



# Effects of turbulent intensity and droplet diameter on spray combustion using direct numerical simulation



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## HIGHLIGHTS

- Heptane spray combustion in a slab layer is studied by means of DNS.
- Turbulence is proved to be of advantage to evaporation.
- The log-normal distribution is reasonable for the scalar dissipation rate PDF.
- The fraction of premixed combustion in spray combustion is examined.

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## ABSTRACT

Direct numerical simulation (DNS) of heptane reacting sprays in a slab region is performed to investigate the effects of turbulence and droplet size on the evolutions of spray combustion. The gas phase is simulated using an Eulerian approach; while the droplets are treated with a Lagrangian method. The coupling between the two phases is considered. It is shown that the mean normalized squared droplet diameter decreases linearly for the cases studied, featuring the  $d^2$  law. Turbulence is proved to be of advantage to evaporation while droplet diameter greatly affects the evaporating rate and the evaporation lifetime. The conditional evaporating rate is found to increase linearly with the mixture fraction. The log-normal distribution for the scalar dissipation rate is examined, and reasonably good agreements are obtained between the DNS results and the model predictions. A parameter characterizing the amount of burning in premixed regime,  $W_p$ , is analyzed. Two stages of combustion are identified for the base case: most of the burning occurs in a non-premixed fashion following auto-ignition, and then premixed combustion becomes prevalent. It is shown that the fraction of premixed combustion generally increases with turbulent intensity and decreases with droplet diameter.

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## 1. Introduction

Many combustion devices operate with liquid fuel injection, including gas turbines, internal-combustion engines and furnaces. There are complex interactions between the gas phase and liquid phase in spray combustion. Better understanding of these interactions helps to improve the performance of combustors to maximize efficiency and minimize pollutant emission. In realistic turbulent spray combustion, the processes of droplet dispersion, droplet evaporation, turbulent mixing and chemical reaction occur simultaneously and are tightly coupled. It is difficult to deal with the underlying problems as a whole. To focus on some of them, it is useful to perform direct numerical simulation (DNS) studies of spray combustion in relatively simple configurations.

DNS is a powerful tool in that it captures all the turbulent and chemical scales without any closure models, which is critical to understand the turbulence-chemistry interactions. Recently, some DNS studies of spray combustion have been conducted [1–12]. Various aspects concerning spray combustion were investigated and insightful achievements were attained. Réveillon and Vervisch [1] used 2D-DNS to analyze a spray jet with co-flowing preheated air, and a large variety of reaction zone topologies was revealed by varying controlling parameters. Réveillon and Demoulin [2] studied the effect of turbulence on the preferential segregation and the evolution of the resulting mixture fraction field of a reacting spray with DNS. Watanabe et al. [4] carried out a 2D-DNS study of a spray flame formed in a laminar counterflow. The effects of strain rate, equivalence ratio, and droplet size were considered. Luo et al. [5] investigated spray flames with 3D-DNS in a swirling combustor using one-step irreversible reaction. They found that premixed flames contributed more the heat released, although non-premixed flames had volumetrically a higher contribution.

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In purely gaseous combustion, some combustion models based on the solution of the mixture fraction, such as conditional moment closure (CMC) and steady laminar flamelet (SLF), have been validated for a wide range of applications. But in spray combustion the mixture fraction is no longer a passive scalar as evaporation strongly modifies the mixture fraction field. The CMC method has been integrated in spray combustion modeling [13,14] and the sub-models for reacting sprays were studied using DNS database by Seo and Huh [15,16], and Wang et al. [17] *a priori*. They found that the closures developed for the presumed probability density function (PDF), conditional scalar dissipation rate and conditional reaction rate in purely gaseous combustion were also valid in spray combustion. Additional models for the conditional evaporating rate have been proposed by Sreedhara and Huh [18]. Two-phase reacting flows were studied by Lederlin and Pitsch [19], and Knudsen and Pitsch [20] in the context of large eddy simulation (LES) using the flamelet approach, which was extensively used in single-phase combustion. However, it is necessary to test the validity of the flamelet concept in the existence of evaporating droplets.

Although there have been some progresses on DNS of spray combustion, the details of the evaporation and combustion processes in spray combustion are not well understood yet. In the present work, spray combustion in a slab layer is investigated using DNS. The main objective is to examine the effects of turbulence and droplet size on the droplet evaporation and flamelet characteristics. The contributions of premixed and non-premixed combustion are analyzed as well. The remainder of the paper is organized as follows: Section 2 introduces the computational method for spray combustion. Section 3 gives the details of the simulation setup. The DNS results are presented and discussed in Section 4. Finally, some conclusions are made.

## 2. Numerical methods

The liquid phase is treated using a point-source approach. Droplet rotation, distortion and inter-droplet interactions are neglected. The droplets are assumed to be spherical and properties of the fuel are constant inside the droplets. Heptane is chosen as the fuel. The properties for heptane are referred to Miller et al. [21]. The governing equations for the position  $\mathbf{X}_i$ , velocities  $\mathbf{V}_i$ , mass  $m_i$  and temperature  $T_i$  of the  $i$ th droplet are as follows:

