Direct numerical simulation, analysis, and modeling of the evaporation of multiple fuel droplets in a hot turbulent flow

By C. Duwig†, G. Lupo†, A. Gruber‡, L. Brandt†¶, P. B. Govindaraju, T. Jaravel AND M. Ihme

We perform and analyze a direct numerical simulation (DNS) of more than 14,000 spherical droplets evaporating in a hot turbulent channel flow. Four-way coupling of the droplet motion with the turbulent carrier phase and interface-resolved evaporation dynamics allow us to draw a qualitative and quantitative comparison with a large-eddy simulation coupled with lagrangian particle tracking (LES/LPT) of the same flow configuration, pointing out the mechanisms that cause the latter method to deviate from the DNS.

1. Introduction
Evaporation of liquid fuel is common in most energy and propulsion systems, with a decisive impact on flame stabilization and chemical emissions. With the rise of alternative fuels for power generation and transport applications, new challenges are encountered in the design and engineering of stable, reliable, and low-emission fuel injectors and burners. Despite its industrial importance, droplet evaporation in hot turbulent flows has not yet been thoroughly explored, and the scientific community lacks detailed understanding of its complex physics. Traditional optical measurement techniques are affected by reflections on the interface and fail to provide sufficient insight to build models. Computational studies have been limited to single-phase turbulent flows, where droplets are represented as point particles without consideration of mutual interactions, due to computational limits and lack of adequate numerical methods. The last restriction has recently been lifted, and some new techniques have shown promising capabilities for accurately capturing dispersed particle flows, with researchers from the Linné FLOW Centre at KTH, Sweden, among the most active actors (Lupo, 2017; Niazi Ardehani et al., 2018).

This study aims to take these new methods one step further and address droplet transport and heat exchange in a turbulent flow with simultaneous evaporation. Some of the remaining fundamental questions are the following: How do droplets cluster during evaporation in a turbulent flow? How do turbulence and global mass transport affect local droplet evaporation? How do we model evaporation/turbulence interaction? How do we model droplet/droplet interaction during evaporation?

Our objective is to contribute to answering these four questions by analyzing the database obtained within the HeTS (heat and mass transfer in dilute spray) project and featuring direct numerical simulation of multiple-droplet evaporation in a hot turbulent channel flow.

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A1 All physical and transport properties are constant.
A2 The flow is incompressible.
A3 Gravity is neglected.
A4 Droplets remain spherical.
A5 The fluid motion inside the droplets is neglected.
A6 Temperature is uniform on the droplet surface.
A7 The gas phase is ideal.
A8 The inert gas is insoluble in the liquid phase.
A9 Thermodynamic equilibrium prevails at the droplet surface.
A10 The surface tension effect on vapor pressure (Kelvin effect) is neglected.
A11 Viscous dissipation is neglected.
A12 Soret and Dufour effects are neglected.

Table 1. Assumptions.

2. Presentation of the HeTS database
As a milestone towards the numerical computation of realistic turbulent evaporating sprays, we have performed the first DNS of a turbulent channel flow that includes interface-resolved heat and mass exchange with a dispersed phase consisting of more than 14,000 droplets. The endeavor has been framed in the HeTS project.

2.1. Presentation of the DNS-IBM method
We perform the DNS with our KTH in-house immersed boundary method (IBM) code (Lupo, 2017). The method solves for spherical droplets of varying size in a dilute spray, which is typical for a large range of engineering applications. The a-priori knowledge of the droplet shape makes the method computationally cheaper than other multiphase techniques such as volume of fluid or level set. The underlying assumptions are listed in Table 1.

The governing equations for the gas phase are the Navier-Stokes equations, the energy equation, and the transport of the vapor species, which written in non-dimensional form read

\[ \nabla \cdot \mathbf{u} = 0, \quad (2.1) \]

\[ \frac{\partial \mathbf{u}}{\partial t} = -\mathbf{u} \cdot \nabla \mathbf{u} - \nabla p + \frac{1}{Re} \nabla^2 \mathbf{u}, \quad (2.2) \]

\[ \frac{\partial T}{\partial t} = -\mathbf{u} \cdot \nabla T + \frac{1}{Re Pr} \nabla^2 T + \frac{\phi \Delta c_p}{Re Sc} \nabla T \cdot \nabla Y, \quad (2.3) \]

\[ \frac{\partial Y}{\partial t} = -\mathbf{u} \cdot \nabla Y + \frac{1}{Re Sc} \nabla^2 Y. \quad (2.4) \]

