

# Influence of residence and scalar mixing time scales in non premixed combustion in supersonic turbulent flows

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## 1 Introduction

The description of non-premixed combustion in supersonic turbulent flows still offers challenging issues from both the physical modelling and numerical points of view. In supersonic reactive flows, the essential influence of self-ignition phenomena is well known, and even in the absence of any pressure discontinuity, the mechanism of viscous dissipation is likely to influence the early development of chemical processes. This phenomena is the direct consequence of the conversion of kinetic energy into enthalpy which is no longer negligible in high Mach number flows. A large amount of valuable information has been gathered to address theoretically, numerically and experimentally this specific aspect. Several experimental test rigs have been designed and studied, and in many of them hydrogen is injected into a main flow of air which can be vitiated or not. For sufficiently high preheated air flows, self-ignition conditions are reached inside the mixing layer that develops between the two supersonic streams. Such conditions are obtained in the experiments reported by Beach [1] and by Cheng and coworkers [2] which are retained as relevant test cases for the purpose of the present study. In our previous analyses [3, 4] chemical kinetics as well as associated finite rate chemistry effects have received considerable attention but it seems worth recognizing that the representation of flow time scales, such as residence and mixing time scales, still requires further work. The present modelling study is devoted to this peculiar point.

## 2 Lagrangian intermittent framework for high speed non premixed combustion

Non premixed turbulent reactive flows featuring finite rate chemistry effects are represented within a two scalar joint Probability Density Function (PDF) strategy. The MIL framework retained here is based on the consideration of the mixture fraction  $\xi$  together with 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, the Lagrangian evolution of fluid particles issuing from either oxidizer or fuel stream is given by the following set of equations  $d\xi/dt = (\tilde{\xi} - \xi)/\tau$  and  $dY/dt = (\tilde{Y} - Y)/\tau + \omega_Y$  where  $\tau$  is a *micromixing* time scale taken equal to the mixture fraction integral time scale  $\tau_\xi = \tilde{\xi}''^2/\tilde{\epsilon}_\xi$ . Within the MIL framework, it is assumed that the chemical reactions are sudden: particles need a finite time to ignite during their evolution towards the mean composition but then instantaneously jump from the IEM mixing line to the equilibrium line. This approximation introduces a strong but clearly-stated functional dependence between the two variables  $\xi$  and  $Y$ . The resulting trajectory  $Y^{\text{MIL}}(\xi)$  allows to express the joint scalar PDF as  $\tilde{P}(\xi, Y) = \tilde{P}(\xi)\delta(Y - Y^{\text{MIL}}(\xi))$ . The pathline  $Y^{\text{MIL}}(\xi)$  is fully determined through the knowledge of the mixture fraction values that correspond to the jump positions, i.e.,  $\xi_{j-}$  and  $\xi_{j+}$ . By comparing chemical time scales with flow time scales, the MIL framework allows to delineate an inflammable domain  $[\xi_{j-}; \xi_{j+}]$  in the mixture fraction space, see for instance [5], and this feature makes it well-suited to describe the effects associated with

finite rate chemistry and/or ignition [6]. Besides, following the early work of Luo and Bray [7] who suggested that such a classical conserved scalar presumed PDF method can be modified to deal with high speed combustion by replacing the static enthalpy with the stagnation enthalpy, the model has been recently extended to supersonic combustion [3]. The objective with such an extension is to include the ignition phenomena associated with the conversion of kinetic energy into thermal energy *via* the viscous dissipation heating. We briefly recall now the main features of the closure proposed in [3]. They are: (i) to approximate the Lagrangian evolution of the total enthalpy  $h_t(\xi)$  by the IEM trajectory, i.e., through  $dh_t/dt = (\tilde{h}_t - h_t)/\tau$ , (ii) to deduce from the levels of both the static enthalpy and the mean static pressure  $\bar{p}$  the value of an auto-ignition time scale  $\tau_{ig}$  for each value of the mixture fraction  $\xi$ . (iii) This self-ignition time scale value  $\tau_{ig}$  is compared to the residence time of the particule  $\tau_{res}$ <sup>1</sup> and this allows to delineate a possible domain of spontaneous ignition in the mixture fraction space. Such a direct comparison between the particle age (or residence time)  $\tau_{res}$  and tabulated chemical induction time  $\tau_{ig}$  takes into account the added functional dependence to velocity through the estimation of static enthalpy  $h(\xi)$  from the total enthalpy  $h_t(\xi)$ . The extended closure has been found able to represent self-ignition phenomena that can result from viscous dissipation effects in supersonic mixing layers [3]. Based on the sudden chemistry assumption that relates the progress variable  $Y$  to the mixture fraction field  $\xi$  through  $Y = Y^{ML}(\xi)$ , the joint scalar PDF  $\tilde{P}(Y, \xi)$  can be simply expressed from the single knowledge of the marginal PDF of the mixture fraction  $\tilde{P}(\xi)$ . It is presumed to be a classical beta function PDF whose estimation can be performed through the calculation of  $\tilde{\xi}$  and  $\tilde{\xi}''^2$  from the following set of transport equations:

