SOOT PREDICTION IN A MODEL AERO ENGINE COMBUSTOR WITH MULTIPHYSICS APPROACH

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Abstract
The main objective of this paper is the assessment of a new multiphysics approach (THERM3D) where reactive CFD, radiation and heat conduction calculations are computed sequentially with a separate solver in a dedicated framework. Therefore, a set of numerical analyses performed on a high pressure test rig are reported. In this context, the importance of taking into account radiative phenomena in order to correctly predict reactive flow fields and pollutant emission in sooting flames is highlighted. Particularly, soot formation and oxidation largely depend on temperature field, leading to an indirect coupling with radiative emissions, showing great differences on soot distribution and emission, due to different rates of formation and oxidation of soot parcels, when radiative calculation is not computed.

Test case
The investigated test case is the DLR-FIRST combustor [1,2]. The rig consists of a combustion chamber of square section, surrounded by a stainless steel pressure housing, as shown in Figure 1. Both are equipped with four quartz windows which provide optical access to the internal reactive flow.

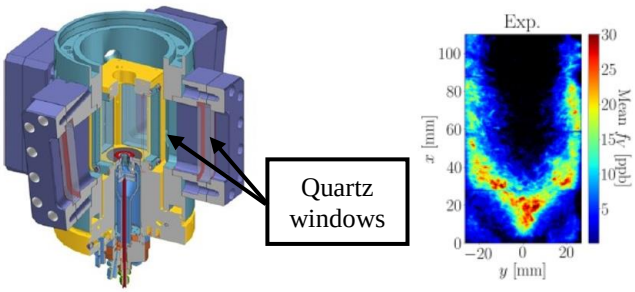

Figure 1. Test case design and soot volume fraction experimental map (adapted from [2,3]).

Air is supplied to the combustion chamber by means of an annular swirled nozzle which enclose the gas fuel injection (Ethylene, C_2H_4). The gap between the chamber and the pressure housing is fed by air to ensure the cooling of combustion chamber

windows. For more information regarding the rig, the reader is addressed to [1] and references therein. Several cases at high pressure have been investigated in [1]. In Table 1, the conditions of the considered operating point are reported.

Table 1. Considered operating point.

P [bar]	Φ [-]	$P_{primary}$ [kW]	$Q_{air,c}$ [slm]	$Q_{air,r}$ [slm]	Q_{fuel} [slm]	Q_{oxi} [slm]	$Q_{air,c}/Q_{air,r}$ [-]	Q_{oxi}/Q_{air} [-]
3	1.2	32.2	140.8	328.5	39.3	187.4	0.3	0.4

Experimental measurements include gas temperature using Coherent Anti-Stokes Raman Spectroscopy (CARS) [3], time averaged soot distributions and instantaneous soot volume fraction maps [1].

Description of the methodology (THERM3D)

In this work, a new in-house multiphysics tool developed in ANSYS Fluent framework is presented. The main feature of this methodology is to compute three different simulations to solve reactive CFD, radiation and heat conduction in a sequentially manner [4]. As shown in Figure 2, the exchange of specific source terms in the conservation equations and the use of proper boundary conditions allow to take into account interactions among the simulations, according to [5, 6, 7].

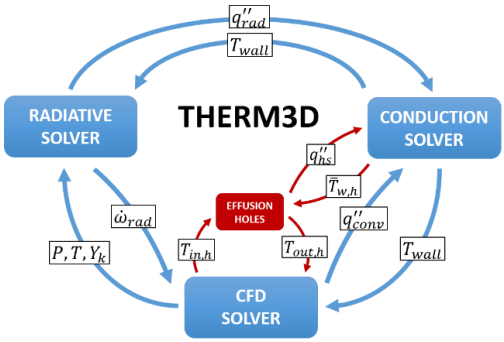

Figure 2. Schematic representation of the THERM3D methodology [4].

Considering the different characteristic scales and the different computed equations, each simulation is performed with the most suitable mesh and numerical setup for the considered physical phenomena, leading to a decrease of the computational time of the entire simulation.

Numerical setup

The results of four different simulations are reported in this work. Firstly, THERM3D (T3DR case) and CHT (CHTR case) solutions were computed together with a flametube calculation (FTR case) without solid domain, employing the

radiation model. Then, a THERM3D without radiative calculation was performed (T3D case) to highlight the weight of radiation in this coupled problem.
All simulations were computed with the commercial code ANSYS Fluent v17.1 using a RANS approach and the realizable k-ε model [8] was considered to take into account turbulence effects. Figure 3 shows the employed computational domain together with boundary conditions assumed for gas phase. Top-hat profiles were adopted for velocity, temperature, mixture fraction and progress variable at inlets, whereas a static pressure was imposed at flametube outlet, according to data reported in Table 1. All walls were treated as smooth with a no-slip condition for velocity. Particularly, quartz windows were considered as transparent to radiation. A constant temperature (313 K) and HTC (121 W/m^2K) value was applied on the cold side of the quartz windows for T3DR and CHTR cases, using the method explained in [9]. A uniform temperature of 900 K was imposed at gas-solid interface for FTR calculation.

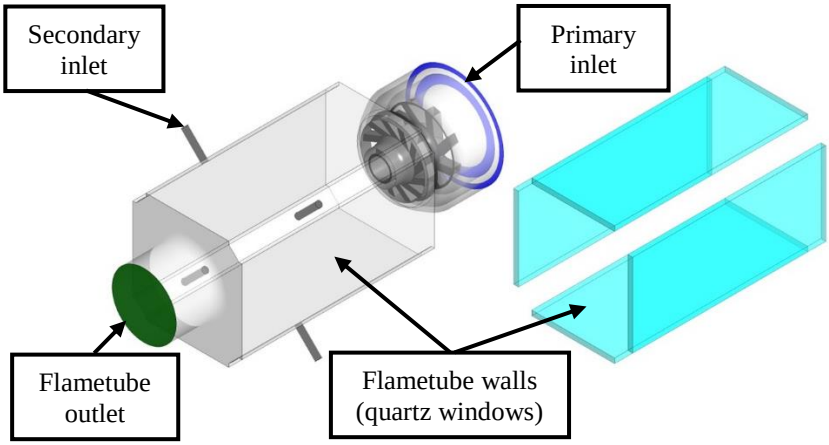

Figure 3. Flametube and solid computational domain.

