Effects of droplet preferential segregation in turbulent flows on the mixture fraction topology

J. Réveillon & F. X. Demoulin
CORIA, University and INSA of Rouen, Saint Etienne du Rouvray, France

Abstract

The objective of this paper is to determine the simultaneous effects of the turbulence on the dispersion of an evaporating spray and the mixture fraction evolution. Three-dimensional simulations are carried out following two stages leading to various physical analysis. First, the mixing between the initially randomly dispersed phase is considered with non-evaporating particles. Following their Stokes number and the turbulence properties, the formation of clusters of particles is analyzed (formation delay, cluster characteristic size). Once the particles are in dynamical equilibrium with the surrounding turbulent flow, evaporation phenomena are considered through the analysis of the mixture fraction evolution.

1 Introduction

In industrial systems dedicated to transport or energy transformation, a combustion chamber is generally fuelled by a spray of evaporating liquid droplets. The modeling of such chambers, involving the combustion of a two-phase flow or of a gaseous mixture issued from evaporation of a spray, is of primary importance to improve, the output of the considered device and to predict pollutant formation while maintaining a reasonable development cost.

One of the input parameter of any non-premixed turbulent combustion model is the mixture fraction variable \( Z \), which describes locally the mixing between the evaporated fuel and the gaseous oxidizer. The objective of this paper is to determine the simultaneous effects of the turbulence on the spray dispersion and the mixture fraction evolution. Thus, main characteristics of the mixture fraction field (fluctuation intensity levels and characteristic length scales) can be estimated directly from local properties of turbulence (rms, length scales) and spray parameters (Stokes number, liquid equivalence ratio).
Multiple interactions may be defined between turbulent flow, spray dispersion and vapor micro-mixing. To reduce the number of varying parameters, a configuration very close to the one used by Eswaran and Pope [1] for their reference study dedicated to the turbulent mixing of purely gaseous flow has been extended to two-phase flow simulations [2]. Thus, a forced isotropic homogeneous turbulence, with statistically stationary properties, is used as carrier phase. A recently developed forcing scheme allowing mean stable properties of the turbulence (energy, dissipation, integral length scale) has been introduced in a spectral formulation describing the evolution of an incompressible gas phase. The dispersed spray evolution is modeled thanks to a Lagrangian formulation describing the position, the velocity and the mass of any droplet embedded in the gas phase. Because of the weak mass loading ratio and to maintain stationary turbulence properties, the coupling between both liquid and gas phases is done through mass exchange terms only and the action of the spray on turbulence is not considered in this work.

2 Numerical system and geometry

Details of computational procedure may be found in [3]. The following three-stage procedure has been employed to analyse all interactions between the turbulent flow and the dispersed phase. Vorticity contours and dispersing particles have been plotted in Fig. 1 to illustrate both Eulerian and Lagrangian resolutions.

Stage 1: statistically stationary turbulence

In this preliminary stage, forced turbulent gaseous phase evolves solely until its statistical properties reach a steady state thanks to the forcing procedure that conserves the mean kinetic energy $k$ equals to the prescribed one [3]. The energy spectrum allows us to determine a reference wave number $\kappa_0$ corresponding to turbulence scales that contain most of the kinetic energy.
Stage 2: spray dynamical equilibrium

Several eddy turn over times after the turbulent flow reaches its stationary state, $N_d$ mono-dispersed non-evaporating particles are randomly embedded in the computational domain with a null initial velocity. The drag force sets particles in motion and very soon the spray reaches a dynamical equilibrium with the turbulence (Fig. 1-(b)). Droplet dispersion is characterized by the Stokes number $St = \frac{\tau_p}{\tau_\kappa}$ [4], which indicates the ability of droplets to capture local variations of carrier phase velocity. Turbulence properties being fixed, simulations have been carried out by modifying the $\tau_p$ parameter leading to 12 different Stokes numbers varying between 0.025 and 11.

