A TURBULENT COMBUSTION MODEL BASED ON LARGE SCALE MOTION COUPLED TO PERFECTLY STIRRED REACTOR COMPARED TO A PARTIALLY STIRRED REACTOR

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Abstract. *The effectiveness of the turbulence-chemistry interaction model is of paramount importance in Computational Fluid Dynamics (CFD) codes. In this work, a turbulent combustion model suitable for large eddy simulation (LES) is formulated. The main feature of the model is to include detailed chemistry keeping, however, the computational effort under acceptable level. The proposed model is based on a PSR model, where the residence time is defined upon the eddy characteristic time. This formulation avoids non-physical results on grid cells with the same spatial averaged values of mass fraction, but showing different mixing grade at molecular level. In the proposed model, the eddy characteristic time is derived from the large-scale motion, which is not modelled if one performs a LES calculation. The proposed model is compared to a Partially Stirred Reactor, where the equation of the Probability Density Function is solved by stochastic method. The comparison between PSR and PaSR models shows that the proposed PSR residence time is able to mimic the turbulent mixing. Comparison with experimental data of temperature at an axial position of maximum temperature in a free jet flame shows that the proposed model is able to reproduce the major features of the turbulent mixing, without the prohibitive computational costs associated with the PaSR model.*

Keywords*: Combustion, diffusion flames, methane flames, PSR-Model, PaSR-Model*

1. Introduction

The strong interaction between chemical kinetics and turbulence poses a great challenge to computational fluid dynamics (CFD). In order to be able to accurately predict reacting flows inside furnaces and combustors the computational model needs to properly account for the interaction between chemistry, turbulent mixing and heat exchange. A turbulent combustion model must be physically consistent and must demand feasible CPU time. At the two frontiers of these possibilities are the PSR model and the hybrid LES/transported scalar PDF equation (Raman et al., 2004)(Hinz, 2000). Between these two limits is the presumed PDF model, which is, however, very limited concerning the chemistry model.

In the most used turbulent combustion models the reactions are assumed to be in equilibrium or assumed to react at an infinitely fast rate. Since CFD codes solve for either the time-averaged equation or only a filtered length scale, the subgrid fluctuations in scalar space need to be modeled (Peters, 2000). The simplest approach is to assume complete mixing inside the computational cell. This is equivalent to assume the computational cell as a Perfectly Stirred Reactor (PSR). This model works fine if the reaction time scale is slow compared to the mixing time scale. However, for combustion simulations, which involve fast reactions, this assumption leads to faster reactions and shorter flame lengths. Another class of methods uses a presumed probability density function (PDF) for the scalars to reduce the mixing rate inside the cell. Normally a Beta-PDF is parameterized as function of the mean value and variance of the mixture fraction (Kuo, 1986). The more general method is the stand-alone transported PDF, which solves the transport equation of the joint velocity-composition PDF (Pope, 1985). This leads to a transport equation that accounts for the scalar distribution at all scales in the extended multidimensional velocities-scalars space. The main advantage of these methods is that the reaction terms appear closed.

In a recent work Raman (2004) has investigated a partially premixed methane-air flame using hybrid finite-volume/transported PDF method. It was used the detailed chemistry mechanism GRI2.11 and GRI3.0 (Smith et al.). In the mixing model of the PDF transported equation, the mixing model parameter $C\phi$ was varied from 2.4 to the PSR limit (a very high value of $C\phi$) and the main conclusion, concerning mixing model, is that a subgrid model including finite mixing time is necessary.

Yaga *et. al* (2000) has simulated a gas turbine combustor using Large Eddy Simulation (LES). He has constructed an eddy characteristic time derived from large-scale motion to calculate the combustion reaction rate using an eddy dissipation concept (EDC) model (Magnussen and Hjertager,1976). The methane-air reaction mechanism used by Yaga et. al (2000) is a very simple global mechanism containing three steps. The distributions of temperature, CH4 and CO mole fraction downstream of the centreline of the combustion chamber show a reasonable agreement with experimental data. Turbulent LES combustion has been addressed also by Colucci *et al.* (1998). In this reference, the PDF method is applied in the framework of LES. Results of a mixing layer are compared for the three used models: Direct Numerical Simulation (DNS), LES without subgrid model for the scalar fluctuations and LES-PDF. The presented results indicated that the LES-PDF model gives the better results compared to the DNS simulation. The computational effort of the LES-PDF method remains however as a critical issue.

