D3.2 COUPLING SOOT WITH ALL TURBULENT COMBUSTION MODELS
Version 1.0

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Change Log

Version	Author	Description of Change
V0.1	Eduardo J. Pérez, Federica Ferraro, Abhijit Kalbhor	Initial draft
V0.2	Daniel Mira, Christian Hasse, Sadiki Amsini, Jeroen van Oijen	Review
V1.0	Ruud Eggels	Final version

Table of Contents

Executive summary

This document contains the description of the coupling and integration of the soot models with the turbulent combustion models applied in the project according to the following sections:

- Description of the turbulent combustion models.
- Description of the soot models.
- Coupling of the soot models with the turbulent combustion models.

Carrying out such coupling positions the consortium in place to tackle the turbulent flames simulations scheduled in the project.

1. Introduction

ESTiMatE targets to contribute to the prediction of soot in terms of chemical evolution and particle formation in conditions relevant to aero engine operations. In particular, the application of advanced combustion and soot models in the frame of Large Eddy Simulations (LES) is one of the main objectives of the project.

In this deliverable, belonging to WP3, the coupling of the different turbulent combustion models with the soot models applied in the project is described. The models have been implemented in different codes used by the partners, namely, Alya, and OpenFOAM, as detailed in the following. Similar models are implemented in the ITD leader code, PRECISE-UNS.

The turbulent combustion models are:

a) Based on the Flamelet Generated Manifold (FGM) there are two variants differing on the treatment of the Turbulence Chemistry Interaction (TCI):
   - Based on presumed-shape Filtered Probability Density Functions (FPDFs) by using a beta function, implemented in Alya.
   - Eulerian Stochastic Fields (ESF), implemented in OpenFOAM.

b) Conditional Moment Closure (CMC), implemented in Alya.

Regarding the soot models two advanced models are considered:

a) Discrete Sectional Model (DSM), implemented in Alya.
b) Split-based Extended Quadrature Method of Moments (S-EQMOM), implemented in OpenFOAM.

A brief description of the codes is given in the following:

a) Alya: the multi-physics code Alya has been developed at BSC and belongs to the

PRACE Benchmark Suite for HPC applications. Alya is based on the Finite Element Method (FEM), has been highly optimized and tested independently in most of the European supercomputer platforms.

b) OpenFOAM: OpenFOAM is a free, open-source CFD software written in C++ for HPC applications, based on the Finite Volume Method (FVM), that has a large user base across most areas of engineering and science, from both commercial and academic organizations. The present OpenFOAM code is an extended in-house version from TUDa.

The soot and some of the combustion models have been already described in previous deliverables of the project (2.3, 2.4 and 3.1), in which the validation for the models was gathered. Therefore, this document contains a brief description of the models and then, addresses their coupling and their application for turbulent cases.

2. Description of turbulent combustion models

In the following a brief description of the combustion models used in the project is given.

2.1 Based on the FGM

The Flamelet Generated Manifold (van Oijen and de Goey, 2000) is a turbulent combustion model based on the flamelet concept, which describes the turbulent flame as an ensemble of one-dimensional laminar flames called flamelets. In the FGM the set of all possible flamelet states under the variation of some degrees of freedom or controlling variables are stored in a table or manifold as a function of such controlling variables. These variables are transported in the flow and the thermochemical state at each point of the domain is retrieved by reading the value from the manifold for the local n-tuple defined by the controlling variables. When accounting for the TCI two different approaches have been considered in the project as described in the following.

2.1.1 Based on presumed-shape FPDFs

In this approach the turbulent quantities are obtained by averaging the values from the manifold according to some FPDF, whose shape is parametrized as function of the controlling variables. In particular, the beta B and Dirac delta δ functions are used in this work.

The controlling variables used to solve the turbulent flow are the filtered mixture fraction $\widetilde{\xi}$, its variance $\widetilde{\xi''^2}$, the filtered progress variable $\widetilde{Y_c}$ and its variance $\widetilde{Y_c''^2}$ and,

occasionally, the level of enthalpy $\tilde{i}$ (normalized enthalpy) if heat loses are included. The domain defined by these variables is discretized in a regular mesh and, the thermochemical states from the flamelet solutions are integrated for the FPDFs that can be obtained from the combination of all the possible 5-tuples of these variables, being the integrated values stored in a look-up table.
During the LES, the filtered variables that define the thermochemical state at each point of the physical mesh are obtained by reading and interpolating the values from the look-up table for the corresponding values of $(\widetilde{\xi}, \widetilde{\xi''^2}, \widetilde{Y_c}, \widetilde{Y_c''^2}, \tilde{i})$.

