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Framework of Coherent Structure Method (CSM) for LES Simulation of Isothermal and Reacting Swirling Flows

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In this work the Coherent Structure Method (CSM) is used for the simulation of the sub-grid scale (SGS) stress tensor for large eddy simulation of isothermal and reacting turbulent flows. The CSM framework modifies the Smagorinsky coefficient C_s as a function of local flow conditions. It reduces its value where a large coherence of the velocity flow field is detected. In this way the modelled dissipation is reduced and RMS values of velocity, temperature and main species' fluctuations is better reproduced when compared to standard Smagorinsky framework, where C_s is kept constant on a predefined value.
Validation is performed by comparing simulation results with available experimental results of an unconfined swirling premixed natural gas/air flame performed by Schneider et al. in 2005. The simulated flame is the 30 kW lean-premixed PSF-30 flame and according to the authors, this flame contains important characteristics of the industrial flames.

1. Introduction

Turbulent premixed combustion is one of the main divisions in the field of combustion, both on the laboratory and the industrial scale. During the last decade, computational fluid dynamics (CFD) has become a mainstream tool for solving problems related to fluid motion, from atmospheric boundary layers (Blocken et al., 2007) to application in cement industry (Mikulčić et al., 2012). Considering the level of detail in description of turbulence in computational fluid dynamics (CFD), three main approaches can be distinguished: direct numerical simulation (DNS), large eddy simulation (LES) and Reynolds-averaged Navier-Stokes (RANS) approach. Real meshes, especially those describing the real industrial geometries, are still not feasible for solving in DNS framework due to large number of computational cells and RANS framework exhibits strong dependencies on large number of modelling closures. Therefore, LES framework stands as good choice for simulation of real-world applications, if the size of the domain is too big for DNS and level of detail in the solution is higher than what RANS can provide. In LES, part of the solution comes from directly resolved scales of turbulence (larger eddies) and part from sub-grid scale (SGS) modelling.
Numerous LES simulation results of premixed flames have been published so far, with various combinations of SGS turbulence and combustion model closures. Lean methane premixed turbulent flames were simulated with linear eddy mixing (LEM) model (Sankaran and Menon, 2005), strongly swirled unconfined flames (Freitag and Janicka, 2007) and methane-air swirling flames (Schneider et al., 2005) have also been presented. The successful attempt for applying LES in internal combustion engines is presented (Richard et al., 2007). Furthermore, extension is made in describing the unsteady phenomena which couldn't be captured with RANS, like cyclic variability around phase averaged mean (Vermorel et al., 2009) or knock and pre-ignition phenomena (Lecocq et al., 2011). Transient flame-vortex interactions in LES have been investigated (Di Sarli and Di Benedetto, 2013), as well as relative influence of SGS combustion sub-model (Di Sarli et al., 2012).
This work investigates applicability of Coherent structure method (CSM) as the SGS framework for turbulent transport in turbulent premixed combustion. It is inherently included in all equations of the

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mathematical model. Methodology is validated on a swirling laboratory flame, the TECFLAM combustor (Schneider et al., 2005).

2. Methodology

The mathematical model consists of conservation equations for mass, linear momentum, energy and scalars, as well as constitutional relations, all adopted to the LES framework. Filtering of the equations is done implicitly, meaning that the computational mesh is actually a filter. Conservation equations for mass and linear momentum are commonly known and therefore not presented in this work. Turbulent viscosity appearing in momentum equation represents diffusion from all scales in SGS levels and can be calculated as $\tilde{\mu}_t = \mu_{SGS} = \bar{\rho}(C_S \Delta_x)^2 \left|\tilde{S}\right|$. Common values of C_s are 0.2 for a homogeneous and isotropic turbulence and around 0.1 for a flow in a pipe. As an alternative, Smagorinsky parameter can be defined locally in the domain by using various SGS functions. In this work Coherent Structure Method (CSM) is used. Conservation of energy is presented in Eq(1)

$$\frac{\partial\left(\bar{\rho}\tilde{h}\right)}{\partial t} + \frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{u}_j \tilde{h}\right) = +\frac{\partial \bar{p}}{\partial t} + \frac{\partial}{\partial x_j}\tilde{u}_i \tau_{ji} + \frac{\partial}{\partial x_j}\left(\left(\lambda + \tilde{\lambda}_t\right)\frac{\partial \tilde{h}}{\partial x_j}\right) + \bar{\rho}\dot{q} \tag{1}$$

Thermal turbulent diffusion is obtained from turbulent viscosity $\tilde{\lambda}_t = \tilde{\mu}_t / \left(\bar{\rho}\,\mathrm{Pr}\right)$. Source term for enthalpy should be obtained by combustion and species transport model.

