# A Generalized Turbulent Combustion Model for Large Eddy Simulation of Turbulent Premixed Flames

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**Abstract**

The aim of this work is to propose a unified (generalized) closure of the chemical source term covering all the regimes of turbulent premixed combustion. The deliverable is a Localized Turbulent Scales Model (LTSM) for Large Eddy Simulation of turbulent premixed flames. This model founds on the estimation of the local reacting volume fraction of a computational cell, that is related to the local turbulent and laminar flame speeds and to the local flame thickness.

## Introduction

A synthetic way to look at turbulence / combustion interaction consists in mapping combustion regimes. In fact, due to the complexity of multi-scale interaction between turbulence and chemistry, several combustion regimes may occur. Regime determination, i.e., the identification of the spatial structure and morphology of the reacting flow, is important for combustion modelling. Combustion regimes have been theoretically investigated for many years in premixed combustion [1]. They are mapped in two dimensional diagrams showing regions where the flow structure will feature flamelets, pockets or distributed reaction zones. Just as typically, these diagrams do not include the effect of important flame physics such as heat losses, flame curvature, viscous dissipation and transient dynamics, all affecting quenching. Furthermore, the effect of the Lewis number on quenching produced by stretching is not considered.

## Modelling the Favre Filtered Chemical Source Term

The Favre filtered chemical source term in the energy and single species transport equations is here modelled as $\widetilde{\omega}_i \approx \gamma^* \omega_i^*$, $\gamma^*$ and $\omega_i^*$ being the local reacting volume fraction of the computational cell and the reaction rate of the $i-th$ chemical species, respectively.

The local reacting volume fraction is defined as $\gamma^* = \mathcal{V_F}^*/\mathcal{V}_\Delta$, $\mathcal{V_F}^*$ and $\mathcal{V}_\Delta$ being the reacting and the total volumes of the computational cell. In particular, the suggested Localized Turbulent Scales Model (LTSM) estimates the local reacting volume fraction $\gamma^*$ assuming that a flame front having a surface area $\mathcal{A_F}$ and thickness $\delta_F$ is contained in a computational cell volume of characteristic size $\Delta = \mathcal{V}_\Delta^{1/3}$, i.e.,

$$\gamma^* = \frac{\mathcal{V_F}^*}{\mathcal{V}_\Delta} \approx \frac{\mathcal{A_F}\delta_\mathcal{F}}{\mathcal{V}_\Delta} \approx \frac{\mathcal{S_T}}{\mathcal{S_L}}\mathcal{A_L}\frac{\delta_\mathcal{F}}{\mathcal{V}_\Delta} \approx \frac{\mathcal{S_T}}{\mathcal{S_L}}\Delta^2\frac{\delta_\mathcal{F}}{\Delta^3} = \frac{\mathcal{S_T}}{\mathcal{S_L}}\frac{\delta_\mathcal{F}}{\Delta} \; . \tag{1}$$

This expression has been obtained with two main assumptions. The first is that within a wrinkled flame front the iso-surfaces of the progress variable are parallel [2]. The second assumption is that the ratio between the

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turbulent and the laminar flame surface areas scales as the ratio between the associated flame speeds , i.e., $\mathcal{A}_{\mathcal{F}}/\mathcal{A}_{\mathcal{L}} \equiv \mathcal{A}_{\mathcal{T}}/\mathcal{A}_{\mathcal{L}} \approx \mathcal{S}_{\mathcal{T}}/\mathcal{S}_{\mathcal{L}}$. With this modelling, subgrid flame front wrinkling and curvature effects are synthesized in this ratio. It is reminded that the laminar flame speed can be estimated as $\mathcal{S}_{\mathcal{L}} \approx (\alpha/\tau_{ch})^{1/2}$, the laminar flame thickness as $\delta_{\mathcal{L}} \approx (\alpha\,\tau_{ch})^{1/2}$, and that these two expressions imply $\delta_{\mathcal{L}}\,\mathcal{S}_{\mathcal{L}}/\alpha = 1$. The quantity $\alpha = k/(\rho C_p)$ is the thermal diffusivity, with $k$ being the thermal conductivity, $\rho$ the density and $C_p$ the specific heat at constant pressure.

