



POLITECNICO DI MILANO

DIPARTIMENTO DI CHIMICA, MATERIALI E INGEGNERIA CHIMICA "GIULIO NATTA"

SMARTCATs COST Action

Short Term Scientific Mission Report

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Details of STSM

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I hereby confirm that Erica Quadarella, Politecnico di Milano-Italy, has spent a period (from 2017-08-13 to 2017-08-19) at the Université Libre de Bruxelles-Belgium, within the framework of a Short Term Scientific Mission (STSM) under the SMARTCATs COST Action CM1404.

Thanking you,

Yours Sincerely,

Alessandro Parente

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Introduction

This STSM was used for setting up a collaborative work between Université Libre de Bruxelles, Brussels, Belgium (ULB) and Politecnico di Milano, Milan, Italy (PoliMi) in order to investigate the role and influence of some parameters (which determine the chemical and mixing time) on the simulation of Sandia Flame D with the PaSR model. The latter one, for the description of turbulence-chemistry interaction, can give a comprehensive description of turbulent combustion systems since is able to well discriminate the contribution of the chemical and turbulent times. For this reason, it is very interesting to study the role of this model and compare the results of the simulations with the ones obtained with the EDC model [1], which assumes that small turbulent structures (i.e. fine structures) govern reaction rates.

The numerical code edcSMOKE was used which is based on the OpenFOAM framework.

Finally, further improvements regarding the PaSR code in edcSMOKE were discussed concerning the possibility to calculate the chemical characteristic time relying on reactions and no longer on species. It is therefore also important to continue this collaboration between the two groups to develop this new part of the code for the improvement and a more faithful reproduction of the results.

Activities

This STSM started with the study of PaSR model for the description of chemistry-turbulence interaction. For this purpose, different articles and thesis that dealt with the subject have been taken into account [2] [3] [4] [5]. The basic idea of the PaSR is that reactions occur in certain regions of the domain (comparable to the *fine structures* described in the EDC model) over a time corresponding to the one characteristic of chemistry. Subsequently, what have been reacted is mixed over a time dictated by turbulence along with unreacted species in the remaining domain (Fig. 1)

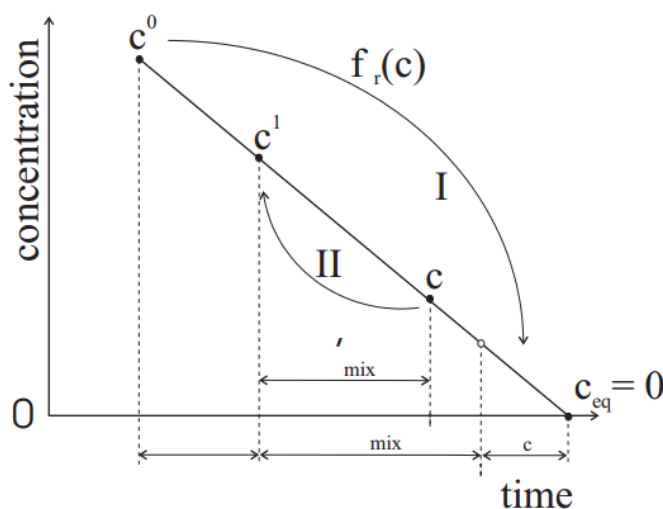


Figure 1. Schematic representation of the PaSR mechanism

The reacting zone is treated as a perfectly stirred reactor (PSR).

It is therefore possible to distinguish between three different concentrations:

- c^0 : initial averaged concentration inside the whole cell
- c : unknown concentration in the reaction zone on a sub-grid level in the reactive fraction of the cell
- c^1 : is the variable which is transported, thus it is the final averaged concentration in the whole cell.