$$\frac{\partial \tilde{\rho} \tilde{\xi}}{\partial t} + \frac{\partial}{\partial x_k} \left( \tilde{\rho} \tilde{u}_k \tilde{\xi} - \tilde{\rho} \frac{\nu_t}{Sc_t} \frac{\partial \tilde{\xi}}{\partial x_k} \right) = 0 \quad (1)$$

$$\frac{\partial \tilde{\rho} \tilde{\xi}''^2}{\partial t} + \frac{\partial}{\partial x_k} \left( \tilde{\rho} \tilde{u}_k \tilde{\xi}''^2 - \tilde{\rho} \frac{\nu_t}{Sc_t} \frac{\partial \tilde{\xi}''^2}{\partial x_k} \right) = 2 \tilde{\rho} \frac{\nu_t}{Sc_t} \frac{\partial \tilde{\xi}}{\partial x_k} \frac{\partial \tilde{\xi}}{\partial x_k} - 2 \overline{\rho \epsilon \xi} \quad (2)$$

where molecular diffusion terms are neglected with respect to their turbulent counter parts.

In the previous equations, the corresponding turbulent scalar transport terms are closed by using the turbulent eddy viscosity  $\nu_t = C_\mu k^2 / \tilde{\epsilon}$ , with  $C_\mu = 0.09$ , and the turbulent Schmidt numbers are set to their usual value  $Sc_t = 0.7$ . In the present study, the standard  $k$ - $\tilde{\epsilon}$  approach is retained to model the turbulence. In order to account for compressibility effects, the pressure dilatation term that appears in the turbulent kinetic energy transport equation is closed as a function of  $M_t$ , the turbulent Mach number based on the turbulent kinetic energy, following the strategy introduced by Zeman et al. [8]. The dissipation rate of the turbulent kinetic energy  $\tilde{\epsilon}$  is modelled as the sum of two contributions. The first one is the classical solenoidal contribution  $\tilde{\epsilon}_s$  which is considered to be unaffected by compressible effects: a classical modelled balance equation is retained for this term. The second term is associated to the compressible or dilatational dissipation rate  $\tilde{\epsilon}_c$  and it is estimated as a function of the turbulent Mach number  $M_t$ . Equation (2) also requires to provide a closure for the mean scalar dissipation rate (SDR)  $\overline{\rho \epsilon \xi} = \overline{\rho D (\partial \xi'' / \partial x_k) (\partial \xi'' / \partial x_k)}$  with  $D$  the scalar molecular diffusivity (Lewis number effects are not addressed in the present study). The issue associated with its modelling is considered below. Finally, from the knowledge of  $\tilde{\xi}$  and  $\tilde{\xi}''^2$  as obtained from Eqs.(1) and (2), the estimation of the presumed beta PDF for the mixture fraction  $\tilde{P}(\xi)$  can be performed at each point of the computational mesh.

## 2.1 Local and average residence time

Ignition and stabilization of supersonic jet diffusion flames are driven by the competition between local residence time  $\tau_{res}$  and chemical induction time the value of which is critically influenced by prelim-

<sup>1</sup>This is the time elapsed since it left either the oxidizer or fuel injection stream. Its closure is discussed in the next section.