To characterize droplet dispersion and preferential concentration, a density $\xi(x,t)$, describing the local mass of liquid per unit of volume has been defined. To make easier the spectral analysis of physical properties, the Eulerian computational grid has been used and $\xi(x,t)$ is determined by considering droplets accumulated in a control volume around each node. A mean

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**Figure 2:** Statistically stationary spray properties. (a) spray relaxation time ($t_\infty$) necessary for the spray to be in equilibrium with the turbulent carrier phase; (b) final ($t > t_\infty$) stationary level of particles slip velocity rms ($w'_\infty$).
reference number density is defined by \( \xi^0 = N_d/L^3 \). Note that in the following \( \langle \rangle \) stands for the mean over the Eulerian grid whereas \( \tilde{\langle \rangle} \) is the mean over the Lagrangian particles or droplets.

Stage 3: liquid phase evaporation and micro-mixing

Once the spray is in dynamical equilibrium, droplet evaporation start following saturation laws. To describe the mixing between gaseous fuel and oxidizer, a specific definition of the mixture fraction is chosen. A normalization is introduced using the saturation limit: \( Z = Y_F/Y^s \). In this non-reactive work, \( Z \) is thus bounded between 0 and 1 and it is of practical interest for analyzing the correlations between the evaporating spray and the mixing.

3 Results and discussion

Although homogeneous turbulence is a straightforward configuration, the addition of an evaporating dispersed phase allows us to be at the midpoint of many ill-know interactions between turbulence, spray, mixing and combustion. As described in the introduction, for the sake of clarity this paper focuses on the correlations between mixture fraction topology and droplets preferential segregation. The analysis of flame ignition and propagation or model closures will be the purpose of future works. In a first part, equilibrium regimes of non-evaporating droplets are depicted before evaporation takes place. It leads to the apparition of a gaseous fuel whose mixing with oxidizer is then detailed.

3.1 Solid dispersion

Equilibrium of the spray with its surrounding carrier phase is detected through the Lagrangian statistics of the slip velocity \( \tilde{w}_k = (u(x_k,t) - v_k) \), where \( u \) is the gas velocity at the droplet location and \( v \) is the droplet velocity. Because of the homogeneous nature of the turbulence and the dispersion, the mean value of the slip velocity defined by \( \tilde{w} = \frac{1}{N_d} \sum_{k=1}^{N_d} w_k \) remains equal to zero. However, the slip velocity root mean square \( w'' \) evolves toward a stationary value \( w''_\infty \) corresponding to their equilibrium with the surrounding gas. Because particles are initially randomly distributed in the computational domain with a null velocity, \( w''/u' \) is equal to one at time \( t = 0 \), \( u' \) stand for the r.m.s. of the gas velocity. Then, depending on particle Stokes number, \( u'' \) reaches a steady state (Fig. 2-(a)) in less than \( 0.2 \tau_0 \) (eddy turn over time) for small Stokes number \( (St = 0.35) \) and no more than \( 1 \tau_0 \) are needed for larger values \( (St = 7) \). This aspect is an important point because, in more complex configurations like combustion chambers, even if delays are short, droplets are most certainly already in equilibrium when evaporation takes place. In figure 2-(b) are plotted the final mean stationary values of the slip velocity rms : \( w''_\infty \). It starts from zero when droplets are small enough to follow all the velocity fluctuations of the flow and it increases regularly to reach asymptotically the unity that would correspond to droplets too heavy to be moved by the carrier phase \( (St = \infty) \).
To study the preferential concentration of discrete particles in turbulent flows several approaches were used, see for instance [4, 5, 6, 7]. In this study droplets dispersion and preferential segregation have been analyzed from an Eulerian point of view thanks to the local liquid density $\xi(x,t)$. Instantaneous fields of $\xi$ have been plotted in figure 3 for three Stokes numbers ($St = 0.17$, $St = 1.05$ and $St = 5.6$) along with the corresponding vorticity field. These four fields have been captured at exactly the same time after droplet dispersion has reached a stationary value ($t > t_\infty$). Without any statistical analysis, it is possible to notice the dramatic impact of the particle inertia on their dispersion properties. In fact, even with a small Stokes number, particles tend to leave vortex cores and segregates in weak vorticity areas because of their inertia. This phenomenon may be seen in figure 3-(b) and -(c) where $\xi$ is represented for $St = 0.17$ and $St = 1.05$. This last case shows a normalized liquid density $\xi/\bar{\xi}_0$ ranking between 0 (no droplets) and 5 (five times the mean density). As it will be shown later, density fluctuations reach a maximum when $St = 1$. When $St = 0.17$, segregation is already clearly visible (maximum : 2.5) although there is more intermediates density areas (Fig. 3-(b)). When the $St = 1$ limit is 'broken', the spray topology tends to be totally different than for $St \leq 1$, see Fig. 3-(d). Indeed, kinetic times become large enough for the

