Large-eddy simulation of an evaporating and reacting spray

By T. Lederlin and H. Pitsch

1. Motivation and objectives

1.1. Evaporative spray modeling for large-eddy simulation (LES)

In a combustion chamber simulation, filling the gap between injection of liquid fuel and combustion modeling resides in the proper calculation of two-phase flow phenomena, which are basically atomization of a liquid fuel sheet, droplet interactions and fuel vaporization. In this report, we will focus on the last two topics, which constitute spray modeling. A preliminary analysis of the flame resulting from this spray will also be given.

The simulations presented here are performed with the unstructured code CDP, developed at the Center for Turbulence Research. The Favre-filtered LES equations for the gas phase are solved for a low-Mach number, variable-density, reacting flow of a mixture of fuel vapor and oxidant, with mixture fraction \( \bar{Z} \), and two-way coupling between the gas and liquid phase (the description of the combustion model is presented in Sec. 1.3):

\[
\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \bar{u}_j}{\partial x_j} = \bar{S}_m,
\]

\[
\frac{\partial \bar{\rho} \bar{Z}}{\partial t} + \frac{\partial \bar{\rho} \bar{u}_j}{\partial x_j} \left( \frac{\partial \bar{Z}}{\partial x_j} \right) = \frac{\partial q^2}{\partial x_j} + \bar{S}_Z,
\]

\[
\frac{\partial \bar{\rho} \bar{u}_i}{\partial t} + \frac{\partial \bar{\rho} \bar{u}_i \bar{u}_j}{\partial x_j} = -\frac{1}{V_c} \sum_k \frac{dm_p^k}{dt} \left( \bar{\mu} \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} - \frac{2}{3} \frac{\partial \bar{u}_k}{\partial x_k} \delta_{ij} \right) + \bar{\tau}_{ij} \right) + \bar{S}_i,
\]

where \( \bar{S}_Z, \bar{S}_m \) and \( \bar{S}_i \) are the mass, mixture fraction and momentum source terms, respectively, expressed as

\[
\bar{S}_Z = \bar{S}_m = -\frac{1}{V_c} \sum_k \frac{dm_p^k}{dt}
\]

and

\[
\bar{S}_i = -\frac{1}{V_c} \sum_k \frac{d}{dt} (m_p^k \bar{u}_p^k).
\]

\( k \) is the index of a droplet with velocity \( \bar{u}_p^k \) and mass \( m_p^k \), contained in the control volume \( V_c \). In Eq. (1.3), \( \bar{\tau}_{ij} \) denotes the subgrid stress tensor and is modeled as

\[
\bar{\tau}_{ij} = \bar{\rho} (\bar{u}_i \bar{u}_j - \bar{u}_i \bar{u}_j) = 2 \bar{\mu} \bar{S}_{ij} - \frac{1}{3} \bar{\rho} q^2 \delta_{ij}
\]

with

\[
\bar{\mu} = C_{\mu} \bar{\rho} \Delta^2 \sqrt{\bar{S}_{ij} \bar{S}_{ij}}
\]
and the isotropic part of the subgrid stress \( q_j^2 \) is absorbed into the pressure. In Eq. (1.2), \( q_j^2 \) denotes the subgrid flux of the mixture fraction and is modeled as

\[
q_j^2 = \bar{\rho}(\tilde{u}_j \tilde{Z} - \bar{u}_j \bar{Z}) = \bar{\rho} \alpha \frac{\partial \bar{Z}}{\partial x_j},
\]

(1.8)

with

\[
\bar{\rho} \alpha \bar{Z} = C_\alpha \bar{\rho} \Delta^2 \sqrt{S_{ij} S_{ij}},
\]

(1.9)

The coefficients \( C_\mu \) and \( C_\alpha^Z \) are obtained using the dynamic procedure of Germano et al. (1991).

1.2. Evaporation model of Lagrangian droplets

Droplet dynamics are simulated using a Lagrangian point-particle model, described in greater detail by Apte et al. (2003). It is assumed that (1) the density of the droplets is much greater than that of the carrier fluid, (2) the droplets are dispersed and collisions between them are negligible, (3) the droplets are much smaller than the LES filter width, (4) droplet deformation effects are small and (5) motion due to shear is negligible. Under these assumptions, the Lagrangian equations governing the droplet motion become:

\[
\frac{d\mathbf{x}_p}{dt} = \mathbf{u}_p
\]

(1.10)

and

\[
\frac{d\mathbf{u}_p}{dt} = \frac{1}{\tau_p} \left( \mathbf{u}_{g,p} - \mathbf{u}_p \right) + \left( 1 - \rho_g / \rho_p \right) \mathbf{g},
\]

