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Investigation of initial droplet distribution and importance of secondary breakup model on lean blowout predictions of a model gas turbine combustor

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Abstract: In the present work, the importance of secondary droplet breakup and the impact of the initial droplet distribution on lean blowout (LBO) predictions is investigated to determine the sensitivity and robustness of the prediction to spray boundary conditions and secondary breakup models, respectively. This is accomplished using large-eddy simulations of a model gas turbine combustor, operating near the LBO limit. The flow field and gas phase chemistry is solved using an unstructured Navier-Stokes solver and a flamelet/progress variable formulation, respectively. Liquid spray is modeled using a polydisperse droplet injection and a Lagrangian spray evaporation model. Simulations with and without stochastic modeling of droplet breakup are performed. An analysis of the droplet Weber number indicates that large diameter droplets are above the critical Weber number and should undergo secondary breakup. The present study demonstrates that secondary droplet breakup has a significant impact on the predicted droplet distribution and temporal evolution of the flame. Due to the large computational requirements of the current simulations, an ad-hoc approach to determining the initial droplet SMD and diameter is not feasible and a secondary droplet breakup model is required to reproduce the experimental trends.
Keywords: ***Lean blowout, Spray, LES***

1. Introduction

Modern gas turbines operate at lean conditions to reduce emissions. Lower operating temperatures are obtained in the combustor chamber due to lean combustion with a corresponding reduction of NOx emissions. However, at lean conditions gas turbines are susceptible to blowout as the flame stabilization mechanisms are weakened. In previous large-eddy simulations (LES) of a referee-rig combustor, secondary droplet break-up was incorporated using a stochastic approach. The need for a secondary breakup (SBU) model was justified due to the large velocity gradients experienced by the droplets near the injectors. In this region, the Weber number was found to be between 2 and 20 [1], which is above the critical Weber number, $We_c = 6$, where droplet breakup is observed experimentally. The previous simulations produced stable flames with accurate axial and radial droplet velocities for a range of fuels. However, the Sauter mean diameter (SMD) calculated was severely under-predicted at all axial locations, suggesting the droplet breakup was over-predicted by the SBU model. The first objective of the current study, is to investigate and quantify the impact of the SBU model on the droplet SMD. The second objective is to determine if the modeling of the spray can be simplified. Specifically, by modifying the spray boundary conditions in such a

way that the SBU model is not required. This work is motivated in an attempt to simplify boundary conditions for an extensive comparison between multiple LES-combustion codes at different research institutions. Removal of the SBU model is motivated by the observation that the SBU occurs very close to the injector exit where very little chemical activity occurs. Thus, by reducing the SMD at the injector based on a priori information, the effects of SBU can be mimicked without requiring the introduction of SBU models in the LES-combustion codes.

2. Flamelet/Progress variable aproach

In the present work, closure of the filtered mean chemical reaction rate is provided by the Flamelet/Progress variable (FPV) combustion model [2, 3]. In the FPV approach the chemical reactivity and flame dynamics are incorporated using a steady flamelet model and the species mass fractions are retrieved from tabulated chemistry.Thus, in the FPV approach the chemistry is tabulated as a function of the filtered mixture fraction, $\widetilde{Z}$, its variance and a filtered progress variable, $\widetilde{C}$. The filtered mean mass fractions of any species ($\widetilde{Y_k}$) can then be retrieved using

$$\widetilde{Y_k} = \int_0^1 Y_k(Z,C)\widetilde{P}(Z,C)dZ, \tag{1}$$

where $\tilde{P}(Z,C)$ is the joint probability density function (PDF) of Z and C, which can be rewritten as $\tilde{P}(Z)P(C|Z)$, where $P(C|Z)$ is the conditional PDF of C given Z. In the current work, a β-PDF is assumed for $\tilde{P}(Z)$ and a Dirac delta function is applied to model $P(C|Z)$[2]. In the present study, the progress variable is defined as $C = Y_{CO2} + Y_{CO} + Y_{H2} + Y_{H2O}$.

3. Spray and Secondary breakup models

A Lagrangian framework is chosen to model the spray behavior with the droplet velocity computed using the Basset-Boussinesq-Oseen (BBO) equation. The droplet diameter at the injector is prescribed using a Rosin-Rammler distribution based on a precalculated SMD. Evaporation of the liquid droplets is modeled using equilibrium calculations of isolated droplets [4].

