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Large Eddy Simulation of Spray Combustion in a Swirl-Stabilized Gas Turbine Burner

Mirko Salewski*, Christophe Duwig†, Vladimir Milosavljevic‡, Laszlo Fuchs§

Division of Fluid Mechanics, Lund University, Sweden

The combustion of sprays in the complex geometry of a gas turbine combustor is studied using Large Eddy Simulation together with Lagrangian Particle Tracking. The reacting flow case including combustion is compared to a flow case without combustion with otherwise identical boundary conditions. The differences in the dependent variables are shown to be large: In the case with combustion, the temperature and density fields change strongly due to the heat release, resulting in corresponding changes in the velocity field and the spray dispersion. The low densities in the recirculation zone in the case of reacting flow allows fluid to push the recirculation zone downstream. Secondly, the low densities result in a reduction of the spray dispersion. Additionally, in the non-reacting flow and in the reacting flow, the computed results are demonstrated to be highly sensitive to the droplet injection diameter.

Nomenclature

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
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<tbody>
<tr>
<td>DNS</td>
<td>Direct Numerical Simulation</td>
</tr>
<tr>
<td>GT</td>
<td>Gas Turbine</td>
</tr>
<tr>
<td>LES</td>
<td>Large Eddy Simulation</td>
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<tr>
<td>LPT</td>
<td>Lagrangian Particle Tracking</td>
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<tr>
<td>ODE</td>
<td>Ordinary Differential Equation</td>
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<tr>
<td>PDF</td>
<td>Probability Density Function</td>
</tr>
<tr>
<td>POD</td>
<td>Proper Orthogonal Decomposition</td>
</tr>
<tr>
<td>PSR</td>
<td>Perfectly Stirred Reactor</td>
</tr>
<tr>
<td>PVC</td>
<td>Precessing Vortex Core</td>
</tr>
<tr>
<td>RANS</td>
<td>Reynolds-Averaged Navier-Stokes</td>
</tr>
<tr>
<td>RMS</td>
<td>Root mean square</td>
</tr>
<tr>
<td>SGS</td>
<td>Subgrid-scale</td>
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<tr>
<td>SMD</td>
<td>Sauter Mean Diameter</td>
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<tr>
<td>WENO</td>
<td>Weighted Essentially Non-Oscillatory</td>
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</table>

I. Introduction

Spray combustion is routinely applied in a wealth of engineering applications: For example, stationary gas turbines (GT) can produce heat and electricity by burning liquid fuels in plants with heat-power coupling cycles. Airborne GTs, reciprocating engines for cars or ships, or rocket engines with liquid propellants are examples for the application of spray combustion for transportation. Stationary GTs may be operated with gaseous fuels as well, but any transportable spray combustion energy conversion system will usually be required to use liquid fuels as the fuels have to fit in a tank. If one compares the emission levels of GTs operating with gaseous fuel with those with liquid fuels, it becomes clear that using liquid fuels is often

*PhD  †PhD, Research Associate  ‡PhD, Associate Professor  §PhD, Professor, AIAA member
the show-stopper for achieving ultra-low emissions, e.g. NO\textsubscript{x} levels.\textsuperscript{1} Despite this widespread usage of multiphase flows with combustion and their importance for the environment, there are several phenomena which are still poorly understood. An example is the atomization of the liquid jet to a fine spray, which leads to droplets of sizes which vary in order of magnitude and which also vary in time.\textsuperscript{1}

Simulation of spray combustion in a GT combustor geometry is uncertain due to the large amount of modeling required. The modeling difficulties regarding the fact that these flows are multiphase flows are for example atomization, secondary droplet breakup, droplet collision, multi-component fuel evaporation, and aerodynamic droplet interaction and droplet deformation.\textsuperscript{2} Secondly, the modeling of turbulent combustion is difficult as several chemical time scales are even smaller than the smallest mixing time scales and strong non-linearities are present, e.g. the reaction rates or the heat release which may additionally fluctuate strongly. As the flow occurs in a cavity, the heat release fluctuations may lead to strong acoustic modes which may destroy the burner. Lastly, there are typical difficulties in modeling even a single-phase flow in a GT burner: The geometry is complex and the boundary conditions are uncertain; the Reynolds number is high, and therefore the flow is turbulent with interacting coherent structures in the energy-containing range of the turbulence spectrum; the flow topology is highly sensitive to these. Accurate modeling of the turbulence in turn is highly important for predicting the dispersion of droplets, the scalar mixing and the combustion.