(1.11)

where \( \mathbf{x}_p \) is the position of the droplet centroid, \( \mathbf{u}_p \) denotes the droplet velocity, \( \mathbf{u}_{g,p} \) the gas-phase velocity interpolated at the droplet location, \( \rho_p \) and \( \rho_g \) are the droplet and gas-phase densities and \( \mathbf{g} \) is the gravitational acceleration. Note that the direct effect of subgrid-scale fluctuations on the particle motion is neglected. This effect might be important in some cases, as shown by Fede & Simonin (2006) or Miller & Bellan (2000), and will be investigated in a subsequent study. The droplet relaxation time scale \( \tau_p \) is given as:

\[
\tau_p = \frac{\rho_p d_p^2}{18 \mu_g (1 + a R_{cp}^b)},
\]

(1.12)

where \( d_p \) is the diameter and \( R_{cp} = \rho_g d_p (\mathbf{u}_{g,p} - \mathbf{u}_p) / \mu_g \) is the droplet Reynolds number. The above correlation is valid for \( R_{cp} \leq 800 \). The constants \( a = 0.15, b = 0.687 \) yield the drag within 5% from the standard drag curve. The Lagrangian equations governing droplet temperature and mass become

\[
\frac{dm_p}{dt} = - \frac{m_p}{\tau_m},
\]

(1.13)

and

\[
\frac{dT_p}{dt} = \frac{1}{\tau_c} \left( T_{g,p} - T_p^* \right) - \frac{1}{\tau_m} \frac{\Delta h_v}{C_{p,l}},
\]

(1.14)

where \( \Delta h_v \) is the latent heat of vaporization, \( m_p \) the mass of the droplet, \( T_p \) its temperature, \( T_p^* \) the temperature at the droplet surface, \( T_{g,p} \) the temperature of the gas phase at the droplet location and \( C_{p,l} \) is the specific heat of the liquid. The diameter of the droplet is obtained from its mass as \( d_p = (6 m_p / \pi \rho_p)^{1/3} \). Here, \( \tau_m \) and \( \tau_c \) are the droplet
lifetime and the convective heating time scale, respectively, expressed by
\[
\frac{1}{\tau_m} = \frac{12}{d_p^2} D^* \ln(1 + B) Sh
\]  
(1.15)
and
\[
\frac{1}{\tau_c} = \frac{12}{\rho_p d_p^2 C_{p,t}^*} \frac{k_s^* \ln(1 + B)}{B} Nu.
\]  
(1.16)
\(D^*\) and \(k^*\) are the mass diffusivity and heat conductivity, respectively. The superscript \(s\) stands for droplet surface, \(Sh\) and \(Nu\) are the Sherwood and Nusselt numbers given by
\[
Sh = 1 + \frac{0.278 Re_p^{1/2} [Sc_s^{1/3}]}{\sqrt{1 + 1.232/Re_p [Sc_s^{1/3}]}}
\]  
(1.17)
and
\[
Nu = 1 + \frac{0.278 Re_p^{1/2} [Pr_s^{1/3}]}{\sqrt{1 + 1.232/Re_p [Pr_s^{1/3}]}}.
\]  
(1.18)
The transfer coefficient \(B\) is obtained as
\[
B = \begin{cases} 
Y^*_F - Y_{F,g,p} (1 - Y^*_F) & \text{if } T_s^* < T_b \\
C_p^* (T_g,p - T_s^*) / \Delta h_v & \text{if } T_s^* \geq T_b 
\end{cases}
\]  
(1.19)
where \(T_b\) is the droplet boiling point and \(Y_{F,g,p}\) the fuel-vapor mass fraction interpolated at the droplet location. The Clausius-Clapeyron equilibrium vapor pressure relationship is used to compute the fuel mass fraction at the droplet surface. Liquid properties are evaluated using the \(1/3\)rd rule for reference mass fractions and temperature. To effectively reduce the number of particles tracked, a hybrid particle-parcel scheme (Dukowicz 1980) is used: The idea behind this approach is to collect all droplets in a particular control volume and group them into bins corresponding to their size and other properties. These bins are then used to create parcels or numerical particles by conserving mass, momentum and energy. This method has been used in this work to speed up the establishment of the flow (with a number of droplets per parcel up to 20) but all the statistics presented in Sec. 3 have been subsequently calculated with 1 particle per parcel.