2.1.2 Eulerian Stochastic Fields

In the Eulerian Stochastic Fields (ESF) method the transport equation of the Favre-filtered joint scalar probability density function $\widetilde{P}(\phi)$ (FDF) is solved. For this purpose, the FDF is represented as an ensemble of N_s Eulerian stochastic fields for each flamelet table controlling variables ϕ_α. The stochastic fields evolve according to a set of stochastic differential equations following the formulation by Valiño (1998) and Valiño et al. (2016). Here, Eulerian stochastic fields for the mixture fraction and the progress variable are considered.

From the solution of the stochastic fields, it is then possible to obtain the moments of the respective marginal subgrid FDF via ensemble averaging, e.g., for the mean $\widetilde{\phi}_\alpha$ and variance σ_α^2:

$$\tilde{\phi}_\alpha = \frac{1}{N_s}\sum_{n=1}^{N_s}\xi_\alpha^n$$

$${\sigma_\alpha}^2 = \frac{1}{N_s}\sum_{n=1}^{N_s}\left(\xi_\alpha^n - \bar{\phi}_\alpha\right)^2 .$$

2.2 Conditional Moment Closure

The Conditional Moment Closure (Klimenko and Bilger, 1999) is a turbulent combustion model first devised for non-premixed combustion and, then, extended to premixed combustion based on conditioning the reacting scalars to a relevant variable (mixture fraction ξ for non-premixed combustion or progress variable Y_c for premixed combustion) as a way to simplify the complexity of the chemical source term calculation

in the context of a turbulent reacting flows. In the project ESTiMatE the model is restricted to non-premixed combustion.

Because of the conditioning, a new dimension in the mixture fraction direction (η) has to be added solving, therefore, the equations in a 4-dimensional space (x, y, z, η) and time. Denoting the conditioning operation as $\langle \cdot \,|\, \xi = \eta \rangle$, which is abbreviated simply as $\langle \cdot \,|\, \eta \rangle$, and the conditional species mass fractions as $Q_i = \langle Y_i \,|\, \eta \rangle$, the CMC transport equation for each of the species of the mechanism reads

$$\overline{\rho}\widetilde{P}\frac{\partial Q_i}{\partial t} + \overline{\rho}\widetilde{P}\langle \overrightarrow{u} \,|\, \eta \rangle \cdot \nabla Q_i = \nabla \cdot (\overline{\rho}\widetilde{P}(D_\xi + D_{sgs})\nabla Q_i) + \overline{\rho}\widetilde{P}\langle N \,|\, \eta \rangle \frac{\partial^2 Q_i}{\partial \eta^2} + \overline{\rho}\widetilde{P}\langle \dot{\omega}_i \,|\, \eta \rangle \qquad i = 1, \ldots, N_{spec}$$

where $\overline{\rho}$ is the density, $\widetilde{P}$ is the filtered probability density function (FPDF), $\langle \overrightarrow{v} \,|\, \eta \rangle$ is the conditional velocity, D and D_{sgs} are the laminar and subgrid mass diffusion coefficients, $\langle N \,|\, \eta \rangle$ is the conditional scalar dissipation rate, $\langle \dot{\omega}_i \,|\, \eta \rangle$ is the conditional chemical source term and N_{spec} is the number of chemical species. For all the variables Favre filtering is used except for the density.

For the terms that require modelling the following well-known models are used

- $\langle N \,|\, \eta \rangle$ according to the Amplitude Mapping Closure.
- $\langle \overrightarrow{v} \,|\, \eta \rangle = \langle \overrightarrow{v} \rangle$
- $\widetilde{P}$ according to a B (beta) function.
- $\langle \dot{\omega}_i \,|\, \eta \rangle$ assuming a first order closure.

The unconditional variables are computed by averaging conditional quantities according to the FPDF at each physical point in the domain. Such FPDF is parametrized according to the filtered mixture fraction and its variance, whose transport equations are solved in the flow, following a beta function.

