Partially Premixed Combustion in Spray Flames

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1 Introduction

Many industrial devices dedicated to propulsion systems or energy transformation inject liquid fuel with a gaseous oxidizer to feed the chamber where turbulent combustion takes place. Numerical simulation is widely used along with experimental studies to evaluate and improve the global features of such devices. Many works [1] have been devoted to numerical simulation and modeling of turbulent combustion of purely gaseous flames. Although many difficulties remain [2], the main features of such flames are now well known and various models have been proposed, however many difficulties still exist when performing two-phase flow simulations.

The objective of this work is to seek out combustion regimes in turbulent sprays, and particularly partially premixed combustion. To this end, 2D direct numerical simulation (DNS) has been used in association with a Lagrangian solver for the dispersed vaporizing phase. By varying the sprays properties in term of droplet density and size, many flame topologies and combustion modes are observed in the simulations.

2 Numerical procedure and flow configuration

The resources required to perform a full DNS of both the turbulent gas-phase motion and the detailed properties of a liquid phase are too great for actual computer facilities, in addition the physical description of the liquid-gas interface is still an open question. Nevertheless, it is possible to realize a DNS in which the flows around and inside an individual drop are not fully resolved, instead closures are retained for the liquid phase and its evaporation rate [3]. The droplets are local sources of fuel, properties of which are calculated in a Lagrangian context. The spray is then viewed as a collection of individual droplets convected by the turbulent flow. Expressions are chosen for the drag force and for the vaporization rate according to a model for the heat transfer within the drop [4, 5]. The drag force and the source of mass due to evaporation enter the momentum equations solved in an Eulerian context. The droplets also affects the turbulent flow and



Figure 1: Computational domain

a two-way coupling is necessary [4]. The treatment of this two-way coupling limits DNS to dilute sprays observed at some stage in real devices [6].

The spray source terms appearing in the Eulerian equations are evaluated by volume averaging the contributions of the droplets within each cell of the Eulerian grid. The Lele's PADE scheme [7] and the boundary conditions of Poinsot and Lele [8] have been used to solve the gas phase transport equations on a Cartesian mesh. This scheme is sixth order in space and third order in time.

A one step Arrhenius law irreversible chemistry is retained. The computations are performed with a Zel'dovitch number $\beta = 8$, a stoichiometric mixture fraction point $Z_s = 0.0625$ and a heat release parameter $\alpha = (T_{burnt} - T_{fresh})/T_{burnt} = 0.66$, where T_{fresh} and T_{burnt} denote the temperatures on the two sides of a reference stoichiometric unstrained premixed front.

Turbulent jets simulations are conducted on 2D Cartesian grids. Fig. 1 displays a sketch of the whole computational domain. The configuration consists of a spray surrounded by two flapping co-flow (Strouhal number equal to 0.6) of preheated air. Flow instabilities are shortly generated after injection and ignition occurs in developed turbulence.

There is a large number of parameters involved in the problem (velocity profile, droplets carateristics, turbulent mixing times ...). Two generic simulations have been retained and are discussed for the same mass fuel rate. All quantities are normalized by the maximum inlet flow velocity and the inlet jet width.

1. In the case denoted as LARGE, the diameter of the n_1 injected droplets per unit of time is $\Theta_1 = 9.26 \, 10^{-3}$ (for a jet width of $1 \, cm$, $\Theta_1 \approx 100 \mu m$. The number of droplets n_1 has been determined so that the fuel mass fraction in the injection channel would be 0.125 if the droplets were instantaneously vaporized. 2. In the case denoted as SMALL, $\Theta_2 = 5.55 \, 10^{-3}$ and to conserve the inlet mass fuel rate, one uses $n_2 = n_1 \Theta_1^3 / \Theta_2^3$.



Figure 2: Left: CASE *LARGE*, snapshot of the energy heat release (isocontours). Right: CASE *SMALL* Vaporizing droplets (dots) and heat release (isocontours).



Figure 3: 1D cut along a spanwise direction at six diameters of the inlet. W_e : Energy heat release. Y_F : Vapor of fuel mass fraction. Y_O : Gaseous oxidizer mass fraction. Left : case *LARGE* (predominant premixed combustion); right : case *SMALL* (predominant diffusion combustion). The data have been referenced by their maximum value in the profile.

3 Flame structure

Both simulations *LARGE* and *SMALL* have been conducted in reacting cases with the same chemical parameters. As soon as mixing between vapor of fuel and oxidizer is sufficient, combustion starts with triple points surrounding the spray. Three flames emerge from each triple point: A rapidly vanishing lean premixed flame on the oxidizer side, a trailing diffusion flame and a rich premixed flame, both connected to the triple point. Combustion is therefore organized in a hybrid regime as shown figure 2.



Figure 4: Two snapshots (A and B) of the energy heat release (isocontours) and the vaporizing droplets (dots). Local zooms show a burning ring of droplets (A') and flame complex interactions and extinctions (B'), case LARGE.

CASE LARGE: The quite large vaporization time implies the presence of vaporizing droplets on the jet centerline, between the mean iso-stoichiometric lines. Therefore, in addition to the stoichiometric diffusion flame, a strongly reactive partially premixed (rich) flame develops along the whole droplets trajectories (Fig. 2-left). Remaining fuel burns in a diffusion regime behind this partially premixed flame. The combustion mode is thus complex, combining triple flames with rich partially premixed combustion close to the stoichiometric condition, due to the slowly vaporizing drops.

CASE SMALL: The droplets are smaller and their very fast heating leads to rapid vaporization. Then, the fuel vapor mass fraction is far from stoichiometry and the rich premixed flame is close to flamability limit and therefore much weaker (Fig. 2-right).

Confirmation of this analysis is given by figure 2. This figure presents spanwise profiles of the energy source term W_e , the vapor of fuel mass fraction Y_F and the gaseous oxidizer mass fraction Y_O . Fig. 2-left shows the predominant premixed combustion regime of the case with large droplets. In Fig. 2-right, the premixed flame is almost negligible compared to the diffusion flame.

Figure 4 presents the flame at two successive times (LARGE simulation). The droplets are also shown, some are crossing the computational domain without being totally vaporized. A large variety of flame topologies is observed, pockets of burning droplets behind the diffusion flame (A') or multiple interactions between premixed and diffusion flames (B'). Local extinctions and edge flames [9] may be detected as well.

4 Conclusion

A Lagrangian model for two-phase flows has been applied with a combustion DNS code including finite rate chemistry.

It has been shown that the combustion regime around a liquid spray strongly depends on the droplets size and distribution. Very different combustions mode may be observed and are directly related to the properties of the spray injector.

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