



# Direct numerical simulation of spray evaporation and autoignition in a temporally-evolving jet

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## Abstract

This work investigates spray evaporation and autoignition in a temporally-evolving jet by means of Direct Numerical Simulation (DNS). The impact of shear on evaporation and spray autoignition mechanisms is quantified by comparing droplets evolving in a high-speed jet flow or in a nearly quiescent environment. Comparisons are based on the topology of the reaction fronts, as characterized by mixture fraction, scalar dissipation rate, flame index, as well as fields of temperature and heat release. The impact of local equivalence ratio, droplet diameter and jet velocity have been investigated by varying these parameters. The results reveal that the temporally-evolving jet is a promising numerical configuration to study spray-turbulence interaction, evaporation, mixing, and auto-ignition mechanisms. It is observed that the autoignition delay time strongly depends on the droplet diameter and jet velocity, while it is far less sensitive onto the equivalence ratio. With high shear, ignition occurs on the lean side, peak heat release being found near stoichiometry in a premixed combustion mode. In the absence of shear, ignition occurs simultaneously over a broad range of mixture fractions, and peak heat release is found for a rich mixture involving both premixed and nonpremixed flames. It is also noticed that the conditional mean of the scalar dissipation rate shows non-monotonic behavior when varying jet velocity.

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## 1. Introduction

Spray combustion is commonly encountered in many industrial devices, such as: gas turbines, diesel

engines, direct injection gasoline engines, and furnaces. A better understanding of liquid-fuel combustion is thus necessary to improve fuel efficiency and control emissions of these applications. Spray combustion includes many physical aspects, in particular evaporation and ignition/autoignition. For a better understanding of such complex phenomena and to develop improved models, detailed investigations are required, typically relying on experiments and Direct Numerical Simulations. DNS has been employed to investigate reactive droplets

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and spray combustion for almost two decades, considering many aspects and configurations. With growing computer power, different modeling levels have been combined, considering either single-step mechanisms [1–9], detailed kinetics in 2D simulations [10–12], or, more recently, detailed chemistry in 3D simulations [13–17]. Three configurations have been mainly considered: (1) Spray dispersion and ignition in homogeneous conditions and/or in flow with zero mean-flow velocity [1,4,9,10,12–16], (2) Spatially-evolving jets [2,3,7,8,17], and (3) Temporally-evolving jets [11]. Common conclusions of all these references are that the equivalence ratio and droplet size are the most critical parameters controlling spray combustion mode and ignition. Although these studies answered many questions, the impact of different operation conditions and configurations has not been sufficiently clarified yet [7]; more specifically, the effect of shear is not completely clear. This paper discusses the impact of shear on evaporation, mixing, and auto-ignition of liquid n-heptane droplets by comparing two cases: droplets evolving in a fast, temporally-evolving jet, compared to moving droplets in a nearly quiescent environment. Chemistry is systematically represented by a skeletal kinetic mechanism. Flame topology is characterized by flame index, mixture fraction, scalar dissipation rate, temperature and heat release. Thanks to a parametric study, the impact of equivalence ratio, droplet diameter and jet velocity on spray evaporation and autoignition is finally quantified. This paper is organized as follows. Section 2 introduces the governing equations and models. Numerical setups and configurations are discussed in Section 3. The DNS results and statistics are discussed in Section 4, before concluding in Section 5.

## 2. Numerical and mathematical approaches

In this work, all droplets, that are smaller than the grid resolution, are modeled as point droplets with diameter  $a$ . The Navier–Stokes equations are solved in the low-Mach number regime. Cantera 1.8 is used to describe chemical reactions and molecular transport processes in the gas phase. The continuous (gas) phase is solved by DNS in a standard manner (Eulerian frame), as described in [18]; whereas, the disperse (droplet) phase is tracked in a Lagrangian frame (Discrete Particles Simulation, DPS) [12,19]; hence, these simulations can be categorized as DNS-DPS. Two-way coupling between both phases is implemented via the exchange of mass, momentum and energy. The droplet equations rely on the model first introduced by Abramzon and Sirignano [20], with four different subscripts and superscripts:  $\infty$ ,  $F$ ,  $f$ , and  $L$ , which are standing for variables in the far-field gaseous region, properties of fuel vapor in film region, mixture variable in film region, and liquid properties,

respectively. The implemented equations describing droplet location, momentum, mass transfer, and heat transfer read as follows:

$$\frac{d\mathbf{X}_k}{dt} = \mathbf{V}_k, \quad (1)$$

$$\frac{d\mathbf{V}_k}{dt} = \frac{\mathbf{U}_\infty - \mathbf{V}_k}{\tau_{v,k}}, \quad (2)$$

$$\frac{da_k^2}{dt} = -\frac{a_k^2}{\tau_{a,k}}, \quad (3)$$

$$\frac{dT_k}{dt} = \frac{1}{\tau_{T,k}} \left[ T_\infty - T_k - \frac{B_{T,k} L_v}{C_{p,f}^F W_F} \right]. \quad (4)$$

In Eqs. (1)–(4),  $\mathbf{V}_k$  and  $\mathbf{U}_\infty$  are the velocity of the  $k$ th droplet and of the surrounding gas at droplet location  $\mathbf{X}_k$ . Also,  $T_\infty$ ,  $T_k$ ,  $L_v$ ,  $W_F$ ,  $C_{p,f}^F$  and  $B_{T,k}$  are mixture temperature in far-field, liquid droplet surface temperature, molar latent heat of droplet vaporization, molar mass of the fuel, specific heat of the fuel vapor in the film region and heat transfer number, respectively. The properties and variables in the film region are computed based on the one-third rule [11,20] and have the subscript  $f$ , as mentioned above. Motion and evaporation of the droplets is characterized by three characteristic time scales: momentum relaxation time ( $\tau_{v,k}$ ), evaporation delay ( $\tau_{a,k}$ ) and heating delay ( $\tau_{T,k}$ ):

$$\tau_{v,k} = \frac{\rho_L a_k^2}{18 \mu_f \left(1 + \frac{1}{6} \text{Re}_k^{2/3}\right)}, \quad (5)$$

$$\tau_{a,k} = \frac{\text{Sc}_k \rho_L a_k^2}{4 \text{Sh}_k \mu_f \ln(1 + B_{m,k})}, \quad (6)$$

$$\tau_{T,k} = \frac{\text{Pr}_k C_{p,L} \rho_L a_k^2}{6 \text{Nu}_k C_{p,f} \mu_f \ln(1 + B_{T,k})}. \quad (7)$$

In these equations, the characteristic time scales are computed as a function of various dimensionless numbers: the droplet Reynolds number,  $\text{Re}_k = \rho_\infty |\mathbf{U}_\infty - \mathbf{V}_k| a_k / \mu_f$ , the Spalding mass transfer number ( $B_m$ ) and the heat transfer number ( $B_T$ ),

$$B_{m,k} = \frac{Y_{s,k} - Y_{F,\infty}}{1 - Y_{s,k}}, \quad (8)$$

$$Y_k^s = \frac{W_F}{W_F + W_O(P_\infty/P_{\text{sat},k} - 1)}, \quad (9)$$

$$B_{T,k} = (1 + B_{m,k})^\theta - 1, \quad (10)$$

$$\theta = \frac{C_{p,f}^F \text{Sh}_k \text{Pr}_k}{C_{p,f} \text{Nu}_k \text{Sc}_k}, \quad (11)$$

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