In this study we model the above mentioned effects: A strongly swirling multiphase flow with turbulent combustion in a complex geometry. The turbulent flow is simulated by Large Eddy Simulation, in which the flow is approximated by simulating the large-scale motion and neglecting the small-scale motion. The multiphase flow is modeled using an Eulerian formulation for the continuous phase and Lagrangian coordinates for the dispersed phase. This Lagrangian Particle Tracking has compared to Euler / Euler the advantage that one can model physical processes on the droplet level. For example, one can introduce submodels for evaporation,\textsuperscript{3–5} breakup,\textsuperscript{6–8} and collision,\textsuperscript{3, 9, 10} droplet deformation,\textsuperscript{11, 12} or aerodynamic fourway interaction.\textsuperscript{11, 13, 14} In the present case we apply full two-way coupling, i.e. there are source terms in all transport equations. The combustion is modeled by writing the heat release as a function of the mixture fraction and the local temperature.

This particular flow occurs in GT combustors operating in the partially premixed flame combustion mode: The swirling fluid is carried outwards by centrifugal forces, and this leads to a low pressure in the region near the symmetry axis of the combustor. In the radial direction the resulting pressure gradient is
balanced by centrifugal forces, but in axial direction the flow is driven towards the low pressure region, leading to a recirculation zone. This phenomenon occurs at strong enough swirl and is called vortex breakdown. Vortex breakdown depends strongly on the burner geometry and the radial distribution of the velocity field. Predicting flows with vortex breakdown is highly relevant for the operation of GTs from an engineering point of view.

The flame will on average remain in the shear layer of this recirculation bubble, since the turbulent flame speed matches the flow speed somewhere in the shear layer. This type of flame anchoring is widely used in GT combustors.\textsuperscript{1} Fig.1 shows the geometry of the present combustor and the recirculation zone which is visualized in blue as an isosurface of the instantaneous axial velocity. The combustor is designed with a smooth expansion (as opposed to a rapid expansion) and therefore there are no external recirculation zones. This design ensures a long recirculation zone to efficiently recirculate the burned gases. This recirculation provides the heat for the chemical reactions to occur.

The flow is inherently unsteady due to the Kelvin-Helmholtz instabilities in the shear layer surrounding the recirculation zone. The recirculation bubble is drawn away from the symmetry axis and rotates together with the swirling flow. This phenomenon has been dubbed precessing vortex core (PVC).\textsuperscript{15,16} The existence has been amply confirmed experimentally\textsuperscript{17–19} and by numeric simulation.\textsuperscript{20,21} In swirling flows with combustion, the PVC may result in heat release fluctuations and ultimately in combustion instabilities. This unsteadiness itself makes large eddy simulation (LES) an essential tool to study swirling flows with vortex breakdown. With respect to Lagrangian particle tracking (LPT), the turbulence model is highly relevant as well, for the dispersion of the droplets depends mainly on the large scales of turbulence.\textsuperscript{22,23} Whereas in Reynolds-averaged Navier-Stokes the effect of the large scales on droplet dispersion has to be modeled, these scales are resolved in LES and are computed as a solution of the filtered Navier-Stokes equations.

We study the dispersion of the droplets in the turbulent flow and mixing and combustion of the computed mixtures. A case with non-reacting flow (no combustion) is compared to the same flow with combustion of the fuel/air mixture. It is shown that the flow topology is so different in the dependent variables, that it may be misleading to use experimental data obtained for a non-reacting flow to predict the behavior of the reacting flow. Additionally, a parameter sensitivity study is performed, in which the assumed injection droplet size is varied. The computed results are highly sensitive to the droplet injection diameter, showing that additionally work in determining this parameter accurately is required.

II. Governing Equations and Numerical Methods

The governing equations are the Navier-Stokes equations for the continuous phase and Newton’s law for the dispersed phase. This approach is referred to as Lagrangian Particle Tracking or Euler / Lagrange framework. The governing equations for the continuous phase are complicated further due to the chemical reactions one has to account for in flows with combustion.

A. Continuous Phase

The non-dimensional continuity, momentum, energy, and mixture fraction transport equations (Equations (1) to (4)) for Newtonian fluids with constant diffusivities are described in Eulerian framework. The equations are valid for flow in the limit of low Mach number to be described below. The transport equations for the temperature and for the fuel fraction are integrated to compute the mixing of evaporated gases. The continuous phase volume fraction $\alpha_c$ is assumed to be unity (point particles).

