

Experimental and Numerical Studies on the Autoignition Process of Fuel Droplets

Christian Eigenbrod, Jens König, Osamu Moriue, Stefan Schnaubelt, Torsten Bolik

Center of Applied Space Technology and Microgravity, ZARM,
University of Bremen, Am Fallturm, D-28359 Bremen, Germany

Abstract

Spontaneous ignition of liquid fuels dispersed in hot air under elevated pressure plays a predominant role in diesel engines and gas turbines. While in the first case autoignition is a prerequisite for proper engine operation in the latter case it has to be avoided to happen prior to entering the main combustion area. The common aim for a mostly perfect premixture of prevaporized fuel in air requests for a detailed knowledge of the primary physical and chemical processes in spray combustion. The study discussed hereafter focus on single droplets as the most fundamental element of spray ignition. Experiments on n-heptane droplets of different initial size under varied pressure and temperature applying interferometry and PLIF of formaldehyde are compared to results from direct numerical simulations incorporating liquid and gas phase simulation as well as low- and high temperature chemical reaction kinetics. For the preparation of simulations of technical fuels, a new binary model fuel for kerosene JET-A has been developed that realizes the same staged ignition behaviour and induction times as the technical fuel.

Autoignition of heterogeneous systems

Whenever alkane fuels have to reside partially or fully mixed in an oxidizing atmosphere at high temperatures, ignition can occur in a multistage mode, subsequently following completely different schemes of oxidation. This behaviour is experimentally well known for premixed gases [1] and for multiphase systems [2]. Fig. 1 exemplary shows the temperature history of an igniting n-dodecane droplet and indicates the definition of induction times referred to hereinafter. If the fuel is supplied in liquid phase, heating, vaporization, mixing

and subsequent ignition and combustion takes place in a transient field of temperature and concentration. The understanding and modeling of the process requires a consequent coupling

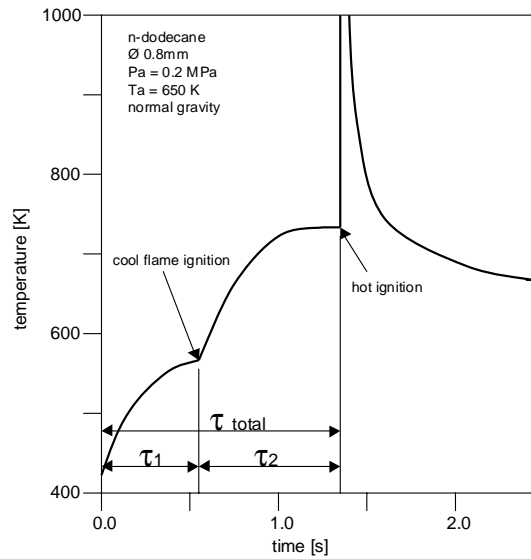


Fig. 1: Temperature history of two-stage ignition

τ_1 = cool flame induction time

τ_{total} = total induction time

τ_2 = cool flame burning lifetime

of the physical processes with a suitable chemical kinetic of the fuel covering the full range of temperatures encountered in the entire process. Up to now, numerical results are in reasonably good agreement with experiments for homogeneous gas phase ignition only. In particular, the low temperature mechanism is quite complex and proceeds via different submechanisms sensibly governed by temperature. Due to the inhomogeneous temperature and concentration field around a vaporizing droplet, a negative temperature coefficient region in the induction time / temperature diagram, as indicated in Fig. 2 for homogeneous gas phase mixtures [3],

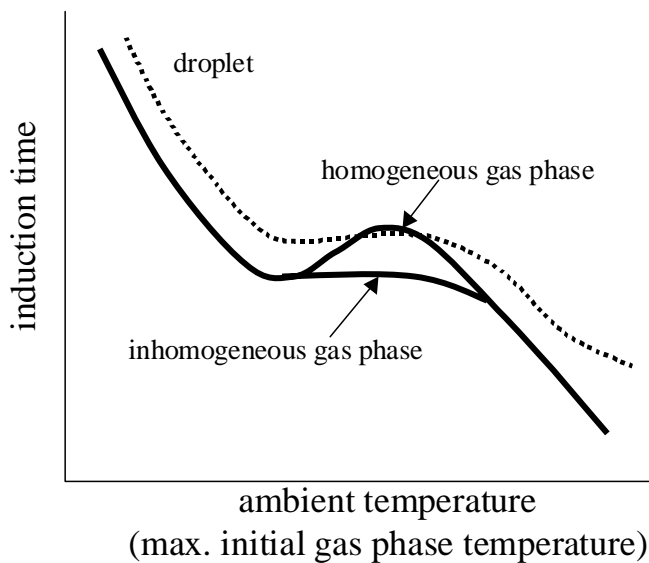


Fig. 2: Difference of induction times for homogeneous, inhomogeneous mixture and a droplet

