

Study of MILD combustion using LES and advanced analysis tools

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Abstract

A cylindrical confined combustor operating under MILD condition is investigated using LES. The combustion and its interaction with turbulence are modeled using two reactor based models, PaSR and EDC. Results show that the Partially Stirred Reactor (PaSR) model yields improved estimation for mean temperature and species mole fractions compared to Eddy Dissipation Concept (EDC). LES data are analysed using advanced post-processing methods such as the chemical Tangential Stretching Rate (TSR), balance analysis and local Principle Component (PCA) analysis. TSR can identify chemical explosive (ignition-like) and contractive (burnt) regions. With the balance analysis of the convective, diffusive and reactive terms in temperature equation, regions with substantial heat release coming from ignition or flame are identified. The local PCA analysis classifies the whole domain into clusters (regions with specific features) and provides the leading species in each cluster. The three analyses correlate well with one another and it is observed that the most chemically active region locates upstream

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(in the near-field). Also, both autoignition and flame-like structures play equally important roles in MILD combustion.

1 *Keywords:* MILD combustion, LES, Reactor-based models, CSP analysis, local
2 PCA

3 **1. Introduction**

4 More than 90% of the world total primary energy supply comes from combus-
5 tion in one form or another. There are challenges to meet future energy require-
6 ment because of the limited fossil fuel resources. Also, the impact of combustion
7 on the environment through emissions of green house gases, CO₂, and pollutants
8 such as NO_x and soot is well-known. Hence, developing efficient combustion
9 technologies with low emissions and fuel flexibility has become imperative. Mod-
10 erate or Intense Low oxygen Dilution (MILD) combustion is a very promising
11 technology and requires a massive recirculation of exhaust gases within the re-
12 action region [1, 2]. The hot exhaust gas preheating reactants helps to stabilize
13 combustion and minimise hotspots, which yields a uniform temperature field and
14 suppresses combustion noise [1]. Also, the temperature rise across the combus-
15 tion zone is only few tens of Kelvin above the background hot gas temperature,
16 typically below 1800 K, inhibiting production of thermal NO_x, CO and soot [1, 2].

17 Various lab-scale burners have been used in experimental studies, including
18 the Jet in Hot Coflow (JHC) burner [3, 4], reversed-flow arrangement having the
19 inlet and outlet on the same side [5] and cylindrical combustor with a converging
20 duct towards the outlet [6]. The effect of hot gas recirculation is included in JHC
21 configuration by using combustion products of an upstream burner. However, this
22 configuration does not account for the effect of internal recirculation as it happens

1 in realistic industrial systems. It is therefore not considered in the current study.
2 The geometry of the other two configurations inherently include the recirculation
3 of hot gases. More spatially uniform temperature field was observed in these
4 configurations compared to JHC case. Also, the combustor in reversed-flow case
5 was well-insulated, but the case in [6] allows heat loss through the wall, which
6 could influence the combustion stability. Hence, conditions achieved in [6] are
7 expected to be representative of practical MILD combustion conditions and thus,
8 this burner is of interest here.

9 Large Eddy Simulation (LES) using a three-stream Flamelet Progress Variable
10 (FPV) formulation was used in [7] to model the JHC flame. This burner was also
11 studied using Partially Stirred Reactor (PaSR) [8] and laminar chemistry (without
12 turbulence-chemistry interaction effects) [8] in the context of LES. All of these
13 studies showed good agreement with measurements. The other two enclosed cases
14 have also been investigated in past studies using tabulated chemistry approaches.
15 The FPV involving counter-flow diffusion flames was extended to include the di-
16 lution effects in [9] and a diluted homogeneous reactor was used in [10]. Both of
17 these approaches use tabulated chemistry and provided results in good agreement
18 with the experimental data. These approaches involve a multi-dimensional lookup
19 table, whose generation is quite tedious and time consuming. Reactor-based mod-
20 els such as PaSR and EDC do not require to consider dilution explicitly since the
21 chemical species of interest (involved in the kinetic mechanism used) are trans-
22 ported. Depending on the size of the chemical mechanism, these methods can be
23 more computationally expensive, compared to tabulated chemistry.

24 The objectives of the present study are (i) to conduct LES of MILD combus-
25 tion in experiment [6] using the PaSR and EDC models for subgrid scale (SGS)

1 combustion, (ii) to analyse the LES data using Computational Singular Perturba-
2 tion (CSP) [11] and balance [12, 13] analyses to identify autoignition and flame
3 regions, and (iii) to apply local Principal Component Analysis (PCA) [14] to ex-
4 tract potential chemical markers for these regions. We believe that this is the first
5 direct comparison of PaSR and EDC models for MILD combustion in a combus-
6 tor with strong internal recirculation zones simulated using LES paradigm. Most
7 importantly, the advanced data analysis tools reveal intriguing features of MILD
8 combustion, providing impetus to further numerical and experimental investiga-
9 tions.

10 This paper is organised as follows. The test case and its numerical modelling
11 are described in sections 2 and 3 respectively. The SGS combustion models are de-
12 scribed briefly in section 4 and the results are discussed in section 5. The analyses
13 to identify autoignition and flame regions are discussed in section 6 and conclu-
14 sions are summarised in the final section.

15 **2. Experimental Configuration**

16 A 10 kW lab-scale MILD combustor investigated in [6] is chosen as the test
17 case for this study. This cylindrical combustor operating at atmospheric pressure
18 has air at 673.15 K entering through a central jet of diameter $d_a = 10$ mm with
19 a bulk-mean velocity of $U_a = 113.2$ m/s, giving a Reynolds number of 17526.
20 Methane at 298.15 K is injected into the combustor through 16 jets with $d_f =$
21 2 mm and $U_f = 6.2$ m/s. The cylindrical combustor has a diameter of 100 mm
22 for a length of 340 mm and then it converges at 15° , as shown in Fig. 1. A strong
23 recirculation region with hot flue gases is achieved aerodynamically because of
24 the converging section.