An extinction or flame stretch factor $\mathcal{G}_{ext} \leq 1$ is also introduced as factor in Eqn. (1) to take into account flame quenching due to subgrid scales. It is modelled according to the so called *quenching cascade model* [3], that compares quite well with experimental and direct numerical simulation data on quenching [4, p. 212-214]. The problem of $\gamma^*$ estimation becomes the problem of estimating the characteristics of the local flame front in terms of its turbulent flame speed, laminar flame speed and thickness (turbulent or laminar) from the filtered conditions of the flow and depending on the related local premixed combustion regime. The local filtered chemical time required to estimate laminar quantities can be calculated as $\tau_{ch} = \rho C_p T/\,|\Delta\mathcal{H}_R|$, where $\Delta\mathcal{H}_R$ is the heat of reaction.

## Vortices / Flame Front Interaction

The interaction between a premixed flame front and eddies has been widely analyzed in literature. Results clearly show that the dissipative Kolmogorov scales $\eta$ cannot quench a flame front [5]. An estimate of the smallest turbulent scale that can affect a laminar flame front without being dissipated can be obtained by considering that the turbulent $l-$scale Damköhler number of second species has to be greater than one, $Da_l^{II} = \tau_{\nu_l}/\tau_{ch} = Pr^{-1}\,(l/\delta_{\mathcal{L}})^2 \geq 1$, where $\tau_{\nu_l} = l^2/\nu$ is the lifetime of the generic vortex of scale $l$, $\nu$ being the dynamic viscosity, $\tau_{ch} = \delta_{\mathcal{L}}/\mathcal{S}_{\mathcal{L}} = \delta_{\mathcal{L}}^2/\alpha$ is the chemical time, and $Pr = \nu/\alpha$ is the Prandtl number. Hence, the smallest surviving scale $l^*$ is estimated as

$$l^* = Pr^{1/2}\,\delta_{\mathcal{L}} = l_\Delta\left(Da_\Delta^I\,Re_\Delta\right)^{-1/2} = l_\Delta Da_\Delta^{II^{-1/2}}\ , \tag{2}$$

where $Re_\Delta = u'_\Delta l_\Delta/\nu$ is the turbulent Reynolds number defined in terms of the local length and velocity macroscales $l_\Delta$ and $u'_\Delta$, $Da_\Delta^I = l_\Delta/\left(u'_\Delta\tau_{ch}\right)$ is the turbulent $l_\Delta-$scale Damköhler number of first species. Turbulent scales larger than $l^*$ will not be destroyed or damped by the flame front.

The smallest surviving scale $l^* \in [\eta, l_\Delta]$, and this is fulfilled for whatever Prandtl number if $l_\Delta \geq l^* \geq \eta \Leftrightarrow Re_\Delta^{-1} \leq Da_\Delta^I \leq Re_\Delta^{1/2}$, observing that $l^* = l_\Delta$ for $Da_\Delta^I = Re_\Delta^{-1}$ and $l^* = \eta$ for $Da_\Delta^I = Re_\Delta^{1/2}$. An important observation is that $l^* \leq \delta_{\mathcal{L}} \Leftrightarrow Pr \leq 1$, and this means that in gaseous combustion ($Pr \leq 1$) eddy-scales smaller than the flame thickness may survive and affect the flame itself, e.g., entering into it (although this has not been proved yet) and thickening it.

