Lagrangian and Eulerian simulations of evaporating fuel spray in an aeronautical multipoint injector

F. Jaegle* B. Cuenot* T. Poinsot ‡

*CERFACS, Av. Gaspard Coriolis
31057 Toulouse, Cedex 01, France

‡Institut de mécanique des fluides de Toulouse
(CNRS-INPT-UPS)
Allée du Professeur-Camille-Soula, 31400 Toulouse, France

Abstract

In an effort to reduce NO\textsubscript{X} emissions of aeronautical engines, staged injection systems that allow optimizing lean combustion processes for different operating points are intensely studied at present. These systems often employ multipoint injection systems where a series of fuel jets is injected perpendicularly to the airflow and subsequently undergoes atomization and mixing. The present work evaluates the capability of two different numerical strategies to simulate multipoint injectors. The evaluation is carried out on a single injector mounted in an experimental rig with optical access. The non-reactive operating condition corresponds to a partial load regime at 4.37 bar and 473 K in the chamber. This allows to study droplet dynamics and evaporating processes under realistic conditions. Measurement data on gaseous and droplet velocities as well as droplet diameter are available.

The gas phase is simulated using the large eddy simulation (LES) solver AVBP, which has repeatedly demonstrated its ability to predict unsteady flows in complex geometries. This gaseous solver is coupled with two different simulation approaches for the liquid phase. The first is a Lagrangian method, the second a mesoscopic Eulerian approach. These methods both rely on identical models for drag and evaporation. Two-way coupling between the gaseous and the dispersed phase is taken into account.

The simulation cases considered include a purely gaseous flow, an Eulerian spray simulation as well as a monodisperse and a polydisperse Lagrangian simulation. The analysis of the results focuses on validation against experimental data but also on the comparison of the performance between the two numerical approaches under identical conditions.
1 Introduction

Large Eddy Simulation has proven to be a powerful numerical tool for the simulation of industrial-scale combustion applications. As a great number of combustion systems rely on the direct injection of liquid fuel, the prediction of two-phase flow phenomena are a crucial ingredient for such simulations. Three major classes of approaches to simulate such problems are widely studied: The first is the direct simulation of the gas-liquid interface using level-set [28], volume of fluid (VOF) [10], ghost fluid methods [8]. This approach allows in particular to simulate primary breakup processes. In terms of computational cost, it is, however, out of reach for industrial-scale applications.

The second, very popular approach is limited to the representation of a dispersed phase, i.e. a set of droplets, which are tracked individually. This representation of a spray is combined with a classical Eulerian approach for the gaseous phase, which includes the exchange of coupling terms in both directions. This method is referred to as the Eulerian-Lagrangian (EL) approach.

The third method assumes that a spray can be viewed as a continuum, for which transport equations can be formulated and solved numerically similarly to the ones of the gaseous phase. As the Eulerian point of view is taken for both phases, it is known as the Eulerian-Eulerian (EE) approach.

The objective of the present work is a comparison of the EL and the EE approaches in a realistic application case, characterized by pressurized and pre-heated (and thus evaporating) conditions in a complex, industrial-scale geometry. Published studies of such comparisons between EL and EE exist but are often limited to academical cases like homogeneous isotropic turbulence, channel flows or generic configurations like bluff-body cases. Furthermore, such comparisons often rely on different codes for EL and EE, which means that the gaseous flow can be influenced by different grids, numerical schemes etc. In the present study, the solver for the gaseous phase is identical for EL and EE, the models (evaporation and drag) for the liquid phase are equivalent and differ only by their implementation and also the grid is the same for all cases considered. To the authors knowledge, comparable studies of industrial-scale applications are limited to the work of Senoner et al. [24].

