Detailed Numerical Simulations of the Auto-Ignition and Combustion of n-Heptane Droplets

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Kurzfassung

Selbstzündungsprozesse von n-Heptan Tropfen in Luft werden für isobare Bedingungen und unter der Annahme von sphärischer Symmetrie simuliert. Unter Berücksichtigung detaillierter Transportprozesse und detaillierter Chemie wird der Einfluss von verschiedenen physikalischen Parametern, wie Druck, Gasphasen- und Tropfentemperatur sowie Tropfenradius, auf die Zündverzugszeit untersucht. Es zeigt sich, dass die Umgebungstemperatur und der Umgebungsdruck die Zündverzugszeit erheblich beeinflussen. Der Einfluss der Tropfentemperatur und des Tropfenradius kann hingegen für die untersuchten Bedingungen vernachlässigt werden.

Abstract

The auto-ignition process of single n-heptane droplets in air is simulated for spherical symmetry and at constant pressure. Using 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 ambient pressure or droplet radius, on the ignition delay time and the location of the ignition is investigated. The gas temperature turns out to be the parameter dominating the ignition process. The ignition delay time decreases with increasing pressure, which can also be observed in homogeneous gas mixtures. This decrease can be described by a power law. The droplet temperature and the droplet radius show a minor influence on the ignition delay time.

1. 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 combustion takes place 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. Because no gravitation and no relative motion of droplet and gas phase (microgravity conditions) are assumed, the considered system has 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. Many experimental studies deal with the fuel n-heptane [1,2,3,4,5]. Numerical simulations have been presented for n-heptane droplets, too [6,7,8,9].

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 vaporization rates of a n-heptane droplet obtained from our numerical simulations are compared with results found in literature. With respect to technical applications, like gas turbines or combustion engines, the influence of ambient physical properties on the ignition process is 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, droplet radius, gas temperature, pressure are varied.

2. Mathematical model

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. To account for the chemical kinetics a reaction mechanism of Golovitchev [10] including 62 chemical species and 572 elementary reactions is used. 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 [11] is used. The liquid phase properties are calculated by the data correlations taken from Reid et al. [12]. 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 [13]. 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 [14].

3. Results and discussion

Simulations are performed for isobaric conditions with an ambient pressure of 1bar and 7bar. At first the vaporization rates of the n-heptane droplets are determined. The temporal evolution of the droplet diameter follows the well known d^2-law $d^2 = d_0^2 - K \cdot t$.

To evaluate the performed simulations the vaporization rate K is compared with different values taken from literature. To allow comparisons with these experimental and numerical results the simulations are performed for a pressure of 1bar. The vaporization rates K are determined for initial ambient gas temperatures of 1200K and 1600K.
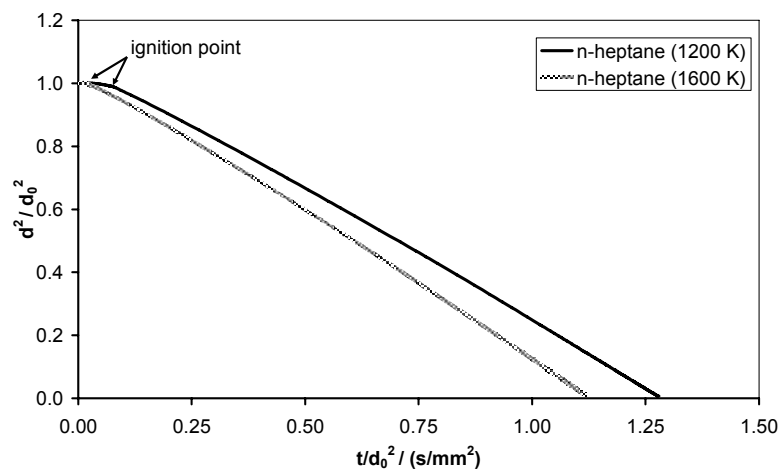

Figure 1: d^2-law of a n-heptane droplet in air (p = 1bar, r_D = 100µm)

In figure 1 one can see the time evolution of the diameter of a n-heptane droplet in air. After ignition the vaporization rates increase. The vaporization rates after ignition are determined to 0.80mm²/s and 0.90mm²/s, respectively. These values comply with the experimental results of 0.85mm²/s [4], 0.758mm²/s [3] and 0.75mm²/s [2] and the numerical result of 0.8mm²/s [6]. A closer comparison of the results is not possible because of the different ambient conditions of the studies.