inary preheating as well as conversion of fluid flow kinetic energy into thermal energy. The value of the local residence time scale  $\tau_{res}$  is nothing else but the time elapsed since the corresponding fluid element has entered the computational domain through a supply injection stream. In the context of chemical engineering, Ghirelli and Leckner [9] recently considered a transport equation for an extensive variable: the *quantity of residence time*, denoted  $\theta$ . It is defined in such manner that  $d\theta$  is the product of an infinitesimal mass  $dm$  and the residence time  $\tau_{res}$  of the corresponding fluid element. For multi-species reactive flows, as those considered herein, the same quantity becomes  $d\theta_\alpha = dm Y_\alpha \tau_{res}^{Y_\alpha}$  for a given chemical species  $\alpha$  with  $Y_\alpha$  and  $\tau_{res}^{Y_\alpha}$  its local mass fraction and residence time values. Following the averaging procedure introduced in reference [9] and, under the assumption of negligible molecular diffusion effects, the transport equation for the average residence time  $\widehat{\tau}_{res}^{Y_\alpha}$  writes:

$$\frac{\partial}{\partial t} \overline{\rho Y_\alpha \widehat{\tau}_{res}^{Y_\alpha}} + \frac{\partial}{\partial x_k} \left( \overline{\rho \tilde{u}_k Y_\alpha \widehat{\tau}_{res}^{Y_\alpha}} - \overline{\rho} \frac{\nu_t}{Sc_t} \frac{\partial}{\partial x_k} \overline{Y_\alpha \widehat{\tau}_{res}^{Y_\alpha}} \right) = \overline{\rho Y_\alpha} + \overline{\Omega_{\theta_\alpha}} \quad (3)$$

where the following notation is used:  $\widehat{\Phi} = \overline{\rho_\alpha \Phi} / \overline{\rho_\alpha} = \overline{\rho Y_\alpha \Phi} / \overline{\rho Y_\alpha} = \overline{\rho Y_\alpha \Phi} / \overline{\rho Y_\alpha} = \widehat{Y_\alpha \Phi} / \widehat{Y_\alpha}$ .

The three terms in the Left Hand Side (LHS) of Eq.(3) represent classical contributions associated to temporal variations, transport by the mean flow field and turbulent transport. The Right Hand Side (RHS) gathers two production terms. The first term reflects the increase in the residence time of an individual fluid element of chemical species  $\alpha$ , i.e. one unit residence time per unit elapsed time. Finally the last term  $\overline{\Omega_{\theta_\alpha}}$  is an average source term induced by chemical reactions. Its instantaneous expression is given by  $\Omega_{\theta_\alpha} = \rho \omega_{Y_\alpha} \tau_{res}^{Y_\alpha}$  for a species consumed by chemical reactions (i.e.  $\omega_{Y_\alpha} < 0$ ) and  $\Omega_{\theta_\alpha} = 0$  for a species produced by chemical reactions (i.e.  $\omega_{Y_\alpha} > 0$ ) where  $\omega_{Y_\alpha}$  is the production rate of species  $\alpha$ . The source term  $\Omega_{\theta_\alpha}$  represents the decrease of *quantity of residence time* due to the consumption of species  $\alpha$ . When the mass of species  $\alpha$  is consumed by chemical reactions, also its *quantity of residence time* will be consumed whereas if species  $\alpha$  is produced by chemical reaction its initial residence time value is zero when it is formed and the corresponding production of  $\theta_\alpha$ , i.e.  $\Omega_{\theta_\alpha}$ , is also zero. For a passive tracer, like the mixture fraction variable, the following transport equation is considered:

$$\frac{\partial}{\partial t} \overline{\rho \xi \widehat{\tau}_{res}^\xi} + \frac{\partial}{\partial x_k} \left( \overline{\rho \tilde{u}_k \xi \widehat{\tau}_{res}^\xi} - \overline{\rho} \frac{\nu_t}{Sc_t} \frac{\partial}{\partial x_k} \overline{\xi \widehat{\tau}_{res}^\xi} \right) = \overline{\rho \xi} \quad (4)$$

Based on the IEM *micromixing* closure  $\tau_{res}$  can be expressed for each value of the mixture fraction:  $\tau_{res}(\xi) = \widehat{\tau}_{res}^{\xi=0} + \tau \ln \left( 1 + \xi / (\tilde{\xi} - \xi) \right)$  if  $\xi < \tilde{\xi}$  and  $\tau_{res}(\xi) = \widehat{\tau}_{res}^{\xi=1} + \tau \ln \left( (\tilde{\xi} - 1) / (\tilde{\xi} - \xi) \right)$  if  $\xi > \tilde{\xi}$ . The quantities  $\widehat{\tau}_{res}^{\xi=0}$  and  $\widehat{\tau}_{res}^{\xi=1}$  denote the values of the residence time as obtained from Eq.(4) written for two passive tracers associated with oxidizer and fuel injection stream condition respectively. The estimation of the *micromixing* time  $\tau$  from the scalar mixing time scale  $\tau_\xi = \xi'^2 / \tilde{\epsilon}_\xi$  is discussed in the next section.

