Soot CFD simulation of a real aero engine combustor

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Soot evolution for a complex fuel is investigated with computational fluid dynamics (CFD). The soot model is evaluated using a Rolls-Royce BR700 annular combustor, based on the Rich-burn/Quick-quench/Lean-burn (RQL) concept. CFD computations are performed at take-off, climb, approach and idle operating conditions. Soot results are examined and compared with published engine data. The implemented kinetic model includes a detailed gas phase, a sectional approach for soot precursors, the polycyclic aromatic hydrocarbons (PAHs), and a two-equation model for soot particles. The models for PAHs and soot cover relevant growth, collision, agglomeration, and oxidation processes, and at the same time represent a good trade-off between accuracy and computational effort. In the steady-state Reynolds-averaged Navier–Stokes (RANS) simulations, finite-rate chemistry (FRC) is utilized for the calculation of chemical source terms. Turbulence is modeled with a standard $k-\epsilon$ approach, and influence on combustion is captured following an assumed probability density function (APDF) technique. A Lagrangian framework is further applied to describe the injection and evaporation of the liquid jet fuel surrogate. The objective of this work is the reproduction of experimentally identified trends, and to gain insight into the soot formation and oxidation of a real aero engine combustion chamber. The calculated Smoke number (SN) and Emission index (EI) at the combustor exit are used as comparative quantities. Good agreement between measurement and simulation is achieved.

I. Introduction

Unwanted by-products of combustion, such as soot, have negative impacts on climate, health, environment, and combustor wall heat load.^{1–5} In conjunction with the increasingly stringent legal regulations a further development of existing combustion technologies is required.⁶ Numerical CFD simulations with validated soot models can support this process and may reduce development costs.⁷ However, the simulation of a real aero engine poses a challenge to numerical combustion simulation.⁸ This includes, in addition to high pressures and temperature, a high degree of turbulence, the liquid injection of the kerosene fuel, the wall film cooling, and the varying local air-fuel ratios, to name only a few of the many complex processes.

To determine the chemical conversion in these simulations, flamelet approaches are frequently applied in literature.^{9–11} Due to its low computational effort, this approach has also already been used in large-eddy simulation (LES) of aero engines.¹⁰ However, the applicability of this method is not given in general, and therefore approaches based on detailed chemistry are also frequently implemented,^{12–14} also to evaluate the applicability and uncertainty of flamelet models. The considerably higher computational cost is offset by element and mass conservation, as well as the inherently and consistently coupled gas phase, PAH and soot chemistry. Modeling soot particles in these simulations presents a particular challenge. Most of the developed and investigated soot models are limited to small hydrocarbon fuels and cannot be directly applied.^{15–17} Some models have already been extended to complex fuels.^{18–20} However, most of them are applied to academic test cases and are not suited for complex CFD simulations, due to their large number

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Figure 1. Discretization of the mass spectrum for gas phase, PAHs and soot model. PAH_i^* denotes a radical belonging to the respective PAH section.

of species and reactions.²¹ Reduction strategies were defined to generate mechanisms tailored to a specific operating condition at the price of losing its general applicability.^{22–26} Thus, in combination with FRC a soot model is required which, on the one hand, is large enough to be used without test case dependent modifications and, on the other hand, requires as little computational effort as possible. Such a model has been developed and investigated in a previous work and is here applied to a more complex test case.^{27,28}

The Rolls-Royce BR700 annular combustor is numerically examined in this work.^{29,30} In this RQL combustion chamber liquid fuel (Jet A-1) is injected into the rich-burn zone by an air-blast injector. For reasons of flame stabilization, spray droplet breakup and a better mixing, the injector consists of three air swirl generators. The fuel is injected using a liquid pre-filmer in between the inner and middle air swirler. The rich conditions in the primary zone lower the temperature levels and thus keep the NO_x emissions low, but also increase the formation of soot. Further downstream, in the quick-quench zone, a rapid mixing with additional oxygen is achieved by primary and secondary dilution air feeds. Thereby, the transition to the lean-burn zone is initiated in which the oxidation of soot is favored at sufficiently high temperatures. Emissions can be kept at a minimum if temperature levels are well balanced between the limits for soot oxidation and thermal NO_x formation. Four operating points (thrust levels), relevant for the International Civil Aviation Organization (ICAO) engine certification, are investigated in this work. These load cases involve take-off (100 %), climb (85 %), approach (30 %) and idle (7 %).