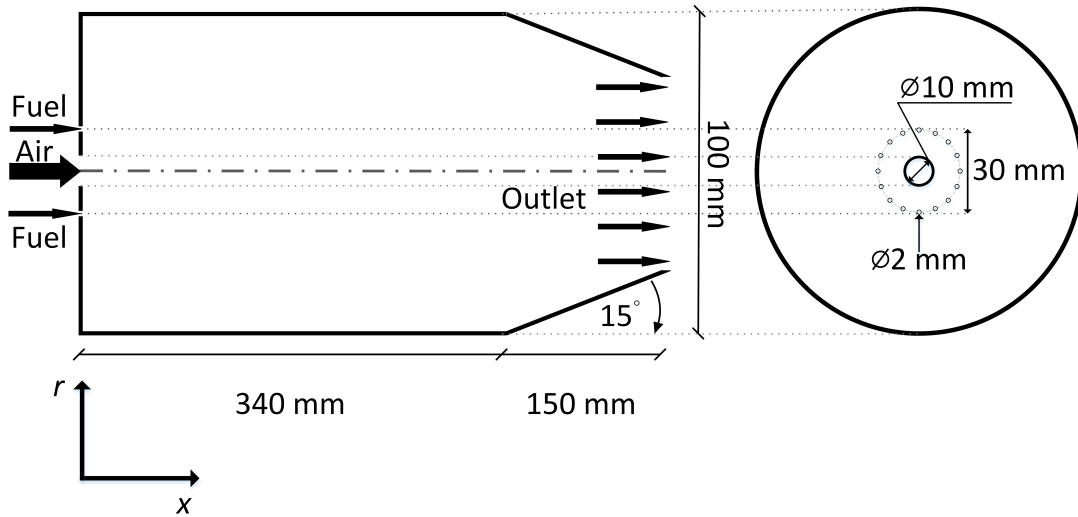


Figure 1: Schematic view of the combustor geometry [6].

1 Several experiments were conducted in [6] with an excess air ratio in the range
 2 of $1.1 \leq \lambda \leq 2.2$. Among these various experimental cases, the case labelled
 3 RUN2 with $\lambda = 1.3$ is under MILD condition and it is selected for this study.
 4 Detailed measurements of mean temperature, dry mole fractions of O_2 , CO_2 , HC,
 5 NO_x and CO are reported in [6]. The mole fractions are measured using stainless
 6 steel water-cooled sampling probes (average repeatability of data within 10%) and
 7 local mean temperature measurements were obtained using 13% rhodium (type R)
 8 thermocouples with uncertainty less than 5% [6]. The radial variations of these
 9 quantities are reported in [6] for several axial locations in the non-converging
 10 section of the combustor.

11 3. Numerical Set-up

12 The schematic shown in Fig. 1 forms the cylindrical computational domain
 13 and it is discretised using O-grid. Three different grids having 2, 4, and 8M

1 cells are considered. The flow rates at the inlet are specified to match the con-
2 ditions of the fuel and air streams. Since the fuel jet Reynolds number is small,
3 no turbulence is specified but the air stream turbulence is specified using a syn-
4 thetic turbulence [15] based inflow generator. The RMS velocity for air stream is
5 $u_{rms} = 20$ m/s, following an earlier study [10] and the length scale specified for
6 the inflow generator is 5.5 mm, 55% of jet diameter. Mean top-hat profiles with-
7 out fluctuation are used for inlet scalar boundary conditions. The no-slip walls are
8 specified to be at 1000 K based on previous studies [9, 10]. The boundary layers
9 are unresolved and represented with wall functions. All the scalar and velocity
10 gradients in the direction normal to the outlet plane are specified to be zero. The
11 simulations are run for $21\tau_{flow}$, where τ_{flow} is the flow through time for the entire
12 combustor length based on U_a . The statistics are collected over the last $8\tau_{flow}$ after
13 allowing the initial transients to leave the combustor. First, a non-reacting flow is
14 simulated using OpenFOAM-2.3.0 [16] software and the above three grids. This
15 code solves Favre-filtered mass, momentum, and energy conservation equations
16 along with filtered transport equations for scalars required in combustion mod-
17 elling. The sub-grid stresses are modelled using one equation (for SGS kinetic
18 energy, \mathcal{K}) model with constant coefficient. Simulation results from the three
19 grids are included in the supplementary material. Detailed analysis of the non-
20 reacting flow results showed that more than 80% (indeed 90% in regions of scalar
21 mixing and combustion) of the turbulent kinetic energy is resolved using the mesh
22 with 2M cells. Moreover, past DNS studies [12] of MILD combustion showed that
23 the reactive structures are broader than Kolmogorov scales and using grid spac-
24 ing of 3 to 5 times the laminar thermal thickness is sufficient for a good LES. In
25 the current case, the estimated laminar thermal thickness [12] is 0.36 mm. The

1 cell size of the 2 M grid ranges from 0.27 to 1.8 mm. Thus, this mesh is appro-
2 priate for the current MILD combustion simulation. The edcSMOKE [17] finite
3 rate chemistry solver is used for the PaSR and EDC sub-grid (SGS) combustion
4 models, briefly described in the following.

5 **4. Combustion Models**

6 Methane-air combustion chemistry is modelled using a skeletal mechanism [18],
7 which was shown to be adequate for MILD conditions in [13] and in [8, 19]. For
8 the finite-rate based LES of a combustion with the current geometry, such mech-
9 anism is considered to be the best to balance between CPU hour requirement
10 and accuracy. Both PaSR and EDC assume that each computational cell con-
11 sists of a reactive structure and a surrounding fluid. Combustion occurs in the
12 reactive structure while surrounding fluid accounts for scalar mixing processes.
13 These mixing processes can be imperfect in turbulent combustion and thus the fil-
14 tered reaction rate, $\bar{\omega}_k$ required for the scalar transport equation is specified using
15 $\bar{\omega}_k = F \cdot \omega_k^*(\tilde{Y}, \tilde{T})$, where $\omega_k^*(\tilde{Y}, \tilde{T})$ represents the reaction rate of species k in the
16 reactive structure. The reactive structure reaction rates are estimated by solving a
17 canonical reactor, typically a perfectly stirred reactor (PSR) or a plug flow reactor
18 (PFR). The residence time in the canonical reactor for this study is set to be CFD
19 time step [8]. The term F in the above equation represents the fraction of the reac-
20 tive structure in a numerical cell and its detail depends on the modelling approach
21 used.

