Two-dimensional and three-dimensional RANS Simulations of a GOX/GCH4 Single Element Combustion Chamber

By H. Riedmann AND O. Knab
Airbus DS GmbH, 81663 Munich, Germany

This report summarizes the Airbus DS CFD activities within the combustion modeling workshop of the SFB-TRR 40 Summer Program 2015. The focus of these activites lies on 2D and 3D RANS simulations of the combustion modeling workshop test case with the Airbus DS in-house CFD tool Rocflam3 and on the comparison with the experimental data. First 2D/axisymmetric simulation results reveal a great dependency on the turbulent Prandtl and Schmidt numbers. Therefore, an important question is how to choose these quantities. This question has been posed to the other workshop participants.
The 3D simulation results are compared with the experimental data and reveal that some subjects should be evolved in order to improve the agreement. In particular the chemistry scheme which is used for combustion modeling in the present simulations is most probably too global to enable a good approximation of the chemistry in this case. This shall be improved in future work.

1. Introduction

While there is longtime experience in the modeling of $\mathrm{H_2/O_2}$ combustion in rocket thrust chambers at Airbus DS, the propellant combination $\mathrm{CH_4/O_2}$ has been put into the focus of CFD modeling research activites quite recently. Therefore, the numerical tools which are used for $\mathrm{H_2/O_2}$ modeling have to be adapted in order to cope with the new propellant combination. The first step is the identification of a suitable chemistry and combustion modeling approach. In addition to that, established setting parameters are put to trial again in order to assess the sensitivity of the simulations on these parameters.

2. Numerical method

The 3D CFD tool Rocflam3 is currently under development at Airbus DS in Ottobrunn as designated successor of the 2D/axisymmetric in-house code Rocflam-II. The continuous gas phase is treated using an Euler description solving the Favre-averaged conservation equations for mass, momentum and enthalpy in three spatial dimensions. The equations are discretized with a Finite-Volume scheme for non-orthogonal, boundary-fitted and block-structured grids according to the pressure based SIMPLE algorithm described by Patankar & Spalding [1] modified to be applicable for compressible flows. In the frame of this work, the transport equations are solved in a steady state formulation. For the discretization of the convective fluxes a 2nd order TVD scheme is applied.
The turbulence model used in this work is the 2-layer $k-\epsilon$ model as described by Chen & Patel [2]. The Durbin realizability constraint [3] is used to complement this turbulence

model.
Rocflam3 comprises several approaches to model the propellant injection. The most common one is the inlet boundary with prescribed mass flow rate and temperature. This boundary condition is well suited for the injection of gaseous and supercritical propellants where a continuum exists. Therefore, it has been chosen for the present test case. While an equilibrium-based PPDF chemistry model is used for H_2/O_2 combustion modeling in Rocflam3, a global chemistry approach is applied in this work as the methane combustion is known to be slower than hydrogen combustion and therefore stronger non-equilibrium effects are supposed to occur. The key element of this approach is computing finite rates for the reactions of the participating species. Therefore, a kinetic scheme has to be established. Due to the high complexity of the elementary reactions in hydrocarbon combustion, reduced mechanisms have to be applied in order to maintain reasonable computational times. A speed-up with respect to the chemical part of the computation can be achieved by considering only a few chemical species reacting globally thus leading to a so called "global chemistry mechanism". As a basis for the global reactions to be solved by Rocflam3, the following universal scheme for hydrocarbon combustion proposed by Westbrook & Dryer [4] has been used:

$$\mathrm{C_nH_m} + \left(\frac{\mathrm{n}}{2} + \frac{\mathrm{m}}{4}\right)\ \mathrm{O_2} \longrightarrow \mathrm{n\ CO} + \frac{\mathrm{m}}{2}\ \mathrm{H_2O} \tag{2.1}$$

$$\mathrm{CO} + \frac{1}{2}\ \mathrm{O_2} \rightleftharpoons \mathrm{CO_2} \tag{2.2}$$