In a first part, the injector and the test configuration are described. The numerical framework is laid out, including the governing equations of the gaseous phase and the liquid phase in a Lagrangian and a Eulerian formulation. In a second part, results from a simulation of the purely gaseous flow are described, followed by the analysis of the evaporating two-phase flow. The analysis comprises the description of spray dynamics and evaporation processes with a strong focus on the comparison between both approaches. For both the purely gaseous and two-phase flow, experimental data are available and allow to assess the accuracy of the obtained results.
1.1 Geometry

The aeronautical injector considered here is an example of a staged architecture that is being studied by many manufacturers for their latest or future combustor concepts. The primary objective is the reduction of NO\textsubscript{X} emissions, which is achieved by lean burning in the primary zone of the combustion chamber. In particular in partial load regimes, this may lead to issues of combustion instabilities or flame blowoff, which can be effectively countered by fuel staging. This method allows to optimize the combustor for stable burning conditions at different operating points.

An isolated, cut-away view of the injector is shown in the left half of figure 1. The two stages can be distinguished from the downstream side as two conical “bowls”, where the central pilot bowl is nested inside the main stage bowl.

![Injector Diagram](image)

**Figure 1:** Staged premixing swirler. Left: cut-away view with highlighted injection system. Right: transparent view with highlighted swirler channels.

The right hand side of figure 1 presents a transparent view in which the three swirler stages are highlighted. Two are of radial type, both leading into the pilot bowl near the center of the configuration. While the innermost one discharges into the pilot bowl at its upstream end, the flow from the second joins it through a circular slot in the conical wall just before the pilot flow exits into the chamber. The third and main swirler is of radial type, slightly inclined relative to the central axis. All three swirler stages are counter-rotating relative to each one’s neighbour, which promotes turbulent mixing in the areas where the flows join.

The bulk of the airflow through the injector (approx. 90 %) passes the main swirler stages. The remaining 10 % is divided between the innermost pilot swirler (3 %) and the outer pilot swirler (7 %). The experimental rig considered here consists of a block-shaped chamber with a square cross-section with the injector mounted on the upstream end and the airflow exiting the chamber through a supersonic nozzle at the downstream end (see figure 2). The flat, lateral surfaces allow for easy optical access. The airflow is fed to the
chamber from a plenum through the injector and a film that is visible in figure 3. The computational domain comprises a certain portion of the plenum and ends shortly after the sonic throat of the exit nozzle.

2 Governing equations

2.1 Gaseous phase

The filtered momentum, total energy and species conservation equations for the gas phase are:

\[
\frac{\partial \rho \tilde{u}_i}{\partial t} + \frac{\partial}{\partial x_j}(\rho \tilde{u}_i \tilde{u}_j) = - \frac{\partial}{\partial x_j}[P \delta_{ij} - \tau_{ij} - \tau_{ij}'] + \tilde{S}_{M,i}^{i-g}
\]  

(1)

\[
\frac{\partial \rho \tilde{E}}{\partial t} + \frac{\partial}{\partial x_j}(\rho \tilde{E} \tilde{u}_j) = - \frac{\partial}{\partial x_j}[u_i (P \delta_{ij} - \tau_{ij}) + q_j + q_j'] + \tilde{S}_{E}^{i-g}
\]  

(2)

\[
\frac{\partial \rho \tilde{Y}_k}{\partial t} + \frac{\partial}{\partial x_j}(\rho \tilde{Y}_k \tilde{u}_j) = - \frac{\partial}{\partial x_j}\left[J_{j,k} + \tilde{J}_{j,k}'\right] + \tilde{S}_{F}^{i-g}
\]  

(3)

where a repeated index implies summation over this index (Einstein’s rule of summation). The index \( k \) refers to the \( k^{th} \) species and does not follow the summation rule.

The symbols \( \rho \), \( u_i \), \( E \) and \( \rho_k \) denote respectively the density, the velocity vector, the total energy per unit mass and the density of the chemical species \( k \): \( \rho_k = \rho Y_k \) for \( k = 1 \) to \( N \) (where \( N \) is the total number of species). Furthermore, \( P \) denotes the pressure, \( \tau_{ij} \) the stress tensor, \( q_i \) the heat flux vector and \( J_{j,k} \) the vector of the diffusive flux of species \( k \).
The superscript \( t \) denotes subgrid-scale terms for the shear stress \( \tau_{ij}^t \), heat flux \( q_{jt}^t \) and species diffusion \( J_{j,k}^t \).