The cross-transport term in Eq. (2.3) is the net enthalpy diffusion due to species diffusion. The liquid phase is treated with global mass and energy balances for each droplet, which give the equations for the droplet radius and temperature, and the Newton-Euler equations for the droplet motion

\[ \frac{dr_s}{dt} = -\frac{\dot{m}}{4 \pi r_s^2 \phi_p}, \quad (2.5) \]

\[ \frac{dT_s}{dt} = g_1(r_s, \dot{r}_s, T_s, t) - g_2(r_s, t) \frac{3 \left( \frac{\dot{q}}{\phi_c} + \frac{\dot{m}}{Ste} \right)}{4 \pi r_s^4 \phi_p}, \quad (2.6) \]
where \( x_c, u_c \), and \( \omega_c \) are the position, velocity, and angular spin velocity of the droplet centroid, respectively, while \( g_1 \) and \( g_2 \) are corrections that account for the fact that temperature is not uniform inside the droplet (Lupo, 2017).

The boundary conditions at the droplet surface (\(|x - x_c| = r_s\)) state the thermodynamic equilibrium and the Stefan flow caused by evaporation. They are uniform (assumptions A4 and A6 in Table 1) and are written as

\[
\begin{align*}
\dot{u} &= u_c - (\phi_p - 1) \frac{dr_s}{dt} n, \\
T &= T_s, \\
Y &= \frac{P_{sat}(T_s)}{P_{tot}}.
\end{align*}
\]

Finally, the heat and mass transfer rates are specified by integrating the fluxes over the droplet surface \( S(t) \)

\[
\begin{align*}
\dot{m} &= \int_S \left( -\frac{1}{ReSc} \nabla Y + uY \right) \cdot n dS, \\
\dot{q} &= \int_S \left( -\frac{1}{RePr} \nabla T \right) \cdot n dS.
\end{align*}
\]

The enforcement of the boundary conditions in Eqs. (2.9)-(2.11) relies on our implementation of the immersed boundary technique (Lupo, 2017): it is an adaptation of the direct forcing developed by Breugem, (2012), to which the following source terms have been added in order to mimic mass, energy, and vapor species inlets that are consistent with the boundary conditions

\[
\begin{align*}
s_{ijk,U} &= -\frac{dr_s \phi_p}{dr_s} \left[ 1 + \cos \left( \frac{\pi r_s}{r_s} \right) \right], \\
s_{ijk,T} &= s_{ijk,U} \left( 1 - \frac{c_p, vap}{c_p} \right) T, \\
s_{ijk,Y} &= s_{ijk,U},
\end{align*}
\]

where \( r_{ijk} = |x_{ijk} - x_c| \) for each Eulerian cell. The source terms are distributed inside the droplet volume and vanish in the gas phase, going smoothly to zero for \( r \rightarrow r_s \).

A second-order central difference scheme is used for spatial discretization. Time integration is performed with a three-step Runge-Kutta scheme.
Table 2. Computational domain and operating conditions.

<table>
<thead>
<tr>
<th>Description</th>
<th>Value</th>
<th>Units</th>
<th>Description</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>(d_0) Droplet initial diameter</td>
<td>80</td>
<td>μm</td>
<td>(N_d) Droplet number</td>
<td>14,081</td>
<td>–</td>
</tr>
<tr>
<td>(L_x/d_0) Streamwise channel length</td>
<td>120</td>
<td>–</td>
<td>(L_y/d_0) Wall normal channel length</td>
<td>32</td>
<td>–</td>
</tr>
<tr>
<td>(L_z/d_0) Spanwise channel length</td>
<td>48</td>
<td>–</td>
<td>(N_x) Streamwise resolution</td>
<td>2304</td>
<td>–</td>
</tr>
<tr>
<td>(N_y) Wall normal resolution</td>
<td>768</td>
<td>–</td>
<td>(N_z) Spanwise resolution</td>
<td>1152</td>
<td>–</td>
</tr>
<tr>
<td>(N_l) Lagrangian points per droplet</td>
<td>1721</td>
<td>–</td>
<td>(T_{\infty}) Initial gas temperature</td>
<td>741</td>
<td>K</td>
</tr>
<tr>
<td>(T_{d_0}) Initial droplet temperature</td>
<td>343</td>
<td>K</td>
<td>(P_{\infty}) Thermodynamic gas pressure</td>
<td>1 atm</td>
<td>–</td>
</tr>
</tbody>
</table>