In its original form all three reactions (Eq. (2.2) is bidirectional) are Arrhenius and thus temperature controlled. The first modification made was to change the main combustion equation Eq. (2.1) to a turbulence controlled one by usage of the Eddy Dissipation Model (EDM) according to Magnussen & Hjertager [5]. Doing so, the results for the general flame behavior and also the wall heat fluxes became significantly more realistic than using only the Arrhenius law. A second modification was made in order to capture water dissociation and recombination effects which occur due to the elevated temperatures, provoked by the usage of pure oxygen as oxidizer:

$$\mathrm{H_2O} \rightleftharpoons \mathrm{OH} + \mathrm{H} \tag{2.3}$$

3. Simulation settings

3.1. *2D/axisymmetric simulation settings*

The first 2D/axisymmetric simulations are performed on a structured grid with a total number of 44840 grid cells. The wall normal resolution is $1\mu m$ at the liner wall and $0.1mm$ at the faceplate. At the liner wall the constraint $y^+ < 1$ is fulfilled for the wall-adjacent grid cells throughout the complete chamber length. The axial resolution in the throat region is $0.25mm$. The grid is visualized in Fig. 1.
At the chamber liner wall the measured temperature profile (see test case description [6]) is prescribed as thermal boundary condition, while the faceplate and the post-tip are supposed to be adiabatic. A mass flow boundary condition is applied at the injector inlet and a supersonic exit boundary condition is applied at the nozzle outlet. At the inflow boundary, the turbulent intensity is set to 20% for methane and 10% for oxygen. Lower values have shown to decrease the numerical stability in this case.
The turbulent Prandtl and Schmidt numbers are varied within the performed studies to

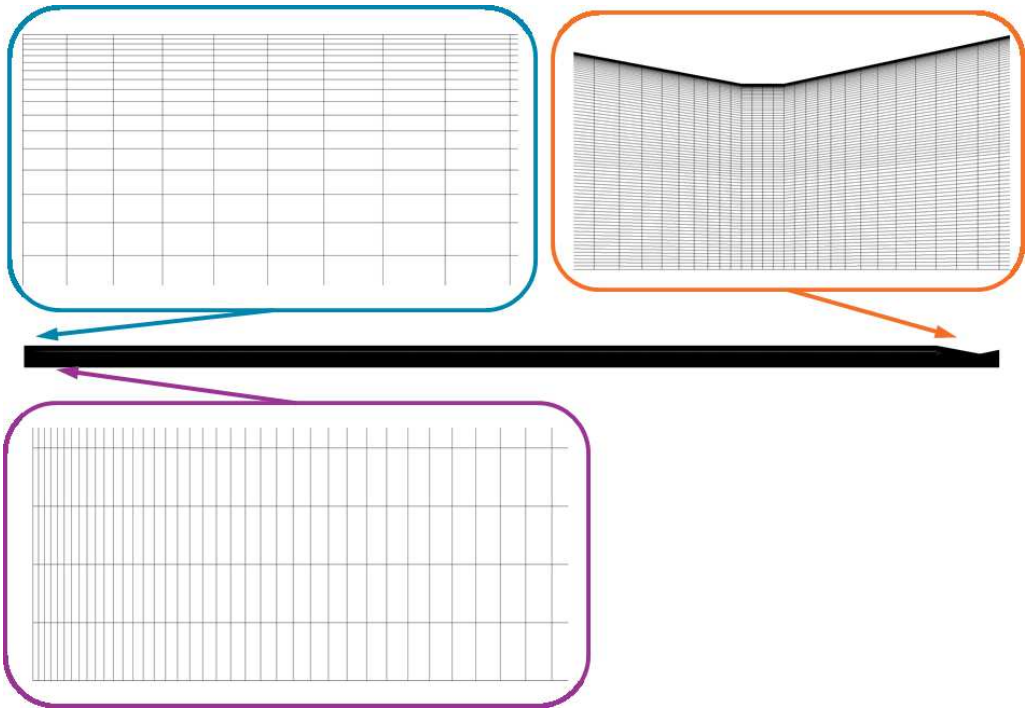

FIGURE 1. Numerical grid used for the 2D/axisymmetric simulations

check the sensitivity of the simulation results on these parameters, see Sec. 4.1.
Later on during the Summer Program, a common grid and common settings have been defined by the participating groups. These have also been used by Airbus DS. See the common combustion modeling workshop report for details.

3.2. *3D simulation settings*

The 3D simulations are performed on a quarter segment of the chamber. The grid resolution in axial and radial direction are adopted from the 2D/axisymmetric simulation resulting in a total number of $2.4 \cdot 10^6$ grid cells. The further settings are also equivalent to the 2D/axisymmetric simulation. Fig. 2 shows the block-structured grid used for the 3D simulations. The blocks where methane and oxygen enter the domain are colored red and blue, respectively.

