Detailed numerical simulation of the auto-ignition of liquid fuel droplets

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Summary. One and two dimensional numerical simulations of the auto-ignition process of single droplets of methanol and n-heptane in air are presented. Detailed models are used to simulate the transport processes as well as the chemical kinetics. Efficient numerical methods are implemented to reduce the computing time. The influence of different ambient parameters on the ignition process is investigated. The ambient gas temperature turns out to be the physical parameter with the largest influence on the ignition delay time. With increasing ambient temperature the ignition delay time decreases. Furthermore, the ignition delay time decreases with increasing pressure following a power law. Two dimensional simulations show the almost exponential dependence of the ignition delay time on the velocity of a gas counterflow. If the counterflow is too strong, the flame is extinguished. Furthermore, the location of ignition is strongly affected by the counterflow velocity.

1 Introduction

A detailed understanding of droplet ignition and combustion is of interest in view of a reliable description of spray combustion. Especially a detailed understanding of the basic physical and chemical processes, like vaporization, transport and chemical kinetics, is required for reliable modelling. 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 droplet ignition 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 numerically. Numerical simulations have been presented for methanol droplets [1, 2, 3] and n-heptane droplets [4, 5, 6, 7]. 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 [8, 9, 10, 11, 12, 13]. Few studies focus on the ignition process of fuel droplets of higher hydrocarbons [5, 6, 7, 14, 15, 16, 17, 18]. Takei et al. [14], Nakanishi et al. [16] and Tanabe et al. [17] have determined ignition delay times of droplets experimentally. Tsukamoto et al. account for chemical kinetics by a one-step irreversible overall reaction [15]. Schaubelt et al. investigate the ignition process of n-heptane and n-decane experimentally and numerically [6, 18]. Morihue et al. simulate the ignition of a fuel droplet in a closed volume [7]. However, the influence of the ambient gas temperature and the ambient pressure on the ignition process in the case of auto-ignition has not been investigated extensively based on detailed numerical simulations. With respect to technical applications, like gas turbines or combustion engines, the influence of ambient physical properties on the ignition process are of major interest. 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 ambient gas temperature, pressure as well as the velocity of a gas counterflow are varied. In the case of the ignition of a droplet pair simulations with different droplet distances are performed. Studies of the ignition and combustion of methanol and n-heptane droplets in air are presented.

2 Mathematical Model

The presented model describes a fuel droplet surrounded by an ambient gas phase. This allows to formulate the governing set of compressible Navier-Stokes equations for a reactive system and equations of state for the gas phase and the liquid phase [19].

\[ \frac{\partial \rho}{\partial t} + \text{div}(\rho \mathbf{v}) = 0, \]  
\[ \frac{\partial \rho_i}{\partial t} + \text{div}(\rho_i \mathbf{v}) + \text{div} \mathbf{j}_i = M_i \dot{\omega}_i, \]  
\[ \frac{\partial (\rho \mathbf{v})}{\partial t} + \text{div}(\rho \mathbf{v} \otimes \mathbf{v}) + \text{div} \mathbf{p} = 0, \]  
\[ \frac{\partial \rho u_i}{\partial t} + \text{div}(\rho u_i \mathbf{v} + \mathbf{j}_i) + \mathbf{p} : \text{grad} \mathbf{v} = 0, \]  
\[ \text{gas : } p = \frac{\rho}{M} RT, \quad \text{liquid : } \rho = \rho(T). \]  

\( t \) denotes the time, \( \rho \) the density, \( \mathbf{v} \) the velocity, \( \rho_i \) the density of species \( i \), \( \mathbf{j}_i \) the diffusion flux density of species \( i \), \( M_i \) the molar mass of species \( i \), \( \dot{\omega}_i \) the