1 *4.1. Partially Stirred Reactor model*

2 The reactive fraction F for the PaSR model, typically denoted using κ [20], is
 3 calculated as

$$F \equiv \kappa = \frac{\tau_c}{\tau_c + \tau_{\text{mix}}}, \quad (1)$$

4 where τ_c and τ_{mix} are the characteristic chemical and mixing time scales respec-
 5 tively in a cell. Here, the chemical time scale for species k is estimated as $\tau_{c,k} =$
 6 $Y_k^* / (dY_k^*/dt)$, which is obtained from a PFR solution. The symbol t denotes the
 7 time. The maximum value of $\tau_{c,k}$ (removing the dormant species) is chosen as
 8 τ_c [21]. The mixing time scale is defined as $\tau_{\text{mix}} = \sqrt{\tau_\Delta \tau_\eta}$, where $\tau_\Delta \simeq \Delta / \sqrt{\mathcal{K}}$ is
 9 the SGS flow time scale and $\tau_\eta \simeq \sqrt{\nu / \epsilon_{\text{sgs}}}$ is the SGS viscous time scale [8]. The
 10 symbols Δ and ϵ_{sgs} denote the LES filter width and SGS dissipation rate of \mathcal{K} .

11 *4.2. Eddy Dissipation Concept model*

12 EDC is based on turbulent kinetic energy cascade [22]. This provides the
 13 fraction of the reactive structures F in the flow [22], as:

$$F = \frac{\gamma_\lambda^2}{1 - \gamma_\lambda^2}, \quad (2)$$

14 with γ_λ estimated as a function of the flow characteristic scales:

$$\gamma_\lambda = C_\gamma \left(\frac{\nu \epsilon_{\text{sgs}}}{\mathcal{K}^2} \right)^{1/4}. \quad (3)$$

15 The model constant $C_\gamma = 2.1377$ is taken from a RANS study [22] as a first
 16 approximation.

17 Compared to PaSR model, EDC utilises only fluid mechanical time scales,
 18 more precisely it involves a ratio of molecular to SGS eddy viscosities, without
 19 involving a chemical time scale to evaluate F .

1 5. Results and Discussion

2 5.1. Streamline profiles

3 The time-averaged streamline profiles on the mid-plane for the two models are
4 shown in Fig. 2, marking the recirculation zones. There are mainly two recircula-
5 tion zones. The smaller one is located at the side corner ($|r| \geq 0.02$ m, $x \leq 0.05$ m)
6 and the larger one, which brings the hot flue gases upstream and heats up the fresh
7 air and fuel mixture, is established in the middle of the domain. Compared to
8 PaSR model, the centre of the large recirculation zone from the EDC is situated
9 more downstream, at around $x = 0.17$ m, while it is at about $x = 0.1$ m for PaSR.
10 Since the same boundary conditions are used for both models, the differences in
11 the streamlines come from combustion effects, showing that the most reactive re-
12 gion for EDC is probably located further downstream than that for PaSR.

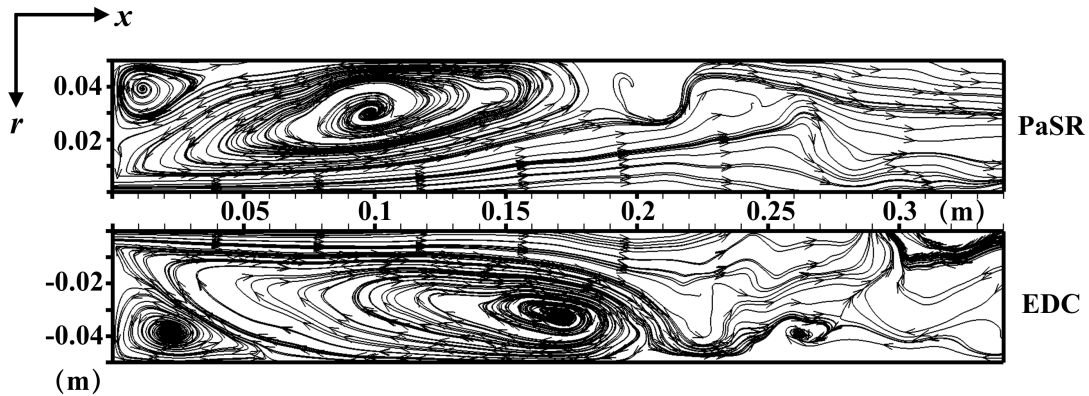


Figure 2: Streamline profiles from PaSR and EDC combustion models

13 5.2. Comparisons with measurements

14 Figure 3 shows the time-averaged temperature fields obtained from the LES
15 using the PaSR and EDC models along with experimental results taken from [6].

1 The symbols in the experimental frame show scalar probe measurement locations.
2 Overall, a reasonable agreement with experimental profile is observed for the
3 PaSR model. However, the penetration of the air jet is over estimated (0.1 m
4 compared to 0.079 m in the experiment) which could be related to the turbulence
5 conditions specified at the air stream inlet. The incoming turbulence and boundary
6 layer at the lip will influence the jet spreading angle and these affect the near-field
7 behaviour, which is also apparent in the results. The high temperature region pre-
8 dicted by the PaSR model spans between $x = 0.1$ m and 0.25 m, while this region
9 extends up to $x = 0.3$ m in the experiment. Hence under-prediction of temperature
10 is anticipated after $x = 0.25$ m. The general pattern of the temperature variation
11 predicted using the EDC is similar to that obtained using the PaSR model but
12 the temperature values are under-predicted by the model as seen in Fig. 3. At
13 $x = 0.11$ m, the PaSR model shows a large temperature gradient while, for EDC,
14 the temperature increase is located at around $x = 0.185$ m. These locations corre-
15 late with the centre of the large streamlines accounting for flue gas recirculation
16 in Fig. 2.