The present work focuses on the formulation of a suitable reaction subgrid model to LES. In the present work a model is proposed and preliminary tested. The proposed model considers the computational cell as a PSR, being the residence time derived from the eddy characteristic time, which in LES is evaluated from the large-scale flow. At the present work no LES simulation is performed. For comparison, a second model, based on the PaSR model (Chen, 1997), is used. The mixing time of the PaSR model is also defined by the eddy characteristic time. This model mimics the molecular mixing processes very well, but is very expensive if CPU time is concerned.

In the next sections, the two turbulent combustion models are formulated and compared each other and also with experimental data, as far as possible.

2. Mathematical Formulation

In the LES method, the large-scale flow is directly calculated, while the subgrid-scale processes are modeled. The time-step of the simulation is set small enough to capture all the time scale of the turbulence. The conservation equations are filtered so that only spatial mean values are available at the grid cells. Therefore, one needs a model to the spatial averaged reaction rate, due the chemical reactions that take place in the molecular level. The LES turbulent combustion model proposed in this work is based on a Perfectly Stirred Reactor Model (PSR), where the residence time is determined upon the eddy characteristic time. If the residence time of the PSR is defined based on the eddy characteristic time, two mixing limits are recovered: in a flame region where the eddy characteristic time is very high no molecular mixing is achieved and conversely, where the eddy characteristic time is very short, turbulent mixing is so intensive that the mixture has a pattern of a perfectly stirred reactor. This formulation avoids non-physical results on grid cells with the same spatial averaged values of mass fraction, but showing different mixing grade at molecular level. In the proposed model, the eddy characteristic time is derived from the large-scale motion, which is not modeled in LES method. A similar procedure to calculate the eddy characteristic time has been successfully adopted by Yaga *et al*. (2000). The proposed model will be, in future work, implemented into a LES solver.

2.1. PSR- Model

In the framework of the proposed model, the computational cell volume can be viewed as a PSR as follows. Figure 1 illustrates the conceptual representation of the grid cell as a reactor chamber. A steady flow of reactants is introduced through the inlet with a given species composition and temperature. The mass flow rate into the reactor is equal the mass flow rate out of the reactor. As the grid cell behaves as an open system, the pressure must be specified and the conservation equations determine the volume outflow. The transient conservation equations are presented as follows.

The global mass conservation in the reactor volume is stated as:

$$\frac{d}{dt}(\rho V) = \dot{m}_{in}^{*} - \dot{m}_{out}, \tag{1}$$

where ρ is the mass density, V is the reactor volume, $\dot{m}_{in}^{*}$ is the inlet mass flow rate and $\dot{m}_{out}$ is the outlet mass flow rate. As the simulation reaches the steady state, the inlet mass flow rate equals the outlet mass flow rate.

The time-dependent equation for mass conservation of each gas-phase species, including the implicit time dependence of ρ through its dependence on the temperature and molecular weight, is

$$(\rho_k V)\frac{dY_k}{dt} = \dot{m}_{in}^{*}\left(Y_k^{*} - Y_k\right) + (\dot{\omega}_k V)W_k \tag{2}$$

where Y_k is the mass fraction of the *k*th species, W_k is the molecular weight of the *k*th species, and $\dot{\omega}_k$ is the molar rate-of-production of the *k*th species by chemical reaction per unit volume. The superscript * indicates inlet stream quantities.

The energy balance for the PSR is determined by

$$(\rho V)\bar{c}_p \frac{dT}{dt} = \dot{m}_{in}^{*}\sum_{k=1}^{K_g} Y_k^{*}\left(h_k^{*} - h_k\right) - V\left(\sum_{k=1}^{K_g} h_k \dot{\omega}_k W_k\right) + \dot{Q}_{liq} + V\frac{dP}{dt}, \tag{3}$$

where $\bar{c}_p$ is the mixture specific heat, h_k is the standard-state specific enthalpy of the *k*th species and $\dot{Q}_{liq}$ is the net heat transfer rate.

