# Effets d'histoire sur la modélisation du mélange dans le contexte LES

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## Résumé :

*L'histoire du mélange joue un rôle à la fois crucial et difficile à modéliser en combustion turbulente non-prémélangée. Une nouvelle approche est proposée basée sur un temps de résidence et un temps caractéristique du mélange subis par les particules d'un élément fluide le long de sa trajectoire. Des équations de transport pour ces temps caractéristiques sont proposées et résolues dans le contexte de la simulation aux grandes échelles appliquée à un jet de combustible dans un coflow d'oxydant . Une tabulation de la chimie construite à partir de réacteurs contrôlés par ces temps de résidence et de mélange est ensuite construite. Cette nouvelle approche est appliquée à la simulation d'une flamme déccrochée stabilisée par des gaz brûlés (Cabra et al [1]).*

## Abstract :

*The time history of mixing is known to play a crucial and non-trivial role in non-premixed turbulent combustion. A new approach is proposed based on a flow residence time and a characteristic time of the mixing which the particles gathered in a fluid element have been submitted to in their flow histories. Eulerian balanced equations for those times are proposed and solved in a Large Eddy Simulation (LES) context for a fuel jet mixing with an oxidizer coflow. In a second part, a Flow-Controlled Chemistry Tabulation (FCCT) is devised with partially-stirred reactors controlled by the residence and mixing times. Finally, LES of a fuel-jet lifted-flame developing in a vitiated oxidizer environment is performed and results are compared against measurements conducted by Cabra* et al. *[1].*

**Mots clefs : Non-premixed combustion, Large Eddy Simulation, Time-History effects**

## 1 Introduction

Large Eddy Simulation (LES) provides a description of the unsteady flow behavior, which is fundamental when it comes to the mixing character of combustion, turbulence intermittency leads to inhomogeneities in the reacting mixture which, in their turn, influence the flame dynamics. However, LES must describe the turbulent structures at a resolution fine enough to allow for a reliable prediction of the subgrid-scale (SGS) mixing dynamics [2], specifically when scalar fields are concerned [3].
Several approaches for turbulent combustion in the LES context exist. The more accurate and complex one is to directly solve for the transported probability density function (pdf) and transported mass-weighted pdf methods [4] are designed precisely to follow the individual history of fluid elements, by tracking the Lagrangian evolution of stochastic particles submitted to modeled forces and sources. The resolved scales of turbulence and chemistry are closed, while only the SGS transports need modeling. To obtain a satisfactory level of accuracy, a large number of particles must be included in the simulation, leading to quite heavy simulations in terms of in memory and cpu time. Alternative methods have been developed aiming at a simplified description of the history using conditioning hypotheses. The multiple-mapping conditioning methods [5] (MMC) based on a sparse-Lagrangian transport by conditioning the mixing model involved in the pdf transport equation with a set of reference variables, or the Conditional Moment Closure relying on balance equations for conditional means [6, 7, 8], or the double conditioning of reactive scalar transport equation [9]. Unsteady flamelet method [10] combines

a topological assumption on the trajectories and a conditioning of the scalar dissipation rate with the mixture fraction, in order to dynamically solve for the flamelet equation. Other approaches consists in fully anticipating the SGS statistics with presumed pdfs avoiding the detailed reproduction of history and, instead, invoking relevant conditioning hypotheses to presume the distributions in the flow. The Presumed Conditional Moments (PCM) formulation [11, 12, 13] is such an approach where the pdfs is assumed to take a specific shape, parameterized by first and second order moments of control variables.

In this latter, so-called presumed pdf approach, the history of the flow is only taken into account through its effect on some statistical properties of the local distribution. The correlations of chemical and mixture parameters cannot be fully reproduced, and strong hypotheses are introduced such as statistical independence between equivalence ratio and progress of reaction. On the other hand, the practical strength of this approach is that, since the shape of the pdf is presumed, the filtered quantities can take a limited range of values, and can thus be computed and tabulated before the LES simulation. A lookup table is then accessed from the computation, making the additional cost due to chemistry marginal.