## 2.2 Mean scalar dissipation rate and integral characteristic scalar mixing time scale

Together with the scalar fluctuations intensity, i.e. the scalar variance level  $\xi'^2$ , the scalar integral length scale  $l_\xi$  will fix the mixing rate at the molecular level  $\tilde{\epsilon}_\xi$ . Such a quantity is known to play a crucial role for non premixed conditions as those considered herein since mixing is a prerequisite before combustion occurs. From a practical point of view, it remains a (very) common practice to close the average SDR that appears in Eq.(2) by invoking a similarity hypothesis between scalar and velocity turbulence spectra which results in the classical approximation  $\tau_\xi = C_\xi \tau_t$  with  $C_\xi$  a modelling constant whose value remains to be determined. However, we know that scalar and velocity fluctuations length scales can display strong differences especially when the largest scales, i.e., the integral scales,

are concerned. Therefore, to avoid any systematic resort to the similarity assumption, we propose to consider a two-equation closure  $\tilde{k}_\xi - \tilde{\epsilon}_\xi$  with  $\tilde{k}_\xi = \tilde{\xi}''^2$  the scalar fluctuations energy.

Considering results obtained from order of magnitude and DNS studies, see for instance [10, 11], we retain the following unclosed transport equation for the mean SDR as a starting point of our analysis:

$$\frac{\partial \overline{\rho \epsilon_\xi}}{\partial t} + \frac{\partial}{\partial x_k} (\overline{\rho u_k \epsilon_\xi}) = \underbrace{-2 \overline{\rho \epsilon_\xi^{ii}}}_{(V)} \frac{\partial \tilde{\xi}}{\partial x_k} - \underbrace{2 \overline{\rho \epsilon_\xi^{ik}}}_{(VI)} \frac{\partial \tilde{u}_k}{\partial x_i} - \underbrace{2 \overline{\rho \epsilon_\xi^{ik}}}_{(VII)} \frac{\partial u_k''}{\partial x_i} - \underbrace{2 \rho D^2}_{(VIII)} \frac{\partial^2 \xi''}{\partial x_i \partial x_k} \frac{\partial^2 \xi''}{\partial x_i \partial x_k} \quad (5)$$

where  $\epsilon_{\xi, u_k}^{ij} = D(\partial \xi'' / \partial x_i)(\partial u_k'' / \partial x_j)$  and  $\epsilon_\xi^{ij} = D(\partial \xi'' / \partial x_i)(\partial \xi'' / \partial x_j)$  denote the cross scalar-velocity and scalar dissipation rate tensors. All the terms in the RHS of Eq.(5) require appropriate modelling. The effects of stretching by turbulence (VII) and local curvature (VIII) are dominant terms [10, 11]. The other two terms in the RHS represent production by mean concentration gradients (V) and by mean velocity gradients (VI).

#### Algebraic closure: linear relaxation model

The mean SDR can be obtained by invoking the assumption of small-scale equilibrium between production and dissipation. Then, Eq.(5) reduces to a balance between turbulent straining (VII) and dissipation contributions (VIII). Using linear estimates we obtain: (VII) =  $-\bar{\rho} \alpha \tilde{\epsilon}_\xi / \tau_t$  and (VIII) =  $\bar{\rho} \beta \tilde{\epsilon}_\xi / \tau_\xi$ , see [12] for further details. Hence, from the equilibrium hypothesis (VIII)=(VII), and we recover the linear relaxation closure  $\tilde{\epsilon}_\xi = \tilde{\xi}''^2 / C_\xi \tau_t$  with  $C_\xi = \beta / \alpha$  the proportionality constant between  $\tau_\xi$  and  $\tau_t$ .