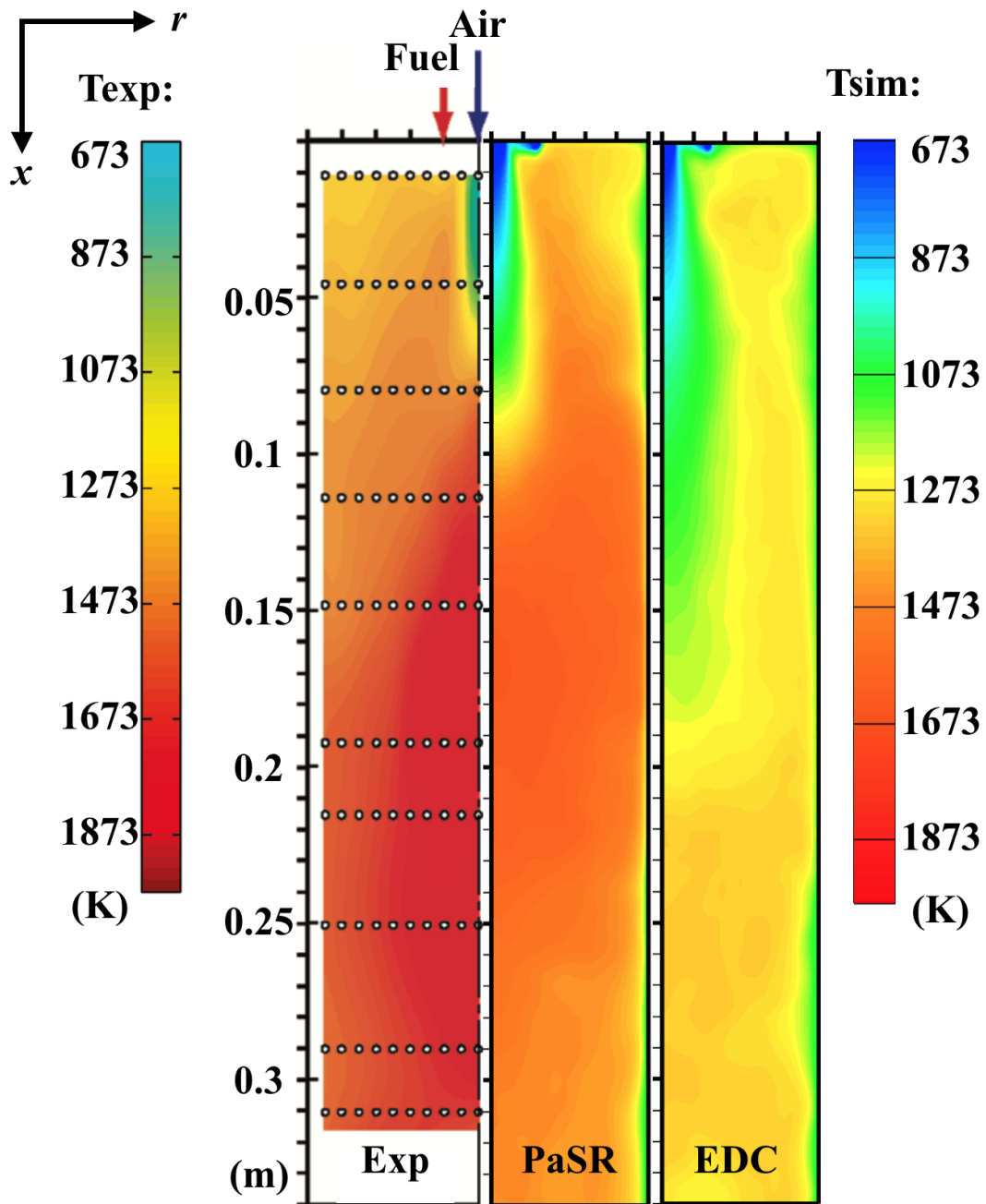


Figure 3: Averaged temperature fields in the mid plane for PaSR and EDC models and measurements.

1 The measured temperature field shows a strong radial gradient for $x \leq 0.15$ m
2 which is also represented in the computational results. For further evaluations, the
3 axial locations of $x = 11/45/79/113/147/310$ mm are considered.

4 The radial variations of mean temperature computed using the PaSR and EDC
5 models are compared to the experimental data in Fig. 4. The results are shown for
6 six axial locations. The EDC under-predicts temperature in general as observed
7 in the previous figure. The values computed using the PaSR model compares
8 quite well with the measurements and this comparison is similar to those obtained
9 in [9, 10]. However, the average temperatures at $x = 310$ mm is underestimated by
10 about 200 K. On the other hand, earlier studies [9, 10] showed an overestimation
11 by about 150 to 200 K.