The work presented in this paper proposes an alternative parameterization of the flow for non-premixed jet flames, which enables a tabulation of turbulent chemistry, but avoids presuming joint pdfs. The idea is to describe not the results of flow mixing history, but properties of this history itself. Two quantities are described : the time duration over which mixing has been acting on a fluid particle, through the computation of a residence time $\tau_{\text{res}}$ ; and the average intensity of turbulence along the fluid particle trajectory, through a characteristic mixing timescale $\tau_{\text{mix}}$. These two timescales are solved by means of two regular Eulerian transport equations. Independently from the run, the pdfs are generated from stochastic simulations of a Partially-Stirred Reactor (PaSR) aiming at modeling the flow dynamics as observed in the LES, conditioned on these $\tau_{\text{res}}$ and $\tau_{\text{mix}}$ along with other flow properties, and tabulated into a lookup table, accessed from the LES. Because the pdfs are generated according to flow characteristics and are conditioned by two timescales of the turbulent history, the method is called Flow-Controlled Chemistry Tabulation (FCCT).

A multi-scale approach is followed [14], at the microscale level, the balance between molecular diffusion and chemistry is described by a flamelet hypothesis [15], a database of canonical combustion problems is projected onto a two-dimensional manifold described by a mixture fraction $Z$ and a progress of reaction $Y_c$. At an intermediate scale, which is still at the subgrid level in the LES, these flamelets interact with turbulence. This interaction is modelled by the stochastic FCCT reactor. Finally, in the LES, the unsteady behavior of the four following parameters is resolved : the filtered mixture fraction $\widetilde{Z}$, progress of reaction $\widetilde{Y}_c$, and residence time $\widetilde{\tau}_{\text{res}}$, as well as the turbulent mixing timescale $\tau_{\text{mix}}$. They are used as input parameters in a four-dimensional lookup table resulting from the Monte-Carlo simulations of the FCCT reactor model, which supply the unclosed Eulerian source terms. This Monte-Carlo simulation is designed to follow the $(\widetilde{\tau}_{\text{res}}, \widetilde{Z})$ response observed in the flow.

A last part of the paper illustrates the implementation of the method in the LES ; the results of a simulation of a lifted methane-air jet flame in a vitiated co-flow are compared with experimental results [1].

## 2 Eulerian description of mixing-time history

**Residence time :**

The evaluation of the local residence time, which is the time a particle has spent in the computational domain since its entry can be obtained through a basic convective-diffusive equation $\tau_{\text{res}}$. The residence time field obeys

$$\frac{\partial \rho \tau_{\text{res}}}{\partial t} + \underline{\nabla} \cdot (\rho \underline{u} \tau_{\text{res}}) = \underline{\nabla} \cdot (\rho D \underline{\nabla} \tau_{\text{res}}) + \rho \, . \tag{1}$$

This residence time is an Eulerian quantity, hence the average over fluid particles within a flow volume.

**Trajectory-averaged mixing time :**

Two mixing times are introduced. The first one, $\tau^*_{\text{mix}}$, is a local mixing time accounting for the SGS mixing effect. It characterizes the intensity of turbulence in the unresolved inertial and viscous ranges

and its subgrid-variance reduction effect [16, 17, 18] :

$$\tau^*_{\text{mix}} = \frac{\Delta^2}{2(D + D_T)} \,, \tag{2}$$

where $\Delta$ is the LES filter size and $D_T \sim \Delta^2(\widetilde{S}_{ij}\widetilde{S}_{ij})^{1/2}$ the modeled SGS turbulent diffusivity, with $\underline{\underline{S}} = 0.5(\underline{\nabla}\,\underline{u} + \underline{\nabla}^t\underline{u})$.

The second one characterises the average mixing level that the particles forming a fluid element have been submitted to in their flow histories,

$$\tau_{\text{mix}} = \frac{\tau_{\text{res}}}{\Theta} \,, \tag{3}$$

where $\Theta$ verifies

$$\frac{\partial \rho\Theta}{\partial t} + \underline{\nabla} \cdot (\rho\underline{u}\Theta) = \underline{\nabla} \cdot (\rho D \underline{\nabla}\Theta) + \frac{\rho}{\tau^*_{\text{mix}}} \,. \tag{4}$$

The FCCT closure discussed in this paper is grounded on the two governing relations (1) and (4). As discussed in the literature [19, 20], non-premixed flames may be more sensitive to the time history of strain and mixing rates than to their local and instantaneous values. For instance, a diffusion and reactive layer submitted to a strain-rate level above the steady quenching value, may not be quenched if this high mixing rate is imposed for a short duration of time. The time history of micro-mixing calibrated through the variable $\Theta$ can thus be an interesting ingredient for turbulent diffusion flame modeling.