cannot be achieved. The zero temperature coefficient region is explained through an appropriate temperature region (lower than ambient) that always exists in the vicinity of a

droplet. This allows for the maximum possible growth of the branched chain of the low temperature reactions during the first stage (during second induction time) regardless of the ambient temperature. Since the second induction time (duration of the first stage) is the time to activate the high temperature reactions and is mainly controlled by the plateau temperature, it does not vary with ambient temperature.

Droplet autoignition does not always show a distinct staged behaviour, but in most technical cases with adiabatic compression ignition happens in a staged regime. Experimentally, for each fuel a characteristic temperature/pressure diagram, depicting the different ignition regimes can be measured. Fig. 3 shows the existence areas for single stage and two stage ignition for n-heptane up to 20 bar.

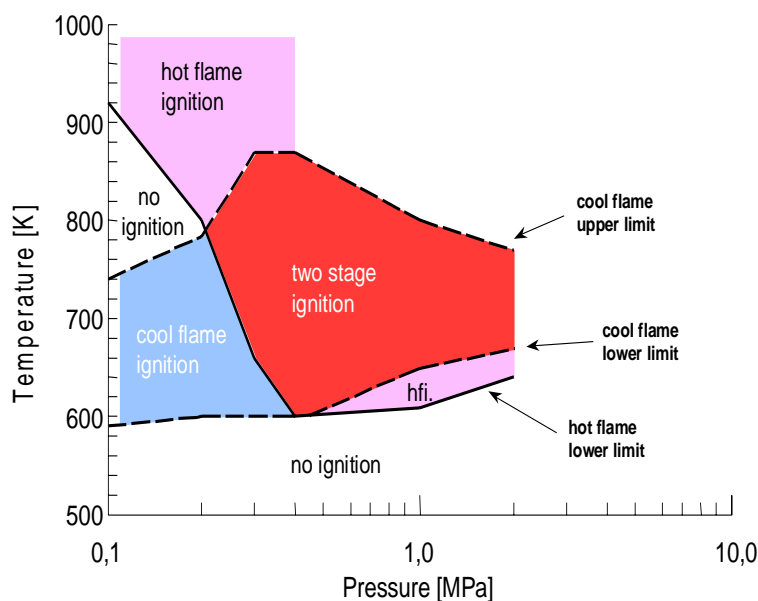


Fig. 3 Ignition regimes of a 0.8 mm n-heptane droplet

Experiments and direct numerical simulation

As the development of numerical tools for single droplets starts with 1-D simulations, μg -experiments were carried out to measure the ignition process of n-alkanes (heptane, decane, dodecane), aromatics (α -methyl-naphthalene, 1,2,4-trimethylbenzene). The results unveiled, that microgravity conditions lead to differing induction times as compared to normal gravity conditions only when the temperature is low and ignition delay times are extremely long. Experiments were performed on ground and in the Bremen drop tower applying the suspended droplet method described elsewhere [2]. The method observes the temperature field evolution around an igniting droplet, suspended at the tip of a thin quartz fibre, by means of a Michelson-type interferometer. At the beginning of each experiment, the fueled quartz

fibre is rapidly lifted into the preheated and pressurized ambient. All experiments were started with droplet diameter between 0.7 and 0.8 mm.

The numerical model assumes spherical symmetry and initial conditions of uniform temperature T_a and pressure p_a in the combustion chamber. The only convective term taken into account is that induced by the evaporation process itself leading to a radial velocity in the liquid and gas phase. The effects of thermal diffusion, radiation, viscosity and kinetic energy are neglected.