Obviously, the reacting term inside the transport equation should depend on the transported variable which is c^1 . Therefore, with some mathematical passages it is possible to get free from the unknown parameter c (belonging to a sub-grid level) in order to get only a c^1 dependence:

$$f_m(c) = \kappa f_m(c^1)$$

where

$$\kappa = \frac{\tau_c}{\tau_c + \tau_{mix}}$$

At this point, it is important to find a method to calculate these two characteristic times. For what concern the chemical one, two different methods have been used to run the simulations and make a comparison. The first one is based on the principle of the *Formation Rates*, in which the chemical characteristic time is calculated as follows:

$$\tau_c = \frac{Y^0}{dydt}$$

where

$$dydt = \frac{Y^* - Y^0}{\Delta t}$$

$Y^* = \text{mean molar concentration inside the reactive zone}$

$Y^0 = \text{mean initial molar concentration inside the cell}$

$\Delta t = \tau_{mix}$

The other more accurate method which has already been implemented for computing τ_c is the one based on the calculation of the *Eigenvalues* of the Jacobian matrix, which is made up of derivatives of the formation rates with respect to species concentration:

$$\begin{pmatrix} \frac{df_1}{dc_1} & \dots & \frac{df_1}{dc_i} \\ \vdots & \ddots & \vdots \\ \frac{df_j}{dc_1} & \dots & \frac{df_j}{dc_i} \end{pmatrix}$$

The smaller eigenvalue is taken in order to calculate the chemical characteristic time as the inverse of that eigenvalue.

What is left, is the calculation of the mixing time which is governed by turbulence. There are many different methods, including the Kolmogorov scale, the integral and the geometric mean. What we have used in the simulations is the second one, that describes the turbulent mixing time as follows:

$$\tau_{mix} = C_{mix} \frac{k}{\varepsilon}$$

where k is the turbulent kinetic energy and ε is the turbulent energy dissipation rate. Unfortunately, C_{mix} is a constant that has not actually been well defined yet. In literature, it is possible to find really different and large ranges of values adopted for this constant. Thus, one of the aims of our simulations was to find the value of C_{mix} which best fits the experimental data.

So, four different values (under the advice of the ULB group) for C_{mix} , ranging from 0.05 to 0.25, were investigated using both the models for the estimation of τ_c .

Before running the simulations, the codes for the different parts of the PaSR were read and discussed in order to understand them and make it easier to change something for further and future improvements of the model. All simulations were run with a "reduced" kinetic mechanism (derived from the POLIMI_1412 [6]) in order to get

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the results of temperature and the main species in a reasonable time. Starting from this solution it will be possible to calculate the NO_x emission just running again the simulation but with the complete kinetic mechanism. The domain was subdivided in a structured grid of about 5000 cells, more refined in the regions of greatest interest (for example near the nozzle and along the centreline of the flame).

Results and discussion

For what concern the simulations with the *Formation Rates* approach for the calculation of the characteristic chemical time, temperature profiles at varying the value of C_{mix} are reported below (Fig. 2):