Following the methods found in the literature and due to the heavy cost involved in solving CMC, two different meshes that represent the same physical domain are typically used: a fine mesh that provides good quality for the LES in terms of the scales solved in the flow for the equations of continuity, momentum, mixture fraction and mixture fraction variance (this block is referred to as CFD), and a coarse mesh where CMC transport equations for species and enthalpy are solved (this block is referred to as CMC). This procedure is not only based on practical reasons but on the fact that the gradients for the conditional variables are much smaller for most of the regions compared to the unconditional variables.

A scheme of the steps followed in solving the LES with CMC is given in Figure 1.

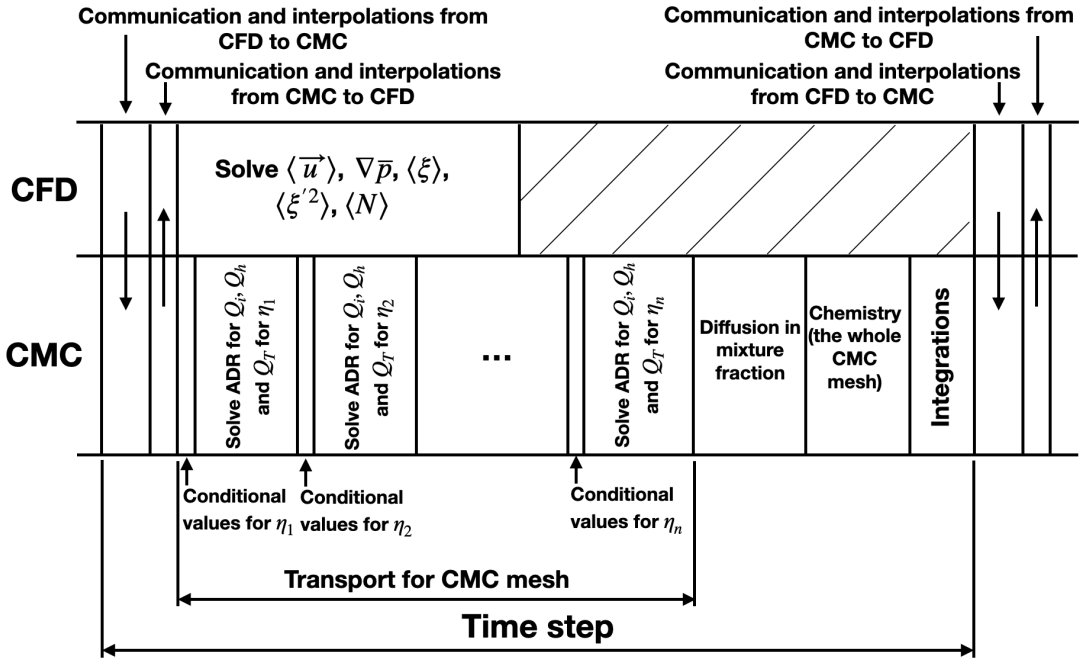

Figure 1: actions to solve one time step in CMC combustion model. Stripped regions represent idle times.

3. Description of the soot models

In the following, a brief description of the soot models used in the project is given.

3.1 Discrete Sectional Model

In the Discrete Sectional Model (Gelbard et al., 1980; Blacha et al., 2012), the population of soot particles at each point of the domain is partitioned into a set of bins according to their size (sections). The soot mass fraction $Y_{s,i}$ for the soot amount with volume ranging between a minimum and maximum values (and related to a specific section) is transported in the flow for all the sections.
The transport equation for each of the sections reads:

$$\frac{(\rho Y_{s,i})}{\partial t} + \nabla \cdot (\rho \overrightarrow{u} Y_{s,i}) = \nabla \cdot (\rho D_{s,i} \nabla Y_{s,i}) - \nabla (\rho \overrightarrow{u}_T Y_{s,i}) + \rho_s \dot{Q}_{s,i} \qquad i = 1,\ldots,N_{sec} \qquad (1)$$

where ρ and ρ_s are the gas and soot densities, respectively, $\overrightarrow{u}$ and $\overrightarrow{u}_T$ are the gas and thermophoretic velocities, respectively, $D_{s,i}$ is the soot diffusion coefficient for section i and $\dot{Q}_{s,i}$ is the source term for soot. A total of N_{sec} transport equations have to be