Liquid Phase Governing Equations

The governing equations for mass and energy in the liquid phase for $r < r_s(t)$ are:

$$\frac{\partial \rho_l}{\partial t} + \frac{1}{r^2} \cdot \frac{\partial}{\partial r} (\rho_l v_l r^2) = 0 \quad (\text{eq. 1})$$

$$\frac{\partial T}{\partial t} = \frac{1}{\rho_l c_{pl} r^2} \frac{\partial}{\partial t} \left| \lambda_l r^2 \frac{\partial T_l}{\partial r} \right| \quad (\text{eq. 2})$$

Gas Phase Governing Equations

The governing equations for mass, energy and species in the gas phase for $r > r_s(t)$ are:

$$\frac{\partial \rho_g}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} (\rho_g v_g r^2) = 0 \quad (\text{eq. 3})$$

$$\rho c_p \left| \frac{\partial T}{\partial t} + v \frac{\partial T}{\partial r} \right| = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \lambda \frac{\partial T}{\partial r} \right) + \dot{q} \quad (\text{eq. 4})$$

$$\frac{\partial \rho Y_i}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \rho_g Y_i v_g) = \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \rho_g v_{D,i}) + \dot{w}_i \quad (\text{eq. 5})$$

The gas phase is considered to be compressible. Thus the cubic equation of state from the Redlich-Kwong type after Peng-Robinson is used.

Initial and Boundary Conditions

i. Liquid phase at $r = 0$:

$$\frac{\partial T}{\partial r} = 0, \frac{\partial \rho}{\partial r} = 0 \quad (\text{eq. 6})$$

ii. Gas phase at $r \rightarrow \infty$:

$$T = T_\infty, p = p_\infty, v = 0, Y_O = 0.21, Y_F = 0, Y_{N_2} = 0.79$$

iii. Interface Conditions at $r = r_s$:

$$\text{mass flux :} \quad \rho \cdot (v - \dot{R}_s) \Big|_{r=r_{s-}} = \rho \cdot (v - \dot{R}_s) \Big|_{r=r_{s+}} = \dot{m} \quad (\text{eq. 7})$$

$$\text{species flux :} \quad Y_i \cdot \dot{m} \Big|_{r=r_{s-}} = Y_i \cdot (\dot{m} + \rho \cdot V_i) \Big|_{r=r_{s+}} \quad (\text{eq. 8})$$

with

$$Y_i \Big|_{r=r_{s-}} = 1 \text{ (i = Fuel) , } Y_i \Big|_{r=r_{s-}} = 0 \text{ (i \neq Fuel)}$$

$$\text{energy balance :} \quad q_T \Big|_{r=r_{s-}} - q_T \Big|_{r=r_{s+}} = \dot{m} \cdot L \quad (\text{eq. 9})$$

$$\text{temperature continuity :} \quad T \Big|_{r=r_{s-}} = T \Big|_{r=r_{s+}} \quad (\text{eq. 10})$$

$$\text{fugacity equilibrium :} \quad f_i \Big|_{r=r_{s-}} = f_i \Big|_{r=r_{s+}} \quad (\text{eq. 11})$$

Gas and Liquid Phase Properties

For the gas phase the binary diffusion coefficient, diffusion velocity, heat conductivity and heat capacity as well as the liquid heat capacity and liquid heat conductivity are calculated temperature and pressure dependent, which can be found in [4,5,6].

Gas Phase Reaction Mechanism

A reduced reaction kinetic for n-heptane with 62-steps (437 elementary reactions, 92 species), which has been developed by the ITM, Aachen, is included into the simulation. In this n-heptane kinetic, special attention has been paid to the low temperature branch with 61 elementary reactions.

Numerical Procedure

According to the effect of a shrinking droplet due to evaporation, the used grid was fixed to the droplet surface. For getting a higher resolution at the drop surface and in the interested region of ignition an exponential grid is applied to the gas phase. The transformed governing equation with the new independent variable $r_s(t)$ are reported in [7].

The resulting algebraic equation system is a stiff differential equation system due to the reaction schemes used. As a consequence a fully implicit multi-order backward differentiation (BDM) method is applied [8]. The equations were discretized by the finite difference method. A typical grid size was about 20 point for the liquid and 70 points for the gas phase.

Fig. 4 exemplarily compares experimental and simulation results of the first- and total induction time of an n-heptane droplet.