The mixture mass density is related to pressure *P* and temperature *T* of the mixture of ideal gases as:

$$P = \rho R T\ , \tag{4}$$

where *R* is the gas constant.

For steady-state conditions, the nominal residence time τ_{res} in the reactor can be related to the reactor volume and the inlet mass flow rate as follows:

$$\tau_{res} = \frac{(\rho V)}{\dot{m}^{*}_{in}}. \tag{5}$$

In the LES calculation, the nominal residence time (τ_{res}) will be given by the values of density, volume and mass flow rate in a local computational cell. In this way, the residence time is defined with the local fluid velocity.

In the proposed model, the characteristic eddy time is estimated by

$$\tau_{mix} = C_{mix}\frac{k}{\varepsilon}, \tag{6}$$

where C_{mix} is a scale constant of the model, k is the turbulent kinetic energy and ε is the dissipation rate of the turbulent kinetic energy.

The LES turbulent combustion model proposed in this work is based on a Perfectly Stirred Reactor Model (PSR), where the residence time is determined upon the eddy characteristic time. The major motivation for this formulation is to avoid non-physical results on computational cells with the same spatial averaged values of mass fraction, but showing different mixing grade at molecular level. In the proposed model, grid cells with the same averaged values of species but in different flame regions, and consequently with different mixing time, will be handled in a different way. The residence time of the mixture in the computational cell is defined as follows:

$$\tau_{PSR} = \tau_{res} - \tau_{mix}, \tag{7}$$

where Eqs. (5) and (6) are used to calculate τ_{res} and τ_{PSR} respectively. This means that the available time to the reactions take place is given by the difference between the residence time of the gas mixture inside the computational cell and the time delay necessary to the mixing occur. Using this formulation of the residence time, two mixing limits are recovered: in a flame region where the eddy characteristic time is very high no molecular mixing is achieved and conversely, where the eddy characteristic time is very short, turbulent mixing is so intensive that the mixture has a pattern of a perfectly stirred reactor. In order to avoid the physically inconsistent negative value of τ_{PSR}, the eq. (7) is used only for values of $\tau_{mix} < \tau_{res}$. In the simulated cases, this condition was always satisfied. However, one should be aware of this restriction of the proposed model. If this condition is not satisfied, it means that no reaction can take place and accordingly the PSR should be by-passed by the reactive mixture.

2.2. PaSR- Model

For comparison with the PSR model, it was used the Partially Stirred Reactor (PaSR) model. The complete set of equation of the model can be found in (Chen, 1997)(Chou, 2004). A detailed investigation of the PDF transport equation, for a single reacting scalar, recovering the PaSR and PSR limits was carried out by (Sabel'nikov and Figueira da Silva, 2002). They have used semi-analytical and numerical solution of the PDF equation in order to investigate the shape of the PDF depending on the ratios between overall residence time, micro-mixing time and characteristic chemical time.

The main step of the PaSR model is the formulation of a transport equation to the joint composition Probability Density Function (PDF) *f* inside the reactor. In turbulent flows the variables assume a random behavior. Hence, simulation methods need to use a statistical approach to the problem. In such an approach, only statistical moments of certain variables are evaluated, such as mean value and variance. Then, a question remains as to how one goes from statistical moments of a variable to its instantaneous values, which are necessary in the thermochemical model. The answer is to compute a joint PDF of the scalar quantities (species and enthalpy). This PDF couples the thermochemical model and the turbulent reactive flow model. In the PDF-Method, the transport equation for the PDF is formulated, starting from the instantaneous conservation equation for mass, momentum, energy and chemical species. After some manipulation of the basic equations and applying statistical operators, one obtains the transport equation for the PDF *f* inside the reactor (or the computational cell):

$$\begin{aligned}\frac{\partial}{\partial}\rho f\left(\underline{\psi};t\right) &= -\sum_{\alpha=1}^{N_\alpha}\frac{\partial}{\partial\psi_\alpha}\left[f\left(\underline{\psi};t\right)\rho S_\alpha\right] + \frac{1}{\tau_{PaSR}}\left(\rho f^{*}_{in}\left(\underline{\psi};t\right) - \rho f_{out}\left(\underline{\psi};t\right)\right) \\ &- \sum_{\alpha=1,\beta=1}^{N_{tot}}\frac{\partial^2}{\partial\psi_\alpha\partial\psi_\beta}\left[\rho f\left\langle\varepsilon_{\alpha\beta}\middle|\tilde{\phi}=\tilde{\psi}\right\rangle\right]\end{aligned} \tag{8}$$

