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Complex chemistry simulations of spark ignition in turbulent sprays

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Abstract

Three-dimensional DNS of two-phase flows with the point-source approximation and with complex chemistry for *n*-heptane has been used to extract physical information on the structure of igniting kernels following localised heat deposition in turbulent monodisperse sprays. Consistent with experiment, small sparks fail to ignite and sprays ignite later than premixed gaseous mixtures. Reaction rates are intense in spherical zones near droplets and much lower in the interdroplet spacing, resulting in a highly wrinkled flame surface. The propagation of these reaction zones was observed. The flame shows a locally non-premixed character, with reactions proceeding at a wide range of mixture fractions, which increases as evaporation progresses. The distribution of various chemical species is presented. The results constitute a database for model validation and physical analysis.

Keywords: Turbulent flame; Spark ignition; Spray; Detailed chemistry; DNS

1. Introduction

Useful physical insight on ignition and flame propagation in sprays has been gained by examining the canonical problems of laminar and turbulent uniformly distributed mono-sized droplets [1–3]. The positive effect of rapid evaporation and the detrimental effect of higher turbulence intensity on ignition performance were demonstrated in several studies [2,4–8]. Those effects were included in the general model for minimum ignition energy for overall lean sprays [9]. Following successful spark ignition, a flame propagates in a uniform cloud of droplets. The concept of effective equivalence ratio, i.e., the gas phase equivalence ratio at the flame front, has been successful in describing the flame speed in a spray over a range of overall equivalence ratio and droplet sizes (i.e., overall rich sprays or lean sprays and large droplets) [7,10–14]. However, this one-dimensional model does not account for numerous observations that the flame speed is affected by the wrinkling of the flame by droplets [10] and by spatial mixture fraction inhomogeneities in the interdroplet spacing which lead to diffusion flames surrounding droplets where chemical reactions are expected to occur at stoichiometry [15–18]. Models have been developed to assess the structure of auto-igniting spherical clusters of droplets, e.g., Ref. [19]. They captured the different structures of group combustion [20], with individual droplet flames for dilute sprays or flames surrounding the cluster for dense sprays.

Recent spark ignition DNS was limited to simple chemistry and fine droplets where strong inhomogeneities could not appear [8]. Furthermore, the role of detailed chemistry in spray ignition and spray flame propagation has received little attention although its effect on laminar flame speed has been demonstrated

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in 1D models [14]. Two-dimensional simulations with detailed chemistry have shown the role of detailed chemistry with low hydrocarbons on premixed [21,22] and non-premixed gaseous spark ignition [23,24]. Wang and Rutland [25] performed two-dimensional DNS of *n*-heptane spray auto-ignition and incorporated detailed chemistry. Nevertheless, 3D detailed chemistry DNS of spark ignition in sprays have not been performed.

In this paper, DNS of spark ignition in a turbulent, uniformly dispersed cloud of mono-sized droplets with high volatility and moderate size is presented in order to explore the flame structure. In the next section, the numerical methods are introduced and then the results and their discussion are presented. We close the paper with a summary of the main conclusions.

2. Mathematical modelling

A Lagrangian point-source formulation has been adopted for the liquid phase. Temperature is assumed uniform inside the droplets and droplet–droplet interactions are neglected. A thin film (subscript *f*) assumption is used to calculate the droplet evaporation and heat exchange with the surroundings [26]. For each droplet *d*, equations for its position $\mathbf{x}_d$, velocity $\mathbf{v}_d$, diameter a_d and temperature T_d are solved:

$$\frac{d\mathbf{x}_d}{dt} = \mathbf{v}_d \tag{1}$$

$$\frac{d\mathbf{v}_d}{dt} = \frac{\mathbf{U}(\mathbf{x}_d,t) - \mathbf{v}_d}{\tau_d^v} \tag{2}$$

$$\frac{da_d^2}{dt} = -\frac{a_d^2}{\tau_d^p} \tag{3}$$

$$\frac{dT_d}{dt} = \frac{1}{\tau_d^T}\left[T(\mathbf{x}_d,t) - T_d - B_{T,d}\frac{L_v}{W_F C_{P_f}} \times \left(\frac{T_{crit} - T_d}{T_{crit} - T_{ref}}\right)^{0.38}\right] \tag{4}$$