Figure 3: (a) Carrier phase vorticity $\tau_0 \sqrt{\omega^2}$ and spray concentration areas $\xi/\bar{\xi}_0$, (b) $St = 0.17$, (c) $St = 1.05$, (d) $St = 5.6$.  

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droplets to cross high vorticity areas leading to a less segregated spray (maximum : 2.5).

The Stokes number dependence of the non-evaporating droplets mean stationary segregation \( \xi'_\infty \) has been plotted in figure 4-(a). As defined above, this parameter is the standard deviation of the field \( \xi \) when droplet are in dynamical equilibrium with the carrier phase (\( t > t_\infty \)). Starting from \( St = 0.17 \) with \( \xi'_\infty/\xi_0 = 0.8 \), a maximum segregation \( \xi'_\infty/\xi_0 = 1.4 \) is observed for a unitary Stokes number before a progressive decay. This parameter informs us on the liquid density level in clusters formed by turbulence. It is also possible to determine their corresponding characteristic size by computing the energy spectrum \( E_\xi(\kappa) \) of the variable \( \xi(x, t) \) when \( t > t_\infty \) and then compute \( l_\xi = 2\pi/\kappa_\xi \) where \( \kappa_\xi \) is the position in spectral space of the most energetic (or fluctuating, in physical space) level. Plotting the \( l_\xi \) dependence with the Stokes number in figure 4-(b) demonstrates the large scale effects of the turbulence on the spray. Information about mean segregation parameter \( \xi'_\infty \) is not sufficient to characterize spray preferential segregation. Indeed for two sprays whose Stokes numbers are 0.17 and 5.6, respectively, a similar mean segregation level equals to 0.8 is found in figure 4-(a) whereas the mean size of the clusters compared to the turbulence integral scale are respectively equal to 0.25 and 0.68. Thus, even if fluctuations levels are similar, liquid density topology is different.

### 3.2 Evaporation and turbulent mixing

Once dynamic equilibrium is reached between the turbulent gaseous flow and the spray of droplets, the evaporation is activated. The amount of vapour of fuel in the gas phase is characterized by mixture fraction \( Z \). Three cases are chosen that correspond to three initial Stokes numbers. They are recapitulated in table 1, cases \( B_\ast \) has a Stokes number close to unity hence segregation is maximum, cases \( A_\ast \)
Figure 5: Evolution of mixture fraction statistics in the domain, characteristic evaporation time: $0.5\tau_0$. Left: mean mixture fraction, right: deviation.

Table 1: Configuration names, $St$ : Stokes number, $\tau_v$ : evaporation delay. Non evaporating case: $\tau_v = \infty$.

<table>
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<th>$St = 0.17$</th>
<th>$St = 1.05$</th>
<th>$St = 5.6$</th>
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<tbody>
<tr>
<td>$\tau_v = \infty$</td>
<td>A</td>
<td>B</td>
<td>C</td>
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<tr>
<td>$\tau_v = 1/2\tau_0$</td>
<td>A$_1$</td>
<td>B$_1$</td>
<td>C$_1$</td>
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<tr>
<td>$\tau_v = 1\tau_0$</td>
<td>A$_2$</td>
<td>B$_2$</td>
<td>C$_2$</td>
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<td>$\tau_v = 2\tau_0$</td>
<td>A$_3$</td>
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and $C_*$ correspond respectively to moderately low and high Stokes numbers. Their initial segregation are about the same initially (figure 4-(a)). The evaporation is studied first in case ($A_1$, $B_1$ and $C_1$) where evaporation delay is equal to $0.5\tau_0$.