In Eq. 8 above, the term on the left hand side (LHS) represents the temporal variation of *f* within the control volume. On the right hand side (RHS) of Eq. (8), the first term gives the transport in the scalar quantities space due to the

chemical reaction and, in case of the enthalpy, radiation losses; the second term gives the convective transport of *f* through the reactor. The third term on the RHS describes the transport of the PDF in the scalars space due to the micro-scale mixing, which requires the use of a mixing model. It is important to emphasize that, for a given value of *f* all the terms in the Eq. (8) are either known or can be directly evaluated, except the last term. This term arise from molecular transport fluctuations in the instantaneous conservation equations. In order to evaluate the average conditional mean value of the dissipation rate ε, one has to know the conditional averages of spatial gradients, that are not directly available if the PDF *f* is known in a single point *x* only. Therefore, the conditional averages of spatial gradients have to be modeled. This is the major difficulty associated with PDF methods. In the present work, the Interaction-by-Exchange-with-the-Mean (IEM) is used. The dimensions of the PDF are large, i.e when using detailed chemistry, and finite-difference solutions of the PDF transport equation are impractical. Pope (1985) developed a Monte Carlo algorithm that makes solving the PDF transport equation feasible for general turbulent reactive flows. Rather than considering the PDF *f* explicitly, the dependent variable in the simulation is represented by an *N*-member ensemble:

$$\phi^1, \phi^2, ..., \phi^n, ...\phi^N \ , \tag{9}$$

where ϕ^n represents a "particle", in fact a stochastic event, out of a total of *N* "particles" inside the reactor.

In the framework of a particle-Monte Carlo method, the PDF evolution inside the PaSR can be written as follows. The overall mass balance for the gas mixture inside de PaSR is

$$\frac{d}{dt}\left(\langle\rho\rangle V\right) = \dot{m}_{in} - \dot{m}_{out} \tag{10}$$

where $\langle\rho\rangle$ is the ensemble-average mixture density. The average properties of the PaSR are obtained from the ensemble of particles inside the reactor. Each particle is regarded as an independent PSR and interacts with others only through the molecular mixing process. Therefore, the conservation of energy and species is applied to an individual particle rather than to the reactor. The species equation for a particle is then similar to that of a PSR:

$$\frac{dY_k^n}{dt} = \frac{1}{\tau_{res}}\frac{\dot{m}_{in}}{\dot{m}_{out}}\left(Y_k - \langle Y_k \rangle\right) + \left(\dot{\omega}_k^n\right)W_k / \rho^n \tag{11}$$

The first term on the RHS of Eq. (11) represents the net effect of through-flow (convection) and molecular mixing of the single particle inside the reactor, the last term stands for the chemical reaction. In the IEM mixing model, the unmixedness or the segregation variable is given as:

$$unmixedness = \frac{1}{1 + \frac{1}{3}\frac{\tau_{res}}{\tau_{mix}}}. \tag{12}$$

The unmixedness determines the statistics over a time-step in the stochastic simulation. As one can see, the eddy characteristic time, which determines the mixing process inside the reactor (Eq. 6), and the residence time are the parameter of the PaSR model. If the mixing time is too long, the unmixedness approaches one, what means that no mixture has occurred inside the reactor. Conversely, if the mixing time is fast enough, the unmixedness approaches zero, indicating that complete mixing was achieved.

The simplicity of using a Monte Carlo method and a scalar PDF permits one to carry out simulations with detailed chemistry without significant computing costs. In the present work the methane combustion is described by the GRI3.0 mechanism, which encompasses 253 reactions and 53 reactive species. Both models PSR and PaSR use the GRI3.0 mechanism.