Secondary breakup is determined heuristically using a stochastic modeling approach to reduce the number of tuning parameters [5, 6]. In this model, droplet breakup is considered to be both a temporally and spatially evolving phenomena, which follows a solution to a Fokker-Plank differential equation,

$$T_j(x,t+1) = \frac{1}{2}\left[1 + erf\left(\frac{x - x_j - \langle\eta\rangle}{\sqrt{2\langle\eta^2\rangle}}\right)\right] \tag{2}$$

where erf is the error function and j is the j^{th} primary droplet. $\langle\eta\rangle$ and $\langle\eta^2\rangle$ are two model parameters which required closure. In the current study, closure of $\langle\eta\rangle$ and $\langle\eta^2\rangle$ are provided via

$$\langle\eta\rangle = -0.1 \quad \text{and} \quad \langle\eta^2\rangle = -0.1 log\left(\frac{We_{cr}}{We_j}\right) \tag{3}$$

4. Experimental and Numerical Details

The design of the referee combustor rig was chosen to mimic a realistic gas-turbine combustion chamber utilizing the Rich-burn/Quick-mix/Lean-burn (RQL) technologies. This burner includes the major characteristics of a real gas-turbine specifically, a complex liquid injection system with multiple concentric swirlers, a multi-perforated liner and two rows of dilution jets. Experimental measurements for different operating conditions and fuels were performed at the Air Force Research Laboratory at Dayton. The present study focuses on the Cat-A2 fuels, which is a conventional petroleum-derived Jet-A fuel. The combustor operates at 2.07 atms with a 3% relative pressure drop across the injection system. A summary of the operating conditions can be found in Ref [1].

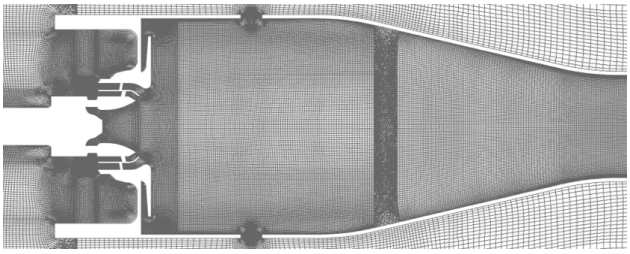


Figure 1: Computational Domain.

Various experimental measurements are available including pressure drop, wall temperature and OH* and CH* chemiluminescence. The present study is focused on the droplet diameter predicted by the simulations which is obtained using phase-doppler particle analyzer (PDPA) [1].
The computational domain consists of a large pressurized plenum, injection system, combustion chamber and exhaust plenum. The mesh is created using mainly regular hexahedral elements with some tetrahedral elements in the injector. The mesh, consisting of approximately 20 million cells, is shown in Fig. 1. Simulations are performed using the low-Mach LES solver VIDA [7], which includes the Lagrangian Spray framework. In the present work, turbulent closure of the sub-grid scale (SGS) turbulence is provided by the WALE eddy-viscosity SGS model [8], with the effusive gas-cooling specified based on experimental measurements. Additional information on the numerical details and equations solved can be found in [1]. Approximately 10,000 CPU hours, using Intel Xeon E5-2680v2 processors, are required for 1 *ms* of simulation time.

Spray boundary conditions are summarized in Table 1. Stable combustion results are taken from previous numerical simulations of the same referee-rig [1]. The updated boundary conditions investigated in the present study where obtained from discussions during the National Jet Fuel Combustion Program (NJFCP). The small differences in injection speed and spray angle was found to not significantly alter the spray characteristics. Thus, no additional stable combustion simulations with updated injection spray and spray angle where undertaken. For all simulations liquid properties are calculated based on NJFCP studies.

Table 1: Summary of spray boundary conditions and model parameters.

	Stable	Updated
Fuel	A2	A2
Spray injection speed	8.6 m/s	8 m/s
Droplet size distribution (SMD)	54 microns	45, 35, 25 microns
Full spray angle	90 degrees	80 degrees
Secondary breakup model	Yes	No

5. Results and Discussions

5.1 Droplet Diameter

In the work of Esclapez et al. [1], simulations of the referee-rig using the same numerical setup and FPV combustion model are performed and the initial droplet size distribution at the injector inlet is obtained from an empirical correlation [9]. This empirical correlation relates SMD to the liquid surface tension, viscosity, mass flow rate, air density and pressure drop across the nozzle. In conjunction with secondary droplet breakup, they were able to obtain a stable flame and good predictions of droplet velocity. However, an under-prediction of the droplet SMD was observed at all radial locations. The applicability of the empirical correlation for the referee-rig at current operating conditions was also stated to be uncertain [1]. Thus, in this section the impact of the initial droplet distribution is investigated. This is accomplished by turning off the SBU-model, and varying the initial droplet SMD. Thus, the impact of the initial droplet diameter on the droplet distribution downstream of the injector and it's impact on flame stabilization can be assessed. In addition, the current simulation predictions are compared to results of the Cat-A2 fuel from [1] to assess the impact of SBU on the droplet distribution.