II. Methodology

The following steady-state RANS simulations are performed with the unstructured finite volume solver Predictive-System for Real Engine Combustors - Unstructured (PRECISE-UNS) developed by Rolls-Royce.³¹ This solver is based on a pressure correction method, initially developed for incompressible, but next extended to compressible, flows. The simulation framework provides several combustion and turbulence models. In this work, a standard $k-\epsilon$ turbulence model is chosen.³² Moreover, this solver provides a Lagrangian framework for spray particle tracking. Therein, a steady-state evaporation model and stochastic methods for turbulent fluctuations are implemented.^{33,34}

The thermo-chemical state in the combustor is defined by transport equations of enthalpy and species mass fractions. Analogously to enthalpy and gaseous molecules, an Eulerian approach is chosen for soot particles. While differential diffusion is considered for the gas phase species and PAHs, soot is diffusively transported by thermophoresis only.³⁵ Species source terms by chemical conversion are calculated by a point-implicit FRC solver, developed at the German Aerospace Center (DLR). Therein, turbulence-chemistry interaction is addressed via an APDF approach.¹³ For this purpose, each reaction rate of the kinetic scheme is averaged over the entire temperature fluctuation range assuming a Gaussian distribution, supplemented by up to two Dirac pulses if required. This calculation is performed in a pre-processing step and the reaction rates, later used in the simulation, are stored in tables. The radiation of certain species is considered by assuming an optically thin medium, whereby emitted radiation is not reabsorbed.³⁶ In view of the dominant pressure, especially for the 100 % load case, a partial violation of this assumption is to be expected. Nevertheless, this method is computationally efficient and may be preferable to a simulation without radiation influence. CO_2 , H_2O and soot are considered as important radiative species.³⁷

A. Chemical and soot modeling

The kinetic scheme of the soot model is composed of the sub models for gas phase, PAHs and soot.²⁸ A schematic representation of these sub models against their molar mass is shown in Fig. 1. The gas phase is based on a skeletal mechanism developed for small hydrocarbons, which has been extended to complex fuels and blends.^{38,39} The scheme covers species up to a molar mass of 100 g mol^{-1} , and thus also aromatic one-

ring structures, e.g., benzene or toluene. The mechanism has been optimized in terms of numerical stability and includes a total number of 112 species and 848 reactions. Subsequently to gas phase species, the PAHs are modeled using a sectional approach. Three sections, logarithmically increasing in size, span over a mass range from 100 to 800 g mol⁻¹. Each of these sections is supplemented by a PAH radical (PAH^{*}), to capture the reversibility of the hydrogen abstraction and carbon addition (HACA) mechanism.⁴⁰ In addition to PAH growth from acetylene, the model also includes the processes of collision and oxidation. Moreover, the interaction between gas phase and first PAH and PAH radical section is defined by additional reactions. Thermodynamic and transport properties for the PAHs are taken from reference species.

In this work, soot particles are described as mono-disperse particles, and therefore transport equations for the soot mass fraction (Y_S) and the soot particle number density (N_S) have to be defined. Following Einstein's summation convention, the transport equations for Y_S and N_S read as follows

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{Y}_S) + \frac{\partial}{\partial x_i}(\bar{\rho}\tilde{u}_i\tilde{Y}_S) = \frac{\partial}{\partial x_i}\left(\frac{\mu_t}{Sc_t}\frac{\partial\tilde{Y}_S}{\partial x_i}\right) + \frac{\partial}{\partial x_i}\left(C_{th}\frac{\mu\tilde{Y}_S}{T}\frac{\partial\bar{T}}{\partial x_i}\right) + \bar{\omega}_{Y_S}, \text{ and} \quad (1)$$