$\mathbf{U}$ and T are the local gas velocity and temperature. T_{ref} is the boiling temperature at the reference pressure p_{ref}, T_{crit} the critical temperature, L_v the molar latent heat of evaporation and W_F the molecular mass of fuel. The relaxation times appearing above are [26]:

$$\tau_d^v = \frac{\rho_L a_d^2}{18\left(1+\frac{1}{6}\mathrm{Re}_d^{2/3}\right)\mu_f} \tag{5}$$

$$\tau_d^p = \frac{\rho_L a_d^2}{4\mathrm{Sh_c}}\frac{\mathrm{PrLe_F}}{\mu_f}\frac{1}{\ln(1+B_{M,d})} \tag{6}$$

$$\tau_d^T = \frac{\rho_L a_d^2}{6\mathrm{Sh_c}}\frac{\mathrm{PrLe_F}}{\mu_f}\frac{B_{T,d}}{\ln(1+B_{M,d})}\frac{C_P^L}{C_{P_f}} \tag{7}$$

with $\mathrm{Re_d}$ the droplet Reynolds number, ρ_L the liquid droplet density, C_P^L is the heat capacity of the liquid and $\mathrm{Le_F}$ the fuel Lewis number. The mass and the temperature Spalding numbers, $B_{M,d}$ and $B_{T,d}$, are calculated by $B_{M,d} = (Y_{F,d}^s - Y_F(\mathbf{x}_d,t))/(1-Y_{F,d}^s)$ and $B_{T,d} = (1+B_{M,d})^\zeta - 1$. $\zeta = (C_P^F\mathrm{Sh_c})/(C_{P_f}\mathrm{Nu_c Le_F})$ where C_P^F is the fuel vapour heat capacity in the film whilst $\mathrm{Sh_c}$ and $\mathrm{Nu_c}$ are modified Sherwood and Nusselt numbers [26]. We consider properties of the volatile fuel *n*-heptane.

For the gas phase, mass, momentum, total energy and $N-1$ species transport equations are solved (N being the number of species appearing in the chemical mechanism used). Temperature-dependent transport coefficient are evaluated through 5th-order polynomials and the molecular viscosity through the expression $\mu = 2.58\times 10^{-5}(T/298)^{0.7}\mathrm{Pr}\ \mathrm{kg\,m^{-1}\,s^{-1}}$, with $\mathrm{Pr} = 0.7$. Diffusion coefficients, $D_\alpha = (\mu\mathrm{Pr})/(\rho\mathrm{Le}_\alpha)$, are found assuming constant Lewis number Le_α for each species α. The values of Le_α for the following species were taken from [27]: 1.11 (O_2), 0.18 (H), 0.73 (OH), 0.30 (H_2), 0.83 (H_2O), 1.10 (HO_2),1.12 (H_2O_2), 1.10 (CO), 1.39 (CO_2), 1.28 (CH_2O), 0.97 (CH_4), 1.00 (N_2). Diffusivity coefficients for the following species were calculated using the Fuller-Schettler and Giddings equation [28]: 2.89 (C_7H_{16}), 1.41 (C_2H_2), 1.00 (CH_3), 1.49 (C_2H_4), 1.80 (C_3H_4), 1.87 (C_3H_6), 2.19 (C_4H_8), 2.72 (C_6H_{12}), 3.09 ($OC_7H_{13}OOH$), 3.08 ($C_7H_{15}O_2$).

Two-way coupling holds between gas and liquid phases. The liquid source terms for mass, Γ_m, momentum, Γ_{U_i} and energy, Γ_E are computed by [29]:

$$\Gamma_m = -\frac{1}{V}\sum_d \alpha_d\frac{dm_d}{dt} \tag{8}$$

$$\Gamma_{U_i} = -\frac{1}{V}\sum_d \alpha_d\frac{dm_d \mathrm{v}_{d,i}}{dt} \tag{9}$$

$$\Gamma_E = -\frac{1}{V}\sum_d \alpha_d\left(C_P^L m_d\frac{T(\mathbf{x}_d,t) - T_d}{\tau_d^T} + \frac{dm_d}{dt}h_F(T_d) + \frac{1}{2}\frac{dm_d\mathrm{v}_{d,i}^2}{dt}\right) \tag{10}$$

where $m_d = \rho_L(\pi a_d^3)/6$ is the mass of droplet d, $h_F(T_d)$ is the fuel vapour enthalpy at the droplet surface and V is the volume of the Cartesian grid cell centred on the DNS node. A weighted summation is done over all the droplets. α_d is the portion of the DNS node volume that intersects a similar volume V centred on the droplet with subscript d. Gaseous properties are similarly interpolated on a droplet by doing a weighted summation over all cells having non-zero α_d. The spherical spark was modelled as a source term of duration t_{sp} in the energy equation, set to reach two adiabatic flame temperature T_{ad}, with a Gaussian radial profile centred in the domain as described in [30].