



Spontaneous ignition of isolated *n*-heptane droplets at low, intermediate, and high ambient temperatures from a mixture-fraction perspective



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ABSTRACT

Detailed numerical simulations of isolated *n*-heptane droplets autoignition have been conducted at pressures of 5 and 10 atm for several values of the initial ambient gas temperature. The ignition modes considered included low-, intermediate-, and high-temperature ignition. The analysis was conducted from a mixture-fraction perspective. For sufficiently low values of the ambient gas temperature, two-stage ignition was observed. Under these conditions, low-temperature reactions played an important role in the transition of the system to a fully burning state. As the initial value of the ambient gas temperature increased, the influence of the low-temperature reactions on the ignition process decreased and eventually became marginal for temperatures above 900 K. Comparisons against homogeneous reactor calculations showed that the ignition location in mixture fraction space could be reasonably predicted for the high-temperature case, whereas discrepancies occurred for the intermediate- and low-temperature ones due to the shift in the maximum reactivity of the system caused by the cool flame appearance. The dependence of the ignition process on the initial droplet diameter was also studied for different values of the initial ambient gas temperature. It was found that, for all cases investigated, a value of the droplet diameter existed for which ignition took the least time to occur. For smaller droplets, the ignition transient was longer and eventually a burning flame did no longer appear when the droplet was initially too small. For the low-temperature case, the minimum ignition delay time was determined by the competition between the quicker ignition of the cool flame and the longer second induction time resulting from the decrease in the droplet size; for the high-temperature case, it was the results of phenomena occurring early during the droplet lifetime.

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1. Introduction

Spray combustion is a topic of great interest in the combustion community due to its relevance to a wide range of practical devices. A thorough understanding of this technology is however hindered by its complexity, which arises from the strong coupling existing between liquid fuel atomization, inter-phase mass and heat transfer, gas-phase mixing under turbulent conditions and chemical reactions. Despite these difficulties, some insight can still be obtained by studying simpler, ideal configurations, so to focus the attention only on certain physical aspects of the problem. One of such configurations is that of an isolated liquid droplet

burning in a stagnant oxidiser in the absence of any convective motion.

Due to its fundamental character, the autoignition and subsequent burning of a liquid droplet has received considerable attention over the last decades, and has also been the topic of a recent review article [1]. Experimental and numerical results are available for a wide range of fuels, including, for example, ethanol [2], methanol [3–5], *n*-butanol [6] and methyl butanoate [7]. Because of their relevance to diesel engine and gas turbine engine combustion, *n*-heptane, *n*-decane and *n*-dodecane [8–18] have received the most attention. Many of these studies have focused on multi-stage (or two-stage) autoignition, which has been first observed experimentally by Tanabe et al. [8] for *n*-heptane and *n*-dodecane. Multistage autoignition is characterized by the appearance of a cool flame prior to the occurrence of the hot flame ignition and is a direct consequence of the existence of both low- and high-temperature

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Nomenclature

C	heat capacity
C_p	heat capacity at constant pressure
\mathbb{D}	mixture-averaged diffusion coefficient
D	binary diffusion coefficient
d	droplet diameter
f	fugacity
h	specific enthalpy
N	rate of scalar dissipation
p	pressure
r	radial coordinate
r_d	droplet radius
T	temperature
t	time
u	gas-phase radial velocity
V	diffusion velocity
W	molar weight
W_{tot}	mass flow rate
X	molar fraction
Y	species mass fraction

Greek symbols

ΔH_v	heat of vaporization
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δ_{ij}	Kronecker delta
κ	thermal conductivity
λ	air-to-fuel ratio
ρ	density
τ_1	first induction time
τ_2	second induction time
τ_t	total induction time
$\tau_{t,\text{ref}}$	reference induction time
ξ	mixture fraction
$\dot{\omega}$	species production/destruction rate

Subscripts

$(\cdot)_0$	initial value
$(\cdot)_\alpha$	quantity referred to α -th species
$(\cdot)_g$	gas-phase quantity
$(\cdot)_l$	liquid-phase quantity
$(\cdot)_{\text{min}}$	quantity corresponding to minimum ignition delay time
$(\cdot)_{\text{MR}}$	quantity corresponding to most reactive conditions
$(\cdot)_{r_d^+}$	quantity evaluated at the droplet radius, gaseous side
$(\cdot)_{r_d^-}$	quantity evaluated at the droplet radius, liquid side

reactions pathways for the oxidation of n -alkanes [11,13]. More recent studies [16–18] have focused on the transition between hot and cool flame burning (and vice versa) in n -heptane droplets under microgravity conditions, with particular emphasis on the kinetic aspects of cool flame combustion.