## 3 Flow configuration and numerics

All simulations thereafter are performed with the structured-mesh SiTCom solver, based on the framework presented in Domingo *et al.* [12], Godel *et al.* [25] and Subramanian *et al.* [13]. The convective terms are solved with a fourth-order skew symmetric like scheme [21] ; the diffusive fluxes are handled with a fourth-order centered scheme. An explicit third-order Runge-Kutta is used as the temporal scheme. Artificial turbulence of the inflow is generated according to the Klein *et al.* approach [22]. Boundary conditions are determined following the 3D-NSCBC formalism [23], including in the BCs a specific heat ratio $\gamma$ computed from the local gas composition. The SGS turbulent fluxes are modeled using the Wall-Adapting Local Eddy-viscosity closure [24]. The laminar viscosity is computed from Sutherland's law ; the laminar and turbulent Prandtl numbers are set to 0.72 and 0.9. The geometry and inlet flows match those of the Cabra *et al.* [1] methane-air experiment. The jet inlet diameter is $D = 4.57$ mm, with a bulk velocity $u_{\text{jet}} = 100$ m.s$^{-1}$, and a uniform co-flow velocity of magnitude $u_\infty = 5.4$ m.s$^{-1}$. The co-flow carries the oxidizer, a mixture of mainly air and $H_2O$ at $T_0 = 1,350$ K ; the fuel, issuing through the central inlet, is a rich mixture of air and methane at $T_1 = 320$ K. In this work, the mesh contains 1,950,000 ; more details concerning LES of this flame under similar conditions may be found in [12, 25].

## 4 $(\tau_{\text{mix}}, \tau_{\text{res}})$ properties

In non-premixed flames, the regions of interest are the zones where the mixing between the inlet streams takes place, which can be characterized by $\widetilde{Z}(1-\widetilde{Z}) \neq 0$, where $Z$ is the mixture fraction (a passive scalar equal to unity in pure fuel and vanishing in the oxidizer stream), and $\widetilde{Z} = \overline{\rho Z}/\overline{\rho}$ is its mass-weighted (or Favre) filtered value. Only the history of the flow in these areas is considered, and the residence and mixing timescale integrations are carried out only there, weighting their source term by $S^+_{\widetilde{Z}} = (1-\delta(\widetilde{Z})) \times (1-\delta(\widetilde{Z}-1))$. In the Large-Eddy Simulation considered in this work, the filtered counterparts of equations 1 and 4. are solved and the trajectory-weighted mixing time is estimated as (Eq. (3)) :

$$\tau_{\text{mix}} = \frac{\widetilde{\tau}_{\text{res}}}{\widetilde{\Theta}} \tag{5}$$

The chemically frozen mixing of fuel and co-flowing streams is first simulated on the 1,950,000-node mesh with longitudinal (resp. transverse) characteristic spacing between 1.57 mm and 4.75 mm (resp. 0.28 mm and 4.4 mm) ; the mesh fineness has an impact on the $\tau_{\text{mix}}$ value, through the cell size $\Delta$ and the SGS turbulent eddy viscosity $D_T$, see Eq. (2).
The structure of the average $\widetilde{\tau}_{\text{res}}$ and $\tau_{\text{mix}}$ fields is illustrated in Fig. 1. It may be seen that the residence time isolines are intersecting the mixing time isolines at close to orthogonal angles. An alternative topology of space is hereby evidenced, indicating that these timescales carry complementary information. This is a favorable argument for using them as conditioning variables.

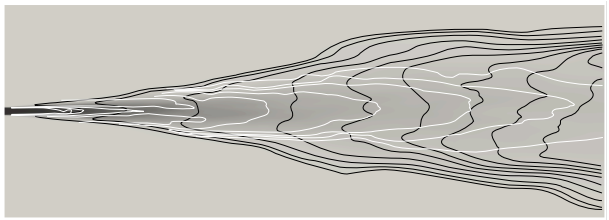

FIG. 1 – Isolines of time-averaged characteristic times. Black lines : residence time. White lines : mixing time.

