Radiation-spray coupling for realistic flow configurations

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1. Motivation and objectives

Designing commercially viable propulsion systems for supersonic aircraft is a major challenge. All modern combustors must balance the need for stability and performance with the goals of efficiency and cleanliness. These competing demands, however, are exacerbated in supersonic situations where the operating conditions are much more severe. Supersonic transport aircraft usually fly in the stratosphere, at cruising altitudes around 60,000–65,000 feet. The engine emissions produced at such high altitude contribute to depleting the ozone layer. Therefore the enhancement of the engine emission characteristics and performance is a vital issue for the supersonic vehicles to become part of the world’s air transportation system. To meet these demands, special combustor design considerations are needed to account for environmental and safety issues.

The Lean Direct Injection (LDI) configuration is a good candidate for supersonic civil transport aircraft, where the combined geometry of a swirler and a Venturi nozzle results in stable combustion of ultra-low NO\textsubscript{x} and soot emissions. Air is injected in a swirler of 60\degree vanes, where it mixes with the fuel droplets to atomize, break up aerodynamically and partially premix in the Venturi before entering the combustor. The combination of the swirler and the Venturi has proven to maximize the atomization performance and minimize pressure drop across the injector (Im et al. 1998). The Venturi nozzle also provides sufficient residence time for the fuel droplets to vaporize and mix uniformly with the swirled air droplets in a lean mixture. The LDI non-reactive flow results were reported earlier (El-Asrag et al. 2007) and only selected results will be presented again for comparison. Here, the reactive multi-physics simulation will be shown for the LDI (Tacina et al. 2001; Yang et al. 2003; Cai et al. 2005). The current paper presents simulations that couple the interaction of turbulence with the important physical processes such as spray/chemistry/radiation in a realistic configuration. Utilizing the single injector LDI as a model for realistic systems, the combustor emission characteristics, radiation coupling, flow/flame interaction, as well as the spray characteristics will be shown and compared with experimental data.

The main emission products of gas turbine engines are soot, nitrogen oxides (NO\textsubscript{x}), unburned hydrocarbons (UHC) and carbon monoxide (CO). The LDI operates under lean conditions. Therefore, soot emissions are not of major concern here. The two major emission products that we will focus on are CO and NO\textsubscript{x}. While CO has known hazardous health effects, NO\textsubscript{x} deplete the ultra-violet protective layer known as the ozone layer. The destruction of the stratospheric ozone (O\textsubscript{3}) by NO\textsubscript{x} can be described chemically by the following mechanism:

\[
\begin{align*}
\text{NO} + \text{O}_3 & \rightarrow \text{NO}_2 + \text{O}_2, \\
\text{NO}_2 + \text{O} & \rightarrow \text{NO} + \text{O}_2.
\end{align*}
\]
It is clear that NO acts as a catalyst for ozone depletion. Therefore, a reduction of NO emissions is vital for high speed commercial transport (HSCT) aircraft.

For hydrocarbon fuels, NO\textsubscript{x} are mainly produced by three well-known mechanisms: the Zeldovich (or thermal) mechanism, the Fenimore HCN pathway and the N\textsubscript{2}O-intermediate route. At high temperatures, the thermal pathway is found to be the most important. While the Fenimore mechanism is more dominant for fuel-rich combustion, the N\textsubscript{2}O-intermediate mechanism is dominant for fuel-lean mixtures at low temperatures. Since gas turbine engines operate at high temperature under lean conditions to minimize soot and CO emissions, the thermal pathway describes NO\textsubscript{x} production in such configurations. As the thermal pathway is a strong function of temperature, accurate prediction of NO\textsubscript{x} requires accurate prediction of temperature inside the combustor. The current study proves that radiation is of paramount importance to achieve this goal. The NO\textsubscript{x} production rate is relatively slower than the other products. Consequently, NO\textsubscript{x} are produced in the post-flame region. This distinct characteristic of NO\textsubscript{x} increases the modeling challenges significantly. The long NO\textsubscript{x} time scale allows for coupling with other slow processes like radiation from gases and particles. Therefore, the radiation coupling is important for accurate results. These issues require the selection of appropriate models to efficiently account for all these processes.