There are several source terms on the right-hand side that account for the coupling from the liquid phase to the gas: \( S_{M,i}^{l-g} = \Gamma \mathbf{u}_l - F_{d,i} \) in equation 1 is the vector of momentum source terms with \( F_{d,i} \) being the force per unit volume the dispersed liquid phase exerts on the gas and \( \Gamma \) the mass transfer rate from droplet evaporation per unit volume. The source term in the total energy equation (eq. 2) takes the form: \( S_{E}^{l-g} = \Pi + \Gamma \frac{u_l^2}{2} - u_{l,i}F_{d,i} \) where \( \Pi \) is the heat transfer rate per unit volume. The source term in the species transport equations (eq. 3) is applied to the equation of the evaporating (or fuel-) species \( F \) only and equal to zero for all other species \( k \neq F \). It has the form \( S_{F}^{l-g} = \Gamma \delta_{k,F} \). The terms \( F_{d,i}, \Gamma \) and \( \Pi \) take different forms for EL and EE and are given in the following paragraphs.

2.2 Liquid phase

The numerical solvers for the liquid phase are based on the assumption of a dilute spray, composed of spherical droplets with negligible interactions such as collisions or coalescence. Furthermore, the ratio between the densities of the liquid and the gaseous phase is considered to be large \((\rho_l/\rho_g >> 1)\), the droplets are supposed smaller than the LES filter width and effects of shear on the droplets as well as secondary breakup are neglected.

Both numerical solvers include the same models for droplet drag and evaporation. Furthermore, both solvers include full two-way coupling. In the following sections, the governing equations of both approaches are detailed. Gaseous quantities, identified by the index ‘\( g \)’ correspond to the filtered quantities of the LES.

2.2.1 Euler-Lagrange

In the Euler-Lagrange (EL) approach, each droplet is tracked individually, leading to a very compact set of equations. The relation between the evolution of a droplet’s spatial coordinate \( x_{p,i} \) and its velocity vector \( u_{p,i} \) is:

\[
\frac{dx_{p,i}}{dt} = u_{p,i}
\]  

(4)

The droplet acceleration is obtained by a simplification of the Basset-Boussinesq-Oseen equation [5]:

\[
\frac{du_{p,i}}{dt} = \frac{1}{\tau_p} (u_{g,p,i} - u_{p,i})
\]  

(5)

where \( u_{g,p,i} \) is the gas-phase velocity interpolated at the droplet location, \( g_i \) the gravitational acceleration and \( \tau_p \) the droplet relaxation time scale, that takes
the form:
\[ \tau_p = \frac{4 \rho_p d_p}{3 \rho_g C_D (Re_p)} \left| u_{g@p,i} - u_{p,i} \right| \]  
\[ (6) \]
where \( \rho_p \) and \( \rho_g \) are the droplet and gas-phase densities, \( d_p \) the droplet diameter, \( Re_p \) the droplet Reynolds number and \( C_D \) the droplet drag coefficient. It is based on Stokes’ law for particle drag [26] with the Reynolds number correction proposed by Schiller and Naumann [22]. The (filtered) gaseous velocity \( u_{g@p,i} \) is interpolated at the position of the particle, which is noted as \( u_{g@p,i} \). In the EL approach, the direct effect of subgrid-scale fluctuations on the particle motion is neglected. This effect becomes significant when the droplet Stokes number based on the Kolmogorov time scale \( \tau_\eta \) approaches unity [7, 16]. However, Apte et al. [2] showed that the direct effect was small for swirling separated flows with subgrid scale energy contents much smaller than those of the resolved scales.