Table 3. Non-dimensional flow parameters.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Definition</th>
<th>Value</th>
<th>Parameter</th>
<th>Definition</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>(Re)</td>
<td>(UL_x/\nu)</td>
<td>5600</td>
<td>(Pr)</td>
<td>(\nu/\alpha)</td>
<td>0.7899</td>
</tr>
<tr>
<td>(Sc)</td>
<td>(\nu/D_{vap})</td>
<td>1.6326</td>
<td>(\phi_p)</td>
<td>(\rho_l/\rho)</td>
<td>32</td>
</tr>
<tr>
<td>(\phi_{cp})</td>
<td>(c_{p, vap}/c_p)</td>
<td>2.2</td>
<td>(\phi_{\alpha})</td>
<td>(\alpha_l/\alpha)</td>
<td>0.00282</td>
</tr>
<tr>
<td>(\phi_{\Delta cp})</td>
<td>(c_{p, vap} - c_{p, inert}/c_p)</td>
<td>0.98</td>
<td>(Ste^{-1})</td>
<td>(\lambda_l/c_{p, T_{\infty}})</td>
<td>0.50538</td>
</tr>
</tbody>
</table>

2.2. Presentation of the flow case

The numerical setup reproduces a channel flow of n-heptane spray in nitrogen. The channel walls are adiabatic, and the domain is periodic in the streamwise and spanwise directions (the streamwise Reynolds number is maintained by a body force in the momentum equation that linearly corrects the streamwise bulk velocity at every time step). Table 2 shows the details of the computational setup. The droplet diameter is chosen such that the droplet Weber number is less than unity (assumption A4 in Table 1). The Eulerian grid resolution and number of Lagrangian points on the droplet surface are chosen in order to guarantee that the droplet initial diameter is resolved by 24 computational points, thus ensuring that both the turbulence in the gas phase and the transport at the droplet interface are fully resolved. The number of droplets gives an initial liquid volume loading of 5%.

The non-dimensional parameters that characterize the momentum, species, and energy balances are shown in Table 3. Aside from \(\phi_{\Delta cp}\), the quantities denoted by \(\phi\) define the ratios between liquid and gas properties. The density ratio of 32 is chosen artificially in order to speed up the convergence of the droplet migration, while still residing in the inertial regime of droplet motion. \(\phi_{\Delta cp}\) accounts for the different heat capacity of vapor and inert gas, which generates enthalpy diffusion in the gas mixture following concentration gradients. The Stefan number \(Ste\) is a measure of the latent heat of evaporation.

3. LES/LPT tool

We perform an LES that reproduces the DNS case. The simulation of evaporating droplets is coupled with the flow solver using the LPT approach, which has been widely utilized
DNS of spray evaporation in hot turbulent channel flows in multiphase flow computations (Riley & Patterson, 1974; Squires & Eaton, 1990). This approach assumes a Lagrangian description of the particles and solves the equations of motion to track their position, mass, and momentum. In contrast to the Eulerian approach, there is no assumption of the existence of unique field representations for particle velocity, which implicitly restricts the maximum Stokes number that can be considered for the dispersed phase. Furthermore, the size of each particle is independent; thus, polydispersity can be handled easily. The coupling of the Lagrangian particles back to the carrier phase is also taken into account, making this a two-way coupled approach.

3.1. Presentation of the LES/LPT method

The LES was performed using the Stanford in-house solver 3DA, a low-Mach-number limit, structured code (Desjardins et al., 2008). A QUICK scheme is used for the discretization of the scalar advection operators, and a second-order central difference scheme is used for solving the conservation equations, in combination with the HYPRE library for solving the Poisson equation. Time integration is performed using a second-order Crank-Nicolson scheme. The hydrodynamic force from all the particles within a cell is distributed to the neighboring grid points using a three-point Gaussian kernel.