\begin{align}
\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} &= \dot{m}_s \tag{1} \\
\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} &= -\frac{\partial \rho}{\partial x_i} + \frac{1}{Re} \frac{\partial}{\partial x_j} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + F_{s,i} \tag{2} \\
\frac{\partial \rho h}{\partial t} + \frac{\partial \rho u_j h}{\partial x_j} &= \frac{1}{Re Pr} \frac{\partial^2 h}{\partial x_j^2} + \dot{Q}_s + \dot{Q}_{chem} \tag{3} \\
\frac{\partial \rho Z}{\partial t} + \frac{\partial \rho u_j Z}{\partial x_j} &= \frac{1}{Re Sc} \frac{\partial^2 Z}{\partial x_j^2} + \dot{Z}_s \tag{4}
\end{align}

\begin{center}
American Institute of Aeronautics and Astronautics
\end{center}
\( \dot{m}_s, \dot{F}_{s,i}, \dot{Q}_s, \dot{Z}_s \) are source terms for mass, momentum, energy, and mixture fraction, respectively. These source terms account for the coupling from the spray to the gas phase. The source terms due to the presence of spray are further described in Section B. The additional source term \( Q_{\text{chem}} \) is the source term due to chemical reactions, i.e., heat release in the flame front. This chemical source term is described in Section C. The Reynolds number is the ratio of convective and diffusive forces given by Equation (5) in which \( L \) and \( U \) are lengths and velocities of the flow, respectively, and \( \nu_c \) is the continuous phase diffusivity. The Schmidt number \( Sc \) (Equation (6)) is the ratio of momentum and mass diffusivities, the Prandtl number \( Pr \) the ratio of momentum and heat diffusivities (Equation (7)).

\[
\begin{align*}
Re &= \frac{UL}{\nu_c} \quad (5) \\
Sc &= \frac{\nu_c}{D_c} \quad (6) \\
Pr &= \frac{\nu_c}{\alpha_c} \quad (7)
\end{align*}
\]

The low Mach number limit in turn does not imply that the density is constant. It may very well change due to heat release or varying molecular composition. As evaporating fuel gases, e.g., heptane, can be 3-4 times as heavy as air, the density differences due to non-uniform mixture fraction can be significant (also by the same factor). The low Mach number assumption removes acoustic waves from the simulated flow, which decreases the mathematical stiffness of the system. The energy equation is thus loosely coupled to the Navier-Stokes equations and can be solved afterwards. One can deduce that in the limit of low Mach number the equation of state becomes simply:24

\[
p_0 = \rho \frac{R_u}{M} T
\]

\( p_0 \) is the operating pressure of the device, \( R_u \) is the universal gas constant, and \( M \) is the molecular mass. The error of using the global operating pressure instead of the local pressure is proportional to the square of the Mach number. The density is thus computed from the local temperature and the local molecular mass.

In the framework of LES, one removes Fourier components with high wavenumber by applying a spatial low-pass filter. The closure problem of LES is evident in the appearance of residual stresses which arise from filtering the non-linear terms. A computational grid can support only Fourier components that have longer wavelengths than the grid size. Thus, if a dependent variable is represented on a grid together with a discrete approximation for the derivatives, the variable is filtered implicitly. If no explicit SGS terms are added, then the numerical scheme should account at least for the small scale dissipation. This is attained for any numerically stable scheme.25,26 However, overly dissipative numerical schemes are highly inappropriate for LES since in addition to dissipation on small scales they may be also too dissipative on the larger scales. This effect can be avoided by choosing appropriate (higher order) discretizations. In addition, the spatial resolution has to be on the order of magnitude of the Taylor micro-scale. With such a fine resolution, the energy transfer among the large scales is dissipation independent and therefore the numerical scheme may act implicitly as a SGS model. However, one should keep in mind that this implicit SGS approach may require a better resolution than a corresponding LES with an advanced SGS model. Nevertheless, even with explicit SGS models (such as the dynamic model), the spatial resolution has to be adequate.25,26 Consequently, the leading term of the truncation error corresponds to a hyper-viscosity that acts as an implicit SGS model. The implicit solver uses fifth-order weighted essentially non-oscillatory (WENO) scheme for the convective terms and fourth-order central differences for the diffusive terms on a Cartesian grid. In regions of complex geometrical features and large curvature of the streamlines local refinements enhance the spatial resolution.