The evolution of the mixture fraction normalized by the saturation value is represented in figure 5-(a). It is clear from this figure that the most segregated case ($B_1$) takes the longest time to be evaporated. The clusters that contain a high number density of droplets are transformed in pockets of high vapour concentration. Since the surrounding vapour concentration can be close to its saturation value, the vapour flux leaving the droplet surface is reduced. Thus the evaporation rate decreases for each droplet located in a cluster. It is even stopped if saturation value of vapour concentration is reached in the cluster. Droplets can be evaporated if they are ejected from the cluster by turbulent motion to reach a place where vapour concentration is low enough. Concerning droplets that stay in the cluster, they evaporate only at a rate that permit to sustain the vapour concentration in the cluster at the saturation value.

The standard deviation of the normalized mixture fraction is shown for the three cases in figure 5-(b). Case $C_1$ clearly evolves from case $A_1$ to case $C_1$. Assuming that mixture fraction fluctuations of the variable $Z$ are mainly due to the presence
of clusters, it confirmed that clusters segregation of case $C_1$ is initially similar to case $A_1$ and then, they become similar to case $B_1$ as the Stokes number is reduced from 5.7 to 1 and lower. This effect may be imputed to the evaporation time that is chosen lower than the time necessary for clusters formation by preferential concentration effect. From figure 2-(a) it can be seen that the spray relaxation time based on initial Stokes number is respectively $0.12\tau_0$, $0.3\tau_0$ and $0.8\tau_0$ for case $A$, $B$ and $C$ to be compared with the evaporation time equal to $0.5\tau_0$.

Normalized evolution of $\xi'$ is shown in figure 6-(a) to characterize segregation rate. Choice has been made to plot results for an evaporation time equal to $2\tau_0$ to clearly show the impact of the evaporation on the droplet segregation. The general trend is a decrease of the segregation level during evaporation; this is due to the mean diminution of the droplet number. But it is possible to notice that for the case $C_3$ segregation is increased first and then decrease. Initial increase of segregation level is due to the evolution of the Stokes number to a level more efficient (close to
the unity) to create cluster. Eventually the segregation level is even bigger for case $C_3$ than for case $B_3$.

Figure 6-(b) shows evolution of the Stokes number averaged on the entire set of droplets not yet evaporated for the three cases. Because droplet sizes decrease due to the evaporation, all Stokes numbers decrease. As shown previously, the most efficient Stokes number for the preferential concentration effect is of the order of unity. For cases $A_3$ and $B_3$, as their Stokes numbers evolve, the preferential concentration effect diminishes. That means that droplets can be ejected from their clusters by turbulence dispersion to be surrounded by vapor-less gas where they are able to evaporate quickly. On the contrary, for case $C_3$, as soon as the mean stokes number is reduced and becomes closer to unity, segregation increases and droplets are ejected from zones of high vorticity to join existing clusters. This explains the initial increase of the segregation; the maximum of segregation is obtained for the dimensionless time equal to unity (see figure 6-(a)). This value corresponds exactly to the end of the period when Stokes number is around the unity, the more effective value for preferential concentration effect (see figure 6-(b)).

The evolution of the mean droplet surface divided by its initial value is shown in figure 7-(a) for the three cases. An additional curve, represented by circle symbols, shows the expected evolution that would be obtained if homogeneously distributed droplets (no clusters) were evaporating in a quiescent flow. Then, evaporation is close to a "d-square" law although the curve is not completely straight since the mean value of the vapor concentration seen by each droplet is not anymore constant but increases as the spray is evaporated. In this case, vapor concentration seen by each droplet is the mean value of vapor over the whole domain. Figure 7-(a) shows the important effect of clusters on the evaporation. Even for the smallest droplets (case $A_1$), an additional time is necessary to complete the evaporation because some droplets are trapped in clusters and cannot be evaporated until they are dismantled.

A possible scenario of evaporation would be: 1) initially the evaporation is very fast since no vapor concentration prevents it. 2) But soon clusters containing a high number density of droplet reach a vapor concentration close to saturation. It reduces dramatically the evaporation rate of the droplets inside the cluster. 3) Droplets leave the saturated area: 3a) they are close to the cluster boundary and because of vapour diffusion, local vapor concentration is lower than the saturation level; 3b) or the turbulent motion ejects the droplet from the cluster, this phenomena is more likely as the droplet Stokes number is large. This scenario is described in figure 7-(b).

References