Among the surviving scales, those smaller than the local flame front thickness may locally enter into it and thicken it provided that $u'_\Delta \geq \mathcal{S}_{\mathcal{L}}$, $u'_\Delta$ being the local *rms* velocity fluctuation. Eddies with characteristic velocity $u'_l \geq \mathcal{S}_{\mathcal{L}}$ will be able to locally wrinkle a flame front. This will be important to model local flame quenching due to turbulence. Hence, given the smallest surviving eddies $l^*$, the smallest surviving and wrinkling eddy $l_w^*$ will be given by the condition

$$\frac{u'_{l^*}}{\mathcal{S}_{\mathcal{L}}} \geq 1 \Rightarrow \frac{u'_\Delta}{\mathcal{S}_{\mathcal{L}}}\left(\frac{l^*}{l_\Delta}\right)^{1/3} = Pr^{1/2}\left(Re_\Delta Da_\Delta^{I^{-2}}\right)^{1/3} \geq 1\ . \tag{3}$$

This means that the surviving scales $l^*$ become $l_w^*$, i.e., able to locally wrinkle a flame front if $Da_\Delta^I \leq Pr^{3/4} Re_\Delta^{1/2}$. Substituting the maximum Damköhler number for the smallest surviving and wrinkling scale into Eqn. (2), the minimum surviving and wrinkling scale $l_w^*$ is obtained, $l_w^*\big|_{min} = Pr^{-3/8}\,\eta \geq \eta$.

| Regime | Scale Condition | | $Da_\Delta^I$ Condition |
|---|---|---|---|
| $\mathcal{V}_\mathcal{R}$ | $\delta_\mathcal{L} \geq l_\Delta$ | $\Rightarrow$ | $Da_\Delta^I \leq Pr^{-1} Re_\Delta^{-1}$ |
| $\mathcal{TTC}_\mathcal{R}$ | $l_\Delta > \delta_\mathcal{L} \geq \eta$ | $\Rightarrow$ | $Pr^{-1} Re_\Delta^{1/2} \geq Da_\Delta^I > Pr^{-1} Re_\Delta^{-1}$ |
| $\mathcal{W}_\mathcal{R}$ | $\delta_\mathcal{L} < \eta$ | $\Rightarrow$ | $Da_\Delta^I > Pr^{-1} Re_\Delta^{1/2}$ |

Table 1: The three main premixed combustion regimes based on the comparison between turbulent length scales and laminar flame front thickness.

| $1 \geq Pr \geq Re_\Delta^{-1}$ | | |
|---|---|---|
| $\mathcal{V}_\mathcal{R}$ | $\mathcal{TTC}_\mathcal{R}$ | $\mathcal{W}_\mathcal{R}$ |
| $Da_\Delta^I \leq (Pr Re_\Delta)^{-1} (\leq 1)$ | $Pr^{-1} Re_\Delta^{1/2} \geq Da_\Delta^I \geq (Pr Re_\Delta)^{-1}$ | $Da_\Delta^I \geq Pr^{-1} Re_\Delta^{1/2}$ |
| | $\mathcal{Z}2_N \subset \mathcal{TTC}_\mathcal{R}$ | |
| | $(Pr Re_\Delta)^{1/2} \geq Da_\Delta^I \geq (Pr Re_\Delta)^{2/7}$ | |

Table 2: Ranges of the premixed turbulent combustion regimes when $1 \geq Pr \geq Re_\Delta^{-1}$, that is the most likely condition in gaseous combustion (also in supercritical condition).

## Premixed Combustion Regimes

Thinking to the interaction between a flame front and turbulent eddies and comparing the local laminar flame front $\delta_\mathcal{L}$, the local turbulent macro-scale $l_\Delta$, and the local turbulent dissipative scale $\eta$, it is possible to identify three main combustion regimes. These regimes are described in Table 1 and they are named $\mathcal{V}_\mathcal{R}$ from $\mathcal{V}olumetric\,\mathcal{R}egime$, $\mathcal{TTC}_\mathcal{R}$ from $\mathcal{T}hickened$, $\mathcal{T}urbulence-\mathcal{T}hickened$, $Corrugated\,\mathcal{R}egimes$, $\mathcal{W}_\mathcal{R}$ from $\mathcal{W}rinkled\,\mathcal{R}egime$.

Theory developed in this work (no details for lack of space) leads to identify premixed combustion regimes based on $Da_\Delta^I$, $Re_\Delta$ and $Pr$ numbers. In particular, depending on the local Prandtl number, there can be four possible conditions: among these, the most likely in gaseous combustion (also in supercritical condition) is $1 \geq Pr \geq Re_\Delta^{-1}$. This is the sole condition analysed in this work and whose combustion regimes ranges are shown in Table 2.

