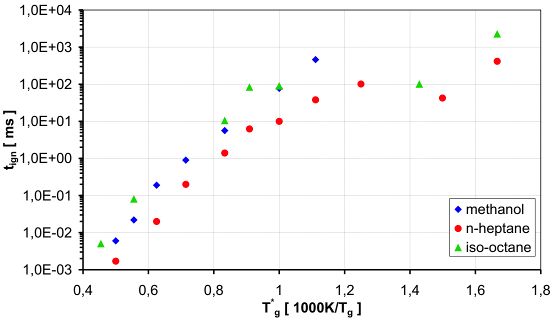

Figure 6: Dependence of ignition delay time on ambient gas temperature ($r_D = 50\mu$m, $T_g = 1200K$)

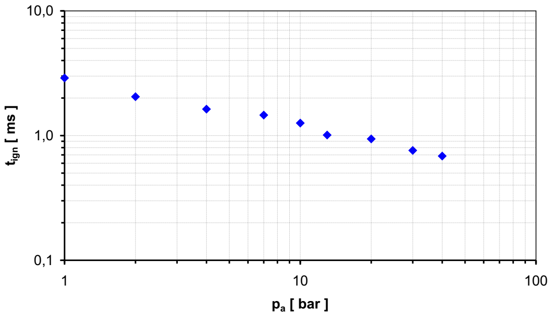

Figure 7: Dependence of ignition delay time on ambient pressure (n-heptane, $r_D = 50\mu$m, $T_g = 1200K$)

to ensure numerical stability the following calculations are performed with a fixed droplet temperature.

The ambient gas temperature is the physical property, which has the largest influence on the auto-ignition process of a fuel droplet. Thus the ambient gas temperature is varied from 600K to 2000K to investigate the influence on the ignition delay time. In figure 6 the Arrhenius plots of the three fuels methanol, n-heptane and iso-octane are shown. All three fuels show the typical exponential dependence of the ignition delay time on the gas temperature with a plateau between 1000K and 700K. Ignition delay times of methanol are only calculated for temperature above 1000K because the reaction mechanism of Chevalier and Warnatz used in this work is devised only for the high temperature domain [17]. The temperature dependence is similar to the case of a auto-igniting homogeneous gas phase. Iso-octane droplets have the largest ignition delay time of the three investigated fuels. Furthermore n-heptane droplets ignite faster than methanol and iso-octane droplets. However the shape of the function graphs $t_{ign}(T_g)$ slightly differ from the shape of the function in the cases of homogeneous gas phase and an offset, varying with temperature, can be observed. Thus it can be stated, that the decrease of the ignition delay times with increasing gas temperature can be attributed mainly to the speedup of the chemical kinetics. However the influence of the vaporization process plays a significant role, too.

In technical applications a multitude of different pressures arises. Hence the influence of the ambient pressure on the ignition delay time is of interest.

In figure 7 a decrease of the ignition delay time with increasing pressure can be observed. This decrease of the ignition delay time follows a power law (c.f. the logarithmic scaling of both axes in figure 7). The exponent of the power law is determined to -0.4.

$$t_{ign}(p) \propto \left(\frac{p}{p_0}\right)^{-0.4} \tag{2}$$

The decrease of the ignition delay can be attributed mainly to the speedup of the chemical kinetics. An analogous change of the ignition delay time can be observed in the case of homogeneous n-heptane/air gas mixtures. In this case the exponent of the power law is determined to approximately -0.6.

In technical combustion chambers the flow field is often turbulent. Thus the droplet is exposed to an alternating gas flow during the ignition process. To investigate the influence of this gas flow the ignition delay times of a methanol droplet at different droplet velocities are calculated. To investigate this regime two-dimensional simulations are necessary. Figure 8 shows the temperature profile of the simulated two-dimensional regime. As one can see, the flame front is not spherical symmetric. In fact it is distorted to a V-shape by the gas flow.

The dependence of the ignition delay time on the droplet velocity is presented in figure 9. For velocities less than 20m/s the ignition delay time is not affected by the gas flow. In fact the ignition delay time remains almost constant despite of variation of the velocity covering three orders of magnitude. However other characteristical properties of the combustion process like the shape of the flame front are influenced by the varying velocity. No ignition occurs, if the velocity is larger than 50m/s. With an increasing droplet velocity the profiles are steepened and accordingly the diffusion fluxes become higher. If the droplet velocity exceeds 50m/s the local strain is so high, that the flame extinguishes.

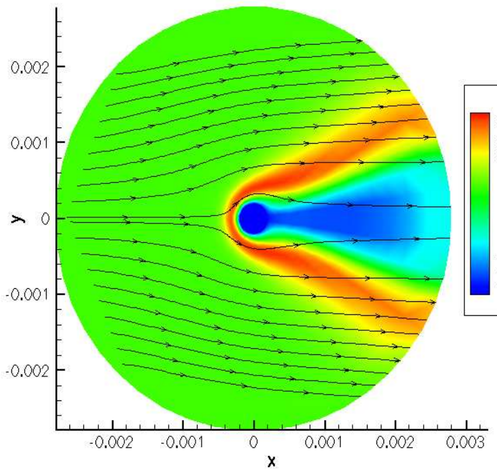

Figure 8: Temperature profile (methanol, t = 10ms, p = 7bar, $r_D = 100\mu$m, $T_g = 1600K$, v = 10m/s)

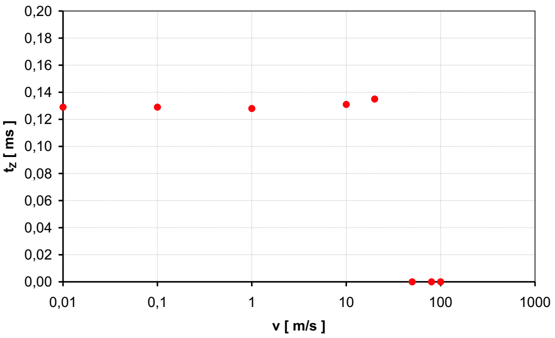

Figure 9: Dependence of ignition delay time on droplet velocity (methanol, $r_D = 100\mu$m, $T_g = 1600K$)

Conclusion

The auto-ignition process of isolated droplets of three different fuels (methanol, n-heptane, iso-octane) in air is investigated. The simulations are performed for isobaric conditions and with detailed models for the vaporization, transport processes and chemical kinetics.

The time evolution of the droplet radius follows the d^2-law in the cases of all fuels. The results of the performed simulations are confirmed by a good agreement of the determined vaporization rates with several experimental and numerical values taken from the literature. The influence of different physical properties on the ignition delay time is studied. The dependence of the ignition delay time on the droplet temperature can be neglected. The ambient gas temperature shows a major influence on the ignition delay times. The ratios of the ignition delay times of the different fuels remain almost the same as in the case of the auto-ignition of homogeneous gas mixtures. However the shape of the Arrhenius plots differ from the homogeneous case. If the ambient pressure is increased, the ignition delay time of n-heptane droplets decreases following a rational law with an exponent of -0.4. The ignition delay time is not affected by the droplet velocity for velocities less than 20m/s. However if the droplet velocity exceeds 50m/s, the vaporized fuel is "blown out" and no ignition can take place.

Further studies will focus on the auto-ignition process of multicomponent droplets [1, 3, 12], like n-heptane/iso-octane droplets to obtain a better description of the influences of technical conditions.

Acknowledgments

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