B. Dispersed Phase

The dispersed phase is described by a probability density function (PDF), or the corresponding droplet distribution function \( f \).

\[
f(\bar{x}, \bar{v}, r, T, y, \dot{y}) d\bar{x}d\bar{v}drdTdyd\dot{y}
\]

The droplet distribution function describes the number of droplets per unit volume at a position between \( \bar{x} \) and \( \bar{x} + d\bar{x} \) which have a velocity between \( \bar{v} \) and \( \bar{v} + d\bar{v} \), a temperature between \( T \) and \( T + dT \), and a radius
between \( r \) and \( r + dr \) with distortion parameters between \( y \) and \( y + dy \) and \( \dot{y} \) and \( \dot{y} + d\dot{y} \). The source terms for the continuous phase are given by the rates of change of mass, momentum, energy, and mixture fraction of all droplets in the incremental volume, respectively. Equations (10) to (13) describe the source terms in Equations (1) to (4), respectively.

\[
\dot{m}_s = -\frac{L}{\rho_c U} \int f \rho_d 4\pi r^2 \frac{dr}{dt} d\vec{u}drdTdyd\dot{y} \\
\dot{F}_{s,i} = -\frac{L}{\rho_c U^2} \int f \rho_d \left( \frac{4}{3} \pi r^3 \frac{dv_i}{dt} + 4\pi r^2 \frac{dr}{dt} v_i \right) d\vec{v}drdTdyd\dot{y} \\
\dot{Q}_s = -\frac{L}{\rho_c U h_{\infty}} \int f \rho_d \left( 4\pi r^2 \frac{dr}{dt} h_{\text{latent}} + \frac{4}{3} \pi r^3 c_p \frac{dT}{dt} \right) d\vec{v}drdTdyd\dot{y} \\
\dot{Z}_s = -\frac{L}{\rho_c U} \int f \rho_d 4\pi r^2 \frac{dr}{dt} d\vec{u}drdTdyd\dot{y}
\]

The radius of the droplets is denoted by \( r \); \( \rho_d \) and \( \rho_c \) are the dispersed and continuous phase densities, respectively; and \( L \) and \( U \) are the length scale scales of the continuous phase. As the number of droplets is too large to permit individual treatment of droplets efficiently, the stochastic parcel method may be applied.\(^{27}\)

A computational particle, a parcel, represents a group of droplets with identical properties. The particle trajectories are calculated in Lagrangian framework. The instantaneous parcel positions \( \vec{x} \) are obtained by integration of the parcel velocities \( \vec{v} \) which in turn are obtained from integration of the parcel accelerations \( \vec{a} \).

\[
\vec{v} = \frac{d\vec{x}}{dt} \quad (14) \\
\vec{a} = \frac{d\vec{v}}{dt} \quad (15)
\]

The instantaneous parcel accelerations are computed from Newton’s law, assuming that the momentum flux due to evaporation is uniformly distributed over the particle surface. Newton’s law is then

\[
\vec{F} = m\vec{a} \quad (16)
\]

All forces except the aerodynamic forces are neglected: Gravitation, gas phase flow acceleration, added mass, the Basset history integral, Magnus -, Saffman -, and Faxen forces. Mach number effects are also neglected. The parcel accelerations are then for spherical, isolated, and rigid droplets (though they can break up):

\[
\frac{d\vec{v}}{dt} = -\frac{3}{4} \frac{\rho_d}{\rho_c D_p} \frac{1}{D_p} C_d \ | \vec{v} - \vec{u} | \ (\vec{v} - \vec{u}) \quad (17)
\]

\( | \vec{v} - \vec{u} | \) is the relative speed, \( \vec{v} \) and \( \vec{u} \) are velocity vectors of the parcels and the gas. \( D_p \) is the droplet diameter. In the present simulation, \( C_d \) is correlated to the parcel Reynolds number as:

\[
C_d = \begin{cases} 
\frac{24}{Re_p} (1 + \frac{1}{3} Re_p^{2/3}) & \text{for } Re_p \leq 1000 \\
0.424 & \text{for } Re_p \geq 1000
\end{cases} \quad (18)
\]

The parcel Reynolds number is defined as:

\[
Re_p = \frac{D_p | \vec{v} - \vec{u} |}{\nu_c} \quad (19)
\]

The dispersion of the droplets depends mainly on the large-scale eddies, and therefore the subgrid scale velocity fluctuations are neglected.\(^{22,23}\)

The atomization of the droplets is modeled by the so-called blob injection,\(^7,8\) i.e. droplets of the largest geometrically possible size. This breakup model is also used for modeling secondary droplet breakup in the entire flow. Further, evaporation is modeled by assuming single-component spherical droplets with uniform properties.\(^3\) Collision and coalescence models are also included.\(^3\) The flow solvers for the continuous phase and the dispersed phase are two-way coupled, i.e. spray and gas mutually interact.
C. Combustion Modeling

Turbulent combustion continues to be a challenge for CFD modeling. It is currently not feasible to use detailed chemical reaction mechanisms together with LES as in a typical flame in a gas turbine there are too many species and chemical reactions present. Furthermore, the chemical reactions have a large spread in their characteristic time scales, rendering the problem mathematically stiff. Instead of the comprehensive reaction mechanisms one identifies the key species and reactions and reduces the reaction mechanisms by neglecting species and reactions which are thought to be of lesser importance. General models cannot be derived as the rates of the chemical reactions are highly (and non-linearly) dependent on the local flow properties.