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{N}_S) + \frac{\partial}{\partial x_i}(\bar{\rho}\tilde{u}_i\tilde{N}_S) = \frac{\partial}{\partial x_i}\left(\frac{\mu_t}{Sc_t}\frac{\partial\tilde{N}_S}{\partial x_i}\right) + \frac{\partial}{\partial x_i}\left(C_{th}\frac{\mu\tilde{N}_S}{T}\frac{\partial\bar{T}}{\partial x_i}\right) + \bar{\omega}_{N_S}. \quad (2)$$

In the equations ρ denotes the density, u_i the i -th velocity component, μ_t the turbulent viscosity, Sc_t the turbulent Schmidt number, C_{th} the thermophoretic coefficient, μ the laminar viscosity, T the temperature, and ω the chemical source term. For Y_S and N_S the thermophoretic coefficient C_{th} is set to 0.55 and the turbulent Schmidt number Sc_t to 0.7. The only difference between Eqs. (1) and (2) is in the calculation of the source term $\bar{\omega}$. While $\bar{\omega}_{Y_S}$ is calculated as a function of molar mass, stoichiometric coefficients, reaction rate and concentration,^{13,41} $\bar{\omega}_{N_S}$ depends on the mixture's density in place of the molar mass. Consistent with incipient soot particles,⁴² the molar mass of soot is set to 1.2 kg/mol. A predefined H/C ratio of 0.5 is assumed for soot particles, leading to a molar composition of 96 C atoms and 48 H atoms. The soot density ρ_S is defined to be 1800 kg m⁻³.⁴³ The average diameter and the surface per unit volume of these soot particles is given by

$$d_S = \sqrt[3]{6 \rho Y_S / (\pi \rho_S N_A N_S)}, \text{ and} \quad (3)$$

$$A_S = \sqrt[3]{36 \pi N_A N_S \rho^2 Y_S^2 / \rho_S^2}, \quad (4)$$

respectively. The model takes into account the processes of inception, collision with PAHs, agglomeration and oxidation. Soot inception takes place through collision reactions of the PAHs which include the PAH₃ and the PAH₃^{*} section. Surface growth is modeled following the HACA mechanism.⁴⁰ In the case of soot, a radical counterpart species is neglected to keep the computational effort as low as possible. However, the influence of a radical soot species is still taken into account by assuming a quasi steady-state which yields

$$k_{S,\text{surface}} = \alpha k r_\chi \chi A_S \quad (5)$$

for the reaction rate of surface processes.⁴⁴ In this equation, α is a function of temperature, k denotes the respective rate coefficient, r_χ the ratio of reactive to stable sites, and χ the density of stable H/C sites (2.32×10^{-19} 1/m²). To obtain an Arrhenius like form for this reaction rate, the α function is defined to be

$$\alpha(T, c_\alpha, T_\alpha, n_\alpha) = c_\alpha (T_\alpha/T)^{n_\alpha} \exp(n_\alpha [1 - T_\alpha/T]), \quad (6)$$

with the coefficients $c_\alpha = 1$, $T_\alpha = 1800$ and $n_\alpha = 40$.⁴⁵ The ratio of reactive to stable sites requires calibration. In an extensive validation of the model over many different shock tube experiments and well-studied laboratory flames, best results have been achieved with a value of 2.5×10^{-3} .²⁸ Since N_S is determined at runtime but already is required in the definition of collision rate coefficients (see d_S), the approach of Di Domenico et al.⁴⁶ is followed, in which the superposition of reactions is used to isolate N_S from a reaction equation. Due to the mono-disperse soot size distribution, the efficiency of soot agglomeration is increased to 3, compared to a sectional approach,²⁸ which is also in agreement with previous works.⁴⁶ Soot oxidation takes place through O₂ and OH, where the dominant path is represented by the latter one. While the kinetic theory of gases is used for the rate calculation of OH with an efficiency of 0.27, the oxidation by O₂ is implemented following the surface process approach given above. Rate coefficients are taken from Fenimore and Jones,⁴⁷ and Appel et al.,⁴⁸ respectively. Moreover, a combination of three OH oxidation reactions,