solved.
The source term for soot includes all the processes in the formation and consumption from all the physical and chemical growth processes associated with soot particles, namely, nucleation, condensation, coagulation, surface growth and oxidation.
Nucleation of nascent soot particles is modelled through the dimerization of two gas-phase PAH species (pyrene molecules (A4) here). The source term for nucleation is calculated only for the first section from the collision rate of two pyrene molecules in the free-molecular regime with unity collision efficiency. Subsequent to nucleation, the incipient soot particles grow in size due to PAH condensation, surface reactions, and particle-particle coagulation. The growth of soot particles by PAH-condensation is modeled by considering Brownian collisions between soot particles and PAH in all the sections. All the collisions are assumed to lead to successful condensation.
The source term for the condensation process is obtained following the Smoluchowski equation described in (Roy, 2014). The coagulation of soot particles is described through Brownian collisions leading to pure coalescence, while particle aggregation is not included. The coagulation source term is calculated for each section based on the model proposed by (Kumar and D. Ramkrishna, 1996). To simplify the computations of collision coefficients in the PAH condensation and coagulation models, a representative mean size is assumed for particles in each section, instead of their size distribution.
Soot surface growth and oxidation processes are described through the standard hydrogen-abstraction-C2H2-addition (HACA) mechanism (Frenklach and H. Wang, 1991). Oxidation of soot through OH and O2 is included in the model.
Finally, the consumption of gaseous species due to soot formation sub-processes is accounted for in the species conservation equations through two-way coupling. In addition to species source terms, the interaction between the soot chemistry and the gas-phase chemistry was accounted for in conservation equations for the total mass and enthalpy.

3.2 Split-based EQMOM

The split-based EQMOM (S-EQMOM) method, recently developed by Salenbauch et al. (2019), is a Quadrature-based Moment Method, which solves only the low-order moments of the soot particle number density function (NDF). Specifically, the S-EQMOM proposes an alternative formulation of the EQMOM approach from Yuan et al. (2012), in which the NDF is approximated by a weighted sum of kernel density functions of a known shape, e.g., gamma or lognormal distributions. In the S-EQMOM the moments of sub-NDFs are considered instead of the moment of the entire NDF. The main advantage of the S-EQMOM over the EQMOM is that the inversion procedure yields a system of equations that is solved analytically and has a unique solution

(Salenbauch et al., 2019), while, in the EQMOM, an iterative and non-unique procedure (Nguyen et al., 2016; Pigou et al., 2018; Yuan et al., 2012) is applied to invert the moments, from low and high order moments of the entire NDF. Therefore, the S-EQMOM formulation greatly improves the stability of the inversion algorithm, allowing a computationally efficient and robust local reconstruction of the soot particle NDF. In the model the soot particles are considered spherical, therefore the vector of the internal coordinates ξ is defined as ξ=[V], leading to a univariate model formulation.

In S-EQMOM the moment inversion procedure consists in analytically calculating the value of the nodes V_{s_α}, the weights w_{s_α}, and the scale parameters σ_{s_α} directly from the first three moments $[m_0^{s_\alpha}, m_1^{s_\alpha}, m_2^{s_\alpha}]^T$ of the N_{sub} sub-NDFs. Note that this corresponds to the inversion of series of one-node EQMOM system using the solution algorithm proposed by Yuan et al (2012).

A generic sub-NDF moment is defined as

$$m_k^{s_\alpha} = \int_{V_{min}}^{\infty} V^k \, n_{s_\alpha}(V) \, dV$$

where s_α is the index of the sub-NDF.

The entire NDF may be then approximated as

$$n(\tilde{V}) = \sum_{\alpha=1}^{N_{sub}} n_{s_\alpha}(\tilde{V}) \approx \sum_{\alpha=1}^{N_{sub}} w_{s_\alpha} \delta_{\sigma_{s_\alpha}} \left(\tilde{V}; \tilde{V}_{s_\alpha}\right)$$

The transport equation for the k-*th* moment of the sub-NDF reads:

$$\frac{\partial m_k^{s_i}}{\partial t} + \nabla \cdot (\vec{u} m_k^{s_i}) = - \nabla \cdot (\vec{u}_T) + \dot{m}_k^{s_i} \qquad k = 1, 2, 3$$

The source term of the moment equation $\dot{m}_k^{s_i}$ includes particle nucleation from two PAH molecules, surface growth by condensation of PAH molecules on soot particles and HACA mechanism, coagulation and particle oxidation by reactions with O2 and OH.

The S-EQMOM model is implemented in a C++ library that can be coupled to any CFD solver through a proper interface. In ESTiMatE interfaces to OpenFOAM and PRECISE -UNS have been developed and validated (see D2.3 and D3.1 for more details).