For accurate chemistry modeling, a detailed Jet-A surrogate mechanism is utilized (Peters 2006). The number of species and reactions considered are 109 and 1118, respectively. Jet-A is known to be a common fuel for gas turbine engines. In the context of LES, the flamelet approach will be used for the chemistry tabulation, which provides an efficient way for coupling of chemistry/turbulence under the assumptions of the flamelet approach. A brief description of the present combustion and spray models is outlined in the next section.

2. Numerical approach and modeling

The simulation is performed by the unstructured LES code CDP. CDP is a set of massively parallel unstructured finite-volume flow solvers developed specifically for large eddy simulation by Stanford’s Center for Integrated Turbulence Simulations as part of the Department of Energy’s ASC Alliance Program. The solver used to perform the simulations reported in this work is the node-based low-Mach number solver (Ham 2007). The LES governing equations and the sub-grid momentum closures are omitted here for brevity. A brief description of the combustion and spray models is presented below.

2.1. Combustion and radiation modeling

The combustion model used is the flamelet/progress-variable (FPV) approach (Pierce & Moin 2004; Ihme et al. 2008). The FPV approach is based on the flamelet concept, which relates the species mass fractions and energy to the mixture fraction through the flamelet equations

$$\rho \frac{\partial \Phi}{\partial t} - \rho \frac{\chi}{2} \frac{\partial^2 \Phi}{\partial Z^2} = \dot{\omega},$$  \hspace{1cm} (2.1)

where Z is the mixture fraction, \( \rho \) is the density, \( \Phi = (T, y_i)^T \) is a vector that contains the species mass fractions \( y_i \) and the temperature \( T \). \( \dot{\omega} \) is the source-term vector and \( \chi \) is the scalar dissipation rate, which represents the inverse of the diffusion characteristic time scale or equivalently the fluid influence on the scalars. The steady laminar flamelet model
(SLFM) tabulates the solution of Eq. (2.1) (without the unsteady term) as a function of the mixture fraction and the stoichiometric scalar dissipation rate $\chi_{st}$. Hence an equation of state (EOS) relating reactive scalars to the mixture fraction and its dissipation rate is written as

$$\Phi = \mathcal{F}_\Phi (Z, \chi_{st}) .$$

(2.2)

The solution of the flamelet equation is represented by the well-known S-shaped curve. Since the abscissa of the S-shaped curve represents variation of $\chi_{st}$, it is obvious that for a certain value of $\chi_{st}$ there exist up to three solutions, the lower stable un-burning solution, the middle unstable solution, and the upper stable burning solution. Therefore, a unique representation of the entire mixture fraction space by the scalar dissipation rate will not reflect all the available solutions.

In the FPV approach a new flamelet reactive scalar $\lambda$ is introduced to describe the reactive state in place of the scalar dissipation rate. As a result, the new state vector is given as $\Psi = \mathcal{F}_\Psi (Z, \lambda)$. This parameter ($\lambda$) is generally called the flame index and is statistically independent of the mixture fraction $Z$ (Ihme et al. 2008). The flame index is defined by a progress variable $C$ that can be a combination of certain species products, temperature, enthalpy or any scalar that can represent the reactive state uniquely on the S-shaped curve. The progress variable here is the sum of the mass fractions of $\text{CO}_2$, $\text{CO}$, $\text{H}_2\text{O}$ and $\text{H}_2$. For each flamelet, the progress variable is a function of the mixture fraction and can be uniquely related to flame index by its value at the stoichiometric conditions $(Z_{st})$ (Ihme et al. 2008):

$$\lambda = C|Z_{st} ,$$

(2.3)

and the reaction progress variable can then be expressed as

$$C = \mathcal{F}_C (Z, \lambda) .$$

(2.4)

Assuming the state vector $\Phi = \mathcal{F}_\Phi (Z, \lambda)$ is obtained by the solution of Eq. (2.1), a joint probability density function (PDF) needs to be evaluated to obtain the Favre filtered ($\bar{\cdot}$) values of the state vector. Since $Z$ and $\lambda$ are defined to be independent variables, by using Bayes’ theorem, the joint PDF at a certain time and space vector can be given as

$$\bar{P} (Z, \lambda; x, t) = \bar{P} (\lambda|Z) \bar{P} (Z) ,$$

(2.5)

where the mixture fraction marginal PDF $\bar{P} (Z)$ is assumed to be a beta distribution (Pierce & Moin 2004) and the conditional reaction progress parameter PDF is a delta function. Since the PDF distribution is characterized by the scalar mean $\bar{Z}$ and the scalar variance $\bar{Z}''^2$, the flamelet tabulation can be written in this form:

$$\Phi = \mathcal{F}_\Phi \left( \bar{Z}, \bar{Z}''^2, \bar{C} \right) ,$$

(2.6)

where $C$ can be obtained from Eq. (2.4). As previously mentioned, for accurate temperature prediction, radiation needs to be considered. Ihme & Pitsch (2008) have extended the above FPV approach to account for radiation as an unsteady process. In this model the total enthalpy $\bar{H}$ including the heat of formation is introduced as an additional variable. Consequently, the extended FPV EOS is written as

$$\bar{\Omega} = \mathcal{F}_\Omega \left( \bar{Z}, \bar{Z}''^2, \bar{C}, \bar{H} \right) .$$

(2.7)

As a result, four parameters have to be computed as part of the LES solution, namely the filtered mixture fraction $\bar{Z}$, the subfilter scalar variance $\bar{Z}''^2$, the filtered progress
variable $\tilde{C}$, and the filtered total enthalpy $\tilde{H}$. Here, the scalar variance $\tilde{Z}_{\tilde{Z}}^2$ is evaluated using an algebraic model (Pierce & Moin 2004), which assumes homogeneity and local equilibrium for the subgrid scales and is given by

$$\tilde{Z}_{\tilde{Z}}^2 = C_Z \Delta^2 \tilde{\rho} |\nabla \tilde{Z}|^2,$$

where the mixture fraction coefficient $C_Z$ is computed dynamically and $\tilde{\rho}$ is the filtered density. Finally, three additional transport equations are solved for $\tilde{Z}$, $\tilde{H}$ and $\tilde{C}$ as follows:

$$\partial_t \tilde{\rho} \tilde{Z} + \nabla \cdot (\tilde{\rho} \tilde{u} \tilde{Z}) = \nabla \cdot (\tilde{\rho} \tilde{D} \nabla \tilde{Z}) + \nabla \cdot \tilde{\tau}_{\tilde{Z} \tilde{Z}},$$

$$\partial_t \tilde{\rho} \tilde{C} + \nabla \cdot (\tilde{\rho} \tilde{u} \tilde{C}) = \nabla \cdot (\tilde{\rho} \tilde{D} \nabla \tilde{C}) + \nabla \cdot \tilde{\tau}_{\tilde{C} \tilde{C}} + \tilde{\omega}_{\tilde{C}},$$

$$\partial_t \tilde{\rho} \tilde{H} + \nabla \cdot (\tilde{\rho} \tilde{u} \tilde{H}) = \nabla \cdot (\tilde{\rho} \tilde{D} \nabla \tilde{H}) - \tilde{q}_r,$$

where $\tilde{D}$ is filtered molecular diffusivity, assuming equal species diffusivity and unity Lewis number, and $\tilde{\omega}_{\tilde{C}}$ is the filtered chemical source term of the progress variable. In the above equations, the residual stresses $\tilde{\tau}_{\tilde{Z} \tilde{Z}}$ are modeled by a dynamic approach (Pierce & Moin 2004). For an optically thin radiation model, the filtered radiation source term is

$$\tilde{q}_r = 4 \sigma \left( \tilde{T}^4 - \tilde{T}_\infty^4 \right) \sum (\tilde{p}_i \tilde{a}_i),$$

where $\tilde{p}_i$ and $\tilde{a}_i$ are the partial pressure and Planck mean absorption coefficient of species $i$, respectively, and $\sigma$ is the Stefan Boltzmann constant. To account for the unsteadiness of NO$_x$ production, the filtered mass fraction of NO ($\tilde{Y}_{NO}$) is computed by solving a transport equation rather than extracting the values from the flamelet tables (Ihme & Pitsch 2008). The filtered LES equation can then be written as

$$\partial_t \tilde{Y}_{NO} + \nabla \cdot (\tilde{\rho} \tilde{u} \tilde{Y}_{NO}) = \nabla \cdot (\tilde{\rho} \tilde{D} \nabla \tilde{Y}_{NO}) + \tilde{\omega}_{\tilde{Y}_{NO}},$$

where the filtered production rate $\tilde{\omega}_{\tilde{Y}_{NO}}$ is closed by assuming scale similarity between the unsteady NO filtered mass fraction and the flamelet tables retrieved value. In the solution procedure the unsteady flamelet equations are solved starting with the steady state solution without radiation. This results in a sequence of transient unsteady flamelets solutions to be stored and tabulated. More details about the FPV and the radiation model can be found in Ihme & Pitsch (2008). The spray models employed are introduced below.