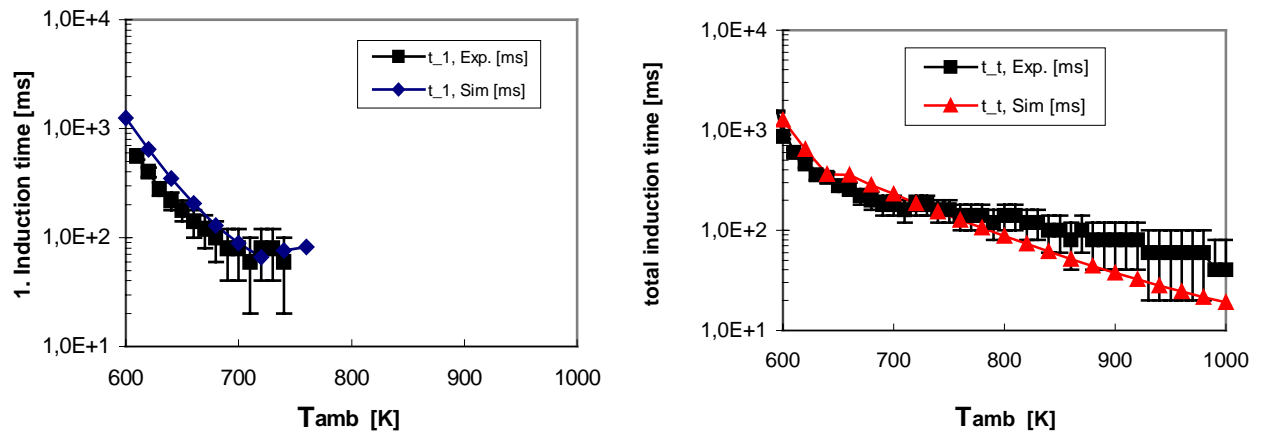


Fig. 4: Comparison of ignition delay times of n-heptane droplets between experiment and simulation, $\varnothing = 0.7 \text{ mm}$, 0.5 MPa

The increasing measurement error towards shorter induction times is mainly caused by the limited time resolution of the recording system (50 f/s). Specifically the zero temperature coefficient behaviour is well matched by the simulation.

Laser diagnostics

As the interferometric method can only deliver induction times with an acceptable error, the application of laser diagnostics was requested in order to get additional information about the instant of ignition (ignition radius) and species concentration data. The LIF of formaldehyde is an appropriate tool as formaldehyde is a suitable tracer for the cool flame establishing in the period between first and total induction time (equal second induction time).