3. Simulation conditions

In order to evaluate the proposed model, experimental data of a turbulent diffusion flame was used. The TNF F flame (TNF, 2004) is a piloted methane-air jet diffusion flame. The fuel consisting of 25 % methane and 75% air forms the inner fuel jet with a diameter of *D=7.2 mm*. The flame is stabilized using a pilot with a diameter of *Dp=18.2mm*. The pilot has a composition corresponding to that of a burnt fuel mixture. The central jet has a bulk velocity (*Uo*) of 99 m/s and the coflow velocity is 0.9 m/s. Experimental data of temperature were taken at the plane *x/D=45*, where the centerline temperature shows a maximum. As in the present work the velocities fields were not simulated, no comparison is made in radial direction of the flame. The PSR network used in the simulation is built with three reactors

located at the positions shown in the Tab. 1. Simulations were also carried out using solo PSR and PaSR volumes defined from the jet inlet up to the position *x/D=45*. A sketch of flow configuration of the flame F is shown on Fig. 1.

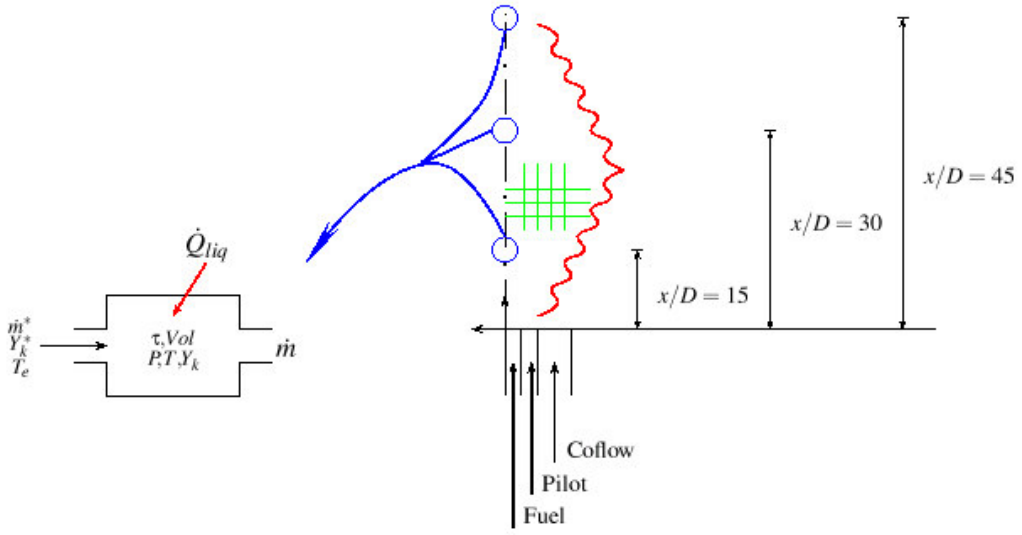

Figure 1 Sketch of flow configuration of the flame F and PSR Model

Table 1 Position of the PSR and PaSR reactors used to simulate the flame F

	Reactor 1	Reactor 2	Reactor 3
PSR-Network	0 ≤ x/D ≤ 15	15 ≤ x/D ≤ 30	30 ≤ x/D ≤ 45
PSR-Solo	0 ≤ x/D ≤ 45	-	-
PaSR- Solo	0 ≤ x/D ≤ 45	-	-

The Fig. 2 shows the axial velocity values taken from experimental data TNF (2004) and from previous simulation using PDF/Finite Volume method (Hinz, 2000). Figure 3 shows the ratio k/ε taken from (Hinz, 2000) and which is used here to estimate the eddy characteristic time (Eq.(6)). From these figures one can estimate both the residence time and characteristic eddy time for the PSR network and for the PaSR model.