In an evaporating spray, the temporal evolution of the droplet mass is given by:
\[ \frac{d m_p}{dt} = -\pi d_p Sh \left[ \rho D \right] \ln (1 + B_M) \]  
\[ (7) \]
where \( Sh \) is the Sherwood number, which is calculated using the formula proposed by Ranz and Marshall [20]. The term \( [\rho D] \) contains the diffusion coefficient of the fuel species, \( D \) and the density of the mixture \( \rho \). It can be expressed by the Schmidt number of the fuel species \( F \) and the viscosity \( \mu \) as \( [\rho D] = \mu/Sc \). The Spalding number for mass transfer, \( B_M \) is expressed as a function of the fuel vapour mass fractions at the droplet surface (index ‘\( \zeta \)’) and the droplet far-field (index ‘\( \infty \)’):
\[ B_M = \frac{Y_{F,\zeta} - Y_{F,\infty}}{1 - Y_{F,\zeta}} \]  
\[ (8) \]
The evolution of droplet temperature is expressed as:
\[ \frac{dT_p}{dt} = \frac{1}{m_p C_{p,L}} \lambda \pi d_p Nu (T_p - T_{g@p}) \frac{\ln(B_T + 1)}{B_T} \]  
\[ (9) \]
with the Nusselt number \( Nu \) corrected by the Ranz-Marshall formula [20]. The heat conductivity in the gas phase is obtained from \( \lambda = \mu C_p / Pr \), where \( C_p \) is the heat capacity at constant pressure of the gaseous mixture and and \( Pr \) the Prandtl number. The Spalding number for heat transfer, \( B_T \) can be related to \( B_M \) the expression
\[ B_T = (1 + B_M) \left( \frac{Sh}{LeF} \right) - 1 \]  
\[ (10) \]
which contains the Sherwood and Nusselt numbers as well as the Lewis number of the fuel species, \( Le_F \).

The two-way coupling terms are calculated as discrete quantities for each droplet and must be translated into volumetric source terms. To do so, particle contributions and summed inside the ensemble of the cells \( D_j \) surrounding a
given node $j$ of the Eulerian grid for the gaseous phase. The volume associated to a node $j$ is noted $V_j$. $\Psi_{j,e}^{(k)}$ is a weight that is calculated from the ratio of the inverse distances from the particle $k$ to the vertices $K_e$ of the element $e$ in which it is located:

$$
\Psi_{j,e}^{(k)} = \frac{\prod_{r \in K_e} |x_{p,i}^{(k)} - x_{n,i}|}{\sum_{r \in K_e} \prod_{m \neq r} |x_{p,i}^{(k)} - x_{m,i}|} \quad (11)
$$

The volumetric force exerted on the gaseous phase is then:

$$
F_{d,i} = \frac{1}{V_j} \sum_{k \in D_j} \Psi_{j,e}^{(k)} m_p^{(k)} \left( \frac{du_{p,i}}{dt} \right)^{(k)} \quad (12)
$$

The mass transfer rate per unit volume is calculated from:

$$
\Gamma = -\frac{1}{V_j} \sum_{k \in D_j} \Psi_{j,e}^{(k)} \left( \frac{dm_p}{dt} \right)^{(k)} \quad (13)
$$

and the heat transfer per unit volume is obtained by the following expression:

$$
\Pi = \frac{1}{V_j} \sum_{k \in D_j} \Psi_{j,e}^{(k)} \left( \frac{dm_p}{dt} h_s,F(T_p) + \lambda \pi d_p Nu (T_p - T) \frac{ln(B_T + 1)}{B_T} \right)^{(k)} \quad (14)
$$

### 2.2.2 Euler-Euler

In the Euler-Euler (EE) method, the spray is considered as a continuum, for which transport equations can be written. The conserved variables are formulated for the so-called mesoscopic quantities (noted with a $\hat{\cdot}$-operator), which represent the conditional ensemble average over all droplets present in a given control volume (Février et al. [9]). In the formulation used here, the spray is assumed to be locally monodisperse. Furthermore, the effects of the random uncorrelated motion are neglected. In the filtered equations used in a LES, Favre filtering is applied to an arbitrary mesoscopic quantity $\tilde{f}$:

$$
\overline{\alpha_l \tilde{f}_l} = \alpha_l \tilde{f}_l \quad (15)
$$

where $\overline{\cdot}$ is the spatially filtered liquid volume fraction. The equation for the conservation of the droplet number density $n_l$ then reads:

$$
\frac{\partial n_l}{\partial t} + \frac{\partial \alpha_l \hat{n}_{l,j}}{\partial x_j} = 0 \quad (16)
$$