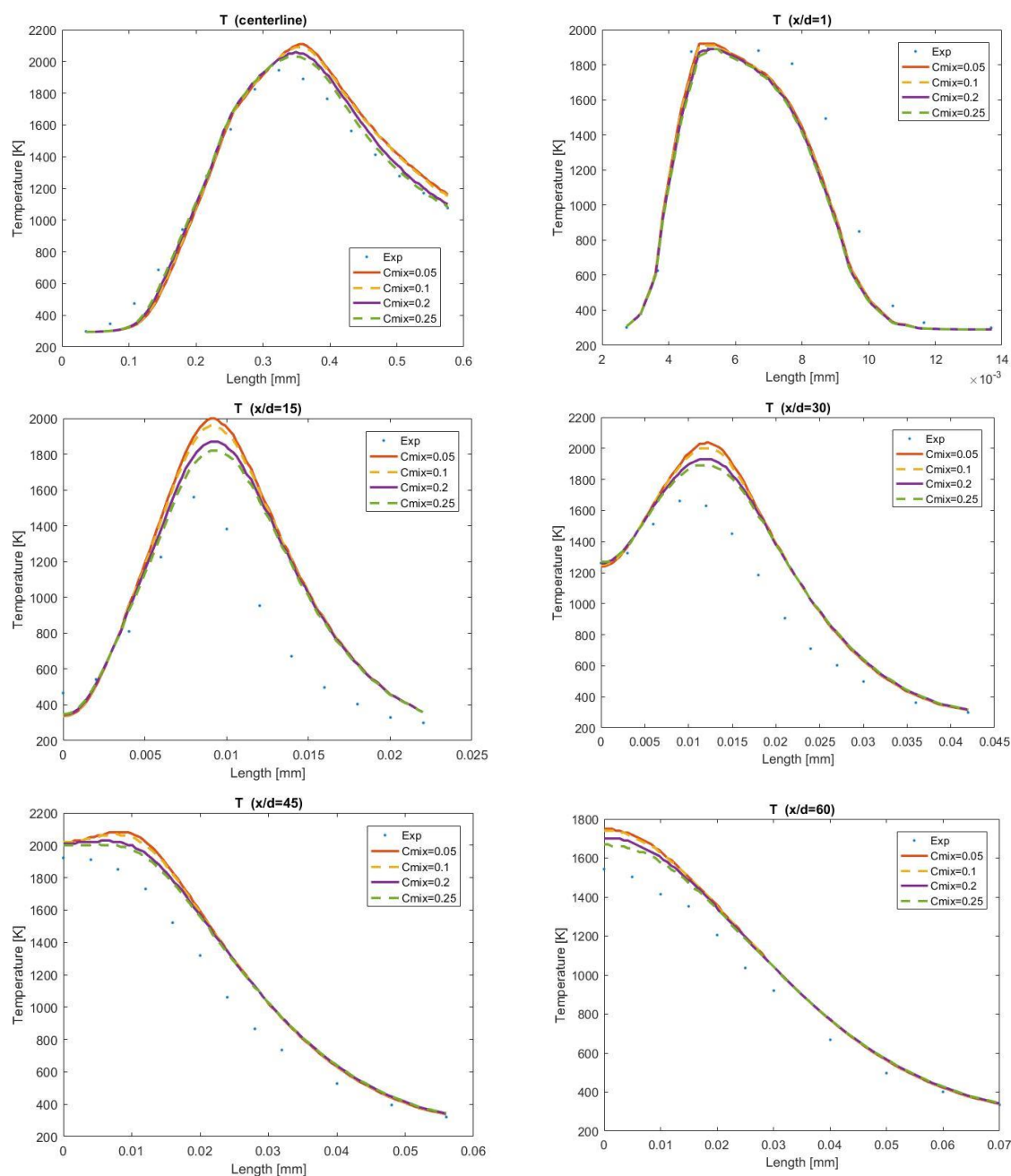


Figure 2. Results with Formation Rate method for τ_c and with different values of C_{mix}

Increasing the value of C_{mix} , temperature's peaks decrease. The best results are for $C_{mix} = 0.2$ and $C_{mix} = 0.25$

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The other method adopted to compute the characteristic chemical time is the one that consider the *Eigenvalues* of the Jacobian matrix. Actually, this is the most rigorous way to calculate τ_c when relying on species. Also in this case, the simulations were run with the different values for C_{mix} and the results are shown below (Fig.3):