4. Results

4.1. *2D/axisymmetric simulation results*

The first 2D simulation results are shown in this section. Thereby, the focus lies on illustrating the influence of the turbulent Prandtl and Schmidt numbers. Fig. 3 shows the the temperature fields for simulations with $Pr_t = Sc_t = 1.2$ and $Pr_t = Sc_t = 0.8$, respectively. One can see that the temperature field significantly depends on these numbers. It is conspicious that the maximum temperature reached in the simulations lies above $4000K$ which is distinctly beyond the adiabatic flame temperature. This is a weakness of the chosen chemistry scheme. Some improvement is necessary at this point.

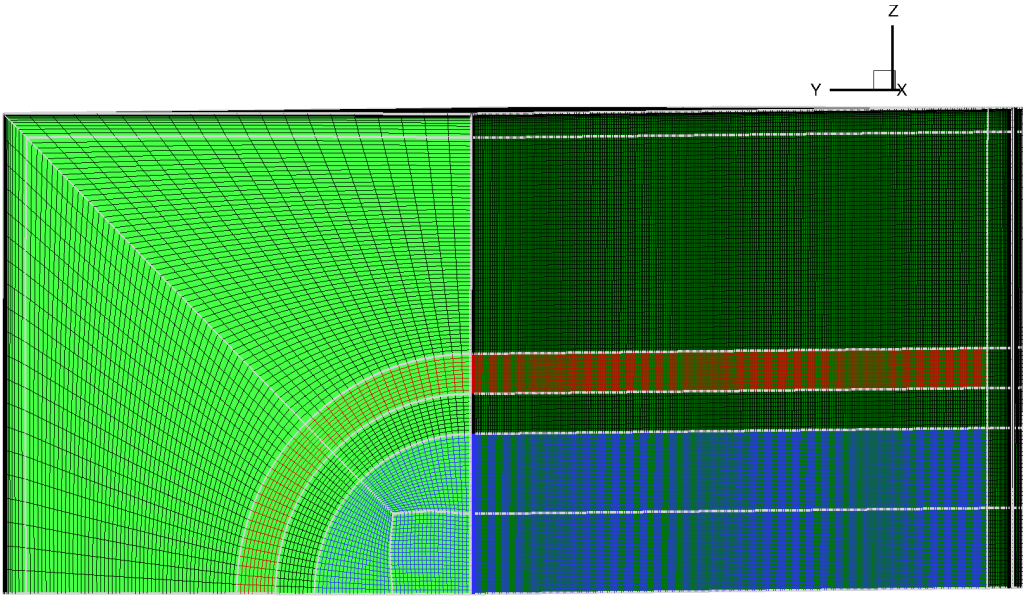

FIGURE 2. Numerical grid used for the 3D simulations

The wall pressure and wall heat flux profiles shown in Fig. 4 and 5 confirm the strong influence of the turbulent Prandtl and Schmidt numbers. Local pressure differences lie in the range of $0.5bar$ ($\approx 3\%$). While the turbulent Prandtl number acts mainly on the heat transfer, the turbulent Schmidt number acts mainly on the mass transfer. Decreasing Pr_t and Sc_t in this special case leads to a better mixing, a higher combustion efficiency, a higher wall heat flux and a higher chamber pressure.
Of course, the turbulent Prandtl and Schmidt numbers should not be used to arbitrarily adapt the measured wall heat flux profile to the experimental data.Their choice should be justified instead. However, it is important to check the sensitivity of the simulation results on these parameters and also to publish the chosen values if simulation results from different CFD codes shall be compared.
At this point it is important to emphasize that the combustion chamber has a square cross section. Thus, a 2D/axisymmetric approximation is difficult to justify. In reality, the flow field is certainly influenced by the three-dimensional flow evolving in the corners of the combustion chamber and this cannot be captured by a 2D simulation. Therefore, 3D simulations are performed in a next step. Nevertheless, it must be pointed out that 2D/axisymmetric simulations are very well suited for extesive parameter studies due to their low computational effort.