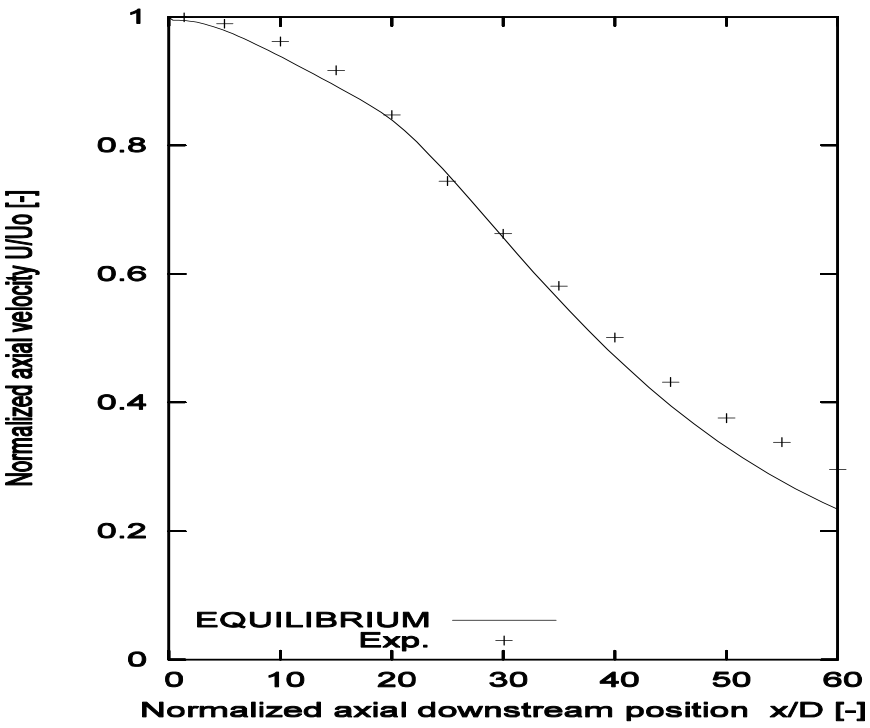

Figure 2 Centreline axial velocity of the flame F. Experimental data from TNF (2004) and simulation from (Hinz, 2000).

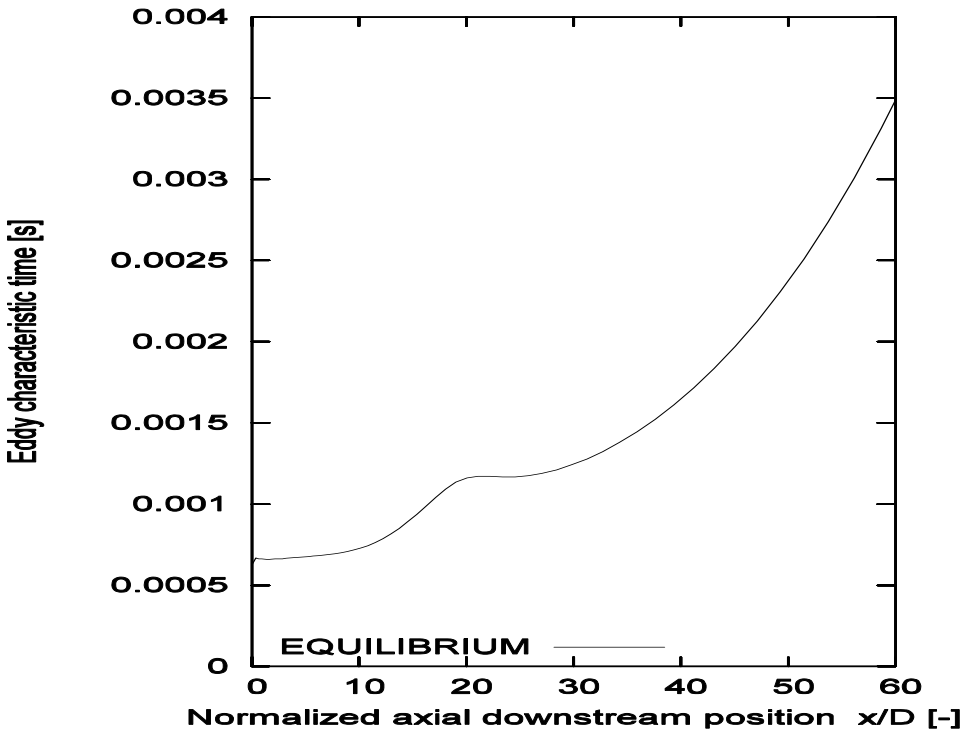

Figure 3 Centreline values of the ratio k/ε taken from (Hinz, 2000) for the flame F.