2.2. Secondary breakup spray model

Jet-A fuel spray droplets are injected from the centerline simplex atomizer. The hollow cone spray has a total angle of 90°. The spray models employed in CDP are described in detail by Apte et al. (2003, 2008a,b). Here, we summarize the most important features.

A stochastic subgrid model for spray atomization is used here. The initial liquid film is approximated by a droplet of size equal to the nozzle diameter. The model views the subsequent particle breakup as a discrete random process, where droplet size is treated as a time-dependent stochastic variable. The temporal and spatial evolution of the particle size distribution is then governed by the Fokker-Plank differential equation. This evolution leads to the formation of new droplets and destruction of the parent ones. The new
droplets position and velocity vectors are tracked by a Lagrangian algorithm in the physical space. Two-way coupling between the gas phase and the liquid droplets is achieved by the source terms in the gas-phase equations, which represent the mutual effect of mixing and momentum/energy transport. These effects are induced by droplet breakup, evaporation and convection by the flowfield. Consequent to the process of droplet breakup and mixing with the gas phase, the liquid phase evaporates under the appropriate conditions. The evaporation model solves a set of ordinary differential equations (ODEs) that describe the variation of the droplet mass and temperature due to evaporation and assumes the non-equilibrium effects inside the droplet volume are neglected. A third-order Runge-Kutta scheme is used to integrate the set of ODEs with the minimum physical drop time scale. The mathematical formulation of the above scheme is omitted here for brevity and can be found in Apte et al. (2008b).

3. Numerical setup

The experimental setup and data are provided by Farhad et al. (2006). The geometry of the single-element combustor is shown in Fig. 1a without the inflow pipe for clarity. Liquid fuel is injected through the center, while air is injected through a swirler with vane angles of 60°. The global swirl number is 1. The swirler is composed of six helical vanes with an effective area of 870 mm². The fuel droplets from the centerline and the swirled air are mixed in a converging-diverging Venturi nozzle. The helical air swirler has an inside diameter of 9.3 mm and an outside diameter of 22.1 mm. The combustor has a square cross-sectional area of 50.8 x 50.8 mm.

The mesh uses 1,072,640 hexahedral elements, which is slightly above the 861,823 element mesh used in the RANS calculations by Farhad et al. (2006); Iannetti & Liu (2008) and about half the LES structured mesh used by Patel & Menon (2008). The unstructured mesh is shown in Fig. 1. The mesh distribution along the z = 0 plane and in the vanes is shown in Fig. 1b, while the y – z plane grid distribution is presented in Fig. 1c. The mesh cells are clustered toward the centerline and toward the walls of the combustor.

An inflow bulk velocity of 20.14 m/s is provided through a tube upstream of the swirl injector. The inflow air is at temperature $T_o = 294$ K and pressure of 1 atm, while the global equivalence ratio is 0.75. The fuel spray has an inflow mass flow rate of 4.15 – 04 kg/s and an initial velocity of 20 m/s. The droplets are injected with a Rosin-Rammler distribution

$$F_m(D) = 1 - \exp \left( - \left( \frac{D}{\delta} \right)^n \right),$$

(3.1)

where $F_m(D)$ is the cumulative distribution function of the droplet diameter $D$, and the parameters $n = 1.34$ and $\delta = 24 \mu m$ are chosen to curve-fit the distribution of the experimental data at the first measured location. An inflow recycling technique is used (El-Asrag et al. 2007) to achieve realistic inflow turbulence. The recycling is done until the inflow profile recovers a realistic inflow turbulent boundary layer. The boundary conditions used are inflow/outflow in the x-direction and walls in the y and z directions.

Statistics are collected over a physical time of 0.032 seconds after the initial transient. Based on the bulk inflow velocity and the full length of the combustor this represents two complete flow-through times. The simulation was performed on a Linux cluster at Stanford University with infiniband interconnection and dual Intel Clovertown (Quad
4. Results and discussion

In this section, two LES simulations are compared to the experimental data. The statistics for the two simulations, with and without radiation, are collected after the same total run time. Unless mentioned otherwise, only the case with radiation is considered for the comparison with the radial experimental data. Almost all the available experimental data are used in the comparison and selected non-reactive flow data are included to show the heat release effect.