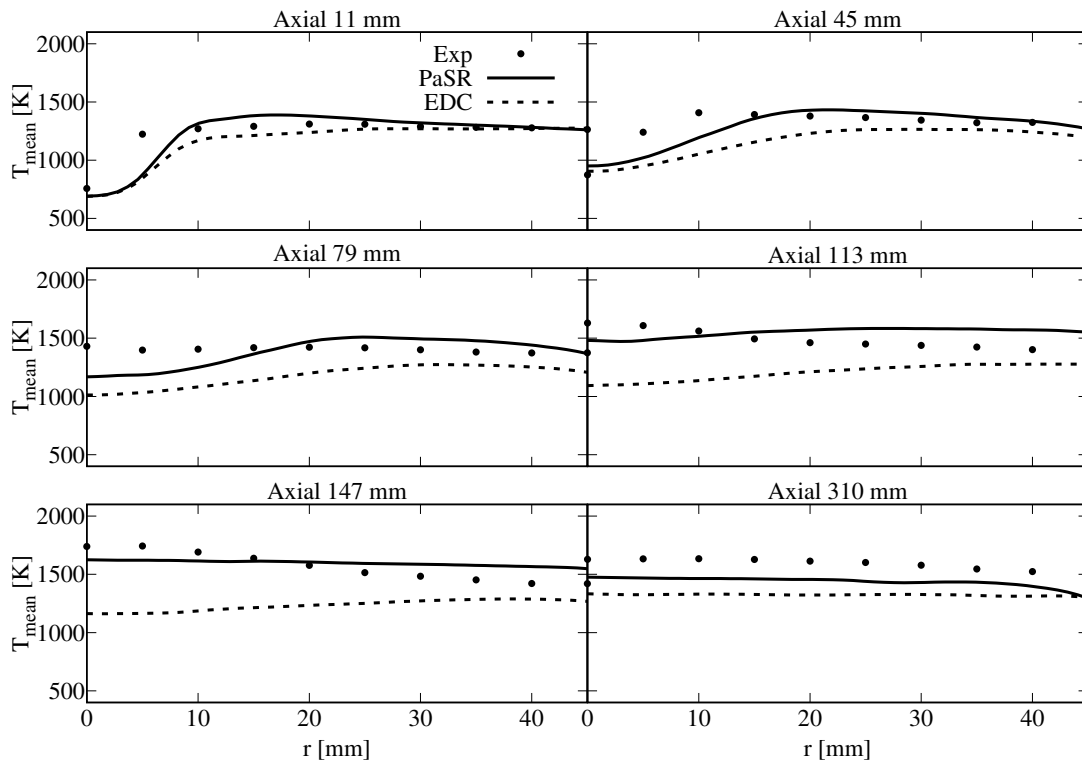


Figure 4: Comparison of computed and measured radial variation of mean temperature at six axial locations.

1 The species mole fraction for O_2 and CO_2 are shown in Figs. 5 and 6. The
 2 computed values of these species mole fractions compare quite well with experi-
 3 mental data for the location $x = 11$ mm and the difference between the PaSR and
 4 EDC models is small. The difference between the models' prediction increases as
 5 one moves downstream with almost no difference for $x = 310$ mm, where the equi-
 6 librium values are expected. A closer scrutiny of the results in these two figures
 7 show a substantial difference between the computed and measured mole fractions
 8 for the first three experimental data points of $r \leq 10$ mm at $x = 45, 79, 113$ and
 9 147 mm, which is also consistent with earlier studies using different combustion

1 models [9, 10]. For the incoming air and fuel stream temperatures, one would ex-
2 pect relatively higher CO₂ values and O₂ mole fractions substantially lower than
3 0.2 in the regions with temperature larger than about 1100 K. The experimental
4 data seem to contradict this and a simple energy balance analysis discussed in the
5 supplementary material suggests that there might be some issues in the measure-
6 ments of CO₂ and O₂ mole fractions in the regions noted above. For these reasons,
7 these specific experimental data points are excluded while evaluating the overall
8 model performance. To conclude, the species mole fraction are well predicted for
9 $x = 11$ mm by both PaSR and EDC models. After $x = 45$ mm, EDC under and
10 over predicts CO₂ and O₂ respectively. The PaSR model works well across the
11 whole domain if one excludes the specific data points noted above.

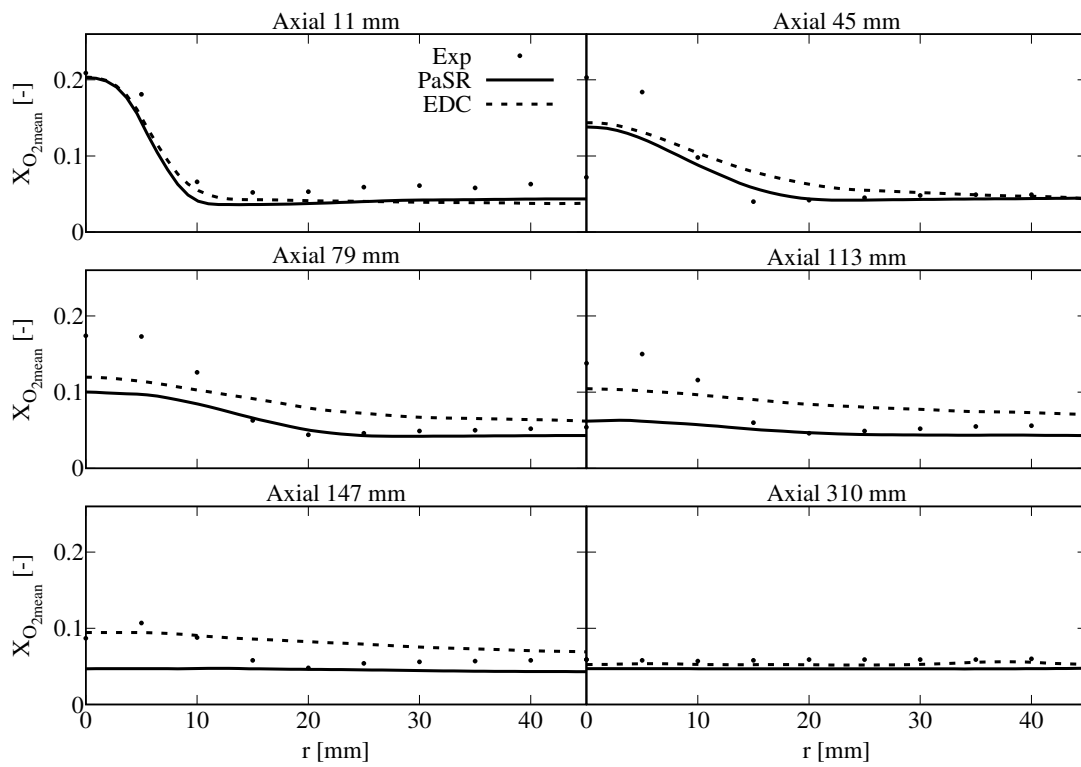


Figure 5: Comparison of computed and measured mean O₂ mole fraction for six axial locations.