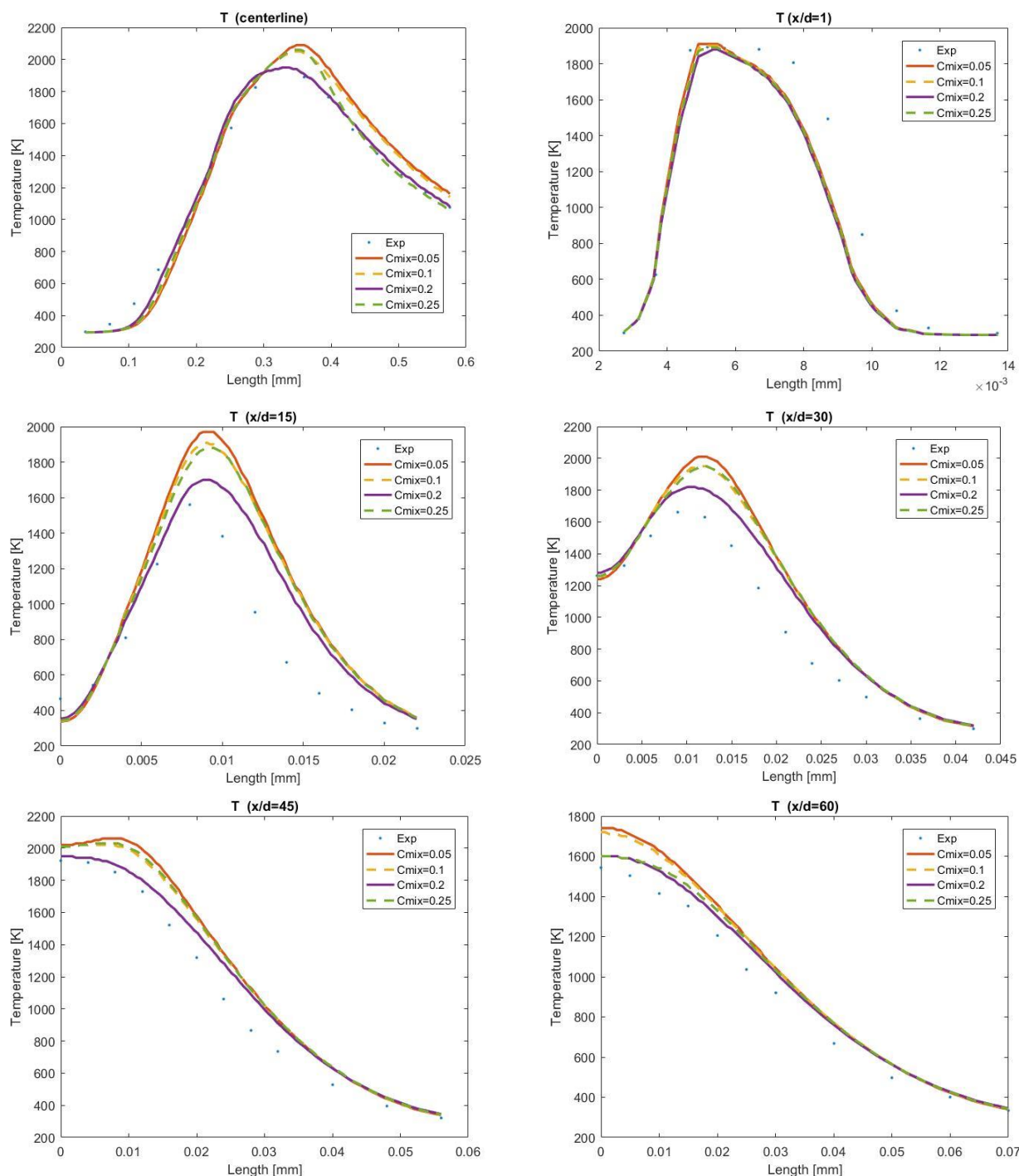


Figure 3. Results with Eigenvalue method for τ_c and with different values of C_{mix}

Also in this case the general trend is of a decreasing temperature peak at increasing the value of C_{mix} , except for $C_{mix} = 0.25$. The best results are obtained with $C_{mix} = 0.2$.

After this kind of analysis, the best results were compared with the one coming from the simulation run with the EDC model (Fig.4):