4.2. *3D simulation results*

The 3D simulation results presented here have been obtained with the turbulent Prandtl and Schmidt numbers set constant to $Pr_t = Sc_t = 0.8$. The temperature field shown in Fig. 6 gives an impression of the three-dimensional flame shape. The mixture ratio fields at distinct axial positions (see Fig. 7) not only show that the flow field is not rotationally symmetric as assumed when performing a 2D/axisysmmetric simulation but also shows that the mixing is weak. If it is underestimated by the simulation, this is a possible reason for the underestimation of the chamber pressure, which lies approximately $1bar$ ($\approx 1\%$) below the measured one. The normalized wall pressure profile visualized in Fig. 8 does

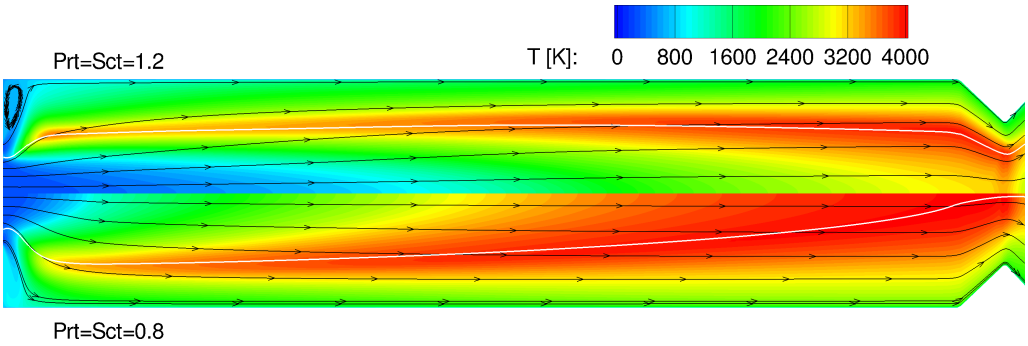

FIGURE 3. Temperature fields and streamlines for 2D/axisymmetric simulations with $Pr_t = Sc_t = 1.2$ and $Pr_t = Sc_t = 0.8$ (x-axis compressed by factor 5)

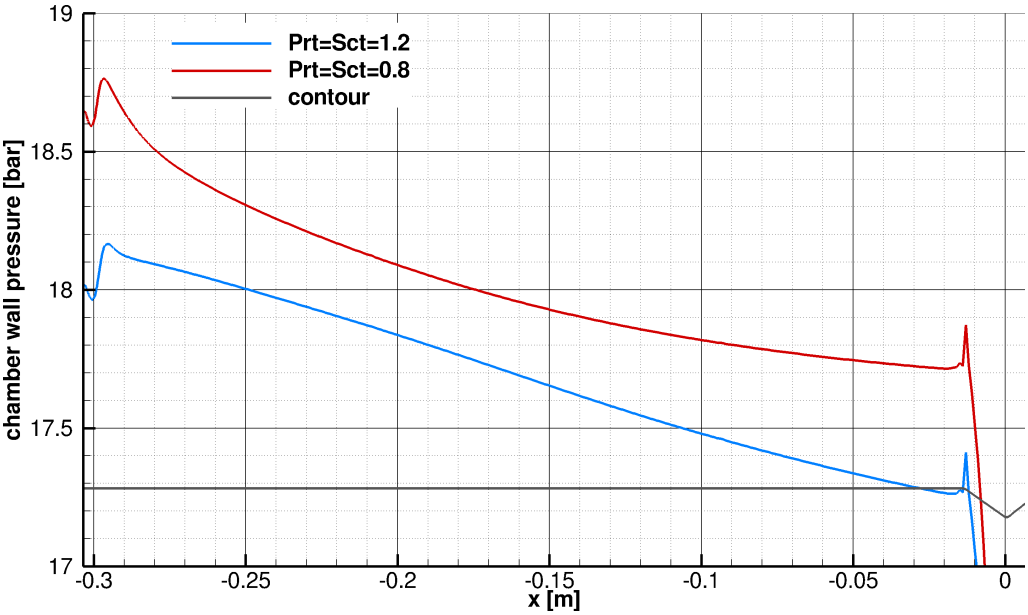

FIGURE 4. Wall pressure profiles for 2D/axisymmetric simulations with $Pr_t = Sc_t = 1.2$ and $Pr_t = Sc_t = 0.8$

not show this underestimation, but compares the shapes of the computed and measured profiles confirming an elongated flame shape by the steadily decreasing profile up to the end of the tube section. The agreement is not perfect but it is satisfactory considering the differences between the absolute values. The underestimation of the wall pressure is supposed to be at least partly linked to the overestimation of the measured wall heat flux, see Fig. 9.

