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Fully resolved DNS of droplet array combustion in turbulent convective flows and modelling for mixing fields in inter-droplet space

Bosen Wang, Andreas Kronenburg*, Giovanni L. Tufano, Oliver T. Stein

Institut für Technische Verbrennung, Universität Stuttgart, Herdweg 51, Stuttgart 70174, Germany

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ABSTRACT

The combustion of droplets in turbulent convective flows is simulated using direct numerical simulations (DNS). The liquid–vapour interface between kerosene droplets and the surrounding air is fully resolved with realistic boundary conditions for mass conservation, heat conduction and species diffusion. The study focuses on the characterisation of the mixing process between the evaporating fuel and the surrounding gas in regions that are dominated by small turbulent scales. For inertial droplets, these regions are characterised by Kolmogorov time scales and the mean relative velocity between droplets and the surrounding gas phase. Scaling laws for quantities of interest that require sub-grid modelling for LES, such as mixture fraction, its conditional scalar dissipation and probability density functions (PDF), are presented and assessed by comparisons with the DNS data. The scaling laws provide satisfactory estimates and are validated for different inflow Reynolds numbers, turbulence intensities and integral length scales, droplet diameters, inter-droplet distances, droplet combustion regimes and various instants of the transient evaporation process. Suitable modelling parameters are extracted from the DNS and functional dependencies of the parameters are suggested. This study demonstrates that the scaling laws are suitable to serve as sub-grid scale models for mixture fraction based approaches such as flamelet, conditional moment closure (CMC) or multiple mapping conditioning (MMC) methods.

1. Introduction

Turbulent spray combustion is the predominant combustion mode in industrial applications such as diesel and gas turbine engines. The liquid fuel is injected from a nozzle into a usually turbulent environment at high speed leading to a rapid disintegration of the spray into droplets and subsequent evaporation [1]. Local inhomogeneities in droplet sizes and distributions lead to inhomogeneities in the local mixing of fuel and oxidiser. Spray combustion can thus not easily be modelled by the existing strategies for diffusion and/or premixed single-phase combustion [2]. The issues related to the mixing of the evaporated fuel vapour with the surrounding gas are manifold. The large turbulent flow scales imposed by the geometry of the combustion chamber tend to be much larger than the inter-droplet distances and lead to significant droplet number density fluctuations. In contrast, small scale mixing at length scales ranging from scales of the order of the particle diameter and Kolmogorov scales to scales proportional to inter-droplet spacing smooth local inhomogeneities during combustible mixture preparation [3]. The characterisation of mixing at different scales is complex, however necessary for accurate sub-grid scale closures for mixture fraction based combustion models. Sub-grid scale closures for very dilute sprays are based on single droplet evaporation models [4,5] and have been validated successfully in the LES context (e.g. [6–8]). For more dense sprays, the combustion and evaporation of different droplets interact and are additionally affected by turbulence. These interactions can strongly influence the mixing characteristics in inter-droplet space and thus combustion. Hence, more advanced closures are needed.

Most experimental investigations studied the correlations between the droplet evaporation rate and turbulence intensity [9,10]. However, these experiments are usually performed for very large droplet diameters. Furthermore, they do not focus on droplet–droplet interactions and cannot capture the interactions between turbulence and mixing that occur at the micro-scale around the droplets. Hence, the vast majority of existing experiments are not entirely suited to address the questions posed in this paper. Instead, direct numerical simulations (DNS) are required to resolve all turbulence–combustion–evaporation interactions in droplet laden flows. A first step are so-called carrier-phase DNS that use a Lagrangian formulation to describe position, velocity

* Corresponding author.
E-mail address: kronenburg@itv.uni-stuttgart.de (A. Kronenburg).

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and mass of droplets that are treated as point sources [11–13]. The gas phase flow field is fully resolved but the droplet surface and the vicinity of the droplet affected by the boundary layer is not fully resolved. The results obtained by carrier-phase DNS may therefore be inaccurate for the analysis of the mixing fields in relatively dense sprays. Particle-turbulence interactions are frequently studied (e.g. [14,15]) but evaporation and combustion are usually omitted. Shinjo et al. [16] demonstrated for quite realistic turbulent configurations that droplets with sizes comparable to the turbulence scales affect the mixing characteristics. However, simple configurations such as droplet arrays are needed to improve our understanding of the more complex interactions between turbulence, combustion, evaporation and mixing in inter-droplet space. Wu and Sirignano [17–19] used fully resolved three-dimensional DNS to simulate burning droplet arrays. They studied effects of droplet spacing, relative velocity and ambient pressure on flame structure transition as well as surface temperature and burning rates of droplets, but the study was restricted to laminar convective environments. Cho et al. [20] used a similar method to study the effect of oxygen concentration and geometrical arrangements of droplets on burning characteristics in the RANS context. However, the instantaneous interactions between droplets and turbulence were not captured.