The conservation equation for liquid mass becomes:

$$
\frac{\partial \rho_l \alpha_l}{\partial t} + \frac{\partial \rho_l \alpha_l \hat{u}_{l,j}}{\partial x_j} = -\Gamma \quad (17)
$$
The term $\Gamma$ describes the mass transfer per unit volume of the spray. It is the Eulerian equivalent to equation 7:

$$\Gamma = \rho_l \bar{\alpha}_l \left[ \pi \bar{d} Sh \left[ \rho D_F \right] ln \left( 1 + B_M \right) \right]$$

The equation for the liquid phase momentum is:

$$\frac{\partial \rho_l \bar{\alpha}_l \hat{u}_{l,i}}{\partial t} + \frac{\partial \rho_l \bar{\alpha}_l \hat{u}_{l,i} \hat{u}_{l,j}}{\partial x_j} = -\Gamma \hat{u}_{l,i} + F_{d,i} + \frac{\partial \tau_{l,ij}}{\partial x_j}$$

$$F_{d,i} = \frac{\rho_l \bar{\alpha}_l \tau_p}{\tau_p} (u_{g,i} - \hat{u}_{l,i})$$

where the droplet relaxation timescale $\tau_p$ is obtained by equation 6 and $\tau_{l,ij}$ is a subgrid stress tensor that is modeled using a Smagorinsky formulation [25] for the trace-free part together with a Yoshizawa formulation for the trace [17].

The conservation equation for the liquid phase sensible enthalpy $h_{s,l}$ is:

$$\frac{\partial \rho_l \bar{\alpha}_l \hat{h}_{s,l}}{\partial t} + \frac{\partial \rho_l \bar{\alpha}_l \hat{u}_{l,i} \hat{h}_{s,l}}{\partial x_i} = -\Pi$$

which is based on the same derivation as the evolution of droplet temperature in the Lagrangian formulation (equation 9). In the present implementation, the subgrid-scale terms for liquid phase sensible enthalpy are assumed to be negligible. The term $\Pi$ on the right-hand side is the heat transfer per unit volume between liquid and gaseous phase. In the Eulerian framework, it takes the form:

$$\Pi = -\Gamma h_{s,F} (\bar{T}_l) + \lambda \pi \bar{d} Nu (\bar{T}_l - T_g) \frac{ln(B_T + 1)}{B_T}$$

In both EL and EE, the viscosity $\mu$ and the heat capacity at constant pressure $C_P$ depend on properties of the gaseous mixture surrounding the droplet. In the scope of the evaporation model, these properties that vary between the droplet surface and the far-field are assumed to be constant and evaluated using the 1/3-rule (Hubbard et al. [11]).

3 Numerical methods

3.1 Numerical methods for the gaseous phase

The gaseous LES solver AVBP explicitly solves the compressible Navier-Stokes equations with a centered scheme that achieves up to third-order accuracy in both time and space [6]. In the present work, the second-order accurate Lax-Wendroff scheme [18] is used due to its lower numerical cost and sufficient accuracy for the gas phase. To damp spurious oscillations, second-order and fourth-order artificial viscosities are applied [15]. A standard Smagorinsky formulation [25] is used to model subgrid-scale turbulence. Inlet and outlet boundary conditions are imposed using the NSCBC method [19]. Solid boundaries are modeled...
using logarithmic wall laws [23, 12]. The gaseous AVBP solver can be combined with two different modules for the dispersed, liquid phase that shall be described in the following.

3.2 Numerical methods for the dispersed, liquid phase

Euler-Lagrange

The interpolation of gaseous properties to the droplet is based on a linear least-squares operator. For time advancement, the Lagrangian solver relies on a first-order forward-Euler method. Since the timestep is determined by the acoustic CFL for the gaseous solver, first order accuracy is deemed acceptable for the temporal resolution of the liquid phase equations. To reduce computational cost and memory requirements, droplets can be grouped into “parcels”. This can be justified for cases with large numbers of droplets. In the present work, a parcel contains 10 physical droplets.