The reacting volume fraction $\gamma^*$ in Eqn. (1) will have to be modelled differently depending on the combustion regimes shown in Fig. 1. The effect of surviving scales that may thicken the flame front is modelled by means of the Zimont's model [6]. In this Section the effect of quenching due to turbulent scales, i.e., the $\mathcal{G}_{ext}$ function, is not taken into account. Hence, attention is posed on $\gamma^* = \frac{\mathcal{S}_\mathcal{T}}{\mathcal{S}_\mathcal{L}} \frac{\delta_\mathcal{F}}{\Delta}$.

For subgrid turbulent combustion (here $Re_\Delta \geq Pr^{-13/6}$ with $Pr \leq 1$) $\gamma^*$ is modelled as

- $\mathcal{V}olumetric\;\mathcal{R}egime$

$$\gamma^* = 1 \tag{4}$$

- $\mathcal{T}hickened\;\mathcal{R}egime$

$$\gamma^* = \frac{\delta_\mathcal{L}}{\Delta} = \left(Pr\, Re_\Delta\, Da_\Delta^I\right)^{-1/2} \leq 1 \tag{5}$$

$$\gamma^*\big|_{max} = 1 \qquad \gamma^*\big|_{min} = (Pr\, Re_\Delta)^{-9/14} \leq 1$$

- $\mathcal{T}urbulence\text{-}\mathcal{T}hickened\;\mathcal{R}egime$

$$\gamma^* = \frac{\mathcal{S}_\mathcal{T}}{\mathcal{S}_\mathcal{L}}\bigg|_\mathcal{Z} \frac{\delta^*_\mathcal{F}}{\Delta} = \mathcal{A}_\mathcal{Z} \left(Pr\, Re_\Delta\, Da_\Delta^{I^{-7/2}}\right)^{1/2} < 1 \tag{6}$$

$$\gamma^*\big|_{max} = \mathcal{A}_\mathcal{Z} < 1 \qquad \gamma^*\big|_{min} = \mathcal{A}_\mathcal{Z}\, (Pr\, Re_\Delta)^{-3/8} < 1$$