1.2.1. Locally linearized droplet equations

If the time scale associated with particle motion is small compared to the flow time scale, typically for very small droplets, the frozen-field assumption allows for the simplification of the Lagrangian equations:

(1) Consider the droplet acceleration equation:
\[
\frac{d\mathbf{u}_p}{dt} = \frac{3}{4} C_D Re_p \frac{\mu}{\rho_p d_p^2} \mathbf{u} - \mathbf{u}_p.
\]  
(1.20)

For a locally frozen field (quasi-steady), assume that \(\mathbf{u} \neq \mathbf{u}(t)\). Then let \(\Phi = \mathbf{u} - \mathbf{u}_p\) and \(\tau_p = \frac{4 \rho_p d_p^2}{3 \mu} (C_D Re_p)^{-1}\); this yields
\[
\frac{d\Phi}{dt} + \frac{\Phi}{\tau_p} = 0
\]  
(1.21)
and
\[
\Phi(t_0) = \Phi_0.
\]  
(1.22)
the solution of which is
\[ \Phi(t) = \Phi_0 e^{-(t-t_0)/\tau_p}. \] (1.23)

(2) Consider the droplet mass equation:
\[ \frac{dm_p}{dt} = -\dot{m}_p. \] (1.24)

For a locally frozen field, we assume \( \dot{m} \neq \dot{m}(t) \). By integrating Eq. (1.24) we get
\[ \int_{m_0}^{m} dm = -\int_{t_0}^{t} \dot{m} dt, \] (1.25)
which gives \( m = -\dot{m}(t - t_0) + m_0 \). Then the characteristic time associated with vaporization is obtained when \( m(t) = 0 \) (i.e., \( \tau_l = m_0/\dot{m} = \frac{1}{6} \pi d_p^3 \rho_p / \dot{m} \)) and
\[ m(t) = m(t) \left[ 1 - \frac{1}{\tau_l} (t - t_0) \right]. \] (1.26)

(3) Consider the droplet temperature equation:
\[ \frac{dT_p}{dt} = \frac{h}{m} \frac{\pi d_p^2}{C_p} (T - T_p) - \frac{\dot{m}}{m} \Delta H_v, \] (1.27)
where \( \frac{h}{m} \frac{\pi d_p^2}{C_p} \) and \( \frac{\dot{m}}{m} \) are the heating and droplet-life time scales, respectively. Then Eq. (1.27) becomes
\[ \frac{dT_p}{dt} = \frac{1}{\tau_c} (T - T_p) - \frac{1}{\tau_l} \frac{\Delta H_v}{C_p}. \] (1.28)

Let \( \theta = T - T_p \) and assume a frozen field, \( T \neq T(t) \); this yields:
\[ \frac{d\theta}{dt} + \frac{1}{\tau_c} \theta = \frac{1}{\tau_l} \frac{\Delta H_v}{C_p}, \] (1.29)
with the initial condition \( \theta = \theta_0 \), the solution of which is
\[ \frac{\theta(t) - \frac{\tau_c}{\tau_l} \frac{\Delta H_v}{C_p}}{\Theta_0 - \frac{\tau_c}{\tau_l} \frac{\Delta H_v}{C_p}} = e^{-(t-t_0)/\tau_c}. \] (1.30)

The frozen field assumption becomes valid and is applied at the end of the droplet lifetime.

1.2.2. Thermal two-way coupling

With the flow solver used in this study, only two scalar equations (for mixture fraction \( Z \) and a progress variable \( C \)) are solved and the other scalars, such as temperature and mass fractions, are extracted from a flamelet table parameterized by \( Z \) and \( C \). Thus, the evaporative cooling effect (or reverse thermal coupling) is accounted for during the generation of the flamelet table. In the absence of combustion, a linear relationship between temperature and mixture fraction is sought. For this purpose, as first proposed
by Peters (1992), the droplet is treated as a source of pure fuel vapor \((Z = 1)\) at \(T_1\), with enthalpy \(h_1\), so that

\[
h_1 = h_L = h^0_{f,L} (T_{ref}) + \int_{T_{ref}}^{T_1} C_p L dT,
\]

(1.31)

where the subscript \(L\) denotes the liquid phase and \(h_f\) is an enthalpy of formation. By choosing \(T_{ref} = T_1\), \(h_1\) is simply given by

\[
h_1 = h^0_{f,L} (T_1).
\]

(1.32)

The hypothetical temperature \(T_2\) that would be attained from the total evaporation of the fuel (i.e., until \(Z = 0\)) corresponds to an adiabatic cooling and

\[
h_2 = h^0_{f,vap} (T_1) + \int_{T_1}^{T_2} C_p_{vap} dT.
\]

(1.33)

During this adiabatic process, the enthalpy of the vapor is conserved, so that \(h_1 = h_2\) or

\[
h^0_{f,L} (T_1) = h^0_{f,vap} (T_1) + \int_{T_1}^{T_2} C_p_{vap} dT.
\]

(1.34)

\(C_p_{vap}\) is expressed with a polynomial correlation, which is straightforward to integrate and the enthalpies of formation \(h_f\) at \(T_1\) are taken from tables.