## 5 FCCT modeling

The mass-weighted space filtering operation is defined in Large Eddy Simulation as :

$$\widetilde{Q}(\underline{x}_0) = \frac{\int_{\underline{x}} \rho(\underline{x}) Q(\underline{x}) \mathcal{G}_\Delta(\underline{x} - \underline{x}_0) \mathrm{d}x}{\int_{\underline{x}} \rho(\underline{x}) \mathcal{G}_\Delta(\underline{x} - \underline{x}_0) \mathrm{d}x} \,,$$

where $\mathcal{G}_\Delta$ is a filter function used to damp fluctuations at lengths smaller than $\Delta$. Assuming that $Q$ may be conditioned by a set of parameters $\underline{\psi}$, thus writing $Q(\underline{\psi})$, $\widetilde{Q}$ may be computed from the joint pdf $p(\underline{\psi}; \underline{x})$ :

$$\widetilde{Q}(\underline{x}_0) = \int_{\underline{\psi}} Q(\underline{\psi}) p(\underline{\psi}; \underline{x}_0) \mathrm{d}\underline{\psi} \,.$$

The Flow-Controlled Chemistry Tabulation approach stems from the idea that the residence time $\widetilde{\tau}_{\text{res}}(\underline{x}, t)$ and mixing timescale $\tau_{\text{mix}}(\underline{x}, t)$, introduced in Section 2, are relevant conditioning variables for the turbulence-chemistry interaction. They are adjoined with the set of parameters $\underline{\widetilde{\phi}} \equiv (\widetilde{Z}, \widetilde{Y}_c)$ (equivalence ratio or mixture fraction and progress of reaction) which allow for a description of chemistry, to form the conditioning variables $\underline{\psi} \equiv (\underline{\widetilde{\phi}}; \widetilde{\tau}_{\text{res}}, \tau_{\text{mix}})$ from which it is assumed all unclosed filtered quantities may be described with : $\widetilde{\overline{Q}} = \widetilde{Q}^{\text{FCCT}}(\underline{\widetilde{\phi}}; \widetilde{\tau}_{\text{res}}, \tau_{\text{mix}})$.
Like in all models based on a reduced conditioning of the variables, a formulation of these FCCT fields must be explicited. While the presumed pdf methods assume an explicit expression of the distributions from the data of the averages $\underline{\widetilde{\phi}}$ and variances $\widetilde{\phi_i'' \phi_i''}$, here, they are dynamically generated in preliminary Monte-Carlo computations of a Partially-Stirred Reactor.
The PaSR simulations aim at reproducing representative evolutions of the considered reactive flow, by the emulation of three processes : a mixing process (*i.e.* turbulent mixing), a reaction process (combustion chemistry) and an injection process (engulfment). The joint-$\underline{\phi}$ distributions are monitored and tabulated to form a chemical table. Then, during the run, this table is accessed from the LES flow solver as a lookup table and provides the terms needed to close the filtered equations. One of the key points is to select an injection process that is representative of the flow studied, and reproduce the $(\widetilde{\tau}_{\text{res}}, \widetilde{Z})$ typical response discussed above. The details of the reactor injection procedure may be found in [26].

## 6 LES of a jet flame

Large Eddy Simulation of the vitiated-air jet flame experimentally studied by Cabra *et al.* [1] is performed, the simulation follows the procedure reported in [12], in which the flamelet presumed pdf

lookup table has been replaced by the FCCT one. Along with the Navier-Stokes equations in their fully compressible form, the filtered Eqs. (1) and (4) are solved for $\widetilde{\tau}_{\text{res}}$ and $\widetilde{\Theta}$, and the relation (5) provides $\tau_{\text{mix}}$. A usual convection-diffusion equation is solved for the mixture fraction $\widetilde{Z}$ ; in the Eulerian balance equation for the progress of reaction $\widetilde{Y}_c$ an additional chemical source $\widetilde{\dot{\omega}}_{Y_c} = \widetilde{\dot{\omega}}_{Y_c}(\widetilde{Z}, \widetilde{Y}_c, \widetilde{\tau}_{\text{res}}, \tau_{\text{mix}})$ appears that is read in the lookup table. The thermochemical properties of the flow are also read from the table to ensure energy coupling. The selected numerics and turbulence SGS modeling have been reported above in Section 3.