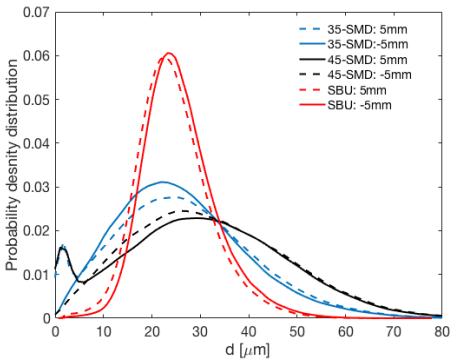


Figure 2: Droplet distribution for four simulations with different spray injector boundary conditions. Red line is obtained from the simulations reported in [1] using the stochastic secondary breakup model. Deflector plate corresponds an axial location of 0 mm.

Figure 2 presents the particle distribution for three simulations at locations downstream of the injector, one closer to the nozzle and one after the deflector plate. As can be seen in Fig. 2, both the 35 and 45 μm simulations without SBU produce very different particle diameter distributions when compared to previous simulations with SBU and a SMD of 56 μm. In the new simulations,

large diameter droplets are allowed to convect downstream, whereas in the previous simulations these droplets would break up. Another interesting characteristic of the new simulation is that there is a noticeable change in the distribution at the two sample locations, with more droplets having larger diameters and a spike in small diameter droplets observed. In comparison, when SBU is included minor changes in the droplet particles is observed between the two locations. Thus, when SBU is included in the simulation it fully defines the diameter within the swirler. Without SBU the boundary conditions chosen for SMD at the injector have a larger impact and could be tuned to better reflect the experimental droplet diameters.

5.2 Impact on LBO simulations

In the previous section, the inclusion of a SBU model is shown to have a appreciable impact on the droplet distribution and SMD profiles downstream of the injector. However, from this analysis it is unclear what impact these changes have on the LBO predictions. In particular, it is unclear if the simulations with the updated boundary conditions will produce stable flames and reproduce the correct experimental characteristics. In this section, the transient flame structure is analyzed to determine the impact of removing SBU and reducing the injector droplet SMD. Figure 3 shows the time evolution of the temperature, droplet position and droplet temperature for three different injector SMD. As a reference, the simulations using an SMD of 56 μm with SBU produced a stable flame as reported in [1].

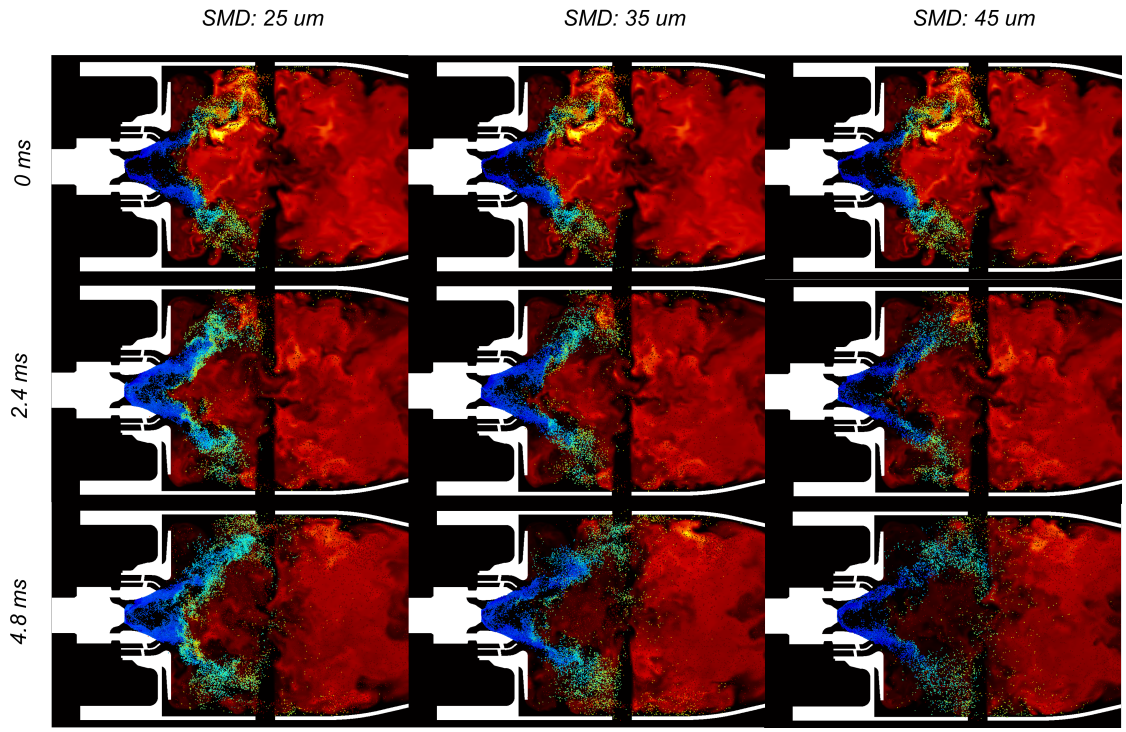
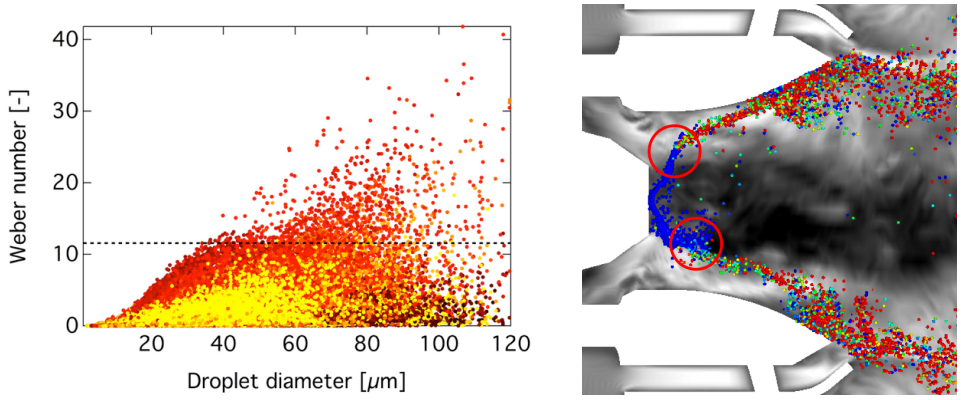