1.2.3. **Validation of the model: evaporation of an isolated droplet**

Before running a full simulation of an evaporating spray, it is interesting to check the accuracy of the evaporation model on a single isolated droplet. The case of a 1-mm Jet-A droplet, initially at 300 K, evaporating in quiescent air at \(P = 1\) atm and different temperatures has been investigated by Harstad & Bellan (2004). The results of their detailed, multi-component model are compared in Fig. 1 with the model used in our code CDP. For the range of temperatures investigated, the difference between both models is smaller than the incertitude of the model of Harstad & Bellan (2004). This validates our model itself as well as the numerical procedure used for thermal two-way coupling, presented in Sec. 1.2.2.

1.3. **Fuel properties and combustion model**

In the experiments, the injected fuel is a commercial aviation kerosene Jet-A, which is a mixture of a large number of hydrocarbons and additives. In the LES calculations, kerosene is modeled by a surrogate, *i.e.*, a single *meta*-species built as a mixture of two major chemical components of kerosene, namely n-decane and tri-methyl-benzene. The thermochemical properties obtained from this surrogate are closed to real kerosene properties and are summarized in Table 1. The chemical kinetic mechanism involves 1171 reactions between 132 species (Peters 2006).

In CDP, turbulent combustion is modeled through an indirect mapping, whereby all the thermochemical variables are assumed to be functions of two tracked scalars: mixture fraction \(Z\) that describes mixing of the reactants and a progress variable \(C\) for the extent of reaction (Pierce & Moin 2004). The transport equations for \(Z\) and \(C\) are, respectively, Eq. (1.2) and

\[
\frac{\partial \rho \hat{C}}{\partial t} + \frac{\partial}{\partial x_j} (\rho \hat{C} \hat{u}_j) = \frac{\partial}{\partial x_j} \left( \rho \alpha \frac{\partial \hat{C}}{\partial x_j} \right) + \frac{\partial h^C_f}{\partial x_j} + \rho \hat{\omega}_C,
\]

(1.35)
Figure 1. Evaporation time of an isolated 1-mm Jet-A droplet at 1atm.

<table>
<thead>
<tr>
<th>Composition</th>
<th>Molar weight</th>
<th>Boiling temperature</th>
<th>Liquid density</th>
<th>Heat of vaporization</th>
<th>Liquid heat capacity</th>
</tr>
</thead>
<tbody>
<tr>
<td>80% of n-decane</td>
<td>165 g/mol</td>
<td>606.5 K</td>
<td>781 kg/m³</td>
<td>2.5 × 10⁵ J/kg</td>
<td>2 × 10³ J/kg/K</td>
</tr>
<tr>
<td>20% tri-methyl-benzene</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 1. Summary of surrogate fuel properties.

where \( q_C \) is obtained with the procedure shown in Eqs. (1.8) and (1.9) and \( \tilde{\omega}_C \) is the filtered reaction rate, obtained from:

\[
\tilde{\omega}_C = \int \omega_C(Z,C) \tilde{P}(Z,C) dZ dC. 
\] (1.36)

2. Configuration and boundary conditions

The experimental rig MERCATO is a swirled combustor fed with air and Jet-A liquid fuel. Its features and geometry are shown in Fig. 2. The regimes considered here are presented in Table 2. The flow conditions are different for the reacting and non-reacting cases. For Case II (non-reacting), the air is heated to 463 K to enhance evaporation and reduce the formation of liquid fuel films on the visualization windows. Cases I and II are operated at the same air inlet temperature and with the exact geometry displayed in Fig. 2. For these two cases the flow exits in the atmosphere, while for Case III an additional exhaust pipe is added after the combustion chamber. For Cases I and II, the comparison is performed for the mean and root mean square (RMS) velocity fields of the gas and (for Case II) of the droplets. For Case III, the droplet velocity field and the flame position will be used for comparison. In non-reacting Cases I and II, velocities and size measurements were performed using PDA-LDA. For Case III, droplet velocities are measured using PIV.
LES of spray

Figure 2. The MERCATO configuration (ONERA Toulouse).