Figure 2 shows that combustion starts in a zone located between 40 and 50 diameters downstream of injection.

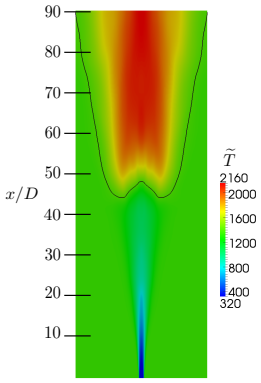


FIG. 2 – 2D view of the averaged temperature field. Line : 1,400 K isoline.

To obtain the statistics of the LES computation and compare them with the experimental means, the fields are collected every 100 iterations (or about $2.5 \times 10^{-5}$ s) and averaged over a 60,000-iteration period, which amounts to about 3.6 $\tau_{\text{box}}$, where the box time is defined as $\tau_{\text{box}} = 90D/u_{\text{jet}}$, with $u_{\text{jet}}$ the bulk fuel-jet velocity.

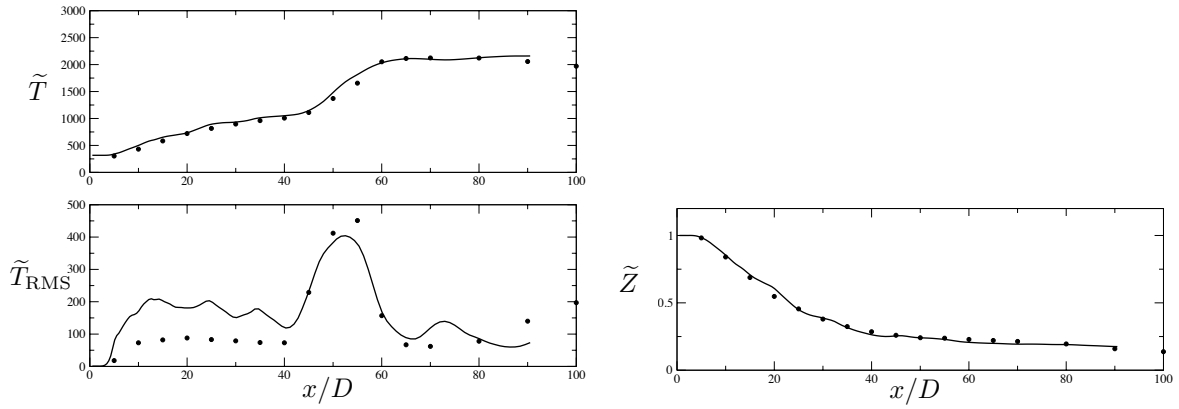


FIG. 3 – Left : Centerline profiles of temperature and temperature fluctuations. Right : Centerline profile of the average mixture fraction. Symbols : measurements ; lines : LES.

In an initial zone extending down to about $40D$, the temperature follows a mixing trend, from the 320 K jet towards the vitiated coflow temperature of 1,350 K. After reaching the axial position of 40 diameters, the temperature then sees an increase over about 20 jet diameters, up to around 2,200 K, an indicator of the presence of the flame, which is reproduced by the LES (Fig. 3). The position of this flame base fluctuates in time, subject to the mixture fraction, residence time and mixing timescale variations. This may be seen on the computed temperature fluctuations whose sharp increase is located where the experimental results position it. Downstream, in the burnt gas at chemical near-equilibrium, the time-averaged temperature conforms to the experimental measurements, remaining constant around

2,200 K. The mixture fraction decay on the jet axis agrees with measurements (Fig. 3).

# 7 Conclusions

A novel chemistry tabulation approach for LES, based on a parameterization by two flow timescales describing the flow mixing history, has been presented. It is formulated through probability density functions which are not presumed, but generated in Monte-Carlo simulations of a Partially-Stirred Reactor, whose behavior is piloted by three processes : turbulent mixing, chemical reaction and inflow/outflow (engulfment). A lookup table is produced, whose coupling with the flow solver is achieved through two timescales, consisting of a residence time and a mixing timescale, and through the transported filtered chemical parameters.

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