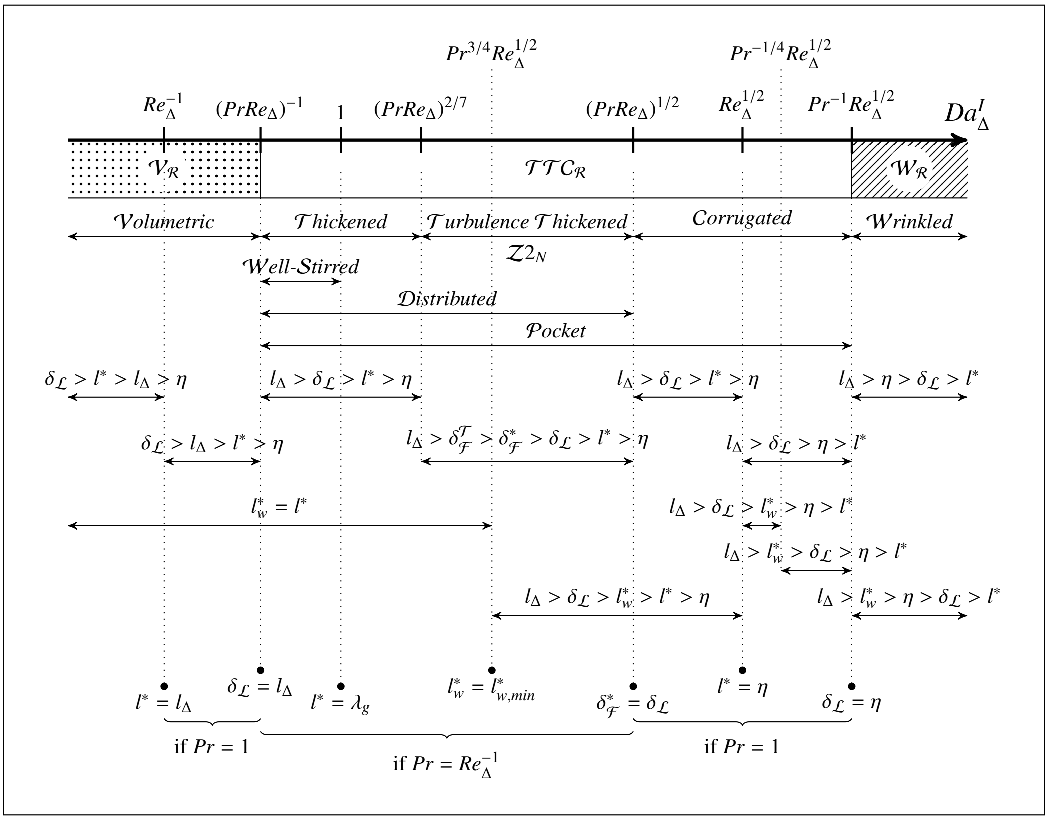


Figure 1: Description of the turbulent combustion regimes for $1 \geq Pr \geq Re_\Delta^{-6/13}$, i.e., for $Re_\Delta \geq Pr^{-13/6}$, with $Pr \leq 1$. Main scales of turbulence and combustion are also compared and ordered. Note that information in this figure are also valid for $1 \geq Pr \geq Re_\Delta^{-1}$, apart from the location of $Da^I_\Delta\big|_{l^*_{w,min}} = Pr^{3/4}Re_\Delta^{1/2}$ that would be located between 1 and $(PrRe_\Delta)^{2/7}$ for $Re_\Delta^{-6/13} > Pr \geq Re_\Delta^{-1}$.

- *Corrugated Regime*

$$\gamma^* = \frac{\mathcal{S_T}}{\mathcal{S_L}}\bigg|_C \frac{\delta_\mathcal{L}}{\Delta} \approx \frac{\mathcal{S_T}}{\mathcal{S_L}}\bigg|_\mathcal{Z} \frac{\delta_\mathcal{L}}{\Delta} = \mathcal{A_Z} Da_\Delta^{I^{-3/4}} < 1 \tag{7}$$

$$\gamma^*\big|_{max} = \mathcal{A_Z}\,(Pr\,Re_\Delta)^{-3/8} < 1 \qquad \gamma^*\big|_{min} = \mathcal{A_Z}\left(Pr^{-2}\,Re_\Delta\right)^{-3/8} < 1$$

having used the Zimont expression for $\mathcal{S_T}$ also in this regime due to the lack of reliable experimental data [7] and the superiority of Zimont model with respect to other models [7].

- *Wrinkled Regime*

$$\gamma^* = \frac{\mathcal{S_T}}{\mathcal{S_L}}\bigg|_\mathcal{W} \frac{\delta_\mathcal{L}}{\Delta} \approx \frac{\delta_\mathcal{L}}{\Delta} = \left(Pr\,Re_\Delta\,Da^I_\Delta\right)^{-1/2} \leq 1 \tag{8}$$

$$\gamma^*\big|_{max} = Re_\Delta^{-3/4} = \frac{\eta}{l_\Delta} \leq 1 \qquad \gamma^*\big|_{min} \to 0$$

having neglected subgrid hydrodynamic effects and Lewis number effects on $\mathcal{S_T}$. This regime appears to be of minor importance to industrial applications [7]. Work is going on to define in this low strain regime (Markstein regime) a $\mathcal{X}$ factor accounting for thermo-diffusive effects that increase or decrease the turbulent flame speed and flame wrinkling: $\mathcal{S_T}/\mathcal{S_L} = 1 - \mathcal{X}$, with $\mathcal{X} > 0$ or $\mathcal{X} < 0$ depending on local curvature, strain and Markstein number signs.