The present study focuses on the modelling of characteristic mixing quantities, such as mixture fraction, its conditional scalar dissipation and its PDF, in inter-droplet space in the presence of interactions between evaporation, combustion and convective turbulent flows. The models for an isolated non-inertial droplet have been discussed by Bilger [21]. However, they cannot directly be applied to convective turbulent flows and to interacting evaporation fields. In this study, the scaling laws derived by Klimenko and Bilger [22] are employed to facilitate the modelling of the characteristic mixing quantities for inertial droplets in convective turbulent flows. We distinguish two different zones in inter-droplet space: a near droplet zone dominated by the quasi-laminar wake of an inertial droplet and a Kolmogorov scale zone determined by small scale turbulence. An earlier study by Zoby et al. [23] used fully resolved DNS to evaluate analytical expressions for mixture fraction, its dissipation and PDF for evaporation without combustion in the near droplet zone. Wang et al. [24] developed the derivations of the scaling laws for the zone determined by small scale turbulence and used similar methods to assess the scaling laws for this zone with the assumption of unity Schmidt number and Lewis number but for evaporation without combustion. The present work continues to use fully resolved DNS to investigate mixing fields in droplet arrays for evaporation with combustion, for both the near droplet zone and the Kolmogorov scale zone. This study also extends the range of turbulent scales and investigated parameters and provides estimates for the modelling constants inherent in the scaling laws. These scaling laws can be used as sub-grid models for any mixture fraction based combustion sub-grid model such as LES-flamelet [25], LES-CMC [26] and LES-MMC [27] for the whole mixture fraction space ranging from the LES filtered cell mean to the value at the droplet surface.

2. Scaling laws

When droplets move relative to the surrounding gas phase in turbulent flows, wake-like structures develop. The zone in the vicinity directly behind the droplet is dominated by a quasi-laminar wake named here “the near droplet zone” (NDZ). Beyond this zone, the Kolmogorov scale fluctuations penetrate the wake. This zone is accordingly called “the Kolmogorov scale zone” (KSZ). The approximate spatial distributions of these two zones in a regular droplet array are illustrated in Fig. 1. These two

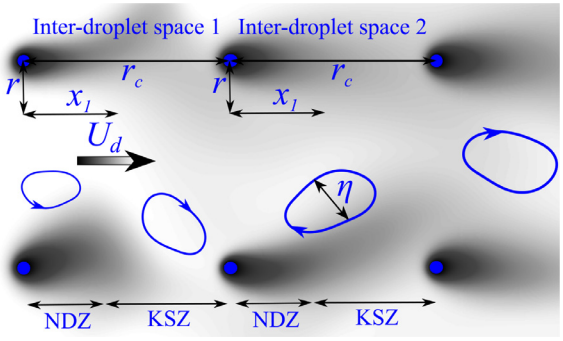

Fig. 1. Schematic diagram of the near droplet zone (NDZ) and the Kolmogorov scale zone (KSZ) in droplets arrays. The circles with arrows represent eddies of the Kolmogorov length scale η.

zones constitute the inter-droplet space. The characteristic mixing quantities will be investigated in the two inter-droplet spaces: inter-droplet space 1 is defined as the space between the first and second droplet layer while inter-droplet space 2 is located inbetween the second and third droplet layer. For these zones, the derivation of scaling laws for the mixture fraction distribution and its conditional scalar dissipation and PDF were presented in earlier studies in [22–24,28]. We only present the final expressions of the scaling laws below, and Appendix A and Appendix B point towards small differences between the derivations presented here and elsewhere [23,24,28]. Klimenko and Bilger [22] proposed that the transition between the near droplet zone and the Kolmogorov scale zone can be based on the relationship between the Kolmogorov time scale τ_η and the characteristic time scale τ, $\tau = x_1/U_d$, where x_1 is the longitudinal downstream distance from the droplet upstream and U_d is the mean relative velocity between droplets and surrounding gas, as shown in Fig. 1. Here, we define a normalised longitudinal downstream distance given by $\hat{x} = x_1/x_u$ where $x_u = U_d\tau_\eta$ is named as the characteristic undulation length of the smallest eddy.

The derivation for the scaling law for mixture fraction in the near droplet zone in axial and radial directions (along x_1 and r, respectively, as visualised in Fig. 1) can be based on the principle of self-preservation for the boundary layer of turbulent wakes [29] and non-dimensional analysis. It is given by

$$f_{NDZ} = f_2 + \frac{J_m(f_d - f_2)}{4\pi\rho D x_1 \phi_n} \exp\left(-\frac{U_d}{4Dx_1\phi_n} r^2\right). \quad (1)$$

Here, f_2 denotes the minimum mixture fraction in the near droplet zone which is related to the average mixture fraction in inter-droplet space and also characterises the interactions between different droplets. The definition of f_2 is given in Appendix A. f_d is the mixture fraction in the liquid phase, J_m represents the evaporation rate of a single droplet, ρ and D are the average density and Favre averaged diffusivity in inter-droplet space, respectively. The parameter r is the radial distance from the droplet center on a plane perpendicular to the flow direction (see Fig. 1). The modelling parameter ϕ_n was suggested as 1 in the derivation by Klimenko and Bilger [22] and it will be calibrated by the DNS results in this study. The expectation of the maximum mixture fraction on each plane perpendicular to the relative mean flow direction in the near droplet zone can be obtained from Eq. (1) for $r \to 0$, viz.

$$f_{max,NDZ} = f_2 + \frac{J_m(f_d - f_2)}{4\pi\rho D x_1 \phi_n}. \quad (2)$$

Similarly, the scaling law for mixture fraction in the Kolmogorov scale zone can also be derived from the principle of self-preservation for the boundary layer of turbulent wakes [29],