# Lagrangian Modeling of Non-Premixed Turbulent Combustion in High Speed and Two-Phase Flows: Application to Rocket Engines Conditions

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### 1 Introduction

High-performance rocket engines, such as the main engine of the European launcher Ariane, usually rely on the separated injection of oxidizer and fuel, the flow velocity of the two streams being fixed to reach the targeted fuel/oxidizer ratio. The dynamics of the resulting non-premixed jet flame is controlled, to a large extent, by the levels of turbulence that are too important to be compatible with a Direct Numerical Simulation (DNS) of the Navier-Stokes equations. To this respect, Reynolds Average Navier-Stokes numerical simulations still remain largely used, and a great modeling effort must be done to provide reliable models able to describe the interaction between turbulence and chemistry in such high speed flows. First, compressible effects associated to shock or expansion waves influence both the fluctuating velocity field and the characteristics of the chemistry by modifying the local levels of pressure and density. Moreover, it is well-known that the mean chemical production rate is also significantly affected by fluctuations of temperature and concentrations so that its closure requires particular attention. In the high speed reactive flows under consideration, the conversion of kinetic energy into thermal energy includes two components: a reversible contribution that corresponds to the heating of the reactants due to local compressions, and an irreversible one that corresponds to viscous dissipation heating. In such turbulent reactive high speed flows, special models must be put forward to take into account its influence that can promote the stabilization of non-premixed flames [1, 2, 3]. In the present study, we present and then subsequently use the developments of a Lagrangian model that includes these supersonic combustion specificities. When two-phase flows are considered, the modeling difficulty is increased by the influence of the spray dynamics onto the composition statistics. In particular, additional unknown terms associated to the vaporization processes appear in the transport equations for the mixture fraction mean and variance and their closure must also be addressed. The present abstract is organized as follows: first the modeling aspects are presented. Then, results of numerical simulations of (i) underexpanded supersonic coflowing reactive jets and (ii) of the 10 bar MASCOTTE test bench are presented in the third and fourth sections. Finally, conclusions and perspectives are drawn in the last section.

# 2 Lagrangian Modeling Strategy

The present model of turbulent combustion is based on the original work of Gonzalez and Borghi, see for instance [4]. It relies on the sudden chemistry hypothesis that introduces a strong but clearlystated functional dependence between the mixture fraction  $\xi$ , and the mass fraction Y of a reactive species, oxygen in the present work. Based on the simplest micromixing closure, i.e. the one given by the IEM (Interaction par Echange avec la Moyenne) model [5], we define a Lagrangian path in the composition space:  $Y = Y_{MIL}(\xi)$  so that the estimation of the joint scalar Probability Density Function (PDF)  $\tilde{P}(Y;\xi; \boldsymbol{x}, t)$  can be simply expressed through the knowledge of the marginal mixture fraction PDF  $\tilde{P}(\xi; \boldsymbol{x}, t)$ . This PDF shape is presumed to be a classical beta function. Such an approach is well-suited to describe the effects associated with finite rate chemistry and/or ignition, and allows to delineate an inflammation domain by comparing flow time scales with chemical time scales as obtained from the tabulation of detailed chemical kinetics [6]. Following Bray et al. [7], the present conserved scalar PDF formalism is extended to high-speed combustion by simply replacing the static enthalpy with the stagnation enthalpy. The validity of such a proposal depends crucially on the existence of a linear relationship between the total enthalpy  $h_t$  and the mixture fraction  $\xi$ , which has been assessed by DNS investigations [7]. The Lagrangian evolution of the total enthalpy together with the knowledge of the velocity field is used to obtain the value of the ignition time scale as a function of the mixture fraction only, but with the added functional dependence on velocity through the consideration of the total enthalpy. A self-ignition domain in the composition space is then delineated using the methodology previously presented in Ref. [8]. It implies the direct comparison between this chemical time scale and an estimated *convection* time scale (or particle age), evaluated as the time needed by a Lagrangian particle to reach a given value of the mixture fraction from its originating stream of pure oxidizer (0) or pure fuel (1). In fact, the Lagrangian history of the particle in the physical space is unknown and the only available information is its composition as well as its Lagrangian evolution in the composition space as given by the postulated IEM trajectory. As a result, the simplest way to evaluate the value of such a time scale is simply to integrate the IEM pathlines, as proposed in Ref. [8].

In this manner, the present formalism simply relies on the knowledge of the mixture fraction mean and variance. Nevertheless, its extension to turbulent reactive two-phase flow situations requires additional phenomena to be considered. Indeed, if chemical reactions do not affect the mixture fraction value  $\xi$ , the evaporation processes that take place in such two-phase flows modify it, and additional evaporation source terms must be considered in the instantaneous equations for the density and mixture fraction in the gaseous phase. Simplest models assume that the chemical species issued from the vaporized phase is instantaneously mixed with the ambiant gas but it is better to take into account the concentration inhomogeneity induced by vaporization: it is higher near the droplets than far away from them. As a result, the mixture can display additional fluctuations of temperature and equivalence ratio that will influence the chemical reaction rate. These added fluctuations induced by the presence of droplets appear naturally in the balance equation of the mixture fraction variance. Indeed, with a mixture fraction defined to be zero in the pure oxidizer, and unity in the pure fuel, it writes:

$$\frac{\partial \overline{\rho \xi''^2}}{\partial t} = -\frac{\partial}{\partial x_k} \left( \widetilde{u_k} \overline{\rho \xi''^2} \right) - \frac{\partial}{\partial x_k} \left( \overline{\rho u_k'' \xi''^2} \right) + \frac{\partial}{\partial x_k} \left( \overline{\rho D} \frac{\partial \xi''}{\partial x_k} \right) + 2\xi'' \frac{\partial}{\partial x_k} \left( \rho D \frac{\partial \widetilde{\xi}}{\partial x_k} \right) \\
- 2\overline{\rho u_k'' \xi''} \frac{\partial \widetilde{\xi}}{\partial x_k} - 2\overline{\rho D} \frac{\partial \xi''}{\partial x_k} \frac{\partial \xi''}{\partial x_k} - 2\left( \overline{\rho \xi \omega_{vap}} - \widetilde{\xi} \overline{\rho \omega_{vap}} \right) - \overline{\rho \xi^2 \omega_{vap}} + \widetilde{\xi} \widetilde{\xi} \overline{\rho \omega_{vap}} \right)$$

where the liquid phase is supposed to be the oxidizer, as expected for the rocket engines test cases considered below. The last four terms in the RHS are unknown correlations associated to the production of fluctuations induced by the vaporization process. In the present study, the liquid phase is assumed to be a spray of droplets, and the final closure is obtained by considering the Lagrangian approach introduced by Borghi [9]: the different terms are evaluated as the sum of the contributions induced by each droplet within the volume V of interest:

1) 
$$\overline{\rho w_{vap}} = \sum_{k} m^k / V$$
 2)  $\overline{\rho \xi w_{vap}} = \sum_{k} \xi_S^k m^k / V$  3)  $\overline{\rho \xi^2 w_{vap}} = \sum_{k} (\xi_S^k)^2 m^k / V$ 

where  $m^k$  and  $\xi_S^k$  denote respectively the vaporized mass flow rate for the droplet k and its composition taken at the liquid surface.

#### **3** Application to underexpanded supersonic reactive jets

A direct application of the computational model described in the previous section consists in simulating the non-premixed turbulent diffusion flame that arises in the highly underexpanded torch jet used as an ignition system in rocket engines. The igniter is located at the centre of the injection plate and it is made of two coflowing streams: a central main jet of vitiated oxygen surrounded by an annular coflowing jet of pure gaseous hydrogen. Since the engine is expected to be ignited in vacuum, the pressure levels can be very low during the transient period that preceeds the injection of the reactants into the combustion chamber and the corresponding Nozzle Pressure Ratio (NPR) values give rise to underexpanded jets featuring several specific difficulties arising among others from the birth of a Mach disk. Favorable conditions for flame stabilization are expected to be reached in the high velocity shear layer that establishes between the central jet and the coflowing jet of hydrogen and behind the Mach disk location. The high level of accuracy required to get a satisfactory description of the gradients in the shear layer has been obtained thanks to the use of the anisotropic mesh adaptation strategy (AMA) of Dolejsi [10] previously described in Ref. [8]. Several NPR values have been considered. The first steps of the transient numerical simulation show that the reactive mixture first ignites in the shear layer. Figure 1 displays three consecutive snapshots of the reaction rate, from the very beginning of the reactive numerical simulation until the final steady-state stabilization of the turbulent non premixed flame. It is noticeable that self-ignition occurs close to the injector exit within the shear layers. Then, the simultaneous decay of turbulent mixing intensity and the presence of hot burned gases make possible the stabilization of a turbulent non-premixed flame within the mixing layers.



Figure 1: Snapshots of the mean temperature field as obtained from the URANS numerical simulation. Figs. a, b: zoom downstream of the injector exit. Fig. c: whole combustion chamber. NPR=16.

### 4 Application to turbulent reactive two-phase flows

The RCM-2 test case presented at the 2nd IWRCM [12] is considered. It has been designed to describe the spray diffusion flame obtained downstream of a single coaxial injector under subcritical conditions. Numerical simulations of the cryogenic 10 bar MASCOTTE test case, studied experimentally at ONERA, are performed following the operating conditions and injector configuration described in Ref. [12]. The overall oxidizer / fuel mass flow rate ratio is 2.11. The injector orifice diameter for the LOx injector is 5mm and it is surrounded by an annular GH2 jet with an annular channel width of 3.2mm. The numerical simulations are performed on a tridimensional mesh corresponding to a 5° cut of the whole test chamber assumed to be cylindrical. The mean and standard deviation measurements of temperature made with a coherent anti-Stokes Raman scattering (CARS) system are available at several radial and axial positions. Moreover, OH emission fields have been collected and a subsequent Abel transformation applied. The computations display a fairly good agreement with both experimental visualizations and previous numerical studies [12]. The results of the non-reactive simulations confirm the ability of the model to describe the mixture composition issued from the vaporization of liquid oxygen. Those obtained from the reactive simulation show that the flame anchors just downstream of the injector, as previously observed in the experiments.

# 5 Conclusions and Perspectives

A Lagrangian model of turbulent combustion in high speed flows has been used in conjunction with an efficient RANS-AMA strategy to simulate high speed turbulent reactive coflowing jets. Its ability to address the high Mach number ignition phenomena associated to the conversion of kinetic energy into thermal energy has been demonstrated and the obtained results are in satisfactory agreement with both underlying physics and available experimental data. For reactive two-phase flows, additional terms that take into account the influence of the dynamics of the spray onto the fuel-oxygen composition statistics have been considered in the final proposal and encouraging results have been obtained for a reference test case corresponding to the combustion of liquid oxygen with gaseous hydrogen in subcritical conditions. The forthcoming steps of the present work concern the interaction of the torch igniter with peripheral LOx/GH2 injectiors and tridimensional numerical simulations are now conducted.

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