First, the time-averaged flow features of the reactive flow will be shown and compared with the non-reactive case with an emphasis on the radiation effect. Subsequently, the mean and root mean squared (rms) values of the gas flowfield, the scalars, and the spray characteristics will be compared to the experimental data.

Due to the swirling flow, an adverse pressure gradient is generated in the axial direction and a vortex breakdown bubble (VBB) is established. The LDI is characterized by a central recirculation zone (CRZ) in addition to recirculation zones (RZs) at the corner of
the dump plane. Three RZs had been observed previously in the non-reactive case (El-Asrag et al. 2007; Patel et al. 2007; Iannetti & Liu 2008). Figures 2a and 2b show an isosurface of mean axial velocity for $\langle U \rangle = 0$ m/s for both the reactive and non-reactive cases. The length of the CRZ in the non-reactive case is approximately twice as that in the reactive one. However, the reactive CRZ has a larger effective bulk diameter. Also, a small toroidal RZ close to the divergent part of the Venturi exists in the reactive flow case as shown by the side view in Fig. 3, which is caused by flow separation. A more compact and stronger reactive CRZ is due to the expansion of the flowfield by heat release effects as shown later.

Figure 4 shows vector plot for the time-averaged total velocity magnitude. Only the projections in the $y = 0$ plane are shown here for clarity. Figure 4a shows that the CRZ starts early inside the divergent part of the Venturi nozzle, in addition to a small RZ observed just downstream of the injector exit. These two small RZs inside the Venturi
enhance mixing and atomization of the spray with the swirling air. However, at the injector exit the droplets and the spray sheet have enough momentum to penetrate this RZ toward the Venturi exit as shown in Fig. 4b. This observation will be assessed later by the axial and radial velocity profiles. Figure 4c shows the velocity magnitude vector plot downstream of the dump. The CRZ has an azimuthal vortex at the location $x = 17$ mm downstream of the dump plane. Figure 4c also shows an additional annular vortex at the burner corners where the second RZ is located. Corner vortices are found to extend along the combustor wall corners up to the exit plane in the $y - z$ plane (not shown here), which will affect the spray droplets’ distribution as shown later.

The instantaneous temperature distribution is displayed in Fig. 5. Figure 5a shows a snapshot of the $y = 0$ plane. Figures 5b-d show three consecutive snapshots at the location $x = 11$ mm. Figures 5a and 5d are at the same time instant. The temperature shows high gradients at the shear layer location and around the CRZ, which leads to
strong mixing. At the edge of the CRZ, fresh cold gases (dark areas) are engulfed into the CRZ. Inside the core of the RZ, the temperature shows nearly uniform distribution due to the strong mixing the fluid undergoes before entering the CRZ.

A comparison of the heat release distribution is illustrated in Fig. 6. The flame without radiation shows locally lower mean values than the case with radiation, for which the heat release is more distributed. The reason is that radiation causes the temperatures to be locally lower, which leads to smaller evaporation rates of the liquid fuel and consequently a lower fuel vapor mass fraction as observed in Fig. 7.

Two snapshots for the spray distribution from the two simulations are shown in Fig. 8. The spray exhibits a 90° cone angle. Some of the spray droplets are trapped inside the corner vortex, which results in an increase in the mean droplet diameter close to the walls. The simulation with radiation shows a wider range of droplet sizes. For the shown instantaneous snapshots, with radiation, droplet size ranges between 0.5 µm and 50 µm, while without radiation the range is between 0.7 µm and 40 µm. This is attributed to a
higher evaporation rate when radiation is not included. Since no primary breakup model is employed here, the spray spectrum shows an intermediate regime, where the spray injected from the nozzle undergoes secondary breakup, followed by a dilute regime where the droplets evaporate. The intermediate regime is mainly inside the Venturi, while the dilute regime extends until all the droplets are evaporated.

The steady state droplet and parcel-size histograms for both cases are shown in Fig. 9. In general, the case without radiation has a lower frequency of particles over the whole spectrum. This will subsequently affect the flow dynamics and the flame structure (as shown earlier). The radiation effect on droplet evaporation can be assessed in Fig. 10. This figure shows the time-averaged rate of droplet mass evaporation at the plane $y = 0$. This value represents the time average of the source term of the droplet mass variation.
Radiation spray coupling

(a) With radiation  (b) No radiation

Figure 8. Instantaneous droplet distribution sized by droplet mass combined with the instantaneous temperature distribution at the $y = 0$ plane.