The mass flow rate into the reactor network was obtained from the experimental set-up of the flame F. The air entrainment was imposed so that an equivalence ratio of 1.0 is achieved at the position x/D=45. The reactors parameters are summarized on Tab 2 and 3 for PSR and PaSR models respectively.

Table 2 – PSR parameters derived from experimental data TNF (2004) and simulations (Hinz, 2000)

Case	C_{mix}	τ_{res} -1	τ_{res} -2	τ_{res} -3	τ_{mix} -1	τ_{mix} -2	τ_{mix} -3	τ_{PSR}	τ_{PSR}	τ_{PSR}
Case 1-PSR	1.0	0.005	-	-	0.0	-	-	0.005	-	-
Case 2-PSR	1.0	0.005	-	-	0.002	-	-	0.003	-	-
Case 3-PSR	1.0	0.005	-	-	0.0013	-	-	0.0037	-	-
Case 4-PSR	0.0	0.0011	0.0013	0.002	0	0	0	0.0011	0.0013	0.002
Case 5-PSR	1.0	0.0011	0.0013	0.002	0.00006	0.00125	0.0016	0.0005	0.0005	0.0004

Table 3 – PaSR parameters derived from experimental data TNF (2004) and simulations (Hinz, 2000)

Case	C_{mix}	τ_{res}	τ_{mix}
Case 6-PaSR	3.0	0.005	0.0039

4. Results and Discussion

Starting from the experimental/simulation data presented at the previous section, the simulations using the PSR and PaSR were carried out. The values of the temperature at the position x/D=45, which corresponds to the higher temperature level at the centreline is compared to the experimental data. The results are presented at the figure 4. Prior to discussing the results, it is important to emphasize that neither the PSR-Network nor the solo PSR and PaSR volumes were designed to exactly fit the experimental data of the investigated flame. Both models PSR and PaSR do not account for the heat and mass transport in the radial direction. Furthermore, the models do not take into account the diffusive transfer process between the reactor and the surrounding flow. One could build a complex PSR-Network in order to better reproduce the fluid movement. Such PSR-Network has been widely used in the literature (Chen, 1997)(Chou, 2004)(Bhargava *et al*., 2002). Using this approach, one gets a network with a large number of parameters used to fit the experimental/numerical data. This is, however, not the issue of the present work. The main goal of the present work is the formulation and evaluation of the applicability of PSR models in the framework of LES codes. Therefore no effort is done to fit exactly the experimental dada. The proposed PSR model will be include, in next work, in a LES code, where the flow movement will be calculated. On the other hand, using a simple PSR-network one can already test the influence of the residence and mixing time. Therefore both models are compared, as far as possible, to the experimental data of the flame F.

The results of the temperature at the position x/D=45 for the six studied cases are show in figure 4. The solid line represents the experimental data. The first three cases are the simulation with a solo PSR volume, which extends from the fuel/air jet exit up to the position x/D=45. The influence of the mixing time is noted, but very small. Case 4 and 5 were obtained for the PSR-Network with values of C_{mix} = 0.0 and 1.0 respectively. In both cases, the temperature at the two first reactors remains unchanged. It means, that no significant reaction takes place inside these two reactors. This result is not confirmed by the experimental value of temperature at the positions x/D=15 and x/D=30. One has to keep in mind, however, that the PSR network does not take into account the mass and heat transfer in radial direction. Once reactions take place at the radial position of stoichiometric mixture, some combustion products and heat are conveyed to the centreline of the jet. This radial transport causes the elevation of the temperature and radical concentrations. These transport processes are not considered neither by the PSR nor PaSR models.