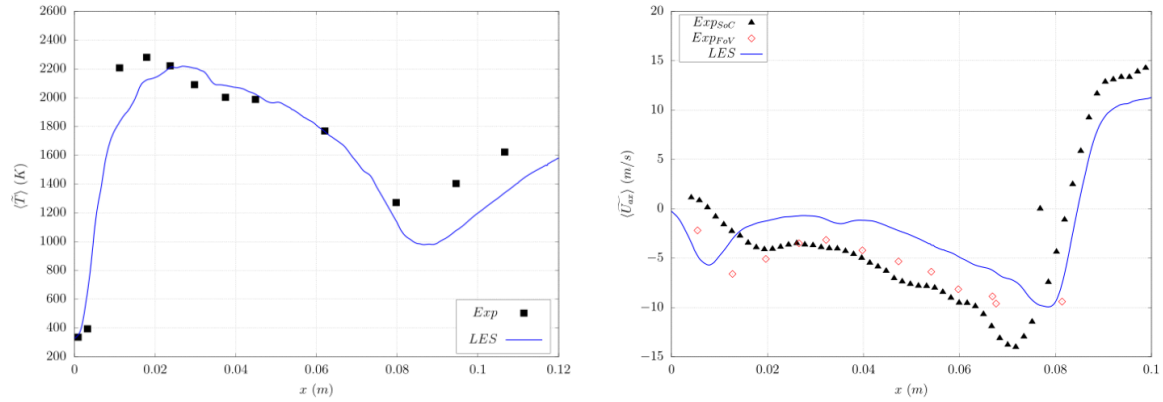

Figure 2: Time-averaged temperature and velocity along the centerline of the DLR combustor. Experimental data are from (Geigle et al. Proc. Combust. Inst., Vol. 36, 2017, pp. 3917–3924).

Results with the S-EQMOM soot model

To evaluate the performance of the S-EQMOM at aero-engine conditions, two test cases are currently investigated:

1. The DLR swirl combustor at elevated pressure with secondary air injection (Geigle et al., 2015) is calculated in OpenFOAM.
2. The BR700 is calculated in PRECISE-UNS.

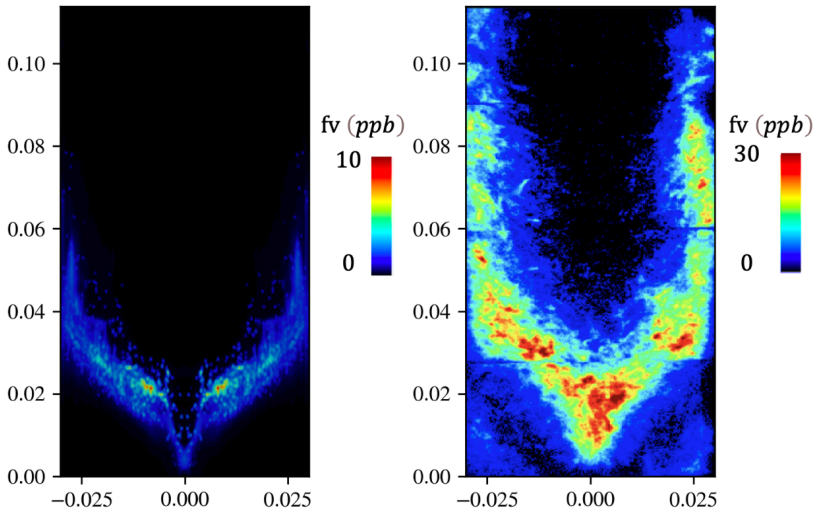

Figure 3. Soot volume fraction from experiments (left) and LES (right) for the DLR combustor.