5. Conclusions

The presented simulation results do not show a satisfactory agreement with the experimental data. The first part of the applied modeling approach which should be revised is the used chemistry scheme. Seven species only are considered and this is most probably not enough to compute the combustion temperature correctly.

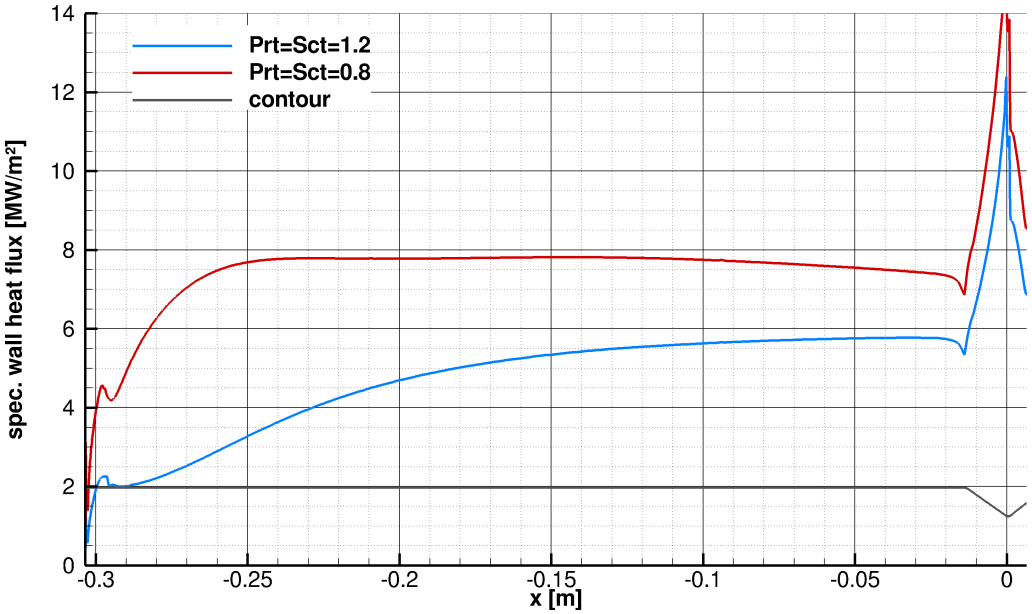

FIGURE 5. Wall heat flux profiles for 2D/axisymmetric simulations with $Pr_t = Sc_t = 1.2$ and $Pr_t = Sc_t = 0.8$

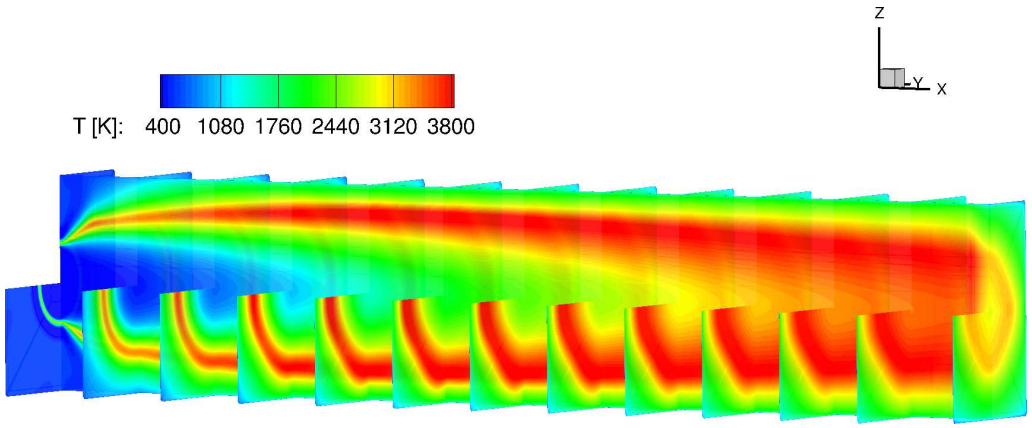

FIGURE 6. Temperature field for the 3D simulation (x-axis compressed by factor 5)

Apart from this open issue, the 2D/axisymmetric simulations have shown the significance of the turbulent Prandtl and Schmidt numbers for the simulation of this test case. It has been clarified how important it is to address the choice of these numbers in order to be able to compare not only simulation and experiment but also simulation results among each other. Unfortunately, no LES simulation result has been delivered during the modeling workshop which better matches the experimental data and hence could be used to evaluate the RANS and URANS specific turbulent Prandtl and Schmidt numbers.