Since the pioneering work of Tanabe et al. [8], there have been several attempts in trying to replicate numerically the multiple ignition stages of n -alkanes droplets observed experimentally. Schnaubelt et al. [11] were among the first to use a complex reaction mechanism to simulate the different autoignition regimes of n -heptane droplets at $p = 5$ atm over the initial ambient temperature range $T_{g,0} = 600$ – 950 K. Their results compared well with their own experimental data and with those of Tanabe et al. One of their main findings was that the first induction time τ_1 (e.g., the time from the start of the simulation to the appearance of the cool flame) is determined mainly from the physics, that is evaporation, transport properties and initial droplet size; on the other hand, the second induction time τ_2 , defined as the time interval between the cool and the hot flame appearances, was found to depend almost entirely on the chemical kinetics. Yang and Wong [12] used a semi-detailed reaction mechanism to simulate n -heptane droplet autoignition at $p = 5$ and 10 atm and over the same temperature range considered by Schnaubelt et al. Their work focused on the implication of the Stefan flow on the disappearance, during droplet autoignition, of the negative temperature coefficient (NTC) region that characterizes the autoignition of homogeneous mixtures. The effect of the initial droplet diameter on the total ignition delay time τ_t , defined as the sum of the first and second induction times, was also investigated. τ_t was found to decrease monotonically with decreasing d_0 until a minimum ignition delay time $\tau_{t,\text{min}}$ was reached for $d_{0,\text{min}}$; for smaller droplet diameters, ignition either did not occur, or occurred at times $\tau_t > \tau_{t,\text{min}}$. Very recently, Cuoci et al. [15] presented results for the autoignition of n -heptane, n -decane and n -dodecane in the pressure and temperature ranges $p = 1$ – 10 atm, $T_{g,0} = 600$ – 1000 K. Experimental ignition diagrams showing the ignition type for given pressure and ambient temperature values were reproduced with good accuracy for all fuels considered. Excellent agreement between simulated and measured first and total

ignition delay times was achieved for n -heptane. The fundamental role of the low-temperature chemistry on the autoignition process of n -alkanes droplets at low ambient temperatures was highlighted.

Although many aspects of n -alkane droplet autoignition have been investigated in great detail, the description of the ignition process and of some limiting phenomena, such as the disappearance of hot-flame ignition for sufficiently small droplets, still deserves some attention. Several studies on single [19,20] and two-phase [21–23] turbulent flow autoignition revealed how ignition kernels develop first at locations where scalar fluctuations are low and the mixture has an optimal composition, which depends on the fuel considered and on the fuel/oxidizer temperatures. In the particular case of n -heptane sprays at initial ambient temperatures below $T_{g,0} = 1000$ K, ignition was found to occur in regions where the mixture was locally rich [23]. The optimal mixture composition for ignition was close to the one corresponding to minimum ignition delay time in perfectly stirred reactor (PSR) calculations for the same nominal values of pressure and initial air and fuel temperatures of the spray; the ignition delay time, however, was longer than the PSR one. Most of the studies on single droplet autoignition have only reported the spatial location at which ignition occurs; no additional information was provided for the composition at the ignition location. An exception is represented by the work of Stauch et al. [14], who investigated numerically the autoignition of n -heptane droplets at $p = 7$ atm for very high values of the ambient gas temperature ($T_{g,0} = 800$ – 1600 K). In their work, ignition always occurred in lean regions, with the local air-to-fuel ratio ranging between $\lambda = 2.4$ and $\lambda = 3.0$. No data, however, was reported for values of $T_{g,0}$ corresponding to two-stage ignition.

It should also be mentioned that a significant class of models for turbulent combustion of sprays are based on a mixture fraction approach. Typically, an equation for the mean and variance of the mixture fraction is solved, with the spray appearing through a mass source term for the former and through some more terms, that require modeling, for the latter; Refs. [24,25,22,26] discuss this in the context of RANS, while Ref. [27] in the context of LES. Supplementary to this, the reactive scalar distributions in mixture

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