In the following the dependence of the ignition delay time of single n-heptane droplets on several physical properties will be investigated. In figure 2 the ignition delay times for simulations with fixed and variable droplet temperatures are presented. At an ambient pressure of 7bar the boiling temperature of n-heptane is 454K. Thus to investigate the influence of the droplet temperature on the ignition delay a low temperature of 379K and a temperature of 450K close to the boiling point are chosen. Additionally simulations with a space- and time-dependent droplet temperature are performed.
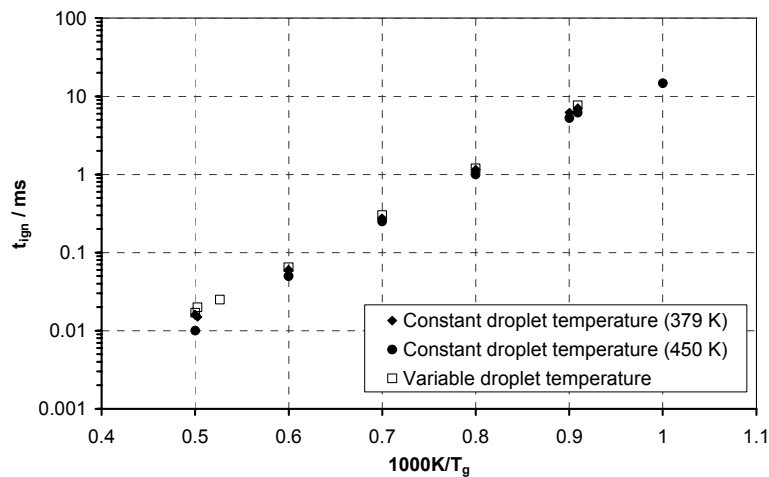
Figure 2: Arrhenius plot of the ignition delay time of different droplet temperatures in the case
of n-heptane droplets (p = 7bar, r_D = 100µm)

One can see the minor dependence of the ignition delay time on the droplet temperature. If
the fixed temperature is sufficiently high, it does not influence the ignition delay time. Thus to
reduce computing time the following calculations are performed with a fixed droplet
temperature.

For the description of technical sprays with statistical droplet size distribution it is of major
interest to determine the influence of the droplet radius on the ignition delay time. Figure 3a
shows the dependence of the normalized ignition delay time t* on the droplet radius. The
ignition delay time t* is defined as the ratio of the ignition delay time and the ignition delay
time of the radius 50µm at the same gas temperature $t^* = t_{ign}(r_D)/t_{ign}(r_D = 50µm)$.
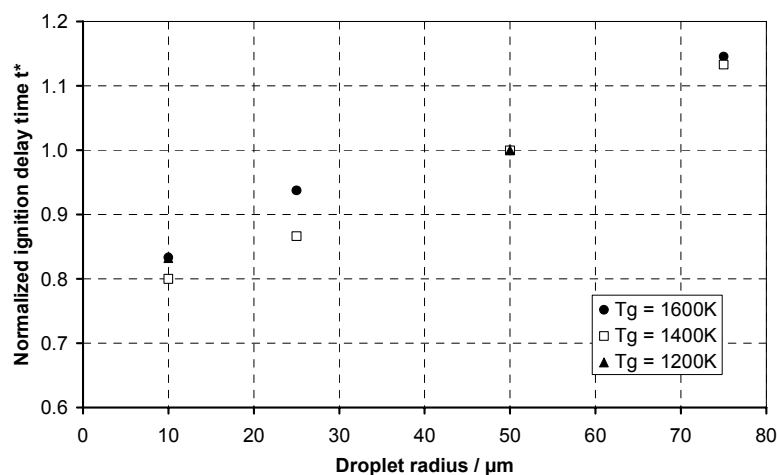

Figure 3: (a) Dependence of the normalized ignition delay time on the droplet radius
(p = 7bar), (b) Arrhenius plot of the dependence of the ignition delay time on
ambient gas temperature (p = 7bar, r_D = 200µm)

A slight increase of the ignition delay time with increasing droplet radius can be detected. Nevertheless the ignition delay times vary in the range of ±20% while the droplet radius is increasing by a factor of 7.5. Thus the droplet radius can be denoted as a parameter with a minor influence on the ignition delay time.