Regarding the test case itself, it must be emphasized that the tests have been performed with a capacitive chamber. Therefore, the hardware temperature has not been in a steady state when the measurements have been conducted. However, the temporal

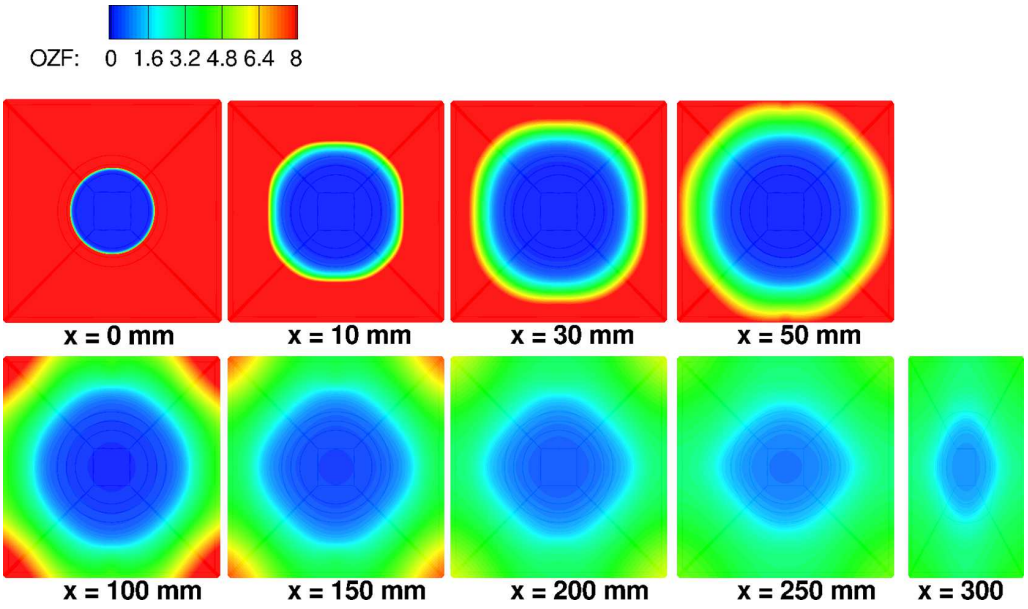

FIGURE 7. Mixture ratio field for the 3D simulation at distinct axial positions ($360°$ visualization)

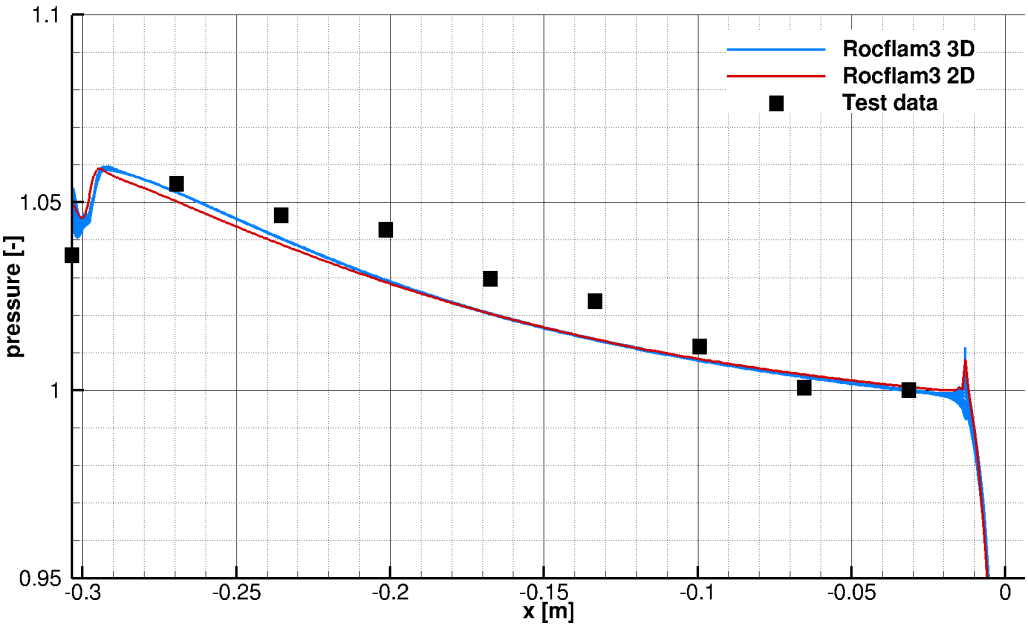

FIGURE 8. Normalized all pressure profile for the 3D simulation

evolution is neglected in steady state simulations thereby necessarily introducing an (at least up to now) unknown modeling error.