Euler-Euler

In the EE framework, the multi-dimensional upwinding scheme PSI [27] scheme is used, as its robustness makes it very well-adapted for cases that include spray injection. For unsteady problems, it is of first order in space and time [1]. Despite its low accuracy, it has proven to yield good results in particle-laden homogeneous isotropic turbulence as well as industrial-scale applications [21, 15].

4 Liquid phase injection

The liquid injection system consists in a series of plain, round jets entering the injector perpendicularly to the airflow where they are atomized. This corresponds to the problem of a liquid jet in a gaseous crossflow that includes complex mechanisms of primary and secondary breakup [29, 4]. Because the basic assumptions (dilute spray, no droplet breakup) do not hold in the near-field of the injection, the Eulerian and Lagrangian methods previously presented become valid only after the resulting spray reaches a fully developed state in the far-field. As it is not the main interest of the present application to capture the near-field effects (i.e. primary and secondary breakup), the objective is to find a simple method, with little or no additional cost and to provide a sufficiently accurate result in the far-field. The relevant quality criteria are a correct spatial distribution of the resulting spray plume (in terms of penetration height and lateral diffusion) as well as a realistic diameter distribution, both locally and spatially. If these criteria are satisfied, the spray that leaves the injector and enters the combustion chamber can be expected to behave realistically in terms of interaction with the turbulent air flow, evaporation and - in reactive cases -
Preliminary studies on the liquid jet in a crossflow case have been carried out by Jaegle et al. [13, 14] using Eulerian and Lagrangian methods in the same numerical framework as in the present study. Different momentum flux ratios \( q = \frac{\rho_l w_{inj}^2}{\rho g u^2} \) between the liquid jet at injection and the crossflow are investigated (ranging from \( q = 2 \) to \( q = 18 \)). This study shows that a simple model for the liquid column region yields good results for the far-field spray distribution (compared to experimental data by Becker et al. [3]). In the Lagrangian framework, despite neglecting secondary breakup, good results for the spatial diameter distribution in the far-field are obtained by injecting a log-normal size distribution that corresponds to the fully developed spray. For the locally monodisperse Euler-Euler method used here, injecting a spatially varying diameter profile is of limited success only for a high momentum flux ratio case \( q = 18 \).

In the present study, the momentum flux ratio has a value of \( q = 0.2 \). Effects of the liquid column can therefore be neglected. Furthermore, in the Eulerian case, a constant diameter is injected as no improvement can be expected from a variable profile based on the findings of the preliminary study. In the Lagrangian formulation, two cases are chosen: in the first one, a monodisperse spray is injected to create conditions that are identical to the Eulerian case for a direct comparison between EL and EE methods. In the second, a polydisperse spray with a log-normal distribution is injected. The Sauter mean diameter of this distribution is based on a correlation provided by Becker et al. [3].

5 Simulation setup

5.1 Grid / boundary conditions

The computational grid is a critical contributor to the quality of the results in the present study. Figure 3 shows an overview of the mesh. It is of unstructured, hybrid type, composed of tetraedral and prismatic and pyramidal elements. The (triangular) prisms form a single, closed layer in all regions where wall functions are used to model the turbulent boundary layer. This layer facilitates the application of wall functions in the no-slip formulation but is is also advantageous in terms of the overall number of cells, because the near-wall grid refinement can easily be controlled by adapting the prism aspect ratio without obtaining an excessive number of near-wall tetraedra.

The grid has several refined zones inside and downstream of the injector. The swirler channels are optimized for the use of wall-functions, with a target for near wall prismatic layer thickness of \( y^+ \approx 100 \). Areas of high grid resolution are located in the pilot and main bowl, stretching outwards in areas where the main shear layers between the counter-rotating swirler stages or between the high-velocity regions and recirculation zones are located. Furthermore, the grid
is refined in proximity of the cooling films.

Grid refinement is significantly relaxed downstream of the high-shear regions at the injector exit as well as inside the plenum. The only focus region related to the two-phase simulations is a local refinement around the multipoint injection. The same mesh is used for all calculations presented in this study, both gaseous and two-phase, regardless of the liquid phase approach. Global parameters of this common mesh are summarized in table 1.