A tetrahedral mesh of 14M elements with three prismatic layers close to the wall was employed for the gas phase simulation whereas heat conduction calculation within solid framework was performed in a hexahedral mesh of 600k elements. Instead, a coarser tetrahedral mesh of 2.6M elements was employed for radiative calculation with THERM3D approach as a result of a previous mesh sensitivity that is not reported for the sake of brevity. Meshes were created in ANSYS Meshing with a global size of 1.15 mm for the reactive gas phase, considering a refinement at injector burner with a sizing of 0.2 mm.
Regarding combustion modelling, the Flamelet Generated Manifold (FGM) was adopted to describe the reactive flow behavior and the flame characteristics [10]. In order to take into account soot formation within the combustor, two additional transport equations for radical nuclei concentration and soot mass fraction were solved according to Moss-Brooks model [11].
The radiative thermal loads are computed by solving the Radiative Transfer Equation

(RTE) in a frozen gas phase solution together with temperature distributions at walls, using Discrete Ordinate (DO) model [12]. RTE solution is parallelly performed in a proper and coarser mesh to balance accuracy and CPU efforts.

Results

Results of the simulated operating condition are here highlighted. First of all, a comparison between temperature fields of each simulation is reported. Then, the significant impact of radiative phenomena on soot emission is evaluated.

Figure 4 shows computed temperature distributions in a plane through the centerline of the combustor. Considering radiative calculation, it is possible to observe a great agreement between T3DR and CHTR approach, whereas slight differences can be noted with FTR solution near the walls, due to the different boundary conditions, and so temperature distributions, at gas-solid interface. When radiation is not computed (T3D), the absence of heat dispersion related to radiative emissions leads to a temperature increase, especially close to swirler outlet and quartz windows.

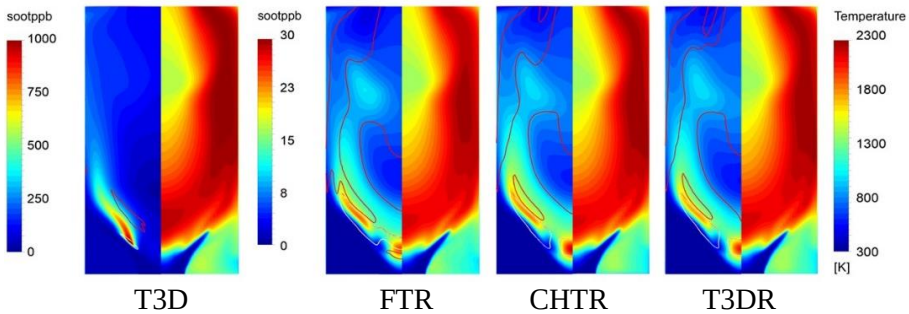

Figure 4. Temperature and soot volume fractions distributions in a plane through the centerline of the combustor.

This fact is also confirmed by a quantitative comparison with experimental data, as shown in Figure 5, where temperature profiles along the centerline of the combustion chamber are reported. A general good agreement can be appreciated with an under-prediction of about 60 K in the first part of the combustor, whereas it is possible to note an over-prediction of about 100 K at 80 mm downstream of swirler outlet, probably due to the employed steady approach.

Considering soot formation, soot volume fraction fields are also reported in Figure 4. The white line is the iso-contour at 15% of soot mass source maximum value (related to soot formation) while the red line is the iso-contour at 15% of its minimum value (related to soot oxidation). Great differences can be observed in terms of values and distributions when radiation is not computed.

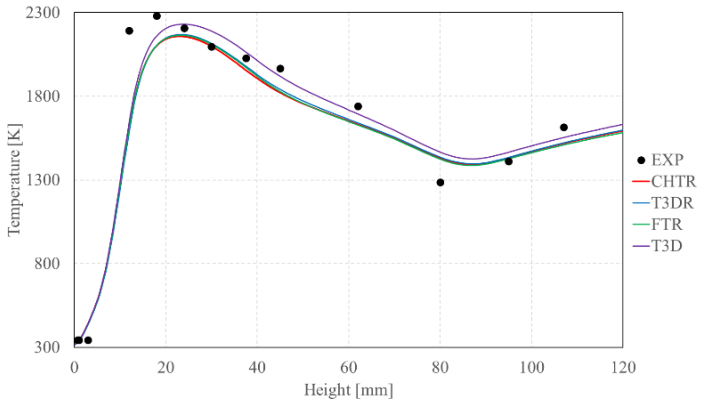

Figure 5. Temperature profiles along the centerline of the combustor.

Consequently, radiative phenomena have a strong impact on soot emissions, related to the non-linear dependence on the temperature of the source terms of soot model equations [11]. While in T3D case soot formation and oxidation are focused in small regions next to swirler outlet, a more uniform distribution of soot oxidation can be observed when radiative calculation is computed.

Nomenclature

P	Power [kW]
Q	Volume flow rate [slm]
p	Pressure [bar]

Acronyms

CFD	Computational Fluid Dynamics
HTC	Heat Transfer Coefficient
RANS	Reynolds Averaged Navier Stokes

Greek

Φ	Equivalence ratio [-]

Subscripts

c	central
r	ring

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