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Numerical analysis of the influence of two-phase flow mass and heat transfer on n-heptane autoignition

Zakaria Bouali [a,b], Cecile Pera [a,*], Julien Reveillon [b]

[a] IFP Energies nouvelles, 1-4 avenue de Bois-Préau, 92852 Rueil-Malmaison, France
[b] CORIA, UMR6614, University and INSA of Rouen, Avenue de l'Université, 76801 Saint-Etienne-du-Rouvray Cedex, France

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ABSTRACT

This paper investigates the influence of liquid fuel presence on the autoignition of n-heptane/air mixtures over a wide range of conditions encountered in internal combustion engines. To this end, evaporating droplet physics and skeletal chemistry mechanisms are simultaneously solved considering a homogeneous constant-pressure reactor. A skeletal mechanism is introduced to account for specific kinetics behavior in the Negative Temperature Coefficient (NTC) region. The impact of mass and heat source terms during evaporation is emphasized by comparing a two-phase flow scenario with a purely gaseous case. The competition between fuel vapor availability and the evaporation-induced gas temperature decrease is specific to two-phase flow autoignition. On the one hand, droplet evaporation delay restricts the gaseous local fuel/air equivalence ratio and consequently the kinetics runaway. On the other hand, temperature reduction due to evaporation may either reduce or enhance chemical reactivity, depending on the local thermodynamic conditions lying either inside or outside the NTC region. By simultaneously accounting for evaporation source terms and skeletal chemistry, we can reproduce the already experimentally observed transformation of the NTC region into a Zero Temperature Coefficient (ZTC) region depending on thermodynamic conditions and droplet size. The ZTC phenomenon appears when combustion heat-release starts before complete droplet evaporation. Since the ZTC behavior can be captured using the point source approach, in which droplets are considered only as zero-dimensional source terms of mass and energy, the present results pave the way for future exploration of NTC chemistry in sprays with a direct numerical simulation of discrete particles considering detailed chemistry and turbulent flows.

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1. Introduction

Injection of liquid fuel in a gaseous oxidizer is the most common technology in industrial combustion devices. Key physical processes include fuel-spray injection and atomization, droplet evaporation, mixture preparation, and combustion (possibly involving autoignition). In this context, a detailed understanding of the basic physical and chemical phenomena involved in two-phase flow autoignition is crucial.

Autoignition is a widely studied and reviewed phenomenon, both on the kinetics side [1] and on the turbulent combustion side [2]. However, most studies are devoted to purely gaseous mixtures. Consequently, numerical [3,4] and experimental [5,6] literature on two-phase flow autoignition is still scarce, and only a few general trends are known. The influence of temperature, pressure, and droplet size is discussed by Aggarwal [7]. Droplet size largely influences the autoignition delay in relation to the available gaseous equivalence ratio. From a qualitative point of view, there are three dominant spray ignition modes and corresponding ignition delays. Spray combustion regimes were classified according to a group combustion number G [8–10]. This dimensionless number may be seen as the ratio between the characteristic evaporation speed and the molecular diffusion speed, or the convective speed of the hot gases inside the droplet cloud (group of droplets). Depending on the droplet distribution inside the cloud, quantified through G (Fig. 1), ignition can occur either individually for each droplet ($G \ll 1$) or around groups of droplets ($G \gg 1$) if droplets are too close to each other to allow for diffusion of heat inside the cloud. A third mode, the spray ignition mode, considers a global ignition of the spray for droplets close to each other but surrounded by a hot atmosphere.

Despite the aforementioned research, there are numerous issues concerning autoignition in sprays that lack answers, particularly in the Negative Temperature Coefficient (NTC) region of hydrocarbon fuels. Within this region, autoignition delay of a purely gaseous and homogeneous mixture increases with temperature. However, the experiments [11,12] have demonstrated that a

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* Corresponding author.
E-mail address: cecile.pera@ifpen.fr (C. Pera).

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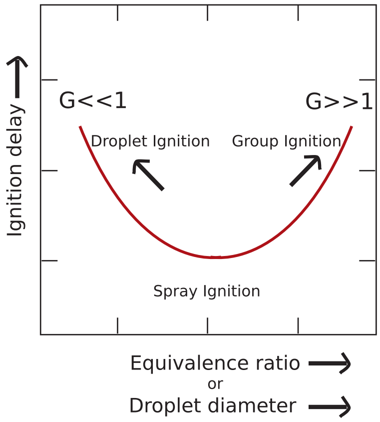

Fig. 1. Qualitative description of the three autoignition modes in sprays, from Aggarwal review [7].

Zero Temperature Coefficient (ZTC) domain is more likely to be observed for two-phase flow (no major influence of temperature on the autoignition delay). The sketch in Fig. 2a shows how NTC and ZTC areas appear on autoignition delay curves. The physics behind the ZTC is not well understood, and its modeling is still a challenge. Few numerical studies [13,14] have investigated this complex issue, and various explanations of the ZTC have been proposed but no consensus emerges.

