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Large eddy simulation of pressure and dilution-jet effects on soot formation in a model aircraft swirl combustor

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ABSTRACT

Soot formation in a model aircraft engine configuration operating at elevated pressures is studied using large eddy simulation (LES) and detailed models for precursor and soot population evolution. Specifically, pressure and secondary oxidation air injection effects on soot formation are simulated. The configuration simulated is a dual-swirl ethylene/air combustor operating at pressures of 3 and 5 bars, with and without secondary oxidation air injection. The inflow conditions are chosen such that for the two different pressures, the only hydrodynamic change is the Reynolds number. Detailed comparisons with experimental data show that the simulation captures gas-phase statistics accurately. Although the spatial structure of soot formation is captured, including some of the trends for different operating conditions, the quantitative comparisons had significant differences. This could be attributed to the large distribution in the measurements or the chemical/physical models for soot formation. Detailed analysis showed that soot mass generation in such devices is driven by acetylene-based surface growth, with strong oxidation zones that significantly reduce net soot emissions. More importantly, soot formation occurs due to a spatially and temporally intermittent phenomena, where a small set of fluid trajectories that deposit fuel-rich pockets into the right gas-phase conditions is responsible for the bulk of soot mass generated. The occurrence of these relatively low-frequency trajectories is due to large scale unsteadiness caused by the strong swirl near the fuel jets. Lagrangian particle trajectory analysis revealed that lower pressure case without sidejet injection encourages entrainment of soot particles into the inner recirculation zone, increasing the residence time and leading to increased soot volume fraction. When pressure is increased from 3 to 5 bar, these particles move through a different mixture fraction-progress variable phase space. Consequently, there is a hydrodynamic scaling mode introduced, which can produce interesting variations from the nominal pressure scaling for soot production. These studies point to an intricate dependence of soot formation on large-scale turbulent flows, which is generally non-universal and not observed in canonical jet flames.

1. Introduction

With increase in operating pressures of aircraft combustors, it is expected that there will be an accompanying increase in particulate emissions [1]. Although modern combustors operate at globally lean equivalence ratios, locally inefficient turbulent mixing can lead to fuel-rich pockets that promote particulate formation. Understanding the role of such mixing processes and the effect of pressure increase on soot emissions is critical for the development of next generation gas turbines. In this context, detailed computational modeling is a useful tool. However, developing predictive computational models for soot is recognized as a formidable challenge [2,3]. Due to the high Reynolds number turbulent flow within an aircraft combustor, soot formation is intricately linked to the turbulence-chemistry interaction associated with both fuel oxidation and soot evolution processes. Although significant progress has been made in the modeling of soot formation in flames [4,5], application of these tools to realistic gas turbine flows and direct comparison with experiments remains sparse. The focus of this work is to use state-of-the-art tools for modeling turbulence, combustion, and soot evolution processes to simulate a model aircraft combustor, operating at elevated pressures. The

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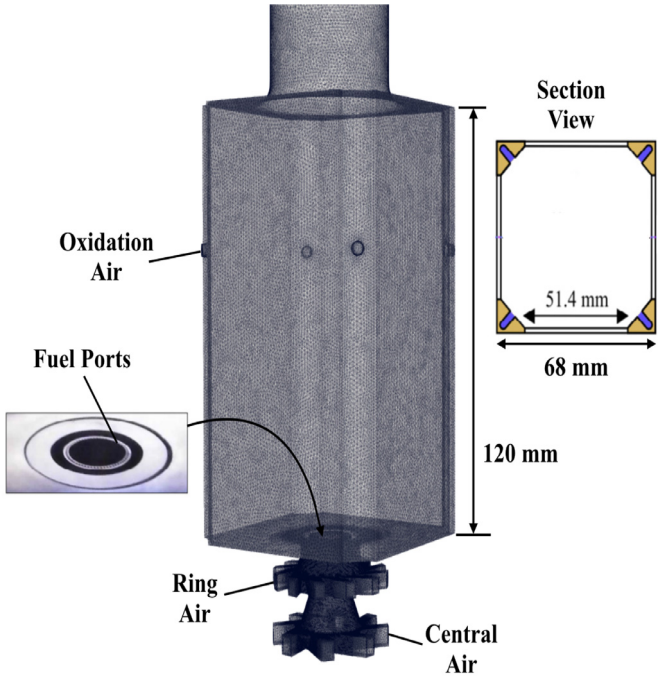

Fig. 1. Combustor geometry and computational unstructured mesh (12 million cells), inlet nozzle details, and planar cross sections at the height of secondary oxidation air injectors.

