FIRST PRINCIPLE AND MODELING OF TURBULENT TWO-PHASE FLOWS

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EXECUTIVE SUMMARY

Aircraft gas turbines often rely on the combustion of high-energy-density liquid fuel to meet weight and volume restrictions. The efficiency of the conversion and the emission of harmful pollutants depend directly on the mixing of the fuel and oxidizer, which itself results from a cascade of mechanisms initiated by the atomization of a coherent liquid stream. In this context, the challenges met by experimental diagnostics are numerous and include the wide range of scales at play, as well as the lack of optical access. These shortcomings have spurred the development of numerical strategies to simulate and model the atomization process. Computational approaches can potentially provide invaluable insight into the effects of fluid properties and nozzle design, as well as control strategies. There are, however, some obstacles to reaching predictive simulation and modeling capabilities, and petascale systems such as Blue Waters are central to achieving this goal.

INTRODUCTION

The reliable prediction of primary atomization and the resultant spray population statistics are vital for the design of low-emissions and stable gas turbine combustors. Atomization of a liquid jet is controlled by unique small-scale physics that rely on the interaction between vorticity generation at the small scales and the interface motion, which in turn is controlled by surface tension forces. Although a critical sub-component of a liquid fueled combustor, the liquid spray breakup resulting from complex fuel injectors is poorly understood. Yet it has a significant influence on the engine performance in terms of emissions, fuel consumption, thermo-acoustic instabilities and durability. The modeling of liquid fuel injectors represents a formidable challenge. The main quantity of interest is the spray penetration, characterized by the droplet number density function that includes the distribution of droplet sizes and velocities. This information is subsequently used to design the primary reaction zone. For instance, insufficient atomization could result in fuel-rich pockets that promote soot formation. Similarly, the nature of atomization will also control ignition tendencies in high-altitude relight conditions. Hence, reliable computational models that predict the final spray properties are indispensable for the successful design of aircraft combustors.

METHODS & RESULTS

Improving the current understanding and the predictive capabilities of primary atomization requires progress in two distinct areas. The first is Direct Numerical Simulation (DNS), which consists of solving the equations that govern the mixing of the liquid and gas without any simplifying assumptions. Hence, it represents the highest achievable level of fidelity. This level of fidelity comes at a price, however, in that the governing equations are very stiff. Tailored (physics compatible) numerical algorithms are therefore required. Also, in the regime of interest, the governing equations (the two-phase Navier-Stokes equations) are chaotic, and feature a wide range of scales, which require the use of extremely large computational meshes. For the foreseeable future, it is, therefore, undeniable that DNS of full-scale industrial configurations will remain scarce. This introduces the second area that requires advances, namely the modeling of primary atomization. Models based on the Reynolds-Averaged Navier-Stokes or the Large Eddy Simulation formalisms are characterized by their reliance on additional modeling assumptions. They, of course, come with a significant reduction in computational cost, the trade-off being their lower fidelity. An additional advantage is their improved controllability over the local instantaneous formulation used in DNS, which is chaotic and therefore harder to optimize or control.

The first component of the project leverages recent and ongoing developments in the field of multiphase computational fluid dynamics, which are unlocking the predictive capabilities of DNS of turbulent two-phase flows, and hence enabling the exploration of the physics of atomization. Reaching the regimes of interest to practical applications, however, requires harnessing the performances of large-scale systems such as Blue Waters. This means, in particular, designing software that achieves good load balancing where conflicting algorithmic requirements meet, e.g. the local application of computational geometry (highly non-linear) in the interface vicinity vs. the global use of iterative linear solvers in implicit and differential algebraic equations. Emerging heterogeneous architectures, in particular the XK nodes on Blue Waters, therefore represent an unprecedented opportunity.

DNS therefore represents a unique tool to quantify the effects of different atomizer designs, or to perform parametric study over low dimensional spaces (given associated computational cost). But it can also provide valuable insight into the modeling of primary atomization. To date, documented studies in this area have mostly been limited to asymptotic limits, or to restrictive phenomenological or empirical hypothesis. Analysis of the very large data sets generated by the DNS software using statistical tools as well as decomposition techniques has proved useful to model single-phase turbulence and combustion, and is, therefore, the second component of the project. Given the volume of the data sets involved, as well as the specificities of the decomposition techniques, this analysis can only be achieved using the fast storage and large bandwidth achieved by the Blue Waters system.

WHY BLUE WATERS

Blue Waters is critical to not only perform the highly resolved simulations required to explore and model primary atomization in canonical flow configurations, but also to push the **frontiers** of current computational infrastructures by leveraging hybrid (i.e. shared and distributed) and heterogeneous (e.g. CPU and GPU) programming, in order to simulate practical engineering applications, and ultimately develop new nozzle designs.