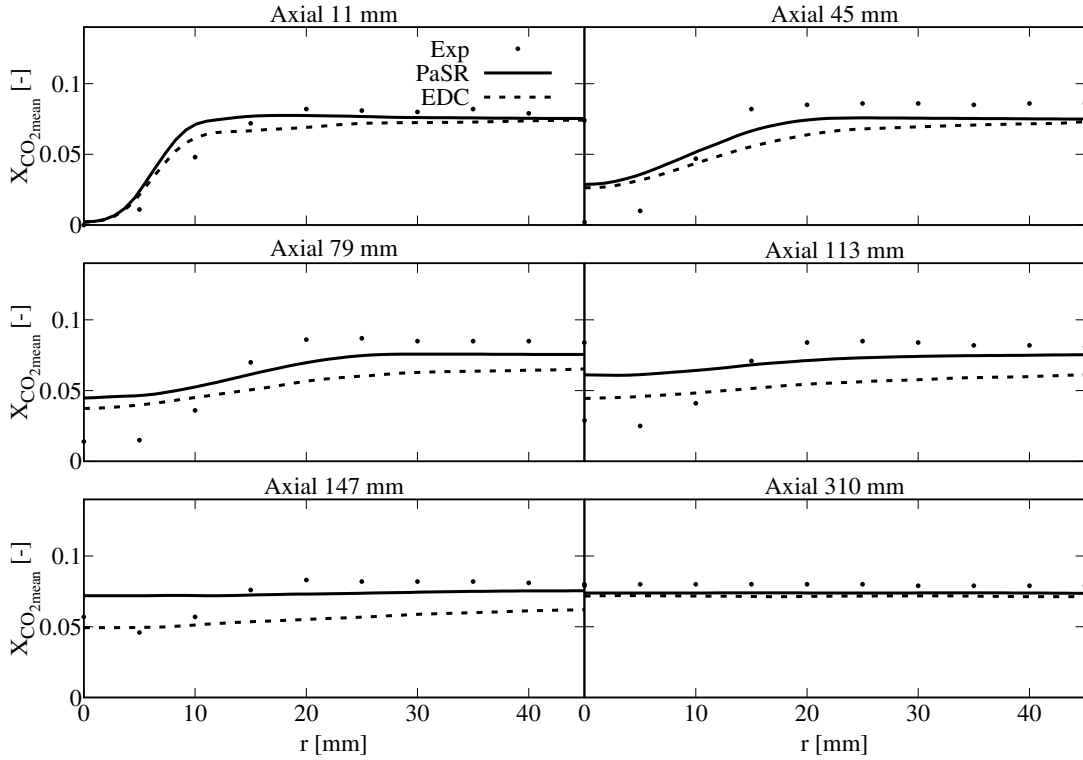


Figure 6: Comparison of computed and measured mean CO₂ mole fraction for six axial locations.

1 **6. Analysis of Reaction Zones**

2 *6.1. Analysis methods*

3 Three methods, CSP, a balance analysis and local PCA, are used to extract
 4 information required to identify ignition- and flame-like regions in MILD com-
 5 bustion. These methods are explained briefly below before presenting the results.

6 *6.1.1. TSR obtained from CSP analysis*

7 The general form of species and energy equations in a homogeneous reactive
 8 system can be expressed with $\partial \mathbf{z} / \partial t = \mathbf{g}(\mathbf{z})$, where $\mathbf{g}(\mathbf{z})$ is the chemical source
 9 vector and \mathbf{z} is N dimensional state vector including N_s , the species mass fractions

1 and temperature: $N = N_s + 1$. The chemical source vector can also be written using
 2 a new set of basis vectors $\mathbf{a}_i(\mathbf{z})$, with $\mathbf{g}(\mathbf{z}) = \sum_{i=1}^N \mathbf{a}_i(\mathbf{z})f^i(\mathbf{z})$, where $f^i(\mathbf{z})$ is the
 3 amplitude of the i -th mode. The term $f^i(\mathbf{z})$ can be further expressed as $f^i(\mathbf{z}) =$
 4 $f^i(\mathbf{g}(\mathbf{z})) := \mathbf{b}^i \cdot \mathbf{g}(\mathbf{z})$ and \mathbf{b}^i denotes the dual basis vector. The bi-orthonormality
 5 condition allows to recover the original representation of $\mathbf{g}(\mathbf{z})$. Based on CSP,
 6 the basis vectors \mathbf{a}_i and covectors \mathbf{b}^i can be approximated to leading order, by the
 7 right and left eigenvectors of the Jacobian \mathbf{J}_g of $\mathbf{g}(\mathbf{z})$, respectively. This set of
 8 basis vectors is traditionally employed in CSP [11] to decouple local time scales
 9 $\tau^i = 1/\lambda_i$, where λ_i are the eigenvalues of Jacobian $\mathbf{J}_g = |\partial \mathbf{g} / \partial \mathbf{z}|$.

10 The tangential stretching rate (TSR) denotes the level of stretching or con-
 11 traction of the dynamics of interest along the direction of a vector field and is
 12 used here to characterize the most *energy-containing* time scales developing in
 13 the chemically reactive system of interest here [23, 24]. This method was used for
 14 turbulent premixed flames [25] and MILD flames [19] in previous studies. The
 15 stretching rate of the reactor dynamics in the direction tangential to the vector
 16 field $\mathbf{g}(\mathbf{z})$ is $\omega_{\bar{\tau}}(\mathbf{g}) := \sum_{i=1}^N W_i(\mathbf{g}) \lambda_i$, with λ_i as the eigenvalue of i -th mode. The
 17 weight, W_i , is

$$W_i(\mathbf{g}) := \frac{h^i(\mathbf{g})}{|\mathbf{g}|} \sum_{k=1}^N \frac{h^k(\mathbf{g})}{|\mathbf{g}|} (\mathbf{a}_k \cdot \mathbf{a}_i). \quad (4)$$

18 It follows that $\omega_{\bar{\tau}}$ is essentially a time scale obtained as a weighted average of
 19 all *energy-containing* time scales with the weight depending on the mode ampli-
 20 tude associated with that scale. The magnitude of the TSR represents the recip-
 21 rocal of the most energy containing time scale of the system, while the positive
 22 and negative sign of TSR, $\omega_{\bar{\tau}}$, indicates an explosive (tendency to react) or non-
 23 explosive/dissipative nature of the dynamics respectively.