2.1 Transport of species

Transport of species is strongly coupled with combustion modelling. Species appearing in thermochemical reactions are transported by scalar equations for all species from the side of reactants and products. Transport equation for fuel mass fraction of k-th species is presented in Eq(2)

$$\frac{\partial\left(\bar{\rho}\tilde{Y}_k\right)}{\partial t} + \frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{u}_j \tilde{Y}_k\right) = \frac{\partial}{\partial x_j}\left(\left(D + D_t\right)\frac{\partial \tilde{Y}_k}{\partial x_j}\right) + \omega_k \tag{2}$$

Fuel source term is negative during the combustion and is calculated from the combustion model. Transport equation for k-th species can be expressed with following equation. In the focus is the reaction rate for fuel (ω_{fu}), described in the next chapter.

Individual reaction rates can be calculated from the fuel reaction rate and stoichiometric coefficients connecting species *i* with reaction *r*. They are obtained from corresponding chemical kinetic mechanisms, (AVL FIRE, 2013).

$$\omega_i = \sum_{r=1}^{N_{reac}} \upsilon_{i,r}\,\omega_{fu,r} \tag{3}$$

Turbulent diffusion term in scalar equations is modelled with relation $\tilde{D}_t = \tilde{\mu}_t / \left(\bar{\rho} Sc\right)$. In this work we are assuming that $Sc = \mathrm{Pr} = 0.7$. This assumption was already used in jet flows (Lubbers et al., 2001).

2.2 Extended Coherent Flame (ECFM) combustion model

Combustion model is Extended Coherent Flame Model (ECFM). ECFM is a topological class of models that tracks the flame front via property called Flame Surface Density (FSD). In this work only a principal equation (Richard, et al., 2007) for FSD is given in Eq(4)

$$\frac{\partial\left(\tilde{\Sigma}\right)}{\partial t} + \frac{\partial}{\partial x_j}\left(\tilde{u}_j \tilde{\Sigma}\right) = T_{res} + P_{res} + S_{res} + C_{res} + S_{SGS} + C_{SGS} \tag{4}$$

Individual terms on the r.h.s. of Eq(4) are representing resolved and SGS contribution to FSD source. Detailed description of the SGS model terms, as well as diffusion coefficient from the resolved transport and control of the flame thickness can be found in reference literature.

With inputs from species transport and combustion model the source term for fuel (Eq(5)) can now be calculated, Eq(5)

$$\omega_{fu} = \rho_{fr} Y_{fu,fr} S_{L,0} \tilde{\Sigma} \tag{5}$$

Source term for enthalpy can be calculated as $\bar{\rho}\dot{q} = \omega_{fu} H_L$. Terms appearing in Eq(5) are unburned density, unburned fuel mass fraction obtained by Eq(4), laminar flame speed, FSD obtained by ECFM and lower heat value of the fuel. Laminar flame speed should be determined locally from empirical relations or $S_{L,0}$ databases which are usually written in the form $S_{L,0} = f(\phi, p, T, EGR)$. Local equivalence ratio Φ can be calculated from the tracers for unburned fuel $Y_{fu,u}$, oxygen concentration Y_{O2} while and unburned gas temperature can be calculated from the unburned enthalpy h_u.

2.3 Coherent structure method (CSM) as the modelling framework of SGS turbulent transport

In 2005, Kobayashi presented model based on coherent structure function (CSF) with a fixed model parameter (Kobayashi, 2005). The proposed approach was successfully applied to non-reactive (cold) flow cases of homogeneous turbulence and channel flows (Kobayashi, 2005), backward facing step and asymmetric plane diffuser (Kobayashi et al., 2008) as well as supercritical flow over the cylinder (Perković et al., 2012). SGS model based on CSF is called Coherent Structure Model (CSM). CSM model is implemented in such way that Smagorinsky closure parameter is now locally adopted according to the local coherence in the velocity field, instead of having constant value. It's formulation is given in Eq(6).

$$C_S \Rightarrow C_{CSM} = C_2 |F_{CS}|^{3/2} F_\Omega \tag{6}$$

In former equation F_Ω represents the energy decay suppression function, $F_\Omega = (1 - F_{CS})$. Coherent structure function is defined as a second invariant of the velocity field (Q) normalized by the magnitude of the velocity gradient tensor (E), i.e. $F_{CS} = Q/E$. Model is closed with constant C_2=1/22, obtained from DNS results of homogeneous isotropic turbulence (Kobayashi, 2006).

3. Simulation setup

The swirler, which is positioned upstream from the combustion chamber, is included into the computational domain to correctly describe mean and turbulent flow of fresh mixture into the domain. Outlet is defined as non-reflecting outflow boundary condition, described in detail in (Lodato et al., 2008). Mesh is well structured, hexahedron-dominated and refined in the flame region, having typical cell size of 2 mm. Further downstream, where flue gases stream towards the exit, the typical cell size is increased to approx. 10 mm. Simulations were performed in CFD application AVL FIRE, v2013.2. From the numerical point of view, second-order upwind MINMOD scheme was used due to good convergence properties and second-order accuracy on refined grids (AVL FIRE, 2013). Integration in time is performed implicitly with time step of 50 µs.