Tanabe et al. [15] have used a 10-step mechanism enabling NTC region representation for gaseous mixtures but neither NTC nor ZTC has been observed in their two-phase flow results. Their studies have suggested that NTC-to-ZTC transition is more likely to be due to temperature and species heterogeneity around particles than to any other droplet characteristics.

Schnaubelt et al. [13] have selected a more detailed kinetics scheme (62 reactions) in order to understand the basic physical and chemical processes of n-heptane droplet autoignition. Despite recovering two-stage autoignition, the ZTC has only been observed within a restricted domain (620–630 K), whereas an experimental ZTC domain has been measured between 700 K and 800 K.

Wolff et al. [16] have studied autoignition of sprays with various droplet diameters (from 10 to 100 μm) over a wide range of thermodynamic conditions encountered in gas turbines. They have pointed out that when the droplet evaporation characteristic time is smaller than the autoignition delay, the particle size does not influence the reaction since autoignition occurs in a homogeneous and gaseous mixture. Nevertheless, the chemical kinetics used in [16] seems to underestimate the NTC phenomenon in purely gaseous conditions, making it difficult to study the NTC-to-ZTC transition in the presence of evaporating droplets.

Yang and Wong [12] have performed computations of n-heptane droplet autoignition with a semi-detailed (116 reactions) mechanism. They have suggested that NTC-to-ZTC transition is due to the Stefan flow effect in addition to a potential temperature and species field heterogeneity. Nevertheless, their results lack a ZTC region, which the authors attributed to a restricted sensitivity of the kinetics in the NTC region. Similarly, Stauch and Maas [17] used a more detailed mechanism (614 reactions) to study the impact of the ignition on the droplet properties evolution.

Finally, Cuoci et al. [14] have carried out detailed simulations of evaporation, autoignition, and combustion of isolated fuel droplets with a complex mechanism (about 200 species and 5000 reactions). They have mentioned that temperature and fuel/air equivalence ratio heterogeneity around the droplet tend to smooth the NTC phenomenon. Nevertheless, their sharp NTC curve remains weak compared to experimental results.

The hypothesis of temperature and mixture heterogeneity around droplets assumed in [12,14] suggests that micro-mixing around droplets must be resolved to capture the NTC-to-ZTC transition. If this hypothesis is correct, it could imply that the use of discrete particle simulations (DPS) coupled with gas direct numerical simulation (DNS) of turbulent spray autoignition using Eulerian/Lagrangian formalism is ill-adapted to capture this phenomenon. In fact, in this approach, droplets are only point source terms within the gaseous phase and no inter-droplet region is resolved. However, DNS + DPS of spray autoignition with a skeletal chemistry mechanism for n-heptane has been recently performed by Wang and Rutland [3,18] using this formalism, and they proved it to be efficient although they restricted their investigations to high temperature chemistry. Consequently, no NTC phenomenon could have been observed.

The objective of the present paper is to analyze how the mass and heat source terms from liquid evaporation influence n-heptane autoignition processes and to determine whether point source models (DPS) are able to capture NTC and ZTC phenomena. It is part of a general study that intents to investigate also the influence of the presence of non-homogeneous temperature fields, local preferential segregation of droplets, and the presence of a turbulent carrier phase [19].

In order to scrutinize the key chemical paths, skeletal chemistry capable of reproducing NTC kinetics is used. The focus is on the

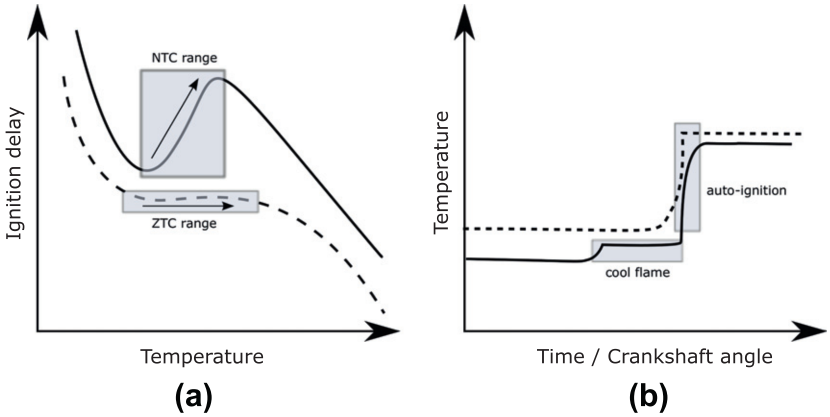

Fig. 2. Sketches of the major autoignition phenomena encountered in combustion chambers. (a) – Negative Temperature Coefficient (NTC) area (gray box, solid line): main autoignition delay increases with respect to temperature. Zero Temperature Coefficient (ZTC) area (gray box, dashed line): main autoignition delay is constant with respect to temperature. (b) – Possible autoignition (AI) processes: (solid line) cool flame AI before main AI or (dashed line) direct main AI. AI delays are defined using maximum temperature gradients.

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