Table 1: Mesh parameters

<table>
<thead>
<tr>
<th>Mesh type</th>
<th>unstructured, hybrid</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cell types</td>
<td>tetraedra (domain volume)</td>
</tr>
<tr>
<td></td>
<td>prisms (domain boundary, areas with wall model)</td>
</tr>
<tr>
<td>Grid nodes</td>
<td>1 619 357</td>
</tr>
<tr>
<td>Grid cells</td>
<td>8 540 311</td>
</tr>
<tr>
<td>Case #</td>
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</tr>
<tr>
<td>--------</td>
<td>----</td>
</tr>
<tr>
<td>Two-phase flow</td>
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</tr>
<tr>
<td>Spray injection</td>
<td>No</td>
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</tbody>
</table>

Table 2: Summary of all simulation cases.

<table>
<thead>
<tr>
<th>Gaseous phase</th>
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</thead>
<tbody>
<tr>
<td>Mass flux (plenum inlet)</td>
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<td>Temperature</td>
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<table>
<thead>
<tr>
<th>Walls</th>
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<tbody>
<tr>
<td>Wall temperature</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Liquid phase</th>
</tr>
</thead>
<tbody>
<tr>
<td>liquid mass flux (Multipoint inj.)</td>
</tr>
<tr>
<td>liquid phase temperature</td>
</tr>
</tbody>
</table>

Table 3: Boundary values, liquid and gaseous phase

5.2 The cases considered

6 Results

6.1 Gaseous flow field

6.1.1 Qualitative description

The flow topology is explained at the in figure 4

6.1.2 Averaged quanities - comparison to the experiment

A validation against experimental data is needed to exclude errors in the gaseous flow that would interfere with the analysis of the spray. Averaged velocity profiles are presented for the axial as well as the tangential component in figures 5 and 6 respectively. These profiles are obtained along three measurement lines located at 10, 15 and 30 mm downstream of the swirler exit (see figure 4).

The main peaks in axial and tangential velocity correspond to the main flow region from the swirler and are well reproduced both in magnitude and position. Secondary peaks on the axial velocity profiles near the lateral walls are created by the cooling films. They are well captured on the first profile and slightly diffused at the 15 mm position. At 30 mm, both peaks have merged and agreement is again excellent.

For the profiles of axial and tangential velocity fluctuations, shown in figures 7 and 8 respectively, agreement is very good. On all measurement positions, the shape and magnitude of the fluctuations is well reproduced. For the tangential
Figure 4: *Instantaneous field of axial velocity on the mid-plane. Position of the measurement lines.*

Figure 5: *Mean axial velocity profiles of the gaseous flow. Comparison of LES results (—), and experimental data (○ ○ ○).*

fluctuations, a slight over-estimation of the peak values can be observed.

Overall, results of the purely gaseous simulations are of very good quality. They match experimental data on first and second order statistics accurately.
This lays an excellent groundwork for the following study of two-phase flow because errors related to the prediction of the gaseous flow can be considered to be negligible.
Figure 8: Tangential velocity fluctuation profiles of the gaseous flow. Comparison of LES results and experimental data (○ ○ ○)
6.2 Two-phase flow results

6.2.1 Qualitative description

Figure 9: Close up views of the multipoint injection. Left: isometric view of the (numerical) particle field in the chamber, polydisperse case. Right: EE results, iso-surface of the liquid volume flux to visualize the spray boundary.

Figure 10: Comparison of EE results with polydisperse EL results. Left: iso-contours of liquid volume flux $\Phi_{lv}[\text{m}^3/(\text{s}\cdot\text{m}^2)]$ on the plane $y = 0$. Right: numerical particles in a 5 mm neighbourhood of the plane $y = 0$.

6.2.2 Averaged quanities - comparison to the experiment

6.3 Computational cost

The computational cost associated with EE and EL methods is an important part of the global comparison. Table 4 lists the key figures of the three simulation
Figure 11: Comparison of polydisperse and monodisperse EL results. Left and right: particles in a 5 mm neighbourhood of the plane $y = 0$, shaded with the particle diameter $d_p [m]$.