Figure 9. Radiation effect on the droplet parcel histogram. (With radiation − − − , without radiation −)

The case without radiation shows higher evaporation rates in the vicinity of the injector and in the flame surface surrounding area due to the reasons discussed earlier.

The LES simulation with radiation modeling is compared with the experimental data next. Figures 11a and 11b show spray droplet mean diameter $D_{10}$ and Sauter mean diameter $D_{32}$. Overall good agreement is observed. At the first three locations a peak value is shown that starts (at $x = 3$ mm) at a radial distance of 8 mm from the centerline and then spreads radially towards the wall. This location is an indication of the spray sheet cone angle. Since the spray droplets directly emitted from the injector have a large droplet size, the profiles show peak values at these radial locations. Downstream of $x = 15$ mm some droplets are trapped in the wall-corner vortex. It is interesting to note that the value of the mean diameter is increasing downstream due to evaporation of the smaller diameter droplets. This is consistent with the experimental data.
Figure 10. Time-averaged droplet mass evaporation rate in (kg/s) at the central $y = 0$ plane.

Figure 11. Radial profiles of droplet arithmetic mean and Sauter mean diameters (Experiment data $\circ$, computation $-$)

The spray droplets’ mean axial velocity distribution is shown in Fig. 12. Good agreement is observed for all locations. Consistent with Fig. 11, the LES shows over-predicted droplet mean axial velocity at the locations of over-prediction in the droplet size. Again, over-prediction is expected at the first few locations, where the small-size droplets are not considered in the experiment.

To show the extent of the centerline RZ and the effect of heat release and radiation on the flow features, the centerline mean axial velocity profiles are shown in Fig. 13. Reactive and non-reactive data from experiments are compared with the LES results with and without radiation. The figure shows that the non-reactive RZ extends to about 100 mm downstream of the dump, while the reactive RZ is stronger and more compact (about 50 mm in length). The expansion of the flow by heat release changes the local velocity and pressure distribution. This local expansion (in the flame region) increases the pressure gradient and leads to faster flow deceleration. This results in a shorter but wider RZ. The CRZ without radiation is over-predicted by about 5 mm due to the change in the flame structure and the spray distribution as shown in Fig. 6.

As discussed below, the LES simulation shows that inside the divergent section of
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Figure 12. Radial profiles of mean droplet axial velocity (Experiment data ◦, computation −)

Figure 13. Comparison of time-averaged centerline axial velocity $\langle U \rangle$. Non-reactive flow (Experiment □, computation −), reactive flow (Experiment ◦, computation with radiation − · −, computation with no radiation · · ·).

the Venturi a small RZ is established, followed by an increase in the velocity due to a sudden expansion after the dump. This is followed by a steep reduction inside the RZ due to the adverse pressure gradient. There are no experimental data inside the Venturi, but the profile captures the initial peak after the dump accurately, which confirms the foregoing physical conclusions. Note that the current simulation captures the centerline profile initial peak. This might be attributed to the realistic inflow conditions used here, as discussed earlier. The deviations near the injector will be discussed later.

The mean and rms axial velocities are shown in Figs. 14 and 15. The first three locations ($x = 3 \text{ mm}$, $x = 5 \text{ mm}$ and $x = 9 \text{ mm}$) are found to be the most difficult to match with the experiment. These locations exhibit high unsteadiness and high measurement errors. The experimental measurements (Cai et al. 2005) use a Phase Doppler Particle Analyzer (PDPA). A problem usually related to the measurements is how to distinguish between the seedings’ particles to measure the gas phase velocity and the spray droplets. In the LDI experimental measurements (Cai et al. 2005) the nominal diameter of the seeding
particles used was 1 µm. To distinguish between the spray and the seeding particles, all particles smaller than 4 µm were used to represent the gas-phase velocity. However, inside the CRZ the small spray droplets just ejected from the nozzle still have high momentum in the positive direction. As a result, the experimental velocity profiles near the exit (i.e., $x = 3$ mm, $x = 5$ mm and $x = 9$ mm) are all positive despite the existence of the CRZ. Therefore, at these locations we expect to under-predict the experimental data. The previous RANS simulation (Iannetti & Liu 2008) shows also higher deviation at $x = 3$ mm, and comparable results at $x = 9$ mm. The LES simulation by Patel & Menon (2008) also shows lower velocity at the location $x = 5$ mm but no data are presented for the other two locations. Starting from the $x = 15$ mm location, the current LES simulation shows good results compared with the experimental data. The CRZ extends to approximately 50 mm downstream of the dump. At the $x = 92$ mm location, the profile shows a nearly uniform velocity that recovers the inflow mass flow rate at the exit cross-sectional area. This uniformity is important in gas turbine engines to minimize the thermal stresses on the turbine blades. A slight deviation is found towards the walls. This can be attributed to the fact that the CRZ in the current simulation is wider than in the experiment. As a result, the flow is more compressed between the CRZ and the walls and the velocity is higher.