<table>
<thead>
<tr>
<th>Case</th>
<th>Pressure (atm)</th>
<th>Air temperature (K)</th>
<th>Liquid flow rate (g/s)</th>
<th>Fuel flow rate (g/s)</th>
<th>Equivalence ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>I: gaseous flow</td>
<td>1</td>
<td>463</td>
<td>–</td>
<td>15</td>
<td>–</td>
</tr>
<tr>
<td>II: gaseous flow + droplets</td>
<td>1</td>
<td>463</td>
<td>300</td>
<td>15</td>
<td>1.0</td>
</tr>
<tr>
<td>III: reacting two-phase flow</td>
<td>1</td>
<td>285</td>
<td>285</td>
<td>26</td>
<td>2.9</td>
</tr>
</tbody>
</table>

Table 2. Summary of regimes.

2.1. Droplet injection

The injection boundary conditions are based on a methodology which takes into account radial, tangential and axial outflow velocity components. Following the empirical correlations of Rizk & Lefebvre (1985), inlet profiles are built from the following parameters: the liquid flow rate, the spray angle and the internal geometry of the Simplex atomizer. For the Lagrangian solver used in CDP, the initial droplet diameter is sampled from a Rosin-Rammler distribution fitted with the experimental probability density function (pdf) of droplet diameters at the first measurement location ($z = 6$ mm). The sampling technique uses the inverse of the Rosin-Rammler cumulative density function. In the case of a more complicated initial experimental distribution, any pdf can be fitted with an acceptance-rejection technique. Both techniques give an accurate result, as shown in Fig. 3.

The droplets are assumed to bounce elastically at the walls and to disappear as soon as they cross the outlet plane.
3. Results

3.1. Case I: non-reacting gas phase

The results show a very good agreement with experimental data for the mean and rms values of the three components of velocity. These results have been presented extensively in the work of Sanjosé et al. (2008) and will not be discussed further here.

3.2. Case II: non-reacting liquid phase

The mean and rms axial velocities of droplets are shown in Fig. 4 and compared with laser-Doppler anemometry (LDA) measurements, at three axial distances from the combustor inlet. The spray angle and the axial velocity are almost perfectly captured by the LES.

Figures 5 and 6, respectively, display the azimuthal and radial components of the mean and rms velocities. In both cases, the mean values are globally good close to the injector nose ($z = 6\text{mm}$). The azimuthal velocity exhibits a good tendency downstream as well as the correct values for the fluctuations. However, the profiles of radial velocity show a larger discrepancy, especially close to the centerline of the combustor. The small number of droplets in this zone makes it difficult to calculate well-converged statistical properties; these results might be greatly improved by running the simulation for a longer time.

The profiles of droplet diameter at the same axial locations are displayed in Fig. 7. Once again the values are globally in good agreement with the PDA measurements, showing the accuracy of the Lagrangian solver used in CDP. However the peaks of the experimental data do not coincide at the first two stations. The results exhibit a typical profile of swirling spray with preferential concentration: It appears clearly that the larger droplets are following the regions of the flow with high shear. It must be noted that the experimental data are noisy in these regions, which makes it difficult to draw conclusions about the LES results. At the $z = 26\text{mm}$ location, the agreement is much better, which is a good indication of the performance of the dispersion and evaporation models.
3.3. Case III: reacting flow

The experimental visualizations of the reacting flow (Fig. 8) do not accurately localize the flame front. From the different locations and colors of the flame, it is clear that the fuel is burning in different regimes, with a partially premixed flame in the central
The initialization of the reacting flow simulation does not reproduce a real ignition process: Starting from a non-reacting velocity field, the domain is artificially filled with burnt gases by setting the progress variable $C$ to one or any other arbitrary high value. Even though this procedure does not correspond to a possible physical mechanism, it provides a fast convergence to a well-established flame. After this stabilization period, the reacting flow has the appearance shown in Figs. 9 and 10 (the number of droplets has been clipped on Fig. 9 for a clearer view). The main characteristics of the reacting flow are well retrieved by the simulation. Most droplets evaporate and burn shortly after injection. Many others cross the flame front and are captured at the walls where they burn in a rich regime. More precise experimental data are still necessary to conclude whether the flame is hanging at the injector wall, as predicted by the LES and evidenced on Fig 9, or stabilized downstream in the swirl region.
4. Conclusion

Large-eddy simulation with Lagrangian spray modeling has been employed to compute the flame of an experimental kerosene-fueled combustor. After a precise validation of the swirling gaseous flow, the spray solver CDP has been shown to accurately predict the important characteristics of the liquid flow: droplet position, velocity and evaporation. These results depend on the number of Lagrangian droplets used to compute statistics and could therefore be improved with a longer simulation. Finally, the reacting flow has been simulated with a flamelet model and the preliminary results on the flame characteristics agree fairly well with the experimental visualization. More detailed measurements are necessary to evaluate the performance of this combustion model in terms of flame stabilization.

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