Figure 2. Rendered simulation domain of the Rolls-Royce BR700 annular combustor (a) and overview of selected cut planes (b). Shown are streamlines from swirl generators (blue), primary (orange) and secondary (yellow) dilution air feeds, effusion wall cooling (green), and contours for significant spray source term (black) and high temperatures (red) in the figure on the left.

each superimposed with a different α function, is used to account for the decreasing oxidation efficiency towards lower temperatures.⁴⁹ A least-square technique was utilized to determine these functions to be $\alpha_1 = \alpha(T, 0.85, 1736.86, 70)$, $\alpha_2 = \alpha(T, 0.45, 2180.37, 70)$ and $\alpha_3 = \alpha(T, 0.97, 2978.08, 16.87)$.

The models for gas phase, PAHs and soot are further supplemented with polyynes and related reactions paths. These species may represent a further PAH and soot growth path, especially at higher temperatures.^{50–52} A more detailed description of the implemented model can be found in the previous validation work.²⁸

III. Numerical setup

The annular combustion chamber BR700 from Rolls-Royce is simulated using the soot model presented above. In this study the four operating points take-off, climb, approach and idle are investigated. Corresponding thrust levels and fuel mass flows are summarized in Table 1. As specified by the manufacturer, combustion chamber pressure and air inlet temperature are reduced with decreasing thrust level, while the air-fuel ratio is increased. To keep the computational effort as low as possible, only a 18° segment with symmetry boundary conditions is considered in the simulations, as shown in Fig. 2a. The chosen section covers one injector and extends up to half the distance to the nearest adjacent injector. The resulting mesh comprises of roughly 200,000 volumes and, despite the application in an unstructured solver, consists of hexahedral and quadrilateral elements only. The computational effort is about 70,000 CPUh per operating point for the chosen grid, gas phase kinetics, and soot model. Since kerosene consists of many different components, and may vary strongly, the fuel is described by a surrogate consisting of only a few important species. Since, the choice of a fuel surrogate may introduce a large uncertainty to the simulation, a surrogate is chosen, which has already been applied in previous works for kerosene where it achieved good results.²⁸ Therein, a blend of 65 vol-% n-decane, 23 vol-% iso-octane and 12 vol-% toluene is chosen as a replacement for real kerosene (Jet A-1).

Table 1. Fuel mass flow boundary condition for the simulations. Given are thrust level (%) and fuel mass flow per segment (g s^{-1}) for the respective operating point.⁵³

	take-off	climb	approach	idle
thrust level	100	85	30	7
fuel mass flow	35.71	29.74	10.72	4.46

Figure 3. Calculated normalized flow field contour plots in different cross-sections (a-d) of the combustion chamber for the take-off operating point (100 %). Superimposed are streamlines starting from the combustor inlet (white), and iso-lines of fuel mass fraction $Y_f=1\%$ (red dashed) and negative velocity perpendicular to the section plane (black dotted).

IV. Results and discussion

A schematic representation of the simulation domain is visualized in Fig. 2a. The geometry is superimposed with streamlines from the swirl generators (blue), primary (orange) and secondary (yellow) dilution air feeds, and effusion wall cooling (green). Corresponding boundary condition surfaces are highlighted in equivalent colors. Moreover, two contour surfaces are shown for significant spray source terms (black) and high temperatures (red). An overview of chosen cross-sections is illustrated in Fig. 2b. The selected cut planes show only a specific part of the complex flow field, but nevertheless, most important processes can be observed.

The magnitude of the velocity field is shown for the 100 % operating point in different cross-sections in Fig. 3. The visible areas of high velocity include the injector streams, as well as the primary and secondary dilution air feeds. As can be seen by the streamlines in Figs. 3a and 3b, the dilution air causes the quenching of the fuel-rich zone. The swirlers favor the flame stabilization and lead to the formation of two main recirculation zones (inner and outer) in the fuel-rich zone. The area of fuel mass fraction $Y_f=1\%$ (red dash-dotted) is located between these recirculation zones, whereby spray droplet breakup, evaporation and mixing is favored. Figure 3c shows that the upper and lower central primary air do not coincide coaxially but push each other apart. This is also apparent from the superimposed iso-lines of negative velocity perpendicular to the section plane, which extend asymmetrically across the cut plane.