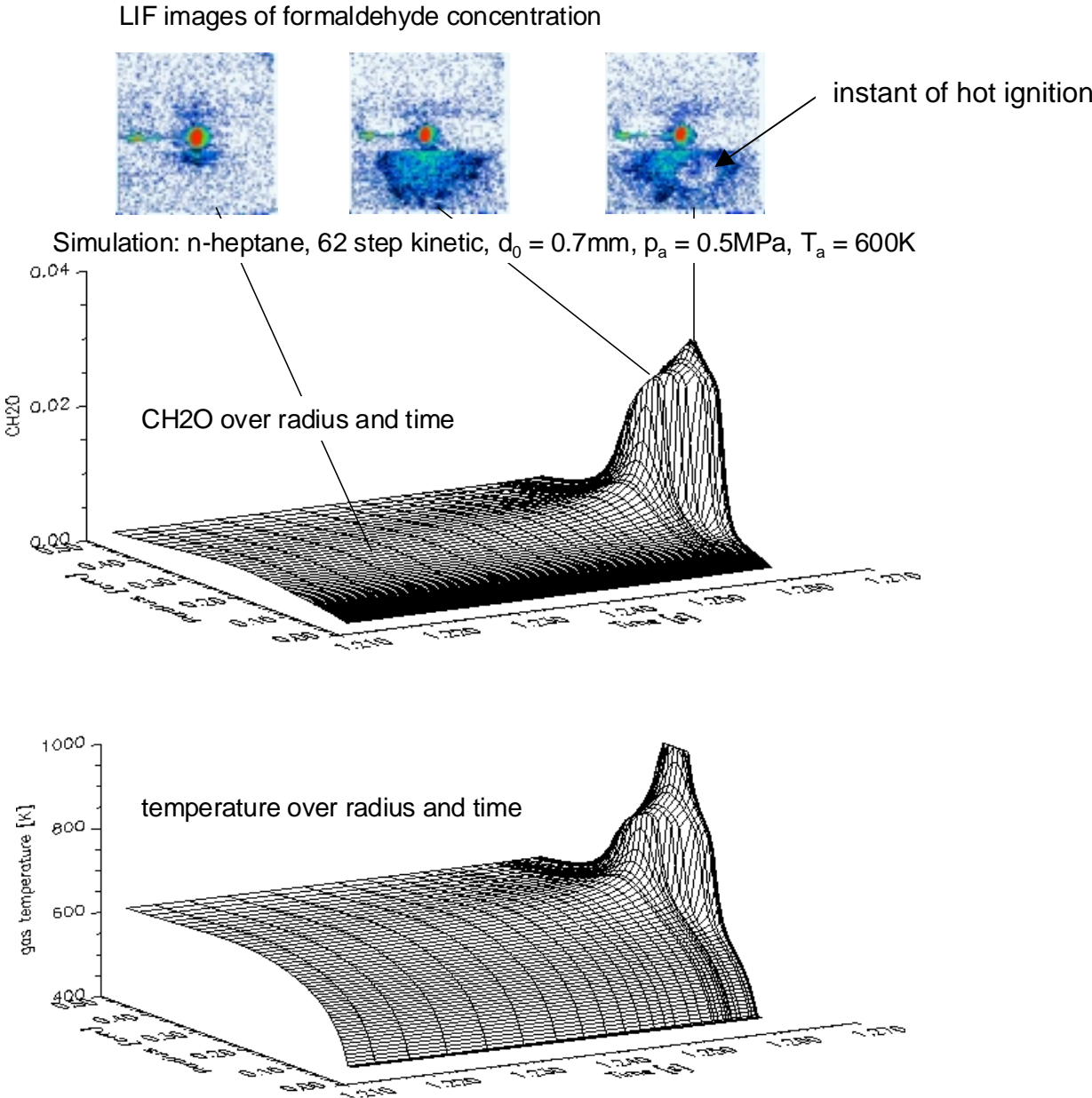


Fig. 5: Comparison of selected LIF images from a high-speed sequence with the simulations

This method also depicts the hot flame ignition very well as this is accomplished by a rapid consumption of formaldehyde along a sharp reaction front. Fig. 5 compares selected LIF images from a high-speed sequence with the simulations.

Model fuel, - comparison kerosene / alkanes, aromatics, mixtures

In order to enable the application of the direct numerical simulation also to technical fuels such as JET-A, a new binary model fuel has been developed. This was necessary, as the existing model fuels (alkanes and alkane/aromatics developed for combustion) did not match the staged ignition behaviour of kerosene. Therefore various n-alkanes (heptane, decane, dodecane), aromatics (α -methyl-naphthalene, 1,2,4-trimethylbenzene) and mixtures between n-alkanes and aromatics of various mass fractions were systematically examined concerning their ignition behaviour and the interacting effects. As a result Fig. 6 compares the selected mixture of 60 % n-decane and 40 % 1,2,4-trimethylbenzene with kerosene JET-A. Both, the first and second induction time of this model fuel is in very good agreement.