![Figure 3. Source terms for the OH, CO, and the temperature transport equation](image)

However, one can summarize the complex chemistry in look-up tables, which are of course only valid for the conditions these have been derived for. Especially, one can use the ansatz of separation of scales and model the flame as laminar flamelets.\(^{28,29}\) These precomputed look-up tables which contain information about the complex chemistry are called flamelet libraries. It has to be emphasized that the use of look-up tables is justified only if the relevant chemical time scales are much faster than the flow time scales. In the present model, one can thus look up the heat release as a function of two scalars, for example the local mixture fraction and temperature. The local mixture fraction characterizes the mixing: \(Z = 0\) means that the local mixture completely originates from the oxidizer inlet and \(Z = 1\) means that the local mixtures stems entirely from the fuel inlet. The temperature characterizes the oxidation state. The temperature is not the only possible choice. One could use any transported variable as long as it is a monotonic function of the oxidation state. The present model represents the combustion process by these two scalars which define the conditions in an ensemble of elementary reactors. The idealized process is called an unsteady perfectly stirred reactor (PSR) and is described by Equations (20) and (21) which are solved before the LES.

\[
\rho \frac{dY_i}{dt} = \dot{w}_i, \quad i = 1, 2, \ldots, N \quad (20)
\]

\[
\rho \frac{dT}{dt} = \dot{w}_T \quad (21)
\]

The initial condition for the \(N\) species and the temperature \(T\) are:
\[ X(t = 0) = \begin{bmatrix} Y_1 \\ \vdots \\ Y_i \\ \vdots \\ Y_N \\ T \end{bmatrix} = Z \cdot X_{fuel} + (1 - Z) \cdot X_{oxidizer} \]  

(22)

These equations are ODE (Ordinary Differential Equations) and are easily solved using chemical packages. One may build the library by solving the equations using the initial conditions for a given \( Z \) within \([0, 1]\) and for given temperatures \( T \) within \([500, 2600]\). The results are then mapped for these conditions. For example, Figure 3 shows the source terms for \( OH \) radicals, carbon monoxide (\( CO \)), and the dimensional source term for the temperature transport equation. The lines show the lines for which there is a chemical equilibrium above the source terms are zero. The source terms are largest well away from the equilibrium lines at high enough temperature.

We used the freeware Cantera for solving unsteady PSR set of equations. The major advantage of this approach over global chemistry is that it contains information about many species (e.g. radicals) and is expected to be accurate for auto-ignition predictions. Of course, the present approach is limited to cases that are relatively close to the original scenario.

One may derive a transport equation for the mixture fraction \( Z \) assuming the same molecular diffusivity for all species.\(^{28, 29}\) This assumption obviously does not account for differential diffusion. In the present case we assume that the turbulent transport is dominant which is consistent with our PSR based approach i.e. that the flow is seen as a collection of well stirred reactors. One combines the transport equations for eliminating the reaction terms and applies the FSFM for subgrid transport closure. A MILES (Monotonically Integrated LES) type closure is applied in the present work.\(^{30, 31}\)

### III. Case Description and Boundary Conditions

Figures 1 and 2 show the overall geometry of the swirl stabilized GT combustor. The inlet conditions are Dirichlet boundary conditions for the velocities, the scalar, and the temperature. The outlet has flux-conservative zero gradient conditions, and the walls have no-slip conditions for the velocities and zero-gradient for the scalars and the temperature.

A major limitation of Cartesian grid based techniques is the difficulty of handling complex geometries. The virtual boundary method\(^{32, 33}\) is a novel advanced technique for enabling simulations of flows in complex geometries on Cartesian grids. The basic idea is to model the wall as a body force ensuring the no-slip condition. In other words, steady walls are replaced by an equivalent body force enforcing zero velocity. The body force \( F \) is:

\[ F = -\alpha \frac{\bar{u}_{LES}(x, t) - u_T(x, t)}{\tau(x, t)} \]  

(23)

where \( \tau \) is the force time-scale, \( d \) is the force distribution (i.e. reads 0 in the fluid and 1 in the solid), \( u_T \) is the wall velocity (0 in case of steady walls) and \( \alpha \) is a relaxation constant. In the present work, \( \tau \) is of the order of the time step and \( \alpha \) is 0.5.