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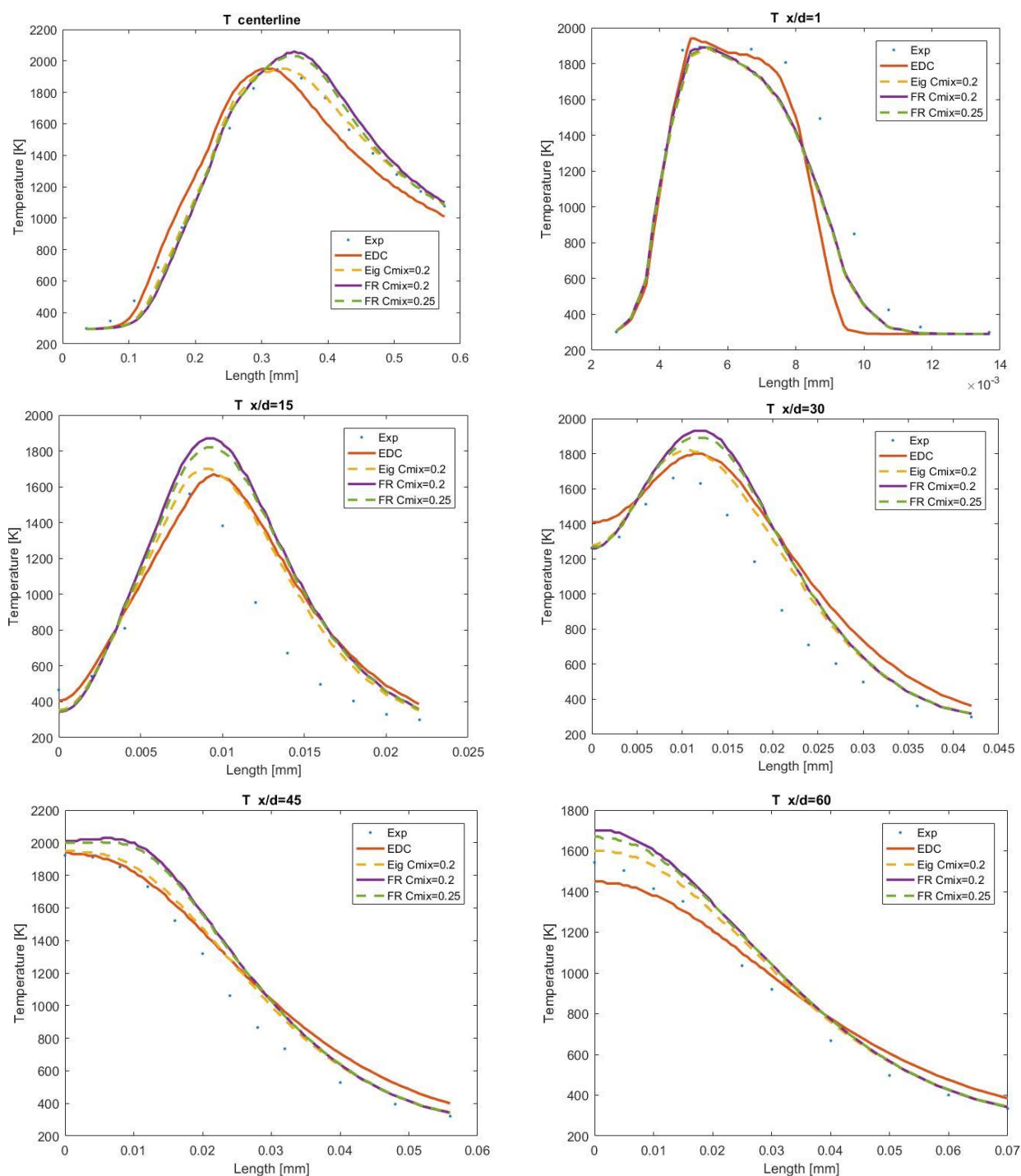


Figure 4. Comparison between results from EDC and PaSR

It can be noted that among the best results from the PaSR model, the one which comes from the *Eigenvalues* method for the calculation of τ_c and with $C_{mix} = 0.2$ is able to better approximate the experimental points. For what concern the comparison with the EDC model, results are quite similar. However, the PaSR seems to better reproduce the trend, especially on the centreline.

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Future works

The PaSR model seems to work well for the reproduction of turbulent combustion systems. However, some points can be improved. In fact, the chemical characteristic time is now computed relying on species. The problem is that in this way we are just looking at the time for the formation or destruction of a species among all reactions. Thus, the time taken by each single reaction to occur is not considered. This issue could be solved starting to rely on reactions for the computation of τ_c and taking no longer into account only one global τ_c but one for each reaction.

It is therefore important to continue the collaboration between POLIMI and ULB in order to modify the code on edcSMOKE and test this new and hopefully more accurate method for computing τ_c .

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