Figure 3: Time evolution of the temperature, droplet position and droplet temperature for three different injector SMD.

For the largest SMD tested, 45 μm, within 2.4 ms the temperature in the recirculation zone begins

to decrease and a larger number of unburnt droplets are observed downstream of the recirculation zone. This trend continues until there are only a few local hot spots within the recirculation zone at 4.8 *ms* and the flame has effectively blown-out. From Section 5.1, it is clear that this process is a consequence of having larger droplets entering the recirculation region compared to the previous simulation. These larger droplets take longer to evaporate, which leads to blowout. From these observations it is expected that the simulations with smaller SMD should sustain combustion longer as they do not contain the same number of large droplets. As can be seen in Fig. 3, both the 35 and 25 μm simulations contain higher temperatures at both 2.4 and 4.8 *ms* with higher temperatures observed in the 25 μm simulations at both times. This supports the idea that a heuristic approach to the selection of the initial droplet SMD and distribution could be applied to improve agreement with the experimental measurements. This approach has the added benefit that it simplifies the modeling, by removing a submodel, allowing for an easier comparison between different combustion models and LES codes.

Unfortunately, this approach has two major drawbacks. First, by removing SBU the physicality of the models is reduced which may lower the model predictability. An additional simulation, with SBU and the critical Weber number set to 12, was performed to determine where SBU is important. The droplet Weber number as a function of droplet diameter and the location where SBU occurs is shown in Figs. 4a) and 4b), respectively. It was found that increasing the critical Weber number from 6 to 12 had no significant effect on the simulations. However, as can be seen in Fig. 4a) even with this higher critical Weber number a significant number of large diameter droplets undergo secondary breakup. Thus, SBU is required to accurately account for the spray physics. Second, an appropriate and fast method for choosing the initial droplet distribution and SMD is not obvious. In the current study, all three SMD tests resulted in blowout with the 25 μm SMD simulation, maintaining combustion the longest. Thus, tuning of the simulations is required which would be very computationally expensive for the current study.



(a) (b)

Figure 4: a) Weber number vs droplet diameter (colored by axial location). Critical weber number set at 12 (dashed line). b) Axial velocity profile with location of secondary breakup (circles)

6. Conclusions

Large-eddy simulations are performed to assess the impact of secondary droplet break up and the initial SMD on the droplet distribution and flame characteristics for a realistic two-phase flow combustor operating near the LBO limit. Large differences in the predicted droplet distribution are observed between simulations with and without a SBU model. With SBU, the droplet distribution is almost indistinguishable at the two axial locations investigated. In contrast, in the simulations without SBU, significant differences between the two locations are observed. Further, large differences in the distribution shapes are seen between the SBU and no SBU simulations, even for simulations with similar SMD at the injector. Thus, in simulations with SBU the droplet distribution appears to be determined strictly by the SBU model and is not sensitive to the SMD chosen at the injector.

The temporal evolution of the temperature, for simulations without SBU and different injector SMD, demonstrate that the stability and flame characteristics of the simulations are sensitive to spray boundary conditions and breakup modeling. In the present work, all three simulations without SBU resulted in blowout. Due to the large computational requirements of the current simulations, it is concluded that an ad-hoc approach to determining the initial droplet SMD and diameter is not feasible. Thus, SBU is required to produce results which are stable and in relatively good agreement with experimental data. However, investigation of the current SBU model is required in order to understand the cause of the under-prediction in the droplet SMD downstream of the injector.

7. Acknowledgements

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