Figure 12: Comparison of EE results with monodisperse EL results. Left: droplet diameter field $d_l [m]$ on the plane $y = 0$, overlaid with the iso-contour marking the clipping diameter. Right: numerical particles in a 5 mm neighbourhood of the plane $y = 0$, shaded with the droplet diameter $d_p [m]$.

cases. The key finding is a significantly higher cost of the EE simulation, where there is almost a factor 2 relative to the polydisperse EL case. Interestingly, the number of particles in the monodisperse EL case is slightly higher compared to its polydisperse counterpart, which leads to a slight advantage of the latter.

The apparent superiority of the EL approach in terms of CPU cost must, however, be relativized. One aspect is the use of the parcel approach for EL, which considerably accelerates the method for high particle numbers. The second is the longer time that is needed to achieve a given degree of statistical
Figure 13: Placement of the sampling locations for histogram data in the y-z plane.

Figure 14: Diameter and Temperature histograms of the monodisperse EL simulation. Samples taken in a series of cubes at 15 mm downstream location and 10 mm (left), 30 mm (middle) and 50 mm (right) lateral distance from the centerline. (see figure 13 for the exact arrangement).

<table>
<thead>
<tr>
<th>CPU times</th>
<th>EE</th>
<th>EL monodisp.</th>
<th>EL polydisp.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of numerical particles</td>
<td>-</td>
<td>1282155</td>
<td>1115579</td>
</tr>
<tr>
<td>Averaging time [s]</td>
<td>$16.1 \cdot 10^{-3}$</td>
<td>$43.6 \cdot 10^{-3}$</td>
<td>$41.5 \cdot 10^{-3}$</td>
</tr>
<tr>
<td>Av. time / residence time [-]</td>
<td>0.412</td>
<td>1.12</td>
<td>1.06</td>
</tr>
<tr>
<td>CPU hours / res. time [-]</td>
<td>473</td>
<td>255</td>
<td>247</td>
</tr>
</tbody>
</table>

64 processors on a SGI Altix ICE 8200 EX (Jade, CINES)

Table 4: Summary of the CPU times of two-phase-flow simulations of the TLC configuration
Figure 15: Diameter and Temperature histograms of the polydisperse EL simulation. Samples taken in a series of cubes at 15 mm downstream location and 10 mm (left), 30 mm (middle) and 50 mm (right) lateral distance from the centerline. (see figure 13 for the exact arrangement).

Figure 16: Comparison of EE results with monodisperse EL results. Left and right: field of the source term for mass transfer $\Gamma [\text{kg}/(\text{m}^3 \text{s})]$ on the plane $y = 0$.

convergence, especially for RMS values. The comparison of averaging time over the residence time in the chamber between EL and EE shows roughly a factor 2 in favour of the EE method although the term “degree of convergence” is somewhat arbitrary. Here, the use of the parcel approach would actually accelerate the convergence of Lagrangian statistics. It depends on the computer resources and the sover scaling characteristics on parallel architectures if this preferrable is advisable or not.
Figure 17: TLC configuration - axial liquid phas velocity profiles. Comparison of (inherently monodisperse) EE-results (—), monodisperse EL-results (- - -), polydisperse EL-results (····) and experimental data (○ ○ ○).

Figure 18: TLC configuration - tangential liquid phas velocity profiles. Comparison of (inherently monodisperse) EE-results (—), monodisperse EL-results (- - -), polydisperse EL-results (····) and experimental data (○ ○ ○).

7 Conclusion

Acknowledgements

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Figure 19: TLC configuration - axial liquid phase velocity fluctuation profiles. Comparison of (inherently monodisperse) EE-results (—), monodisperse EL-results (- - -), polydisperse EL-results (····) and experimental data (◦◦◦).

Figure 20: TLC configuration - tangential liquid phase velocity fluctuation profiles. Comparison of (inherently monodisperse) EE-results (—), monodisperse EL-results (- - -), polydisperse EL-results (····) and experimental data (◦◦◦).
Figure 21: TLC configuration - profiles of the Sauter mean diameter. Comparison of (inherently monodisperse) EE-results (—), monodisperse EL-results (- - -), polydisperse EL-results (····) and experimental data (○ ○ ○).
References


