Numerical modeling of auto-ignition of isolated fuel droplets in microgravity

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Available online 10 July 2014

Abstract

In this work we present and apply a mathematical model to simulate the auto-ignition of isolated fuel droplets burning in microgravity conditions. The aim is to demonstrate the fundamental role of the low-temperature mechanisms on the auto-ignition process and to show that several experimental observations cannot be explained without considering the formation of cool-flames around the burning droplet.

Thus, in order to better clarify the importance of the low-temperature chemistry, a detailed kinetic scheme (with hundreds of species and thousands of reactions) was adopted to model the spontaneous ignition of isolated droplets of *n*-heptane, *n*-decane, and *n*-dodecane in air, in a wide range of operating conditions (with environment temperatures from 600 K to 1100 K and pressures from 1 bar to 20 bar).

The model was able to correctly identify the typical auto-ignition regimes of *n*-alkane oxidation. The comparison with the experimental measurements available in the literature was satisfactory: both first-stage and total induction times were reasonably captured by the numerical simulations. The simulations confirmed that the low-temperature chemistry plays a role of paramount importance in the auto-ignition process. In particular, the competition between low- and high-temperature mechanisms was found to explain the different types of auto-ignition which can be experimentally observed.
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Keywords: Low-temperature chemistry; Cool flame; Detailed kinetics; Microgravity; Droplet

1. Introduction

The combustion of liquid fuels is of great interest in many practical applications, from industrial burners to diesel engines, especially because of their high-energy density per unit volume [1]. In particular, the spontaneous ignition (or auto-ignition) of fuel droplets is a very important process to be controlled effectively. However, the strong interactions between the many physico-chemical processes dominating the ignition of fuel droplets make the study of combustion of liquid fuels a very complex subject. It is thus useful to take apart the overall system and to study simpler and possibly ideal conditions. The most adopted and suitable simplification corresponds to the isolated fuel droplet system with a surrounding gas. Such a system includes all of the existing basic processes occurring in practical combustors, including heat-up, phase-change, diffusion, and chemical reactions. In addition, microgravity conditions further simplify the

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system, because of the spherical symmetry, which strongly reduces the required computational time and memory requirements, especially when complex kinetic schemes are adopted.

The transient behavior of droplet heating and the gas-phase mixture conditions causing the ignition are today quite well understood. Several numerical models were proposed and applied, with particular emphasis on the transient physical processes [2]. From recent works [3–5] it was recognized that a detailed description of the chemical reactions is strictly necessary to predict with reasonable accuracy not only the ignition delay times and the explosion diagrams, but also to better characterize the burning rates. Several efforts have been already devoted to the numerical study of autoignition of isolated fuel droplets with detailed chemistry, but only a few of them adopted low-temperature mechanisms [4,6–8]. The improving knowledge on the chemistry of hydrocarbon oxidation and the increasing availability of computational resources now enable the possibility to simulate the auto-ignition of isolated fuel droplets with very detailed kinetic mechanisms, with hundreds of species.

In this paper we numerically investigate the auto-ignition of isolated fuel droplets of *n*-heptane, *n*-decane and *n*-dodecane in microgravity conditions using a detailed kinetic mechanism (460 species and more than 16,000 reactions). All the simulations are compared and validated with experimental data available in the literature. The final aim is to demonstrate the importance of the low-temperature chemistry during the auto-ignition process. To our knowledge, this is the first work in which the auto-ignition of isolated fuel droplets is numerically modeled using such a large kinetic mechanism.

2. Mathematical model

The mathematical model used to describe the transient evaporation, ignition, and combustion of isolated pure fuel droplets in microgravity conditions was presented and validated in [4]. Here, only its main features are summarized. The numerical model assumes spherical symmetry, because of the microgravity conditions. The conservation equations of energy and mass are solved both for the liquid and gas phases. In addition, the conservation equations of species are solved for the gas phase. Only the ordinary mass diffusion is taken into account in the species equations. Previous simulations including the Soret effect did not show any significant impact on the auto-ignition results [9]. The properties of the liquid are taken from Daubert and Danner's database [10]. The possible presence of internal liquid recirculations is accounted for using the simplified approach suggested in [11].

Chemical reactions in the gas phase are described using a detailed kinetic mechanism (see the next paragraph). The transport properties for species in the gas phase were either taken from the CHEMKIN transport database [12] or estimated following the procedure proposed in [13], while the thermochemical information was obtained primarily from the CHEMKIN thermodynamic database. Radiative heat fluxes were estimated by adopting the approach proposed by Kazakov et al. [14]. The Planck mean absorption coefficients were derived from polynomial expressions for CO, CO_2, and H_2O, which are assumed to be the only molecules influencing radiative transfer. Symmetry conditions are imposed at the center of the droplet. At the liquid/gas interface the continuity of fluxes of heat and species is considered. The far field boundary ($\sim$100 times the initial droplet diameter) is defined using Dirichlet's conditions (i.e. assigned ambient composition and temperature) and remains fixed in the simulations.

The resulting system includes partial differential equations and non-linear, algebraic equations (because of boundary conditions). The partial differential equations are discretized using the finite-difference method, using an adaptive grid fixed on the droplet surface. The resulting system of differential-algebraic equations is solved in a fully-coupled approach using the BzzDae solver (http://www.chem.polimi.it/homes/gbuzzi) [15].

The results reported in this work were based on a grid with 30 and 200 points for the liquid and gas phases, respectively. Simulations with a larger number of points did not show significant differences. The convective and diffusion terms were discretized using the upwind scheme and centered, 2nd order differences, respectively. The simulations were carried out on Intel® Xeon® CPU X5675 @ 3.07 GHz processors.

3. Detailed kinetic mechanism

A general, detailed kinetic scheme, called POLIMI_TOT_1311 and consisting of 460 species and more than 16,000 reactions, was used to describe combustion in the gas phase [16]. The mechanism is freely available on the web (together with thermodynamic data and transport properties) at the following address: http://creck-modeling.chem.polimi.it. The mechanism covers the low- and high-temperature regions of hydrocarbon oxidation. Further details and extensive validation can be found in [16,17] and in the Supplemental material.

4. Autoignition of isolated *n*-decane droplets

Xu et al. [18] performed several experimental measurements about vaporization and auto-ignition of isolated fuel droplets of *n*-decane in