1 6.1.2. Balance analysis

2 The balance analysis considers $\mathcal{B} = |C - D| - |R|$, where C , D and R are
3 the convective, diffusive and reactive terms in a species or temperature transport
4 equation [12, 13]. This quantity varies spatially and $\mathcal{B} < 0$ signifies reaction
5 dominated (ignition-like) regions, $\mathcal{B} = 0$ represents flame-like region because
6 of convective-diffusive-reactive balance and $\mathcal{B} > 0$ identifies unburnt or burnt
7 (convective-diffusive) regions. This analysis was developed and used in past stud-
8 ies of MILD combustion [12, 13] and it is used here along with TSR analysis to
9 gain further insights.

10 6.1.3. local PCA

11 Principal Component Analysis (PCA) [26] is a statistical technique often used
12 for size reduction. It detects the directions which are most active in a multi-
13 dimensional data set, providing a mathematical formulation to select optimal pa-
14 rameters representing the local thermochemical state.

15 For a data set, \mathbf{X} , consisting of n observations of p variables, the Principal
16 Components (PCs), \mathbf{Z} , are defined by the projection of the original data onto the
17 eigenvectors, \mathbf{A} , of the covariance matrix, \mathbf{S} , $\mathbf{Z} = \mathbf{XA}$. The eigenvalue matrix, \mathbf{L}
18 associated to \mathbf{S} quantifies the relative importance of the PCs. Thus a reduced sub-
19 set of PCs with size q is defined: $\mathbf{Z}_q = \mathbf{XA}_q$. Such approach minimizes the amount
20 of information loss in the dimension reduction. Each PC is a linear combination
21 of the variables, with weights defined by the covariance matrix eigenvectors. The
22 global PCA analysis cannot handle highly non-linear systems, like turbulent re-
23 acting systems. Such realization has prompted the development of a local PCA
24 approach, which employs a partition of the data set into clusters (regions), fol-
25 lowed by the local application of PCA in each cluster [14]. Details about the

1 application of local PCA are presented in [14].

2 6.2. Insights gathered

3 The above tools are used on the data from the PaSR model, since both instan-
4 taneous and time-averaged values of κ in Eq. (1) approach almost 1 in regions of
5 high heat release across the whole domain. The TSR values are obtained using
6 CSPTk software toolkit and the values of \mathcal{B} are normalised using $(\Delta T \rho_r S_L / \delta_{th})$
7 for stoichiometric methane-air flame with reactants conditions used in the experi-
8 ment. Figure 7 shows typical variation of $\psi_{\bar{\tau}} = (|\omega_{\bar{\tau}}| / \omega_{\bar{\tau}}) \log |\omega_{\bar{\tau}}|$ in the mid-plane
9 at an arbitrarily chosen time as a color map. Two more time moments are anal-
10 ysed and results show similar distributions. The snap shots are included in the
11 supplementary material. The regions with high heat release rate, \tilde{Q} , are marked
12 using two contours for $\tilde{Q} = 10^8$ and 10^7 W/m³. The contours of normalised \mathcal{B} are
13 shown for three values to mark flame-like ($\mathcal{B}^+ \sim 0$), ignition-like ($\mathcal{B}^+ < 0$), and
14 convective-diffusive regions. These contours for $x > 0.2$ m are not shown since
15 combustion is almost complete by this axial location, see Fig. 3. Values of $\psi_{\bar{\tau}} > 0$
16 indicate the tendency for the local mixture to react and this occurs before ignition
17 begins. Large positive $\psi_{\bar{\tau}}$ appears close to the shear layer between the air and fuel
18 stream in the near-field. There is no substantial heat release in these region and
19 \mathcal{B}^+ is positive. All of these signify convective-diffusive region which is consistent
20 with expectation based on physical considerations. This region is also seen to be
21 intermittent (see the difference between the top and bottom shear layers) because
22 of the strong shear generated turbulence in these areas.

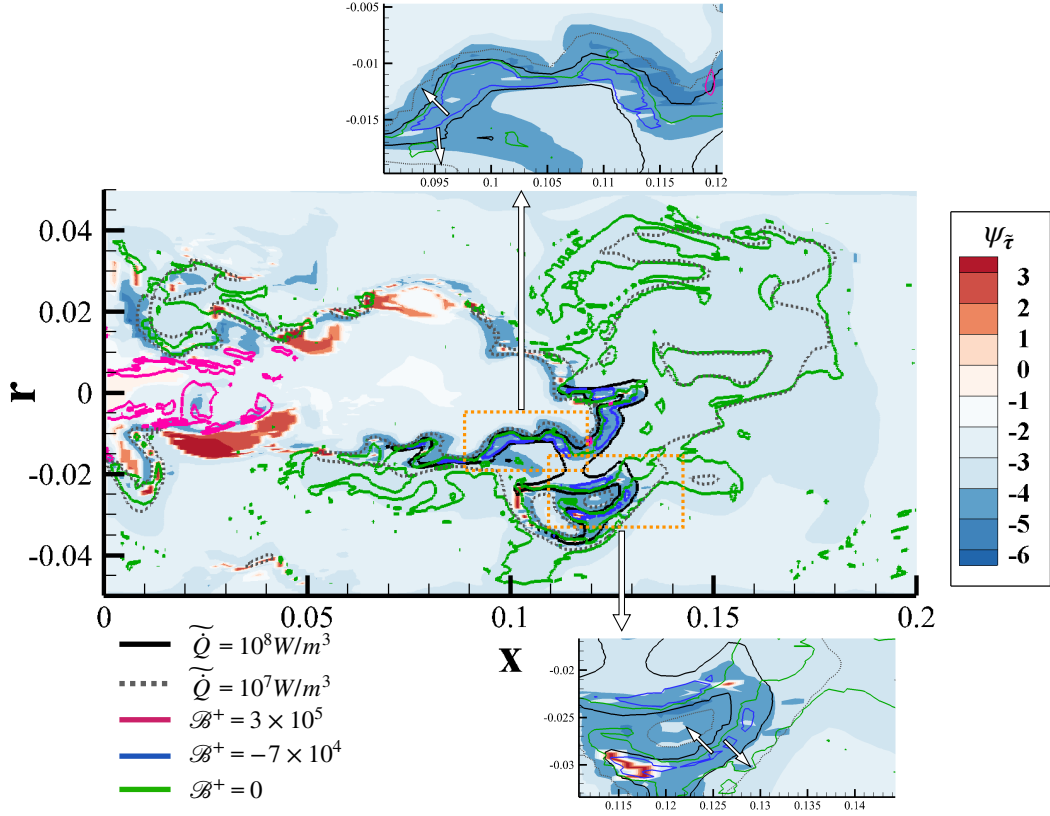


Figure 7: Typical distribution of $\psi_{\bar{\tau}} = (|\omega_{\bar{\tau}}|/\omega_{\bar{\tau}}) \log |\omega_{\bar{\tau}}|$ in the mid-plane is shown along with heat release rate \bar{Q} and \mathcal{B}^+ contours. The unit of the axes is m.