Figure 4. Calculated normalized temperature (left) and soot volume fraction (right) contour plots in cross-section A of the combustion chamber, for the operating points take-off (a), climb (b), approach (c), and idle (d). Superimposed are iso-lines of fuel mass fraction (red dash-dotted), zero velocity (white solid), soot formation (black dashed) and oxidation (blue dotted).

In Fig. 4 the normalized temperature and soot volume fraction contour plots are given for all examined thrust levels. The normalization is achieved with the maximum values taken from the take-off operating point in Fig. 4a. The contour plots of the temperature are superimposed with iso-lines of zero velocity (white solid) and fuel mass fraction (red dash-dotted). The plots for soot volume fraction are superimposed with regions of soot formation (black dashed) and soot oxidation (blue dotted).

Comparing the different operating points for the normalized temperature plots in Fig. 4 shows that the temperature fields in the fuel-rich zone change significantly between the 85 % and the 30 % operating point. The regions of maximum temperature, between inner and outer recirculation zone, shrink with decreasing thrust level and disappear completely in the 7 % case. In addition, areas of maximum temperature move further upstream with decreasing thrust level. This observed trend does not continue with transition from the 30 % to the 7 % load case. In the latter one the temperature in the inner recirculation zone decreases significantly. A similar behavior can be observed for the fuel mass fraction $Y_f = 1\%$ (red dash-dotted) in Fig. 4. With a decreasing thrust level, down to 30 %, the spray cone angle expands, and then collapses slightly in the 7 % case again. The iso-lines for zero velocity $v = 0.0 \text{ m s}^{-1}$ (white solid), which also indicate areas of recirculation, are almost identical across the operating points. As well the lean zones in the rear part of the combustor show apart from the dropping temperatures very similar distributions. The areas of high temperatures wind around the primary and secondary dilution air feeds.

Also deviations occur between the operating points for the normalized soot volume fractions plotted in Fig. 4. Most soot volume fraction is predicted for the 100 % load case in the fuel rich-zone. A very similar distribution is observed for a thrust level of 85 %. Considerably less soot with a distinctly different distribution, is obtained for the 30 % and the 7 % operating points. Differences have also already been found in the temperature plots. The least soot concentration is predicted for the 30 % case. Similar levels are reached in the 7 % case in fuel-rich zone, however, the entire combustion chamber is noticeably more covered with soot. This is also visible by the source term of soot formation (black dashed). While these areas are limited to the fuel-rich zone for the 100 %, 85 % and 30 % case, soot formation almost reaches the lean zone in the 7 % case. Concerning soot oxidation, additional source terms are visualized with blue dotted iso-lines. As expected, oxidation extends over the entire combustor in the 85 % and 100 % operating point. The significantly less formed soot in the 30 % case, leads to a completion of soot oxidation in the first half of the combustor. In the 7 % load case, areas of significant soot oxidation extend further downstream into the lean zone of the combustion chamber, but do not compensate for the increased soot formation.

A. Smoke number and Emission index

Experimental measurements of combustion chambers in aero engines under real operating conditions are usually not publicly available. However, legal regulations require the publication of engine data for the certification. One of these published values is the Smoke number (SN), measured at the engine outlet. Conclusions about the combustion chamber can be drawn by considering the bypass air and turbine cooling. The calculation of the SN in the simulation is obtained with the integrated soot concentration at the combustion chamber exit as follows,

$$C_S = \begin{cases} 0.06949 \text{ SN}^{1.234}, & \text{for } \text{SN} \leq 30 \\ 0.0297 \text{ SN}^2 - 1.803 \text{ SN} + 31.94, & \text{for } \text{SN} > 30 \end{cases} \quad (7)$$

In the equation, C_S denotes the soot concentration with the unit mg m^{-3} . The experimental values are taken from the public ICAO database.⁵³ The SN results for the investigated operating points are shown in Fig. 5a. Regarding the trends, simulation and experiment agree very well. The SN decreases, as the thrust level is reduced to 30 %. The measurement at 7 % shows an increase of the SN, which is also predicted in the simulation. Concerning the values, the best agreement is achieved for the 30 % case. The 85 % and the 100 % thrust levels are slightly underestimated. The highest deviation is observed for the 7 % operating point. Deviations are nearly within one order of magnitude.