The swirl generator and the nozzle for spray injection are resolved by the LES grid through local refinements. Figure 2 shows the detailed geometry of the swirl generator in yellow. The blue color marks an isosurfaces of the instantaneous spray volume fraction. The swirl in the gas phase is generated by flow through the ducts which lead to the combustor at an angle, such that the gas inflow has a tangential velocity component. The spray is injected through a circular injector at an angle such that the droplets are injected in the shear layer around the recirculation zone. In the inner tube there is an airflow to assist the atomization.

The Reynolds number is set to \( Re = 50000 \), the swirl number, defined as the ratio tangential to axial bulk velocities, is \( S = 3 \). The air inlet pressure is set to 18 bar, the temperature to 700 K. In the present computation it is assumed that 97% of the mass flow go through the swirler and 3% go through the atomizer. The liquid fuel is assumed to be heptane which is injected at room temperature. The overall equivalence ratio is rich at \( \phi = 1.6 \).

The droplets are injected at the end of the injection pipe (see Figure 2). As the injector is of annular type, the droplet injection diameter is the width of the gap between the two concentric tubes. They bounce...
elastically off the walls. If droplets reach the outlet, they are destroyed.

The numerical grid has 3.7 million cells which gives a mesh spacing of 0.013 length units on the finest grid.

IV. Results and Discussion

The non-reacting flow without combustion has been investigated in a previous study\textsuperscript{24} in which a parameter sensitivity study to the injection droplet size was conducted. Additionally, the flow dynamics was analyzed by the proper orthogonal decomposition. Spectral data was also presented. This study extends the previous work to include combustion modeling. One may note that even the non-reacting flow has a temperature of about 700K, and thus the evaporation of the droplets must also be modeled.

The dependent variables are compared for non-reacting flow and reacting flow in terms of averages and RMS. This comparison is reasonable due to the fact that experimentalists frequently perform non-reacting flow experiments as a precursor to reacting flow experiments due to the lower costs and due to safety concerns. This transition may be investigated by computational techniques. In the present case, the non-reacting flow is compared to the reacting flow for a droplet injection diameter of SMD = 60µm. Additionally, a parameter sensitivity study is conducted for the reacting flow by comparison to an injection diameter of SMD = 500µm.

A. Comparison of Reacting Flow and Non-Reacting Flow

![Figure 4](image1.png)  
**Figure 4.** Non-reacting case average normalized axial velocity with SMD = 60µm

![Figure 5](image2.png)  
**Figure 5.** Reacting flow case average normalized axial velocity with SMD = 60µm

An overview over the entire flow field is given by Figures 4 and 5 for the non-reacting flow and the reacting...
flow, respectively. The non-reacting flow case has a convex recirculation bubble whereas the windward side of the recirculation zone for the reacting flow case has a concave curvature since the atomization air penetrates the recirculation zone. This penetration is explained further below. Additionally, the exit velocities are higher by continuity in the reacting flow case since the density is lower.

The strong differences in the dependent variables between the non-reacting flow case and the reacting flow case of course originate from the heat release in the reacting case. The only difference in the simulation is the chemical source term \(Q_{chem}\) in the energy transport equation (Equation (3)). It is therefore reasonable to discuss the temperature field first. The discussion of the velocity field, which is usually the most obvious starting point, is referred to later. The same color scaling is used for corresponding figures to enable an easy comparison between the two cases at the expense of detail for the individual fields. For example, Figures 6 and 7 are plots of the average temperature fields for the non-reacting flow and the reacting flow cases, respectively. The scale ranges from 300\(K\) to 1800\(K\) in both cases, for which the flow inlet temperature is 710\(K\). In the non-reacting case without combustion (Figure 6) the temperature decreases near the atomizer outlet to below 400\(K\), since the energy for the droplet vaporization is provided by the gas phase. As there is no combustion, the temperature cannot be higher than 710\(K\) anywhere in the flow field. Contrarily, in the reacting flow case the temperatures increase to above 1700\(K\). The lip between the atomizer and the swirler are under severe thermal load in temperatures of more than 1400\(K\). One can clearly see a cone-shaped region in which the temperature is at about 1200\(K\) which is low compared to the neighboring regions in which the temperature is about 1400\(K\). It is shown later in the discussion that the droplets evaporate in this region, resulting in the temperature decrease. As the non-reacting flow case has temperature differences below 400\(K\), the RMS of the temperature fluctuation is of course much lower compared to the reacting flow case which has differences of over 1000\(K\). Figures 8 and Figures 9 provide this comparison, and large temperature fluctuations can be noted in the reacting flow case near the symmetry axis and at the swirler inlet into the main combustion chamber. The non-reacting flow figures are presented with a different scale in a previous work which allows a closer inspection of the non-reacting flow.\(^{24}\)