The underlying assumptions are the same as in Table 1, except for gas compressibility. The LES/LPT approach solves the governing equations in their dimensional form. The gas-phase calculation is performed for the same quantities as in the DNS, obeying the following equations

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = \dot{S}_m, \tag{3.1}
\]

\[
\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \nabla \cdot \left\{ \mu \left[ \nabla \mathbf{u} + \nabla \mathbf{u}^T - \frac{2}{3} (\nabla \cdot \mathbf{u}) \mathbf{I} \right] + \dot{S}_m \right\} + \dot{S}_a, \tag{3.2}
\]

\[
\frac{\partial (\rho c_T)}{\partial t} + \nabla \cdot (\rho c_T \mathbf{u}) = \nabla \cdot (\kappa \nabla T) + \dot{S}_T, \tag{3.3}
\]

\[
\frac{\partial (\rho Y)}{\partial t} + \nabla \cdot (\rho \mathbf{u} Y) = \nabla \cdot (\rho D_{vap} \nabla Y) + \dot{S}_m, \tag{3.4}
\]

where \(\dot{S}_m, \dot{S}_a,\) and \(\dot{S}_T\) are the source terms of mass, momentum, and energy, respectively, associated with the droplets and described by Vié et al., (2015). The subgrid closure for Eqs. (3.1)-(3.4), when filtered on the LES grid, is the Germano model (Germano et al., 1991).

The dispersed liquid droplets are described by a Lagrangian point-particle method (Miller et al., 1998), and the governing equations for each droplet can be written as

\[
\frac{d\mathbf{u}_d}{dt} = f_1 \left( \frac{\mathbf{u}_g - \mathbf{u}_d}{\tau_d} \right), \quad \frac{d\mathbf{x}_d}{dt} = \mathbf{u}_d, \tag{3.5}
\]

\[
\frac{dm_d}{dt} = -\frac{Sh}{3Sc} \frac{m_d}{\tau_d} \ln \left( \frac{1 - Y_d}{1 - Y_d} \right), \tag{3.6}
\]

\[
\frac{dT_d}{dt} = \frac{Nu}{3Pr} \frac{c_p g f_2}{\tau_d} (T_g - T_d) + \frac{\lambda_d}{m_d c_p} \left( \frac{dm_d}{dt} \right), \tag{3.7}
\]

where \(x_d, \mathbf{u}_d, m_d,\) and \(T_d\) are the droplet position, velocity, mass, and temperature, respectively. \(Y_d\) is the vapor mass fraction in thermodynamic equilibrium with liquid at temperature \(T_d.\) \(\tau_d\) is the droplet relaxation time given by \(\tau_d = \rho_d d^2/18 \mu_g,\) with \(\rho_d\) the
liquid density, \(d\) the droplet diameter, and \(\mu_g\) the gas viscosity. \(u_g, T_d,\) and \(Y_d\) represent the gas velocity, temperature, and vapor mass fraction at the droplet location. \(Nu\) and \(Sh\) are the Nusselt and Sherwood numbers, respectively. \(f_1\) accounts for deviations from Stokes drag, and \(f_2\) represents the Nusselt number correction due to evaporation; these corrections, as well as expressions for \(Nu\) and \(Sh\), are discussed by Miller et al., (1998).

To ensure a consistent comparison between both simulations, thermophysical properties were frozen to the values used in the DNS.

3.2. Presentation of the flow case

On the basis of the DNS case in Section 2.2, a channel flow setup is simulated using a \(48 \times 96 \times 32\) non-uniform grid with adiabatic walls, and periodic in the streamwise and spanwise directions. The streamwise Reynolds number is maintained with a body force, similarly to the DNS. The grid is stretched near the walls, using a hyperbolic tangent profile \((y^+ = 0.93\) for the first cell at the wall). A preliminary single-phase channel flow simulation at \(Re_\tau = 180\) was performed, and the unresolved turbulent kinetic energy was found to be below 0.1%, well in agreement with Pope’s criterion (Pope, 2004). For the droplet-laden simulation, to ensure consistency, the field from the DNS was interpolated onto the LES grid for all quantities to create the initial profile.

4. Results

4.1. Analysis of the DNS data

The analysis of the dispersed-phase statistics shows a remarkable migration of the droplets toward the channel center. Figure 1 shows the local droplet distribution as a function of wall distance and time. The dynamics of the migration are shown in Figure 2(a,b) in terms of the droplet wall normal mean velocity and velocity fluctuation, respectively, as functions of wall distance and time. The droplets undergo a velocity reversal, drifting toward the wall in the beginning but turning toward the centerline soon after. The diminished wall normal velocity fluctuation at the centerline locks the droplets in the central region once they have reached it.