It is observed that $\Delta \equiv l_\Delta$ was assumed in deriving the non-dimensional number dependence in previous expressions, and that all of them guarantee $\gamma^* \leq 1$.

For subgrid laminar or pseudo-laminar combustion, i.e., $Re_\Delta < Pr^{-13/6}$, $\gamma^*$ is modelled as

- *Laminar $\mathcal{V}$olumetric $\mathcal{R}$egime* ($\delta_\mathcal{L} \geq \Delta$): $\gamma^* = 1$.
- *Laminar* (Planar) *$\mathcal{F}$lamelet $\mathcal{R}$egime* ($\delta_\mathcal{L} < \Delta$): $\gamma^* = \frac{\delta_\mathcal{L}}{\Delta} < 1$.

## Model Validation

The LTSM Model has been validated by simulating a test case defined and simulated by these authors using the Direct Numerical Simulation approach [8]. The test case consists in an unconfined and atmospheric Bunsen flame produced by three adjacent rectangular slot burners. The central slot burner injects a fresh mixture of methane, hydrogen and air ($\Phi = 0.7$ with 0.2 mole fraction of hydrogen) at $100\,\mathrm{m\,s^{-1}}$ and 600 K, while the two side burners inject hot combustion products of the same central mixture at $25\,\mathrm{m\,s^{-1}}$. Homogeneous isotropic turbulence is forced at the inlet with $L_{zz} = 0.8$ mm, $L_{xx} = L_{yy} = L_{zz}/2 = 0.4$ mm, $u'_z = u'_x = u'_y = 12\,\mathrm{m\,s^{-1}}$ as spatial correlation length scales and velocity fluctuations. The central jet turbulent Reynolds number is 226, based on the rms velocity fluctuation, $12\,\mathrm{m\,s^{-1}}$, the integral scale, 1 mm, and the kinematic viscosity of inlet fresh reactants, $5.3 \cdot 10^{-5}\,\mathrm{m^2\,s^{-1}}$. The Kolmogorov length scale is $\eta \approx 17.22\,\mu$m. The adiabatic flame temperature is 2071 K. The laminar flame speed and flame front thickness at these conditions are $\mathcal{S}_\mathcal{L} = 0.96\,\mathrm{m\,s^{-1}}$ and $\delta_\mathcal{F} = 0.386$ mm, respectively. Hence, $u'_{rms}/\mathcal{S}_\mathcal{L} = 12.5$ and $L_t/\delta_\mathcal{F} = 2.6$; $Ka_\eta = 503$, $Da^I_{L_t} = 0.21$, thus locating this flame into the broken reaction regime of the standard combustion diagram, where turbulence is expected to strongly influence premixed flame structures.

The chemical mechanism adopted for combustion is a skeletal mechanism having 17 species and 58 reactions [9]. The walls are assumed viscous and adiabatic. Partially non-reflecting boundary conditions were imposed at the open boundaries. The subgrid scale model adopted for the turbulence closure is the dynamic Smagorinsky model. The whole computational domain has 3463885 nodes.

Predicted temperature and velocity components are compared with DNS data, in terms of their time averages and rms fluctuations at different heights above injection (e.g., see Fig. 2). The agreement is good. PDFs of some quantities are also reported in Figs. 3 and 4. Working is going on to validate the main modelled quantities against the same DNS data.