The extremely strong qualitative and quantitative temperature differences result in corresponding changes in the density fields, since the density is inversely proportional to the temperature. The density also depends on the mixture fraction as discussed in Section A. In multiphase flow the density of the continuous phase (or the density ratio) is a highly important parameter, since the motion and breakup of the droplets depends strongly and non-linearly on it. The density in the non-reacting flow case (Figure 10) increases to over 20\(kg/m^3\) near the atomizer in the non-reacting flow case. The density becomes this high because the droplets evaporate in this region, and thus the temperature becomes low. Secondly, the evaporated heptane gas has a higher molecular weight than air, augmenting further the density increase. These effects become clear when one considers the ideal gas law (Equation (8)). The density does not increase to such high values in the reacting flow case (Figure 11) mostly for the obvious reason that the temperatures are so high. Instead, the density near the atomizer is only about half the value of the density in the non-reacting flow case. Secondly, the density is below 5\(kg/m^3\) in the very hot regions of the flow. Especially, the low values on the symmetry axis has profound effects on the axial velocity field and the recirculation bubble. The density fluctuations have about the same size for the non-reacting and the reacting flow cases (Figures 12 and 13, respectively), but in the reacting flow case the region of the largest density fluctuations is further downstream from the atomizer.

Figures 14 to 17 compare the axial velocity average and RMS fields for reacting and non-reacting flows. The non-reacting flow (Fig.14) has a clear recirculation bubble whereas in the reacting flow the atomizing air penetrates straight into the combustion chamber. The penetration occurs due to the fact that the recirculating air in the reacting flow case has low inertia as the density is low. In the non-reacting flow a strong PVC occurs due to which flow enters the swirler intermittently.\(^{24}\) This leads to the large RMS values at the lip between the atomizer and the swirler in Figure 16. This does not occur in the reacting flow case (Figure 16) since the hot air has smaller inertia and therefore cannot enter the swirler intermittently as it is possible for the non-reacting flow case.

Figures 18 to 21 compare the spray volume fractions in terms of averages and rms for reacting and non-reacting flow. One notes that the droplets disperse more in the case of non-reacting flow (Figure 18) as compared to reacting flow (Figure 19). This fact can be explained as a combination of a Stokes number effect and a Weber number effect. Equation (17) reveals directly what is here referred to as a Stokes number effect: The droplet acceleration is proportional to the density of the continuous phase. If one extracts a time scale from this equation, the so-called momentum response time \(\tau_m\), it is clear that this time scale is

\[\tau_m = \frac{\rho_{\text{chem}}}{\rho_{\text{air}} v_{\text{droplet}}}\]

where \(\rho_{\text{chem}}\) is the density of the continuous phase, \(\rho_{\text{air}}\) is the density of the air, and \(v_{\text{droplet}}\) is the velocity of the droplet.
Figure 6. Non-reacting case average temperature in $K$ with $SMD = 60\mu m$.

Figure 7. Reacting flow case average temperature in $K$ with $SMD = 60\mu m$.

Figure 8. Non-reacting case RMS temperature in $K$ with $SMD = 60\mu m$.

Figure 9. Reacting case RMS temperature in $K$ with $SMD = 60\mu m$. 
Figure 10. Non-reacting case average density in $kg/m^3$ with $SMD = 60 \mu m$

Figure 11. Reacting case average density in $kg/m^3$ with $SMD = 60 \mu m$

Figure 12. Non-reacting case RMS density in $kg/m^3$ with $SMD = 60 \mu m$

Figure 13. Reacting case RMS density in $kg/m^3$ with $SMD = 60 \mu m$
Figure 14. Non-reacting case average normalized axial velocity with $SMD = 60\mu m$

Figure 15. Reacting flow case average normalized axial velocity with $SMD = 60\mu m$

Figure 16. Non-reacting case RMS normalized axial velocity with $SMD = 60\mu m$

Figure 17. Reacting flow case RMS normalized axial velocity with $SMD = 60\mu m$
Figure 18. Non-reacting case average volume fraction with $SMD = 60\mu m$.

Figure 19. Reacting case average volume fraction with $SMD = 60\mu m$.

Figure 20. Non-reacting case RMS volume fraction with $SMD = 60\mu m$.

Figure 21. Reacting case RMS volume fraction with $SMD = 60\mu m$.
inversely proportional to the gas phase density. The Stokes number is defined as:

$$St = \frac{\tau_v}{\tau_f}$$

The Stokes number is therefore smaller in the non-reacting flow case which is why the dispersion effect is called Stokes number effect. This is a reformulation of the statement that the droplet acceleration is proportional to the density of the continuous phase.