The DLR combustor is also a benchmark case of the International Sooting Flames workshop. Figure 2 shows the time-averaged temperature and the velocity on the

centerline of the combustor. The simulation results slightly overpredict the experimental data in the inner recirculation zone, identified by the negative velocity, while comparing very well downstream of the secondary air injection. In figure 3 the time-averaged soot volume fraction obtained in the LES is compared with the experimental data. The S-EQMOM model predicts soot presence in the region between the flame front and the inner recirculation zone, similar to the measurements. Quantitatively, the soot volume fraction is under-predicted approximately by a factor of three. This is consistent with previously published LES results with detailed soot models and will be further investigated in the next months. These results were presented to the AIAA SciTech

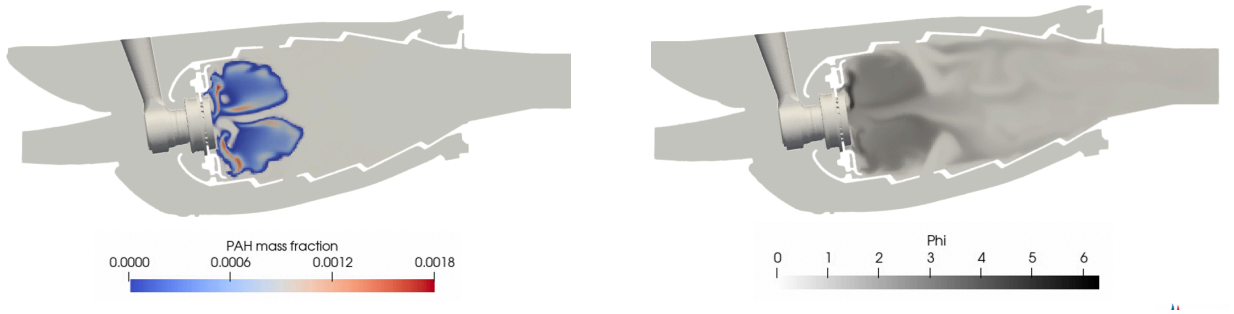

Figure 4: Instantaneous PAH mass fraction and equivalence ratio in the BR700.

2022 Forum (Cokuslu et al., 2022).

LES of the BR700 combustor are currently conducted in PRECISE-UNS using the latest version of the kinetic mechanism provided by UNISTUTT. The mass fraction of the PAH species and the equivalence ratio is shown in Fig. 4. These results verify the implementation of the new kinetic mechanism in PRECISE-UNS and of the PAH transport equation. Simulations with the coupled S-EQMOM will be performed in the next months.

4. Coupling of the soot models with the turbulent combustion models

This section is devoted to the description of the coupling between the soot and turbulent combustion models together with their application to some turbulent flames.

4.1 FGM-beta PDF + DSM

In the present FGM-DSM formalism for LES, transport equations are solved for the filtered soot mass fraction in addition to the control variables. By applying a spatial filter

to Eq. (1), along with closure models for subgrid-scale soot fluxes and thermophoretic fluxes, the filtered equation for the soot section is obtained as:

$$\frac{\partial(\overline{\rho}\widetilde{Y}_{s,i})}{\partial t} + \nabla\cdot(\overline{\rho}\widetilde{\vec{u}}\widetilde{Y}_{s,i}) = \nabla\cdot\left(\overline{\rho}C_{th}\overline{\nu}\frac{\nabla\widetilde{T}}{\widetilde{T}}\widetilde{Y}_{s,i}\right) + \nabla\cdot\left[\overline{\rho}\left(\overline{D}_{s,i}+\frac{\nu_t}{Sc_t}\right)\nabla\widetilde{Y}_{s,i}\right] + \rho_s\overline{\dot{Q}}_{s,i} \qquad i=1,\ldots,N_{sec} \qquad (2)$$

where ν_t, Sc_t are the subgrid-scale turbulent viscosity and the turbulent Schmidt number, respectively. The mean source term $\overline{\dot{Q}}_{s,i}$ for the corresponding soot section accounts for combined contributions from nucleation, condensation, surface growth, oxidation, and coagulation sub-processes. The soot source term is tabulated in the lookup database as a production rate and a linearized consumption rate of soot volume fraction and, subsequently, applied in Eq. (2). During the database creation, 1-D flamelets representative of the combustion type (premixed/non-premixed) are computed with complete soot kinetics using CHEM1D code. In FGM, a manifold representing the thermochemical space, parametrized by controlling variables, is constructed from solutions of laminar flamelets. Turbulence-chemistry interaction is accounted for as explained in section 2.1.1.

The performance of the FGM-DSM framework is studied in a model gas turbine combustor, experimentally investigated at DLR (Geigle et al.). The burner presents a high-pressure Rich-Burn/Quick-Quench/Lean-Burn (RQL) combustion system. In the burner, gaseous ethylene fuel is injected into the combustion chamber through a central annular nozzle surrounded by a concentric swirling primary air coflow. To create an RQL-type region for soot oxidation, secondary air is supplied into the combustion chamber at a specific downstream position.