The rms axial velocity profile is shown in Fig. 16. The rms peaks close to the dump plane at the onset of the shear layer and then decays axially as the shear layer decays downstream. The predicted and experimental axial rms profiles show good agreement. The high rms values at the first three locations confirm the high unsteadiness of the shear layer. For example, at $x = 5$ mm the rms value is around 100% of the corresponding mean value. At the first three locations, over-prediction is noticed at the $y = 15$ mm radial location. The discrepancy with the experimental data at the first three locations is due to the reasons mentioned in the previous paragraph. The LES data predict two rms peaks that start at the radial location $y = 9$ mm at the first axial location. These two peaks spread downstream with the spread of the shear layer. Downstream of $x = 20$ mm, the peaks start to move again toward the centerline following the CRZ surface. After reaching the $x = 46$ mm location, the peaks are completely merged. After this location, no reverse
flow exists and the shear layer is completely diffused. Similar observations apply to Fig. 17, where the radial profiles of the turbulent shear stress are plotted. The shear stress shows antisymmetric radial profiles. Good agreement is shown, with deviations at the first two locations. The zero shear stress at the centerline indicates flow symmetry around the centerline.

Figure 18 shows the mean velocity component in the $y$-direction at different axial locations. The flow is rotating in the clockwise direction (CCW) viewed from the outflow cross-section. The global swirl number is of the order of 1. In contrast to other velocity components, the results show good agreement with the first location at $x = 3$ mm. The flow shows solid body rotation around the centerline downstream of the location $x = 29$ mm. Upstream of this location the flow is rotating around the central RZ.

The focus of the following discussion is the LDI emission characteristics. For supersonic vehicles, the NO emissions directly deplete the stratospheric ozone layer. Therefore, accurate models are required to predict gas turbine emissions. As discussed earlier, NO production is a slow process and it is coupled with other processes that have long char-
characteristic time scales such as radiation. Radiation affects NO in an indirect way through
the change in temperature, which then changes the production rate. As a result, the first
step is to predict temperature accurately. Figure 19 shows the centerline mean tempera-
ture with and without radiation modeling. This figure shows that without radiation the
temperature is over-predicted. This is consistent with earlier observations.

The radiation model employed here is an optically thin model (Ihme & Pitsch 2008).
The model assumes that the medium is gray and neglects the heat lost or gained by wall
absorption and reflection. Figure 20 shows radial temperature profiles at the locations
where experimental data are available. The temperature is under-predicted at the cen-
terline. This may suggest a need for a more accurate radiation model that accounts for
the absorption within the flame, the scattering by the media, and the wall effect.

Figure 21 shows the centerline species distribution for CO. The CO level along the
centerline is captured reasonably well. An initial peak is observed in the rich combustion
region followed by a decay in the CO level as it is oxidized to produce CO$_2$. The centerline
Figure 19. Comparison of the centerline mean temperature $\langle T \rangle$. (Experiment $\circ$, computation without radiation (−) and with radiation (· − ·).

Figure 20. Mean radial temperature profiles $\langle T \rangle$ (Experiment $\circ$, computation −).

NO profile also shows good results (not shown here). The effect of radiation improves the results generally.

Acknowledgements

The authors thanks Dr. Nan-Suey Liu for providing advice, grid and experimental data for comparison. Many thanks to Dr. Anthony C. Iannetti from NASA GRC, Dr. Thomas Lederlin, Dr. Wai Wang and Dr. Andrea Lamorgese at CTR for helpful discussions. The authors also acknowledge Dr. Frank Ham for his valuable support regarding the CDP code.

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Figure 21. Time averaged centerline CO mass fraction profile in ppm $\langle Y_{CO} \rangle$ without radiation (−) and with radiation (−−).


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