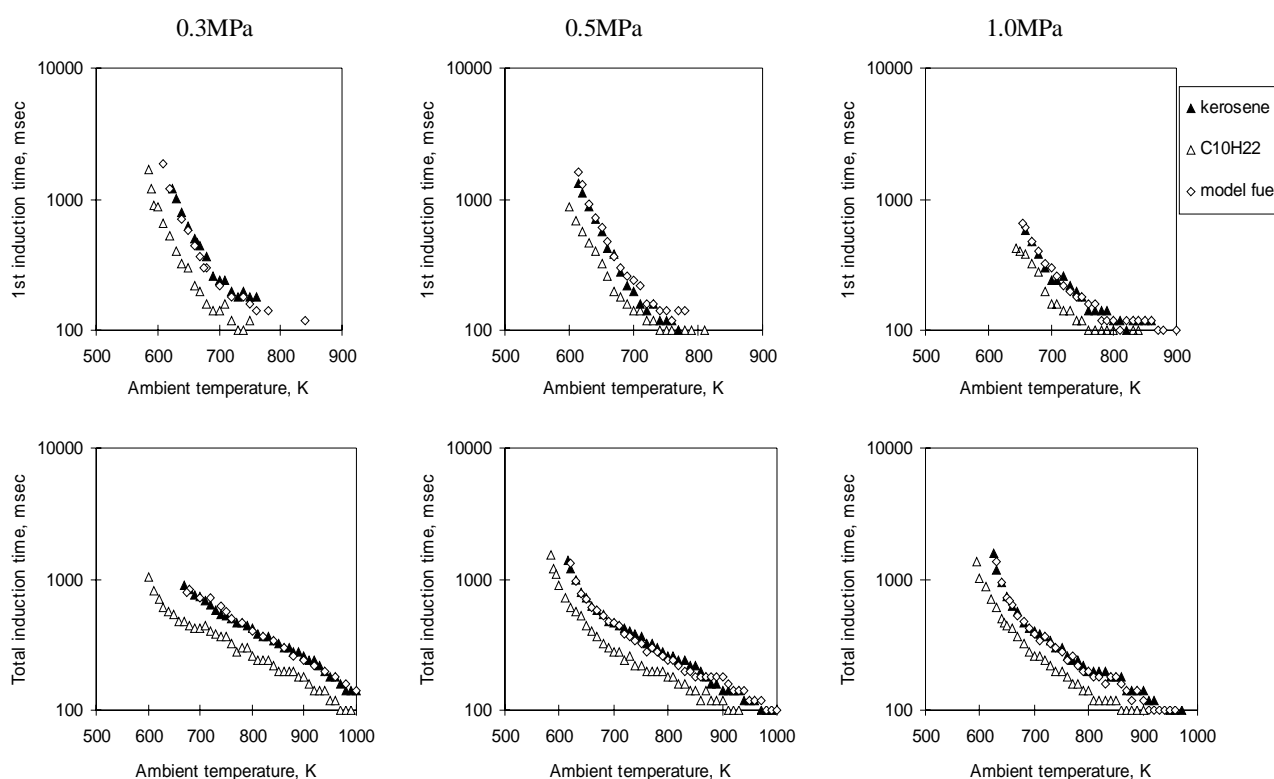


Fig. 6: Comparison of first and total induction times of kerosene with n-decane and the model fuel 60 % n-decane / 40 % 1,2,4-trimethylbenzene

References

1. Müller, U.C.: „Reduzierte Reaktionsmechanismen für die Zündung von n-Heptan und iso-Oktan unter motorrelevanten Bedingungen“, *PHD-Thesis*, RWTH-Aachen, (1993)
2. Tanabe, M., Kono, M., Sato, J., König, J., Eigenbrod, Ch., Dinkelacker, F., Rath, H.J.: „Two stage ignition of n-heptane isolated fuel droplets“, *Combust. Sci. and Tech.*, 1995 Vol. 108, pp.103-119
3. Ciezki, H.K. and Adomeit, G.: „Shock-Tube Investigations of Self-Ignition of n-Heptane-Air Mixtures under Engine-Relevant Conditions“, *Comb. and Flame*, 93, 421.
4. Reid, R.C., Prausnitz, J.M., and Poling, B.E., „The Properties of Gases & Liquids“, McGraw-Hill Book Co., Singapore, 1986, p 741.
5. Oran, E., and Boris, J.P., *Progress in Energy and Combustion Science*, 7: 1-72 (1981).
6. Gardiner Jr., W.C. (Ed.), *Combustion Chemistry*, Springer-Verlag, New York, 1984, p. 509.
7. Tanabe, M., „Spontaneous Ignition of a Single Droplet in High Temperature and High Pressure Surroundings“, *Ph. D. Thesis, ZARM*, (1996).
8. Winslow, A.M., *Journal of Physical Chemistry*, 81: 2409-2413 (1977).

Acknowledgements

The authors thank their partners from the Institute for Physical High Technology, IPHT, Jena and the Institut für Technische Mechanik, ITM, of the RWTH Aachen for their contributions. The related joint national project DROP-COS (Development and Research Program on Pollutant-Reduced Combustion Systems) is supported by the German Aerospace Center, DLR, under grant number 50 WM 9448.