Another parameter for comparison is the Emission index (EI), given in units soot per kilogram fuel. For the mass-based EI (mg/kg fuel) similar trends are achieved in comparison with the SN in Fig. 5b. Absolute deviations increase but are still within 1-2 orders of magnitude. Results for the number-based EI ($\text{\# /kg fuel}$) can be seen in Fig. 5c. While good agreement is achieved for the take-off and climb operating points, approach and idle particle numbers diverge by 1-2 orders of magnitude. Although the deviation in

Figure 5. Measured and calculated SN (a), particle mass (b) and particle number (c) based EI at the combustion chamber exit (cross-section D). Open symbols: experimental data;⁵³ lines with filled symbols: simulation results.

the idle case may be attributed to the overpredicted particle mass, the soot model seems to reflect the trend only partially. Since soot is modeled as a mono-disperse spherical particle in the chosen two-equation model, particle agglomeration and aggregation may be underestimated, which in turn leads to an overprediction of particle number. Measured and predicted SN and EI values are summarized in Table 2.

Table 2. Measured (exp) and predicted (sim) emission values at the combustion chamber exit (cross-section D). Given are thrust level (%), SN (-), particle mass based (mg/kg fuel), and particle number based (#/kg fuel) EI for the respective operating point.⁵³

		thrust level		SN		EI (mass)		EI (number)	
				exp	sim	exp	sim	exp	sim
take-off	100	13.96	7.73	608.50	49.24	3.97×10^{15}	7.39×10^{15}		
climb	85	11.87	6.80	556.50	48.55	5.72×10^{15}	7.33×10^{15}		
approach	30	0.27	0.23	5.60	1.70	9.49×10^{14}	2.38×10^{16}		
idle	7	0.57	7.39	11.20	273.80	1.30×10^{15}	4.17×10^{17}		

V. Summary and conclusions

In this work, an aero engine combustor has been investigated by steady-state RANS simulations. FRC with APDF turbulence-chemistry interaction is utilized to describe the chemical conversion of evaporated fuel, towards soot precursors and finally to soot particles. The kinetic scheme employed here, concludes a detailed gas phase mechanism, a sectional PAH model and an efficient two-equation soot model. Soot tendencies for the operating points take-off, climb, approach, and idle are compared to SN and EI measurements. The observed phenomena, as well as the results of the comparison to the experiments are:

The concept of a RQL combustion chamber is reproduced for all examined operating points. A highly swirled inflow causes the formation of recirculation regions in the fuel-rich zone of the combustor, especially important for reasons of flame stabilization. The areas of high temperature and highest soot volume fraction are quenched by the primary dilution air injection, which together with the secondary air introduces the lean zone, where the oxidation of soot takes place.

The experimentally identified SN trends with decreasing thrust are reproduced well by the model. The operating points of highest thrust (take-off and climb) are very similar. As observed in the experiments, the least soot concentration is obtained for the approach case in the simulation, too. Even the observed increase in soot emission for the idle operating point is reproduced by the model, but also shows the maximum deviation to the experiment. Predicted trends of the mass-based EI are similar to the SN. A diverging trend to the experiment is found for the particle number related EI in the approach and idle case, which is due to the overestimation of the particle mass in the idle case, but also to the soot model used.

Despite many uncertainties, e.g., in fuel composition, turbulence modeling and interaction with chemistry, but also in the experimental values, the model provides good results and clearly demonstrates its applicability, to be used in soot simulations for complex real combustors. The model identifies regions with strong soot

formation and soot oxidation and reproduces mass-based emission trends very well. Further studies with a more complex soot model (sectional approach) may improve the prediction of particle number emission trends.

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