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The auto-ignition of single *n*-heptane/*iso*-octane droplets

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Abstract

Numerical simulations including detailed chemical and physical models are performed to investigate the influence of different physical parameters on the auto-ignition of *n*-heptane/*iso*-octane droplets in air. Simulations are performed for isobaric conditions with an ambient pressure of 8 bar and a droplet radius of 200 μm. The ambient gas temperature ranges from 800 K to 2000 K and the droplet temperature was varied from 300 K to 400 K. Below an ambient temperature of 1000 K the ignition delay time is found to increase with an increasing volume fraction of *iso*-octane. Above 1000 K the ignition delay time appears to be almost independent of the mixture composition of the droplet. The local ignition conditions are also studied. It turns out that ignition occurs at points, where the mixture is lean. This trend is more significant, if the ambient temperature increases. The influence of physical properties of the mixture components, like diffusion coefficients, heat conductivity, heat of vaporization and vapor pressure, is investigated. Furthermore, the influences of simplifying assumptions such as the distillation and diffusion limit are studied.

Keywords: Droplet; Multicomponent; Ignition; *n*-Heptane; *iso*-Octane

1. Introduction

A reliable description and simulation of spray combustion requires a detailed understanding of the underlying physical and chemical processes. Detailed simulations of these processes help to test and to validate assumptions made in the simulation of spray combustion [1–5]. The ignition and combustion of single fuel droplets in a stagnant gas environment is well suited to investigate the basic principles of droplet combustion. Because of these conditions spherical symmetry can be assumed. 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 a detailed understanding of this interaction is necessary. In order to achieve such a detailed understanding, it is of importance to investigate the influence of certain physical parameters on the ignition process.

Single component droplets are not representative for practical applications, because almost all fuels consist of mixtures of hydrocarbons. The modeling of multicomponent fuel droplets is much more ambitious because additional physical processes have to be accounted for. Diffusion inside the droplet might affect the vaporization process and therefore the ignition delay time or the droplet lifetime significantly. Furthermore, a detailed multicomponent vaporization model has to take into account the different vapor pressures of the species and the different enthalpies of vaporization.

Several authors have investigated the ignition and combustion of multicomponent fuel droplets. A number of studies deal with the combustion of droplets of fuel and water [6–9]. Makino and Law have investigated the gasification behavior of burning and vaporizing dodecane/hexadecane droplets [10]. Okai et al. and Shaw et al. have studied the combustion of methanol/dodecanol droplets experimentally [11,12]. The ignition of blended fuel

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Nomenclature

d	droplet diameter (μm)
d_0	initial droplet diameter (μm)
h_{vap}	specific heat of vaporization (J/kg K)
p	pressure (bar)
p_{vap}	vapor pressure (bar)
r	radius
r_D	droplet radius (μm)
RON	research octane number
t	time (s)
t_{ign}	ignition delay time (ms)
t^*_{ign}	normalized ignition delay time
T	temperature (K)
T_D	droplet temperature (K)
T_G	gas temperature (K)

Greek symbol

λ_{loc}	local air–fuel ratio

Subscripts

C_7H_{16}	*n*-heptane
C_8H_{18}	*iso*-octane

droplets, consisting of *n*-heptane and *n*-hexadecane, has been investigated by Takei et al. [13].

In this study the ignition process of *n*-heptane/*iso*-octane droplets is investigated in detail. Previous research, using the present numerical model, was on the ignition behavior of pure *n*-heptane droplets [14]. With the extension to multicomponent droplets consisting of *n*-heptane and *iso*-octane it is possible to simulate droplets with a given research octane number (RON). Here, the influence of the mixture composition on the ignition delay time is investigated for different ambient temperatures. The local air–fuel ratios of the *n*-heptane/*iso*-octane mixture at the starting point of ignition are determined for a wide range of ambient temperatures. Furthermore, it shall be studied, if the modeling of a gasoline droplet by a bicomponent droplet, consisting of *n*-heptane and *iso*-octane, with the corresponding RON leads to reasonable results. Such a modeling can be crucial, because real gasoline consists of a multitude of chemical species with different physical and chemical properties. The physical properties of two mixtures can vary significantly, even though the RONs are equal. Thus, the influence, in terms of sensitivities, of some physical properties, e.g. vapor pressure and heat of vaporization, on the ignition process is investigated. Furthermore, the results of calculations based on detailed modeling of the transport processes in the liquid phase are compared to the results of simulations with almost infinitely fast diffusion (distillation limited vaporization) and with artificially decelerated diffusion (extremely diffusion limited) in the droplet. The validity of the used numerical model has been demonstrated in [14].

2. Numerical model

To investigate the coupling of physical and chemical processes, detailed simulations have to be performed. The chemical and the physical processes are modeled in detail. The chemical kinetics is governed by a large number of chemical species and elementary reactions. In our case of mixtures of *n*-heptane and *iso*-octane the reaction mechanism of Ahmed et al. [15] is used, comprising 94 chemical species and 614 elementary reactions. The physical transport processes in the gas phase as well as in the liquid phase are modeled in detail. Fourier's law is used to determine the heat fluxes [16]. For the calculation of the diffusion coefficients the approximation of Curtiss and Hirschfelder [17] is used. The mixture of the liquid fuels *n*-heptane and *iso*-octane is assumed to be ideal. The liquid phase properties are calculated based on the data correlations taken from Reid et al. [18]. The density of the liquid fuel is determined by the relation of Hankinson and Thomson [19]. The approximation of Latini and Baroncini [20] is used to calculate the heat conductivities, the Rowlinson–Bondi method [21] to calculate the specific heat capacities. The diffusion coefficients are determined by the approximation of Tyn and Calus [22]. For the calculation of the liquid viscosities the correlations of Brulé and Starling and Letsou and Stiel [23] are used. The presence of internal circulation in the liquid phase is ignored. Previous studies showed no significant influence of the internal circulation on the reported results. These observations are in accordance with the findings of Cuoci et al. [24].

The vaporization model is based on a local phase equilibrium. A detailed description of the governing equations and the interface equations of the phase transition can be found in [14]. In the presented case of *n*-heptane/*iso*-octane droplets, surface reactions are not taken into account. The necessary properties to model the phase transition are also taken from Reid et al. [18]. The vapor pressure is calculated using the Wagner equation [25], the enthalpy of vaporization is calculated by the approximation of Riedel and Watson [26–28].

To overcome numerical difficulties due to the discretization of the convective terms, the equation system is transformed into modified Lagrangian coordinates. Uniform pressure is assumed, and therefore the momentum conservation equation is fulfilled trivially [29]. The governing equations of the liquid and the gas phase are solved in a fully coupled way. Efficient numerical methods are utilized to minimize computing time [29,14]. The partial differential equation system is discretized by the method of lines using finite difference techniques. The solution of the resulting