Secondly, this Stokes number effect is augmented by a Weber number effect. The Weber number is defined as:

$$We = \frac{\rho_c D_p U_{rel}^2}{\sigma}$$

$\sigma$ is the surface tension. The droplet size after breakup is determined by their Weber number which is set to $We = 12$. Therefore larger densities may lead to smaller droplet diameters after breakup, though the relative velocity $U_{rel}$ will also decrease due to the smaller Stokes number. In the non-reacting flow case the droplets therefore become smaller. This Weber number effect decreases the Stokes number further in the non-reacting flow case.

Therefore the droplets follow the turbulent eddies more closely in the non-reacting flow case, whereas in the reacting flow case the average droplet trajectories is closer to the ballistic limit. Also the RMS show this trend (Figures 20 and 21): In the reacting case the droplets tend not to disperse into the central region close to the symmetry axis whereas in the non-reacting case some droplets do disperse there. The average droplet distribution explains the position of the main temperature decrease in the non-reacting flow and the reacting flow cases which was discussed above.

The average mixture fraction of the evaporated gases follows from the droplet dispersion (and also couples back on it via the density effects). In the non-reacting flow case the largest mixture fractions occur near the atomizer with local values up to $Z = 0.3$. In the reacting flow case one expects larger peak mixture fractions as the evaporation is more rapid. However, the evaporation is delayed since the breakup of the droplets is less efficient in the reacting flow case due to the Weber number effect described above. The mixture fraction attains the peak values of $Z = 0.5$ further downstream, consistent with the average trajectories of the droplets: The largest fractions of evaporated gases are obviously at the place where most of the droplets evaporate. The large mixture fraction values then lead to larger fluctuation of the mixture fraction for the reacting flow case as compared to the non-reacting flow case (Figures 24 and 25). These large fluctuation in the mixture fraction may lead to a highly unsteady combustion in the reacting flow case.

B. Sensitivity to the Droplet Diameter for Reacting Flow

The sensitivity to the injection droplet size is frequently one of the most important parameter sensitivity studies since the Weber and Stokes numbers both depend on the droplet size. It is currently not possible to determine what size the droplets have at the injection. Experimental data in this dense spray region is not available since optical diagnostics cannot look in regions in which there are too many droplets. This has the consequence for the numerical simulation that one has to study the sensitivity to the assumed droplet size. Figure 26 reveals that for large injection droplet sizes the zone of rapid droplet evaporation is more focussed as can be seen from the more pronounced minima in the average temperature field. In the case with $SMD = 60\mu m$ many droplets evaporate in a relatively even manner along the main droplet trajectory, whereas for $SMD = 500\mu m$ many droplets evaporate further downstream after they have broken up. This fact is related to the well-known $D^2$-law which implies that small droplets evaporate much faster than large droplets. The fluctuation in temperature are significantly smaller for large injection droplet size (Figure 27). The more focussed evaporation is also clearly demonstrated by the average mixture fraction field (Figure 28). Here the peak values are larger in the case with the large droplets at injection. Contrarily, the peak RMS values (Figure 29) are larger for the small droplets whereas the for the large droplets the fluctuations are spread over a larger region, but their peak values are smaller.

V. Conclusions

Large Eddy Simulations of a turbulent flow with spray combustion in a complex geometry is presented. The flow field for a case with combustion is compared to the corresponding flow field without combustion.
Figure 22. Non-reacting case average mixture fraction with $SMD = 60\mu m$

Figure 23. Reacting case average mixture fraction with $SMD = 60\mu m$

Figure 24. Non-reacting case RMS mixture fraction with $SMD = 60\mu m$

Figure 25. Reacting case RMS mixture fraction with $SMD = 60\mu m$
Figure 26. Reacting case average temperature in $K$ with $SMD = 500\mu m$

Figure 27. Reacting case RMS temperature in $K$ with $SMD = 500\mu m$

Figure 28. Reacting case average mixture fraction with $SMD = 500\mu m$

Figure 29. Reacting case RMS mixture fraction with $SMD = 500\mu m$
The combustion has profound effects on several important parameters, for example the position of the recirculation zone, the main droplet dispersion, the mixture fraction distribution, and of course the temperature and the density. Furthermore, the fluctuating values also differ strongly. Additionally, it is shown that the flow field in the reacting flow case is highly sensitive to the droplet injection diameter. Thus there is a need for accurate knowledge and modeling of the droplet injection size.

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References