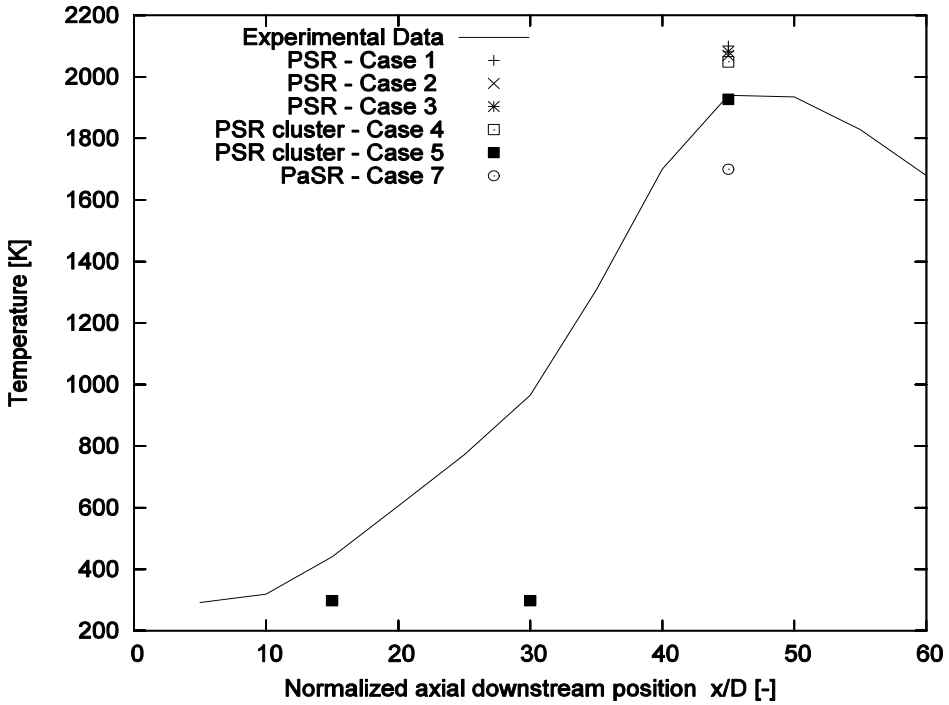

Figure 4 – Axial experimental (solid line) mean temperature and simulation for PSR and PaSR (symbols).

At the position *x/D=45* the result of the PSR-network using variable mixing time (Case 6) gives the same value as the experimental data (*T≈ 1927K*). This means that the eddy characteristic time can be used as a time parameter for the PSR model, better than using the residence time of the flow inside the reactor volume. The mean temperature at the position *x/D=45* obtained with the PaSR model is 1700 K with rms of 500 K. The influence of the mixing time is clear, however the unmixedness in the centreline of the flame was overestimated. If one compares solely the simulations, it is easy to see that the PSR-Network, parameterised by the eddy characteristic time, is able to mimic the unmixedness inside the computational cell, like the PaSR intrinsically does. The computational costs of the models are, however, quite different. While the PSR-Network takes a few seconds, the PaSR needs from 1 up to 2 hours for a single simulation. Such computational costs are prohibitive in the framework of LES, where the flow simulation alone, due to the turbulence time scale, demands a large amount of CPU time.

5. Conclusion

The main goal of the present work is the formulation and evaluation of a turbulent combustion model to be used in LES codes. A network of PSR volumes was proposed, where the residence time inside each reactor is defined upon the eddy characteristic time. For comparison with the PSR-network, a PaSR model is also used. The effect of the eddy characteristic time is compared between the two reactors models. From the results shown, one can conclude that the PSR-residence time, as proposed, can efficiently mimic the turbulent mixing. Although neither the PSR-Network not the PaSR take into account the heat and mass transfer in radial direction, a comparison is done with experimental data of a methane turbulent diffusion flame. The temperature of the different cases are compared at the plane *x/D=45*, where the experimental temperature has a maximum. If one uses a unique PSR volume or even a PSR-Network without considering the eddy characteristic time, the calculated temperatures are higher than the experimental data. On the other hand, using the PSR-residence time, as proposed, a very good agreement is achieved. The comparison between PSR-Network and PaSR shows that, due the prohibitive computational costs, the PSR model should be used LES codes. Alone from the shown results it is not possible to conclude, however, that the model is able to correctly capture all the subgrid effects that appear in LES for turbulent reactive flows.

6. Acknowledgements

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