Modeling Complexities in Turbulent Spray Combustion

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Abstract

Turbulent spray combustion is a common process found in aircraft and automobile engines as well as chemical reactors. Spray combustion is a multilscale multiphysics problem involving the nonlinear interaction of spray evolution and evaporation, gas-phase turbulent mixing, and combustion. A detailed description of this complex process requires models for each of the physical processes involved. In this study, we focus on the development of the multiphase combustion models. Currently, spray combustion models are directly extended from corresponding single-phase combustion models. However, combustion in the presence of evaporating droplets has many unique features that render invalid many of the assumptions underlying the single-phase models. The objective of this work is to introduce a novel probability density function (PDF) based approach, which addresses many of the multiphase combustion modeling challenges. Numerical algorithms and preliminary results are presented here.

Keywords: Spray combustion , large eddy simulation, probability density function, combustion regime.

Liquid fuel based combustion is widely encountered in aircraft and automobile engines as well as chemical reactors. In typical combustors, the liquid fuel is sprayed using an atomizer that produces a fine mist of droplets. The droplets evolve in the background turbulent gas-phase flow and evaporate. This fuel vapor then mixes with the gas-phase oxidizer and reacts in a high-temperature environment. The proper dispersion of fuel inside the combustor is critical in maintaining stability and in reducing emissions. The complete description of the spray combustion system requires models for tracking the spray droplets, gas-phase turbulent flow, and combustion. Since the focus of this work is the modeling of the combustion process, standard and state-of-the-art approaches for the other two components will be used. The spray droplets will be evolved using a Lagrangian approach. The gas-phase turbulent flow will be described using the large eddy simulation (LES) method.

Single-phase combustion models are derived based on the nature of the combustion regime. For instance, the fuel and oxidizer could be molecularly mixed before entering the combustion chamber leading to premixed combustion. If the fuel and oxidizer mix insider the combustor, a non-premixed combustion process is supposed to exist. The controlling parameters and the flame structure are vastly different in the two cases giving rise to very different combustion models. Since the combustion regime is determined by the boundary conditions, the combustion model can be chosen *apriori*. In spray combustion, the fuel is released in vapor form through droplet evaporation, which in itself depends on the physical dispersion of droplets and the rate of liquid evaporation. Both these processes are dependent on the gas-phase turbulence and combustion. Consequently, the combustion regime can change within the reactor due to a number of reasons including the relative rates of evaporation and mixing, effect of droplet inertia on the gas-phase turbulence, and the spatial distribution of the reaction zone [1]. Fig. 1 shows the flame structure for two different droplet structure in a coflowing oxidizer stream. When the droplets are close enough, the flame is pushed outside and a flame front typical of premixed combustion is formed. If the droplets are dispersed far enough, the flame front advances into the inter-droplet spacing leading to a partially-premixed combustion process. While these cases demonstrate the extreme effects, droplet structure and its evolution play a critical role in determining the combustion process. For this reason, a combustion model that presumes the combustion regime will not be fully valid in spray combustion.

In this work, a novel method termed the probability density function (PDF) approach is used [2]. The main advantage in this approach is that the chemical source terms appear closed and do not require modeling. This, in turn, implies that the combustion regime is not fixed in a simulation. While this is certainly advantageous, mixing of scalars has to be modeled and poses a tremendous challenge. In the lecture, models recently proposed by the author to address this issue will be discussed. In the PDF approach, the transport equation for the joint-PDF of all chemical species and other scalars that define the thermochemical state of the system is solved directly. This transport equation is high dimensional and cannot be solved using conventional finite-volume or finite-difference discretization scheme. Typically, a Lagrangian Monte-Carlo method is used. In practical simulations, this PDF solver is coupled with the spray and turbulence models and evolved in a temporally accurate manner. This coupled solver was used to simulate canonical flows in an effort to verify and validate this computational tool (Fig. 2). The nature of information exchange between the solvers is very important in the context of spray combustion. It will be demonstrated that the current techniques for simulating such flows change the underlying physics of the combustion process.

References

[1] V. Raman and H. Koo, "Effect of Droplet Inertia on Evaporation and Spray Combustion", *Submitted to the The 32nd International Combustion Symposium*, 2008

[2] V. Raman and H. Koo, "LES/Filtered-Density Function Approach for Turbulent Spray Combustion", *Submitted to Combustion and Flame*, 2008

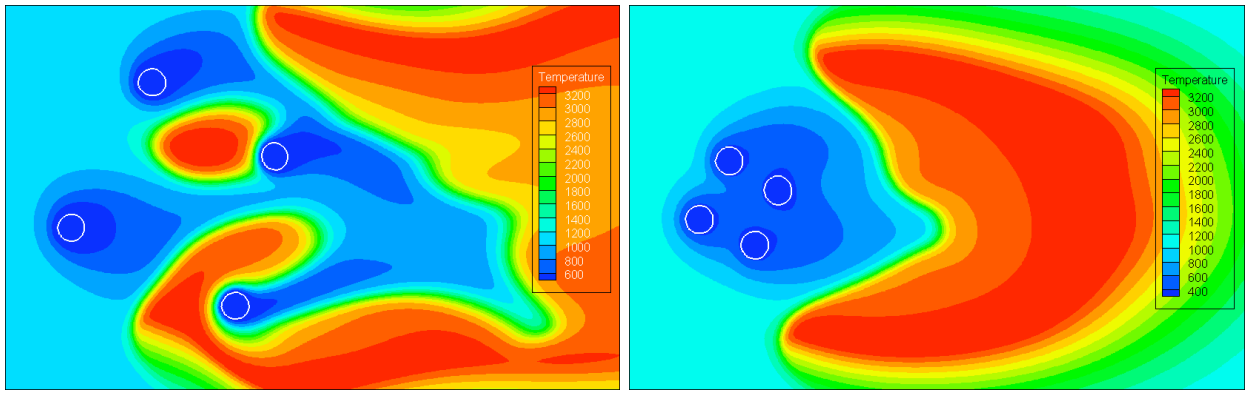

Figure 1: *Multiple droplet combustion with detailed resolution of the droplet interface. Droplets are dispersed closely (right) and (right) far apart.*

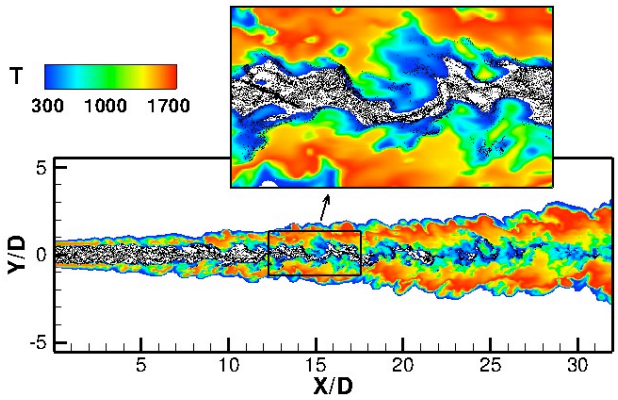

Figure 2: *Spray droplet population superimposed on the instantaneous contours of gas-phase temperature. The inset shows more details about the reaction zone.*