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Assessment of scaling laws for mixing fields in inter-droplet space

B. Wang, A. Kronenburg*, D. Dietzel, O.T. Stein

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

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Abstract

Droplet evaporation and subsequent mixing of the fuel vapor with the turbulent surrounding hot oxidizer has been simulated using direct numerical simulations (DNS). The kerosene droplets are fully resolved with realistic boundary conditions at the liquid–vapor interface to ensure the correct heat and mass transfer between the two phases. The study focuses on combustible mixture preparation in the inter-droplet space at scales larger than the quasi-laminar near droplet zone. The data are analysed with respect to key quantities for mixture fraction based combustion models such as mixture fraction distribution and its dissipation. The DNS is compared with scaling relationships for the wake and for length scales of Kolmogorov size where the wake seizes to be the dominant flow structure. The scaling relationships agree reasonably well with DNS data and they may serve as sub-grid scale closures for combustion models such as conditional moment closure or *flamelets*. Their respective regions of validity are quantified for the different cases of turbulence intensity that are investigated here.

Keywords: Spray evaporation; Turbulent mixing; Mixture fraction; Scalar dissipation; PDF

1. Introduction

Turbulent spray combustion is one of the most important technologies for power generation and transport, but no universal model exists that could predict all details of the fundamental processes associated with spray break-up, droplet evaporation, subsequent fuel–air mixing and combustion. One of the major issues that hinders analysis of these phenomena is the scale separation of the large flow scales imposed by the geometry of the combustion chamber and the small scales at the droplet interface and in inter-droplet space that determine the combustible mixture preparation. Typically, the size of the droplets and the inter-droplet distances are much smaller than the integral length scale, and even the Kolmogorov scale can be larger than – but of the order of – the scales characterising the droplets and their distribution. It can therefore be hypothesized that the interactions between the small scales and the droplets significantly contribute to the details of droplet evaporation and combustion mixture preparation.

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

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Most of the existing relevant experimental investigations study the effect of turbulence intensity on the droplets' evaporation rate [1,2]. They do not, however, address the gas phase characteristics, i.e. the fuel–oxidizer mixing, due to the well known issues associated with gas phase measurements in particle laden flows. Here, only numerical simulations can aid the analysis and direct numerical simulation (DNS) is required to fully resolve the details of the interactions. So-called 'carrier-phase DNS' where the flow field is resolved but droplets are modeled as point sources of fuel may shed light on mixture preparation in very dilute flows [3,4], but local inhomogeneities induced by evaporation of the droplets are not resolved and relatively dense sprays or interactions between the Kolmogorov and the particle scale cannot be analyzed. Wu and Sirignano [5–7] used fully resolved three-dimensional DNS of droplet arrays burning in stagnant and convective environments. Their studies focused on the quantification of the effect of droplet sizes and droplet loading on ignition and combustion, but do not include an analysis of turbulence and local mixture preparation. Particle-turbulence interactions are much more frequently studied (e.g. [8,9]) but particles are usually not fully resolved, the flow is inert and evaporation is omitted.

The present study attempts to close this gap and focuses on the statistical distribution of combustion relevant quantities in the gas phase (in this case mixture fraction) at length scales ranging from the particle scale to the Kolmogorov scale and interparticle spacing, respectively. We will assess scaling relationships [10] for the modeling of mixture fraction distribution and scalar dissipation at these scales. These scaling laws could then be used as sub-grid models for e.g. large-eddy simulations (LES). There, local inhomogeneities of mixing related quantities are not resolved at the Kolmogorov scale but severly affect the accuracy of mixture fraction based combustion models, such as Conditional Moment Closure (CMC) (e.g. [11,12]). Earlier studies by Zoby et al. [13,14] used fully resolved DNS to evaluate the analytical expressions for mixture fracion and its dissipation in the near droplet zone. However, the quasi-laminar near droplet zone does not seem to determine mixture distribution from the droplet to the cell mean. Quasi-laminar approximations as suggested by Bilger [15] vastly overpredict fluxes from the droplet to lower mixture fraction regions and lead to an excessive generation of scalar variance that unduly affects any mixture fraction based model [16]. Turbulence scales larger than the laminar boundary layer but smaller than the grid size must therefore be responsible for transport in mixture fraction space and distribution from the droplet to the (LES-filtered) cell mean. The present work now extends the analysis by Zoby et al. [13] from the near droplet scale to Kolmogorov scales and assesses the range of validity of the different scaling relationships.

2. Problem formulation

The simulations shall resemble droplet evaporation under engine-like conditions. The surrounding hot air is composed of nitrogen and oxygen (79:21 on a molar basis) at a pressure of $p_\infty = 15$ bar and a temperature of $T_\infty = 950$ K. After secondary breakup when droplets are small and evaporation is highest, the drag changes the velocity during the lifetime of the droplet only moderately. This was shown by earlier studies [13,14] where a momentum equation was solved for the droplet velocity. Here, we therefore assume a constant relative velocity during the time of simulation and the mean velocity of the flow is set to $U_d = 0.2$ m/s. To facilitate the analysis, statistically stationary conditions are enforced by temporal invariance of the droplet size. Radiation is neglected and Lewis numbers are set to unity in the gas phase.

The configuration is similar to the configuration by Zoby et al. [13] where regular droplet arrays were investigated. The convective flow (in axial direction) is perpendicular to an infinite droplet array (realized by periodic boundary conditions in cross-stream and spanwise directions) with two droplet layers and a droplet spacing of $r_c = 10$ droplet diameters. The fuel droplets are kerosene and have a diameter of $d = 100\,\mu$m. The entire domain spans 20 droplet diameters in cross-stream and spanwise directions, and extends $10d$ downstream of the second droplet row in the axial direction. The droplet number density can be calculated from the inter-droplet distance as $c = {r_c}^{-3}$.

A homogeneous isotropic turbulent velocity field is superposed to the mean flow at the inflow of the computational domain. The perturbations are calculated from a modified von Karman spectrum and details of the algorithm can be found in Davidson [17] and Billson [18]. The initial integral length scale is limited by half the domain size and limits the range of the turbulent spectrum that can be realized. However, larger scales are expected to transport the droplet cloud as a whole and will not modify interparticle mixing as much as the smaller scales. Three different turbulent fields are fully characterized by the largest scale, the fluid viscosity ($\nu = 8 \times 10^{-6}\,\mathrm{m^2/s}$ corresponding to the hot air stream at 15 bar and 950 K) and the Kolmogorov length scales of $\eta = 1.6d$, $2.2d$ and $2.7d$, respectively. In the absence of shear, these conditions ensure a relatively moderate decay of turbulence as the flow is convected through the domain and turbulence levels conserve more than 50% of their initial value at the outflow plane. The details of the three cases investigated here with the different turbulent fields are given in Table 1. Note that turbulent Reynolds numbers seem low, but they are