#### Mean scalar dissipation rate transport

Improved scalar mixing rate representations require to consider Eq.(5). Various forms of modelled transport equations can be found in the literature but the oldest closures do not include all the terms that were derived and studied through the order of magnitude analysis performed in reference [10]. Based on our previous studies [11] the following closures are retained. The production term associated with mean velocity gradients (VI) is represented by  $C_{P_u} \overline{\rho u_i'' u_k''} (\tilde{\epsilon}_\xi / \tilde{k}) \partial \tilde{u}_k / \partial x_i$  with  $C_{P_u} = 1$  and where  $\overline{\rho u_i'' u_k''}$  is modelled within the Boussinesq's approximation. The expression retained for the production term due to the mean scalar gradient (V) is given by  $C_{P_\xi} \overline{\rho u_k'' \xi''} (\tilde{\epsilon} / \tilde{k}) \partial \tilde{\xi} / \partial x_k$  with  $C_{P_\xi} = 1$ . It is used here in conjunction with a turbulent diffusivity assumption, and the resulting SDR transport equation writes:

$$\frac{\partial \overline{\rho \epsilon_\xi}}{\partial t} + \frac{\partial}{\partial x_k} \left( \overline{\rho \tilde{u}_k \tilde{\epsilon}_\xi} - \frac{\overline{\rho \nu_t}}{Sc_t} \frac{\partial \tilde{\epsilon}_\xi}{\partial x_k} \right) = C_{P_\xi} \frac{\overline{\rho \nu_t}}{Sc_t} \frac{\tilde{\epsilon}}{\tilde{k}} \left( \frac{\partial \tilde{\xi}}{\partial x_k} \right)^2 + \alpha \frac{\overline{\rho \tilde{\epsilon}_\xi}}{\tau_t} - \beta \frac{\overline{\rho \tilde{\epsilon}_\xi^2}}{\tilde{\xi}''^2} \quad (6)$$

$$+ C_{P_u} \overline{\rho} \left( \nu_t \left( \frac{\partial \tilde{u}_i}{\partial x_k} + \frac{\partial \tilde{u}_k}{\partial x_i} \right) - \frac{2}{3} \left( \tilde{k} + \nu_t \frac{\partial \tilde{u}_j}{\partial x_j} \right) \delta_{ik} \right) \frac{\tilde{\epsilon}_\xi}{\tilde{k}} \frac{\partial \tilde{u}_k}{\partial x_i}$$

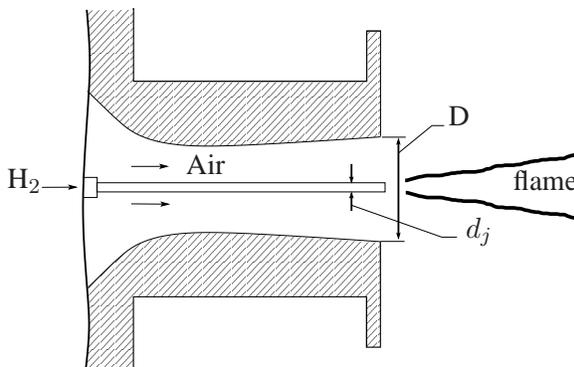


Figure 1: Sketch of the experimental setup [1]

	Hydrogen Jet	Vitiated Air
Mach Number, M	2.00	1.90
Temperature, K	251	1495
Velocity, m/s	2432	1510
Mass fraction :		
$Y_{H_2}$	1.000	0
$Y_{O_2}$	0	0.241
$Y_{H_2O}$	0	0.281
$Y_{N_2}$	0	0.478
External diameter D :		0.0653 m
Injector diameter $d_j$ :		0.009525 m
Injector lip thickness :		0.0015 m

Figure 2: Exit conditions and geometry

### 3 Application to supersonic turbulent coflowing jets

The complete closure discussed above is implemented into the CFD code *N3S\_Natur* [13]. It is applied to two distinct pertaining and well-documented test cases [1, 2] that are often retained in the field of supersonic combustion [15,16], but in this abstract we focus on the experimental configuration described in references [1, 14]. It consists of axisymmetric coaxial jets of H<sub>2</sub> and vitiated air discharging into quiescent atmosphere, see Figs. 1 and 2.