The ambient gas temperature is the physical property that 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 3b the Arrhenius plot of n-heptane droplets is shown.
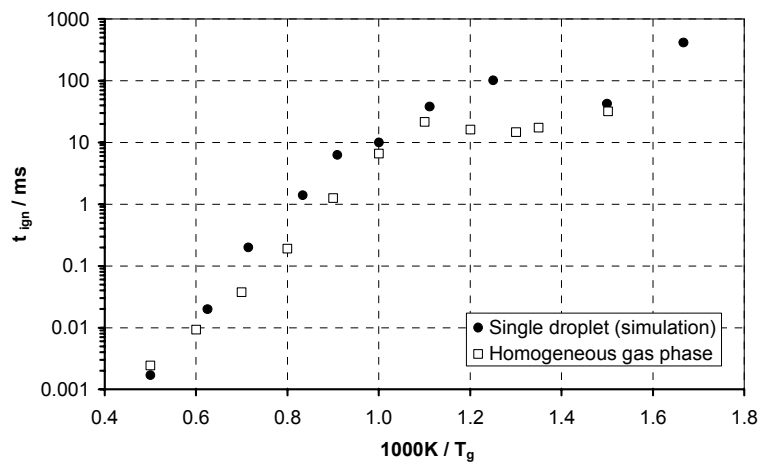

Figure 3: (a) Dependence of the normalized ignition delay time on the droplet radius (p = 7bar), (b) Arrhenius plot of the dependence of the ignition delay time on ambient gas temperature (p = 7bar, r_D = 200μm)

It can be seen that the ignition delay times of the droplets show a behavior similar to the temperature dependence of the ignition delay times of a homogeneous stoichiometric n-heptane/air gas mixture. The ignition delay times increase exponentially with decreasing gas phase temperatures. Compared to the ignition of a homogeneous n-heptane/air gas mixture the ignition of the droplet is delayed due to the transport processes.

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 4 a decrease of the ignition delay time with increasing pressure can be observed. This decrease of the ignition delay time follows the power law $t_{ign}(p) \propto (p/p_0)^{-0.4}$ (c.f. the logarithmic scaling of both axes in figure 4.

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.
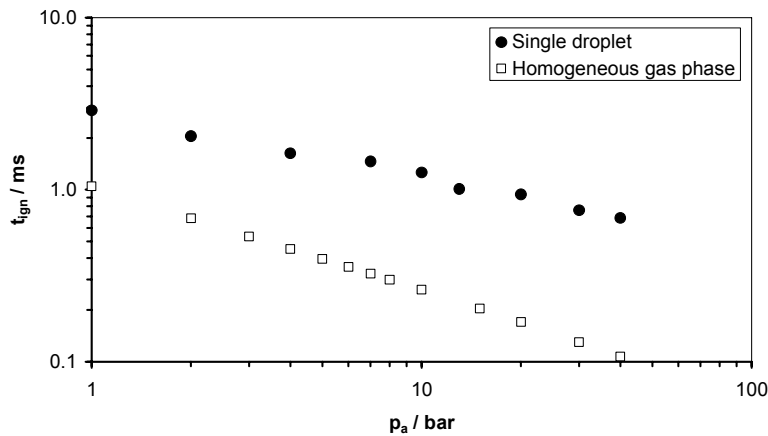

Figure 4: Dependence of ignition delay time on ambient pressure (T_g = 1200K, single

droplets r_D = 50μm, homogeneous gas phase λ = 1)

4. Conclusions

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

The resulting time evolution of the droplet diameter, following a d^2-law, coincides with experimental and numerical results presented in 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 and the droplet radius can be neglected for the considered conditions. The ambient gas temperature shows a major influence on the ignition delay time. Compared to the ignition of a homogeneous stoichiometric n-heptane/air mixture the temperature dependence of the ignition delay time is similar, but the ignition is delayed due to transport processes. The ignition delay time decreases with increasing pressure following a power law with an exponent of -0.4.

Further studies will focus on the auto-ignition process of multicomponent droplets, like n-heptane/iso-octane droplets, to achieve a better description of technical conditions.

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