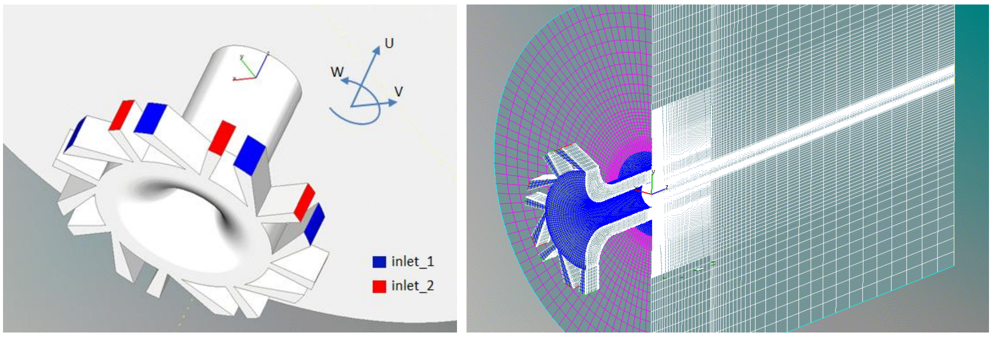

Figure 1: Computational mesh (half of the domain) and detailed view of swirler-chamber connection

4. Results and discussion

Simulation results are validated against experimental data for flame PSF-30. Mean and RMS values of axial and tangential velocity field, as well as temperature field are validated for two axial positions and three approaches for Smagorinsky constant C_s, namely C_s=0.1, C_s=0.2 and C_s=f(CSM). Qualitative analysis, presented in Figure 2, shows that instantaneous flame front is wrinkled and flow field on the entrance to the domain is swirled.

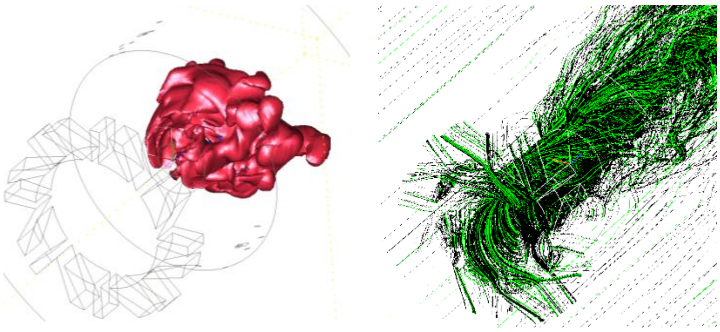

Figure 2: Flame PSF-30 instantaneous iso-surface of reaction rate (RR=0.5 W) and streamlines showing swirl velocity field

Simulations of isothermal flow are used for validation of mean and RMS values of three components of velocity (axial, radial and azimuthal) w.r.t. the values measured in the experiment under isothermal conditions. The importance of this simulation test is to see if the current mesh quality and simulation setup can reproduce velocity field inside the combustion region and if yes, under which ratio of mass flows for '*inlet_1*' and '*inlet_2*', see Figure 1. Results of isothermal flow in Figure 3 show that ratio of 47/53 should be used.

Validation results in Figure 4 show that all three approaches for C_s are in a good agreement with experimental data for both the mean and RMS values of velocities and temperature. Moreover, good agreement with the experiment for axial position of 1 mm indicates that boundary conditions are well resolved. Slightly better performance is seen for the C_s=f(CSM) over other two approaches if RMS values are compared. Reason for that lies in the fact that CSM tends to reduce C_s close to zero in regions with high coherence in the local flow field, which is the case in the centres of the vortices. This reduces SGS model dissipation and fluctuations can be more pronounced.

Negative correlation between C_s and vorticity (as a measure of the local flow coherence) can be seen in Figure 5 for both flames. This means that C_s drops in regions where vorticity is significant.