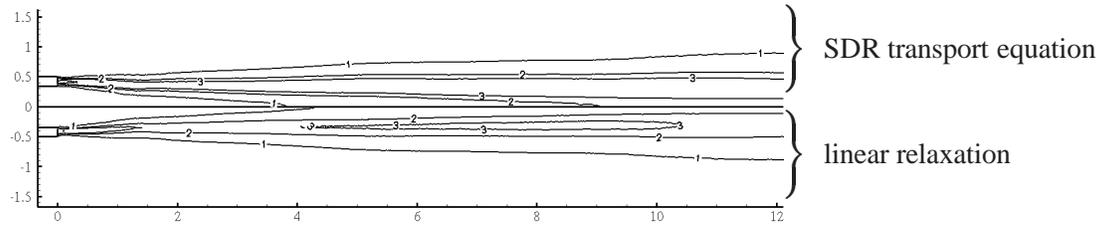


Figure 3: Computed contours of scalar variance. Top: SDR transport equation. Bottom: linear relaxation of scalar fluctuations. Isolines: 1.  $\xi''^2 = 0.0005$ , 2.  $\xi''^2 = 0.005$ , 3.  $\xi''^2 = 0.01$ , 4.  $\xi''^2 = 0.05$ .

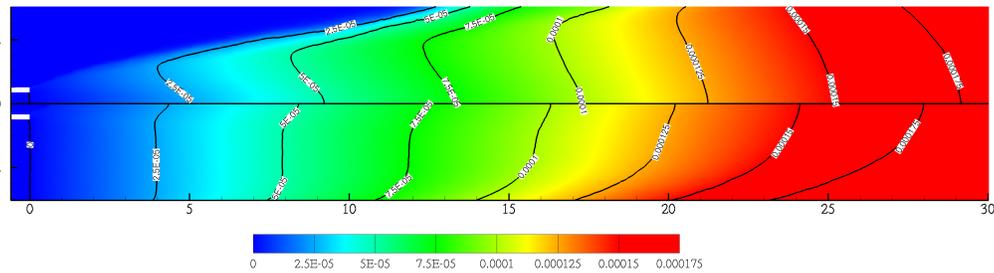


Figure 4: Average fields of the residence time. Top:  $\hat{\tau}_{res}^{\xi=1}$ . Bottom:  $\hat{\tau}_{res}^{\xi=0}$ .

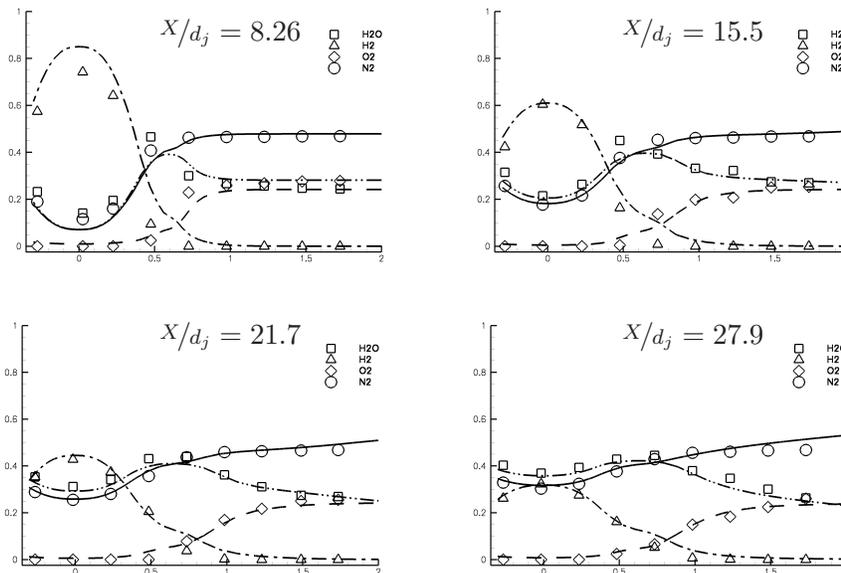


Figure 5: Species mass fraction profiles downstream of the injector exit. Computations vs. experiments.

Some of the results obtained by numerical simulations are now briefly illustrated. Figure 3 reports the contours of scalar variance as obtained from non reactive numerical simulations based on either linear relaxation closure or SDR transport equation as provided by Eq.(6). The results emphasize differences

in the mixture fraction variance field that are likely to affect the development and stabilization of the reactive flow-field. The field of average residence time is depicted in Fig. 4. Finally, computational profiles of species mass fractions obtained at different location downstream of the injector exit are satisfactorily compared with experimental data in Fig. 5. The exhaustive analysis of both residence and scalar mixing time scales influence on the numerical results is the subject of our ongoing work.

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