The droplet migration is closely interlinked with turbulent modulation of the gas phase. The comparison of the asymptotic gas velocity root mean square profiles, shown in Figure 3, to those of the single-phase turbulent channel with the same friction Reynolds number \((Re_\tau = 180\) (Moser et al., 1999), shows that the turbulence level is damped by
the droplets. The higher streamwise velocity fluctuation in the middle of the channel is not turbulence in the gas, but is rather due to the increasing sampling by the gas velocity of the passing liquid droplets and droplet wakes, which gather in the central region.

The centerline migration strongly affects the evaporation dynamics: as the middle region gets saturated with fuel vapor, the concentration gradients at the gas-liquid interface become weaker; moreover, the formation of a local high liquid loading area, characterized by higher heat capacity and thermal inertia, hampers the heat transfer from the gas to the liquid phase, and the droplets cool down by latent heat of vaporization. The net effect is a suppression of the global evaporation rate and the local appearance of condensation events ($\dot{m} > 0$), as shown in Figure 4, which compares the droplet evaporation rate distribution and liquid volume fraction averaged within two different time windows, at the beginning and end of the DNS run. Figure 5 shows the joint probability distribution of droplet evaporation rate and droplet distance from the wall for the final period of the DNS. While the majority of the droplets are clustered in the central region and exhibit a rather homogeneous evaporation rate, a tail of stronger evaporation is found for the droplets close to the wall.

4.2. A-priori analysis of the LPT closures

The LES/LPT framework invokes closures at two levels: the LES subgrid turbulent fluxes and the heat and mass exchange associated with the LPT material points. The interaction between the two closure levels is one way, and limited to the droplet Reynolds number, a
function of the local turbulence, which impacts the LPT fluxes. We can identify \emph{a-priori} three aspects where the LES/LPT framework is lacking: the feedback of the droplet motion on the turbulence, the droplet/droplet interaction, and the parameterization of the LPT closure based on gas flow field quantities.

The first two arise from the coupling between the two phases in the LES/LPT, and call for efforts to include the modelling of four-way coupling effects in the LES/LPT, which indirectly affect the evaporation dynamics, as pointed out in Section 4.1. The last issue is a consequence of the coarse-grained approach of the LES, where the droplet interface is not resolved: the LPT closure must thus resort to film theory for modeling the heat and mass exchange between the continuous and dispersed phases. This introduces the dependence on the gas field values at a hypothetically infinite distance from the droplet, which in the LES/LPT framework are naturally chosen as the values in the Eulerian

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure4.png}
\caption{Comparison between initial and final periods of the DNS. (a) Local liquid volume fraction as a function of the wall distance and (b) probability density function (PDF) of the droplet evaporation rate.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure5.png}
\caption{Joint probability density function (PDF) of droplet evaporation rate and droplet wall distance, normalized with the number of droplets in each wall normal bin, for the final phase of the DNS run ($t = [1.76 \times 10^{-3}, 3.11 \times 10^{-3}]$ s).}
\end{figure}
cell inhabited by the droplet. This is arbitrary, and furthermore neglects any influence of higher-order quantities such as local gradients on the evaporation dynamics.

4.3. Comparison of DNS versus LES/LPT data

Figure 6 compares mean and standard deviation of the droplet diameter between the DNS and the LES/LPT. As expected, after an initial stage, where the trend is similar, the LES/LPT deviates from the DNS solution, over-predicting the evaporation rate, as a consequence of not being able to capture the liquid-phase migration and turbulence modulation of the gas stream, with the associated effects on the phase change dynamics discussed above.

The erroneous prediction of the turbulent intensity renders incongruous the Sherwood number correlation, used in the LPT as a closure for the effect of turbulence on the evaporation rate, as illustrated in Figure 7.

5. Conclusions

We have performed a DNS of evaporation of a large number of droplets in a turbulent channel flow, and compared it to an LES with LPT modeling of the dispersed phase.
The comparison shows that finite-size effects of inertial droplet motion and interaction with the bulk flow turbulence strongly affect the evaporation dynamics. LES/LPT will continue to be, for the foreseeable future, the only affordable approach to numerical simulations of sprays with phase change and/or reaction in realistic flow configurations. Therefore, future work on the improvement of LES/LPT closures must strive toward the inclusion of finite-size effects in the models for momentum and energy coupling of the continuous and dispersed phases.

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