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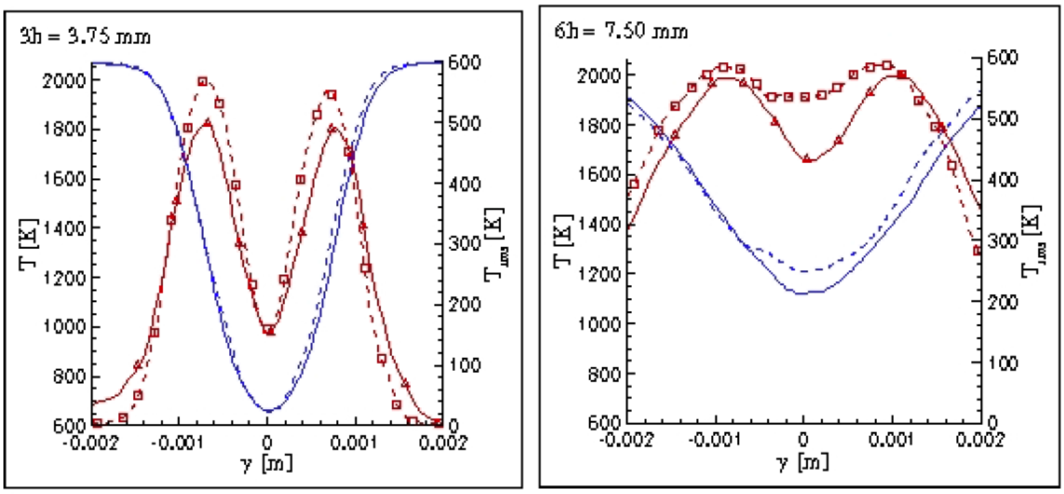



Figure 2: Transversal average and rms temperature profiles at several heights above injection: comparison between LES (solid lines) and DNS data (dashed lines). Lines with symbols are rms fluctuations.

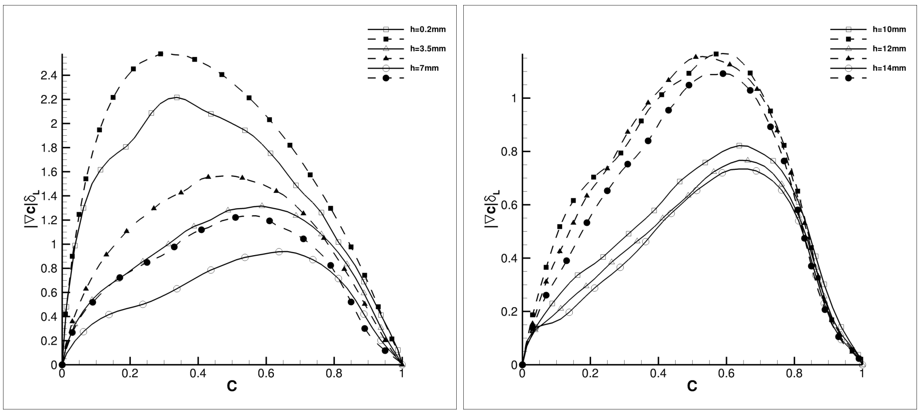
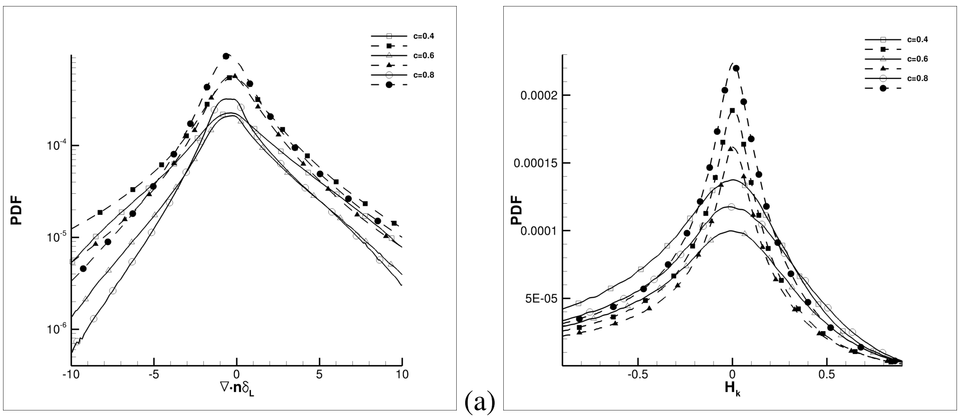



Figure 3: Inverse of the normalized flame front thickness as function of the progress variable: comparison between LES (solid lines) and DNS data (dashed lines).




(a) (b)

Figure 4: Normalized curvature PDF (a) and shape factor PDF (b) for different progress variable levels: comparison between LES (solid lines) and DNS data (dashed lines).