Acknowledgments

This work has been financed by Airbus DS GmbH.

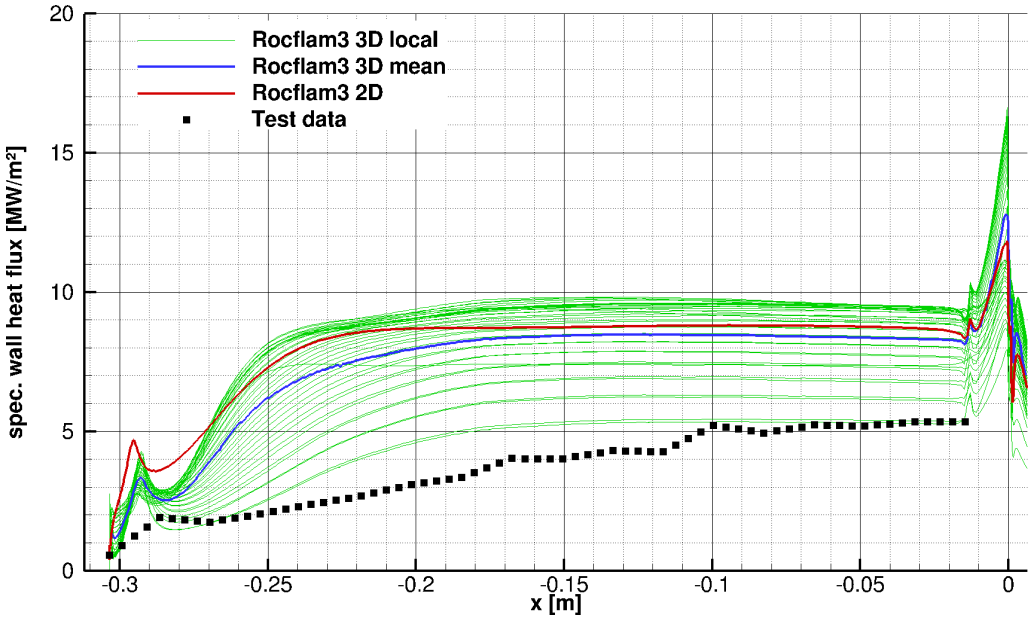

FIGURE 9. Wall heat flux profile for the 3D simulation ($Pr_t = Sc_t = 0.8$)

References

[1] PATANKAR, S. V. AND SPALDING, D. B. (1972). A calculation procedure for heat, mass and momentum transfer in three-dimensional parabolic flows. *International Journal of Heat and Mass Transfer*, **15**, 1787–1806.

[2] CHEN, H. C. AND PATEL, V. C. (1988). Near-wall turbulence models for complex flows including separation. *AIAA Journal*, **26**, 641–648.

[3] DURBIN, P. A. (1996). On the k-epsilon stagnation point anomaly. *International Journal of Heat and Fluid Flow*, **17**, 89–90.

[4] WESTBROOK, C. K. AND DRYER, F. L. (1981). Simplified reaction mechanisms for the oxidation of hydrocabon fuel in flames. *Combustion Science and Technology*, **27**, 31–34.

[5] MAGNUSSEN, B. F. AND HJERTAGER, B. H. (1977). On mathematical modeling of turbulent combustion with special emphasis on soot formation and combustion. In: *16th Symposium (International) on Combustion*, Pittsburgh, Pennsylvania, USA.

[6] CELANO, M. P., SILVESTRI, S., KIRCHBERGER, C., SCHLIEBEN, G., HAIDN, O. AND KNAB, O. (2014). Transregio SFB-TR40 - Test Case 1: Single Element Combustion Chamber - GCH4/GOX. In: *SFB-TR40 TU MÃijnchen*, MÃijnchen, Germany.

[7] SCHLICHTING, H. (1979). *Boundary-Layer Theory*. McGraw-Hill.