1 After $x = 0.05$ m, larger negative $\psi_{\bar{\tau}}$ values appear. Heat release rate larger
2 than 10^7 W/m³ is observed in the regions where $\psi_{\bar{\tau}}$ changes from positive to nega-
3 tive values (see the location at about $x = 0.05$ m and $r = -0.01$ m). The \bar{Q} increase
4 to 10^8 W/m³ by about $x = 0.1$ m where $\psi_{\bar{\tau}} < 0$ start to appear suggesting that the
5 ignition has occurred and these regions are dominated by reactions. Indeed, the
6 values of \mathcal{B}^+ are negative suggesting that these are reaction dominated regions.
7 To see these phenomena clearly, these regions are magnified in the insets of Fig. 7
8 depicting that negative \mathcal{B}^+ appears in the middle of the \bar{Q} contour of 10^8 W/m³,

1 and it expands in the direction of relatively lower \tilde{Q} (10^7 W/m³), indicated by the
2 white arrows. Hence, it is clear that the MILD combustion shares some conven-
3 tional combustion features while having its own distinctive attributes, as observed
4 in past DNS studies [12, 13], which can be captured using the PaSR model.

5 From Fig. 7, different areas with varied features are identified. In order to
6 better characterize the current flame with region-based post-processing tool, local
7 PCA approach [14] is used here. In total eight clusters are used, each one repre-
8 senting a specific area of the system (see Figure 8). In each cluster, one species
9 contributing the most (showing the highest weight) to the first PC is identified. It
10 is observed that cluster 2 marked with OH is located in the region where $\mathcal{B}^+ =$
11 0 and $\tilde{Q} = 10^7$ W/m³. This area represents the flame region, which is consistent
12 with the identification of a flame marker such as OH as principal variable. The
13 region with positive $\psi_{\bar{\tau}}$ value indicates the explosive region of the flame, where
14 the radical pool (H, O and OH) is initiated, before ignition takes place. Cluster
15 5 in this region is characterised by H (followed by O) as the most contributing
16 species, which is again consistent with what is observed in Fig. 7. H₂O₂ is the
17 leading species in cluster 8. This area overlaps with the region showing high heat
18 release, as well as negative $\psi_{\bar{\tau}}$ and \mathcal{B}^+ value. H₂O₂ is considered as an ignition
19 precursor and it well characterises the identified region.

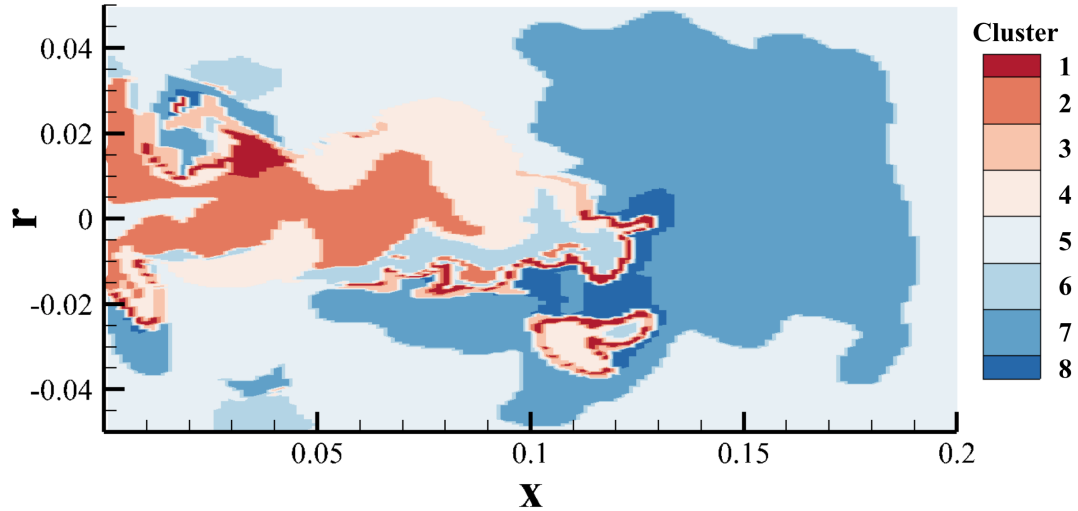


Figure 8: The local PCA map of clusters. The unit of the axes is m.

1 7. Conclusions

2 Turbulent partially premixed combustion under MILD condition inside a cylin-
 3 drical combustor with aerodynamically established recirculation zone is studied
 4 using LES with the PaSR and EDC models for SGS combustion. The computed
 5 temperature and scalar mole fractions are compared to the measurements from [6].
 6 A good overall agreement is observed for the PaSR model and it is comparable
 7 to those observed in past studies using FPV and homogenous reactor-based tabu-
 8 lation combustion models [9, 10]. The averaged temperature and CO₂ mole frac-
 9 tions are generally under-estimated, leading to over-estimation of O₂ mole frac-
 10 tion by the EDC, which could be due to the model parameters (e.g. C_γ) chosen or the
 11 value used for the canonical reactor residence time [27] since they are taken from
 12 past studies. Sensitivities of the EDC results to these parameters are to be explored
 13 in a future study. The LES data from PaSR model is analysed using TSR derived

1 from computational singular perturbation theory and convective-diffusive-reactive
2 balance in T transport equation to identify ignition- and flame-like regions. A
3 good agreement between these analyses are observed. Potential chemical markers
4 (CMs) that can be used in laser diagnostics of MILD combustion are identified
5 using local PCA.

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14 uniroma1.it.

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