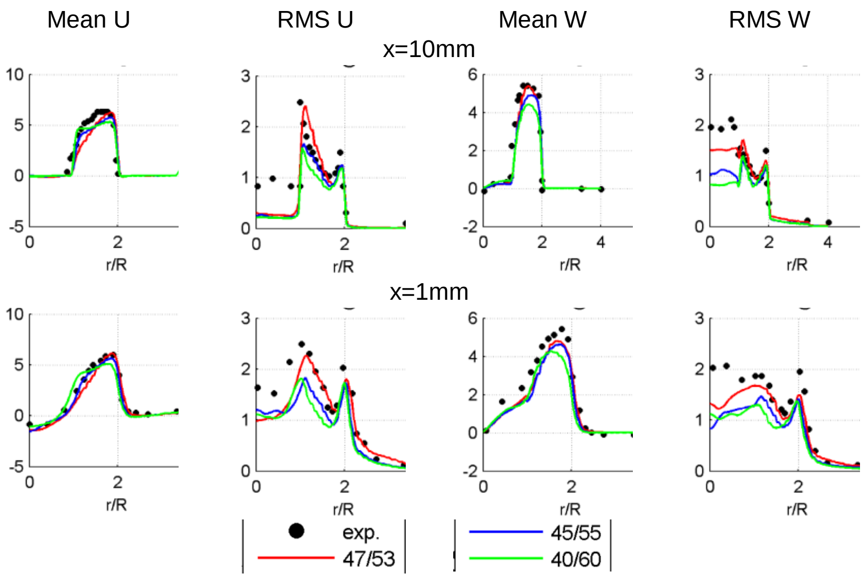

Figure 3: Flame PSF-30 isothermal – comparison between three ratios of 'inlet 1' over 'inlet 2' mass flows for the case Cs=f(CSM) for radial distribution of velocity components (1 mm and 10 mm from the swirler inlet to the combustion chamber)

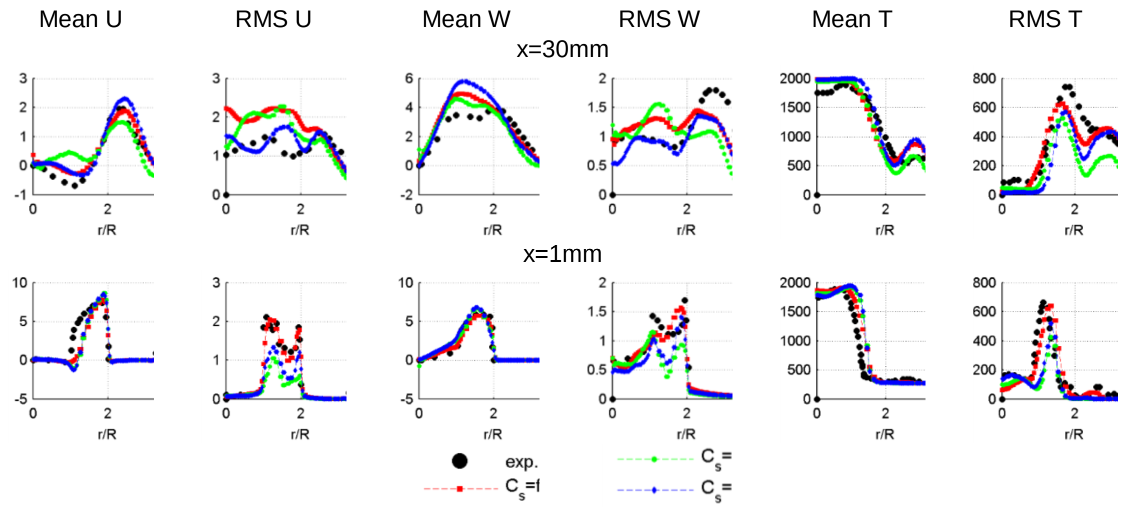

Figure 4: Flame PSF-30 reactive – comparison between three SGS approaches for radial distribution of velocity components and temperature for two axial positions (1 mm and 30 mm from the swirler inlet to the combustion chamber)

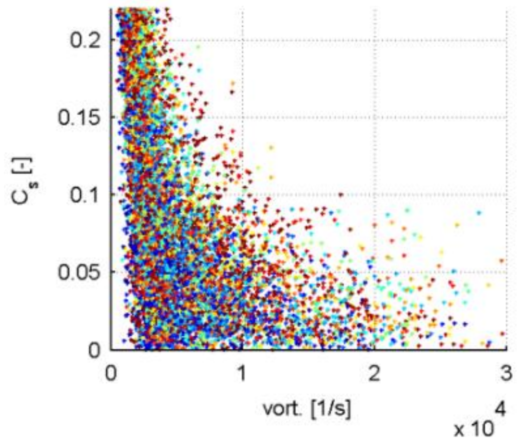

Figure 5: Flame PSF-30 – Scatter plot of Cs vs. vorticity for the approach Cs=f(CSM), coloured by the reaction progress variable

5. Conclusions

A laboratory swirling flame PSF-30 has been simulated in this work by using and comparing three Large eddy simulation turbulent transport frameworks: constant Smagorinsky C_S=0.1 and C_S=0.2, as well as dynamically changed Smagorinsky depending on the local coherence in the flow field, the C_S=f(CSM). The CSM approach outperformed the other two approaches when RMS values are compared. Since CSM is cheap and simple to implement, the recommendation is that it should be used in the industrial applications.

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