A detailed numerical study of the DLR burner is conducted using Large-Eddy Simulation (LES) in collaboration with UPV, TUE, and BSC. The simulations are carried out using multi-physics reacting flow solver Alya. A chemical kinetic mechanism developed by USTUTT (Ramírez et al.) is employed for gas-phase chemistry during flamelet table generation. Prior to sooting flame simulations, the gas-phase flow and mixing characteristics are verified for the LES. The results for time-averaged fields for velocity and temperature show good agreement with the measurements (see Fig. 5). Furthermore, FGM-DSM provided a satisfactory qualitative and quantitative prediction for the soot volume fraction, as can be noticed in Fig. 6.

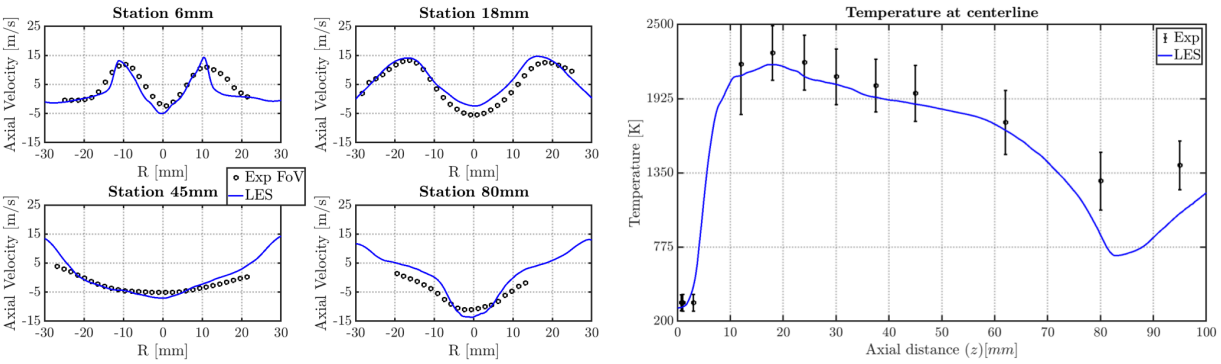

Figure 5. Comparison between simulations and experiments. Averaged axial velocity at radial stations (left). Averaged temperature at centerline (right).

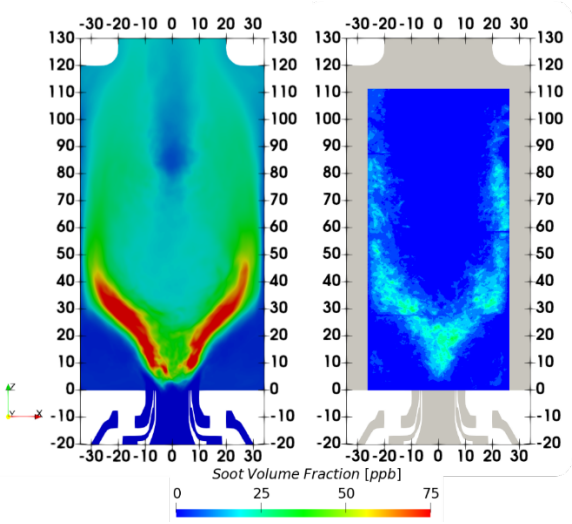

Figure 6. Averaged soot volume fraction. Simulations (left). Experimental measurements (right).

4.2 FGM-ESF + S-EQMOM

The coupling between the FGM-ESF and the S-EQMOM is achieved through the reactive scalar fields involved in the soot physico-chemical processes.

To model the mass transfer between gas- and particle-phase due to nucleation and account for the slow PAH chemistry, a filtered transport equation for the PAH mass fraction is solved, following Mueller and Pitsch (2012),

$$\frac{\partial \bar{\rho}\tilde{Y}_{PAH}}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_i\tilde{Y}_{PAH}}{\partial x_i} = +\frac{\partial}{\partial x_i}\left(\bar{\rho}(\tilde{D}+D_T)\frac{\partial \tilde{Y}_{PAH}}{\partial x_i}\right) + \overline{\dot{\omega}}_{PAH}.$$

Here $\widetilde{Y}_{PAH}$ is the sum of the PAH soot precursors accounted for in the kinetic mechanism.