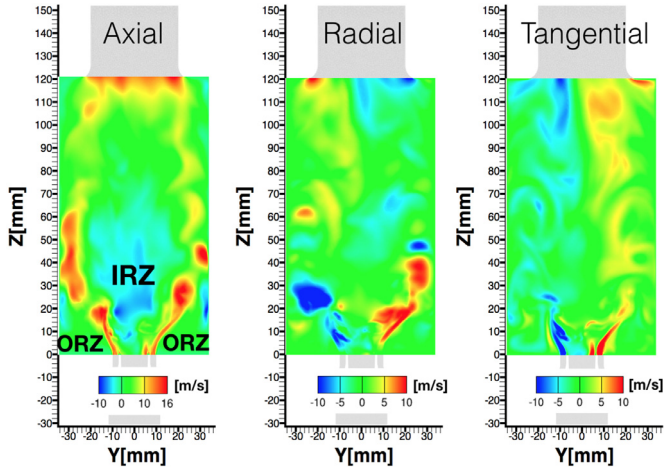

Fig. 2. Instantaneous velocity contours for 3 bar case without sidejet. Locations of inner recirculation zone (IRZ) and outer recirculation zone (ORZ) are specified.

objective is to determine the predictive capability of the models and analyze the challenges in capturing soot formation in complex flows.

It is now accepted that the use of large eddy simulation (LES) is necessary to capture the turbulent mixing driven combustion processes that govern aircraft-type combustors [6]. In particular, LES has been applied to model gas-phase combustion in a variety of aircraft combustor geometries, with very good success in the prediction of the overall flow characteristics [7–11]. In many of these applications, the use of tabulated flamelet approaches has been shown to be accurate for operating conditions far away from blowout or other extinction phenomena [8,12–14]. For this reason, in this work, LES with flamelet approach is used to model the turbulent combustion process. The simulation of soot formation is itself a complex problem. This includes the chemical and physical models that govern gas-phase precursor and particulate-phase evolution [3,15,16], as well as the computational description of

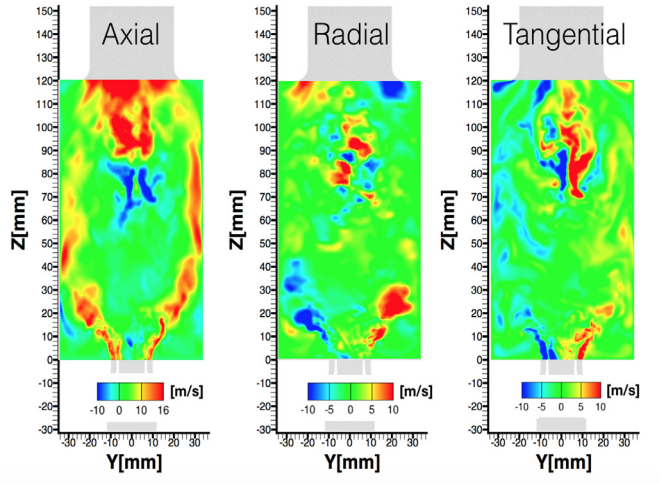

Fig. 3. Instantaneous velocity contours for 3 bar case with sidejet.

the nanoparticle population balance [5,17–19]. Aided by increasing computational power, detailed models as well as the framework for such comprehensive simulations have been developed [3,20–22]. Here, the soot modeling approach of Mueller [3] will be utilized. This method incorporates detailed chemical kinetics for the fuel oxidation and precursor formation, turbulence-chemistry interaction using a presumed-PDF approach [23], and nanoparticle evolution through the method-of-moments [19,24].

Over the last decade, validation studies that utilize high-fidelity experimental data have emerged for sooting flames. The International Sooting Flames Workshop (ISF) [25] provides one such central forum for model validation. An analysis of results presented there and elsewhere [20–22,26,27] provides interesting insights. Canonical jet flames, which are amongst the simplest turbulent flows that support chemical reactions, are found to be a challenging configuration for soot prediction. While there are numerous literature studies demonstrating the accuracy of LES in predicting gas-phase jet flames [6,28,29], similar computational models fail to predict soot concentrations spectacularly, often providing volume fractions that are orders of magnitude lower (or higher) compared to experiments [25]. Part of this discrepancy is due to the high sensitivity of soot formation to gas-phase thermochemical composition. For instance, Mueller and Raman [30] have shown that even small errors in temperature mismatch with experiments can lead to significant errors in soot predictions. Further, models for soot evolution are often formulated based on data from laminar flames, which may not be representative of the conditions seen in a turbulent flame. This includes the range of strain rates, as well as the spatial and temporal variations in the thermochemical composition of the gas-phase, which introduces a history-dependent evolution of the soot particles.

Since different physical and chemical processes dictate soot formation, the relative importance as well as accuracy determine predictive capability. Temperature perturbations resulted in downstream soot volume fraction errors of 30% in turbulent non-premixed piloted jet flames [30], however this was insufficient to explain the discrepancies with experimental data. Other sources of error in turbulent combustion modeling or chemistry mechanism are likely responsible as well. In jet flames burning ethylene fuel, models that employ Polycyclic Aromatic Hydrocarbon (PAH) based precursor chemistry vastly underpredict soot volume fraction [25]. On the other hand, semi-empirical models [31] that rely on acetylene-based nucleation predict much higher soot mass [20]. Since PAH concentrations are highly sensitive to strain rates, it is possible that either inaccurate precursor chemistry or errors in