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

$$\frac{d\mathbf{V}_i}{dt} = f_1 \frac{\mathbf{U}(\mathbf{X}_i, t) - \mathbf{V}_i}{\tau_d} + \mathbf{g}, \quad (2)$$

$$\frac{dm_i}{dt} = -\frac{\text{Sh}}{3\text{Sc}} \frac{m_i}{\tau_d} \ln(1 + B_M), \quad (3)$$

$$\frac{dT_i}{dt} = \frac{\text{Nu}}{3\text{Pr}} \frac{C_p}{C_L} \frac{f_2}{\tau_d} (T_g - T_i) + \frac{\dot{m}_i L_V}{m_i C_L}, \quad (4)$$

where the vector  $\mathbf{U}(\mathbf{X}_i, t)$  is the gas velocity at the droplet position and  $\mathbf{g}$  is the volume force.  $\tau_d$  is the particle time constant and  $f_1$  is an empirical correction to the Stokes drag law.  $T_g$  is the gas temperature at the droplet position. Sc and Pr are the Schmidt and Prandtl numbers of the gas phase, respectively. Nu and Sh are the corrected Nusselt and Sherwood numbers to account for the convection effect on evaporation, and  $f_2$  is a correction for the effect of droplet evaporation on droplet heating. The heat capacity  $C_L$  and latent heat of vaporization  $L_V$  are assumed constant. The heating and evaporation of single-component droplets can be expressed in terms of the mass transfer number defined by:

$$B_M = \frac{Y_F^{\text{surf}} - Y_F}{1 - Y_F^{\text{surf}}}, \quad (5)$$

where  $Y_F$  is the mass fraction of the fuel at the droplet position, and  $Y_F^{\text{surf}}$  is the mass fraction of the fuel at the surface of the droplet, which is obtained using the equilibrium assumption:

$$Y_F^{\text{surf}} = \frac{\chi_{eq}}{\chi_{eq} + (1 - \chi_{eq})\theta}, \quad (6)$$

where  $\theta$  is the ratio of the carrier gas molecular weight to the fuel molecular weight. The surface equilibrium mole fraction of the vapor  $\chi_{eq}$  is related to the saturation pressure  $p_{\text{sat}}$  through the Clausius–Clapeyron equation:

$$\chi_{eq} = \frac{p_{\text{sat}}}{p} = \frac{p_{\text{atm}}}{p} \exp\left(\frac{L_V}{R} \left(\frac{1}{T_B} - \frac{1}{T_d}\right)\right), \quad (7)$$

where  $R$  is the idea gas constant,  $T_B$  is the boiling point of the fuel, and  $T_d$  is the droplet temperature. Detailed validation of the droplet evaporation model can be found in a previous study [31].

The gas phase combustion is based on the solution of the compressible Navier–Stokes equation system:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial X_j} (\rho u_j) = \dot{S}_m, \quad (8)$$

$$\frac{\partial}{\partial t} (\rho Y_k) + \frac{\partial}{\partial X_j} (\rho Y_k u_j) + \frac{\partial}{\partial X_j} (\rho Y_k \cdot (V_{kj} + V_j^c)) = \dot{\omega}_k + \dot{S}_k, \quad (9)$$

$$\frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial X_j} (\rho u_i u_j) = \frac{\partial \sigma_{ij}}{\partial X_j} + \rho \sum_{k=1}^N Y_k g_{k,i} + \dot{S}_{v,i}, \quad (10)$$

$$C_p \left( \frac{\partial \rho T}{\partial t} + \frac{\partial \rho u_i T}{\partial X_i} \right) = \dot{\omega}_T + \frac{Dp}{Dt} - \rho \frac{\partial T}{\partial X_i} \sum_{k=1}^N Y_k V_{k,i} C_{p,k} + \frac{\partial}{\partial X_i} \left( \lambda \frac{\partial T}{\partial X_i} \right) + \dot{Q} + \tau_{ij} \frac{\partial u_i}{\partial X_j} + \rho \sum_{k=1}^N Y_k g_{k,i} V_{k,i} + \dot{S}_T, \quad (11)$$

where  $\rho$  is the density,  $u$  the velocity,  $Y$  the mass fraction,  $V$  the diffusion velocity,  $V^c$  the correction velocity,  $p$  the pressure,  $T$  the temperature,  $\tau_{ij}$  the viscous stress tensor,  $g$  the volume force,  $\dot{Q}$  the heat source term,  $C_p$  the heat capacity at constant pressure and  $\dot{\omega}_T$  the heat release rate. The influence of the droplets is reflected in terms of source terms in the above equations, where  $\dot{S}_m$  is the mass source term,  $\dot{S}_k$  is the mass source term of the  $k$ th species,  $\dot{S}_v$  is the momentum source term and  $\dot{S}_T$  is the energy source term. The source terms contributed by the droplets for the exchange of mass, momentum and energy are expressed as:

$$\dot{S}_m = -\frac{1}{\Delta V} \sum_i \alpha_i \frac{dm_i}{dt}, \quad (12)$$

$$\dot{S}_v = -\frac{1}{\Delta V} \sum_i \alpha_i \frac{dm_i \mathbf{V}_i}{dt}, \quad (13)$$

$$\dot{S}_T = -\frac{1}{\Delta V} \sum_i \alpha_i \frac{dm_i C_L T_i}{dt}, \quad (14)$$

where  $\Delta V$  is the control volume for every node, and  $\alpha_i$  is the distribution coefficient of the  $i$ th droplet source term on the node. In the present study a uniform Cartesian grid is adopted, so that  $\Delta V = \Delta^3$  ( $\Delta = \Delta x = \Delta y = \Delta z$ ).

## 3. Computational details

The simulations are carried out with a DNS code developed in our group. The DNS code is robust and has been applied in studies

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