According to (Mueller and Pitsch, 2012) the filtered source term $\overline{\dot{\omega}}_{PAH}$ is decomposed in three components: a chemical production term $\dot{\omega}^{+}_{PAH}$, which is independent of the species concentration, a chemical consumption term $\dot{\omega}^{-}_{PAH}$, which is linear with the species concentration, and a consumption term representing the mass transfer rate from gas-phase to soot $\dot{\omega}_{nuc}$, which is quadratic with the species concentration,

$$\dot{\omega}_{PAH} = \dot{\omega}^{+}_{PAH} + \dot{\omega}^{-}_{PAH} + \dot{\omega}_{nuc}.$$

The filtered source term is then decomposed as

$$\overline{\dot{\omega}}_{PAH} = \overline{\dot{\omega}}^{+T}_{PAH} + \overline{\dot{\omega}}^{-T}_{PAH}\left(\frac{\tilde{Y}_{PAH}}{\tilde{Y}^{T}_{PAH}}\right) + \overline{\dot{\omega}}^{T}_{nuc}\left(\frac{\tilde{Y}_{PAH}}{\tilde{Y}^{T}_{PAH}}\right)^{2}.$$

where the superscript *T* indicates the value obtained from the flamelet table.

4.3 CMC-beta PDF + DSM

In the current implementation for the coupling between CMC and DSM, the soot mass fractions related to the sections are conditioned to the mixture fraction. After manipulation and simplification of some terms the final transport equations for the conditional soot mass fractions sections $Q_{s,i} = \langle Y_{s,i} \,|\, \eta \rangle$ read

$$\overline{\rho}\widetilde{P}\frac{\partial Q_{s,i}}{\partial t} + \overline{\rho}\widetilde{P}\langle \vec{u} \,|\, \eta\rangle \cdot \nabla Q_{s,i} = \nabla \cdot (\overline{\rho}\widetilde{P} D_{sgs} \nabla Q_{s,i}) - \frac{\partial(\overline{\rho}\widetilde{P}\langle N \,|\, \eta\rangle)}{\partial \eta}\frac{\partial Q_{s,i}}{\partial \eta} + \overline{\rho}\widetilde{P}\langle \dot{Q}_{s,i} \,|\, \eta\rangle \qquad i = 1,\ldots,N_{sec}$$

where the soot mass diffusivity and the thermophoretic effect are neglected. In a similar way than for the chemical source terms, a first order closure is applied for the estimation of the soot source terms.

The model has been applied to the Large Eddy Simulation of a turbulent counterflow flame at atmospheric pressure, corresponding to task 4.2 from the project. Ethylene, diluted with nitrogen, is used as the fuel. The complex chemical mechanism generated during the project in task 2.1 is being used for the current simulations. Simulations are performed in the code Alya. Preliminary results for temperature and soot volume fraction are shown in figure 7.

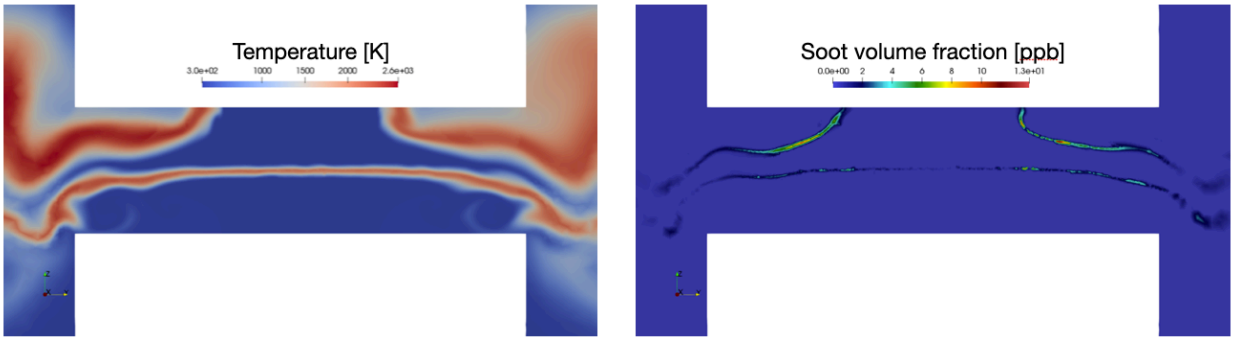

Figure 7. Instantaneous temperature and soot volume fraction fields from CMC for a turbulent counterflow flame.

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