# GT2011-45\$, (

# MODELING OF SOOT AND NOX IN A FULL SCALE TURBINE ENGINE COMBUSTOR WITH DETAILED CHEMISTRY

T. Blacha, M. Di Domenico, M. Rachner, P. Gerlinger, M. Aigner Institute of Combustion Technology German Aerospace Center, DLR 70569, Stuttgart Germany

Email: Thomas.Blacha@dlr.de, Massimiliano.Didomenico@dlr.de, Michael.Rachner@dlr.de, Peter.Gerlinger@dlr.de

# ABSTRACT

A numerical simulation of spray atomization, combustion and soot formation in a full scale turbine engine combustor is presented and discussed in this work. Turbulence has been captured by a two equation turbulence model, chemistry by a detailed kinetic mechanism and turbulence chemistry interactions have been accounted for by an APDF-approach (assumed probability density function approach). For the kerosene fuel a surrogate has been used, consisting of n-decane, isooctane and toluene. The injection of the liquid fuel spray has been included by coupling the gas field CFD code with a spray code. Apart from the n-decane and isooctane reaction paths, the chemical kinetic reaction mechanism accounts for species as heavy as toluene. Polycyclic aromatic hydrocarbons heavier than toluene are represented by a sectional approach, while soot is calculated via soot volume fraction and particle number density. Main flow features are investigated and good agreement with the experimental measurements can be reported.

# INTRODUCTION

In combustion technology pollutants such as soot or nitric oxides have become more and more important during the last decades not only for health and environmental reasons [1–4] but also from the point of engineering [5–7]. For example, in combustion chambers soot may not only lead to locally elevated heat loads onto the walls through heat radiation, but it is also a marker for incomplete and therefore less efficient combustion.

Although soot has already been studied for several decades, it is still far from being completely understood [8]. Nevertheless, recent works show progress being made not only in the case of small laminar flames [9-13] but even in the field of turbulent combustion systems [14–16]. The special challenge concerning turbulent combustion systems is not only due to the fact, that turbulent phenomena (such as turbulence-chemistry interaction) need to be resolved, but it is also a matter of greater dimension ranges that are generally involved and therefore the necessity of very large computational grids. In consequence complex 3D turbulent combustion simulations usually come along with a high computational cost. In order to reduce the latter, empirical combustion models are often used such as eddy dissipation or turbulent flamelet models. However, the formation of pollutants such as soot or nitric oxides is much more complex and cannot solely be linked to a single scalar such as temperature, turbulent time scales or mixture fraction for a universally valid model [17]. In turn, the alternative of finite rate chemistry dealing with soot mechanisms containing several hundred species and thousands of reactions [18] appears to be much too expensive, although finite rate chemistry models generally feature a very big range of universal applicability.

In order to gap this bridge a soot model has recently been proposed by Blacha et al [13, 16, 19] showing good agreement concerning soot predictions in laminar and turbulent test cases. Extending the underlying chemical mechanism to a kerosene surrogate fuel and adding a nitric oxide sub mechanism, the current work aims to predict the formation of pollutants in a real scale turbine engine combustor without the need of any tuning.

#### NUMERICAL MODEL

All calculations were steady and have been performed with the DLR in-house Code THETA. A second DLR in-house Code SPRAYSIM has been coupled to THETA as it has already successfully been done in the past for similar applications in order to capture both spray and chemistry [20].

Based on a given flow field SPRAYSIM traces an ensemble of spray particles in a Lagrangian framework on unstructured grids until their evaporation. The action of gas field turbulence on the liquid was accounted for by the spectral droplet dispersion model of Blümcke [21]. The spray has been modeled using the three compound surrogate mentioned below with a mean Sauter diameter of  $10\mu m$  starting in an annular region above the actual spray nozzle. At the end of a spray tracing calculation SPRAYSIM passes source terms for momentum, turbulence, energy, mass and species mass fractions to the CFD solver THETA. Then, after a given number of iterations by the CFD solver, the new flow field is passed back to SPRAYSIM in order to relaunch a new spray tracing calculation. The whole spray-gas iteration process is continued until convergence is reached.

The CFD code THETA is an incompressible flow solver for finite volume grids which has been optimized for combustion problems. It features a multi grid algorithm, dual grid technique, a finite rate chemistry solver and parallelization via domain decomposition. Turbulence is captured using the two equation k- $\omega$ -SST model by Menter [22] and a RANS formulation for all transport equations. Turbulence-chemistry interactions have been included according to the work of Gerlinger [23] using an APDF approach (Assumed Probability Density Function). While the temperature is presumed to follow a clipped Gaussian function, species fluctuations are represented by a  $\beta$ -PDF according to Girimaji [24, 25].

#### Gas phase chemistry

The chemical kinetic mechanism of the gas phase consists of the base mechanism mentioned in [19] considering molecular species up to benzene and toluene. Furthermore a sub mechanism has been added for a kerosene surrogate fuel consisting of 12% toluene, 23% isooctane and 65% n-decane (molar). The sub mechanism has been derived from the work by Slavinskaya [26] where this surrogate has first been proposed. Although it consists only of three different hydrocarbons, the behavior of Jet A-1 is very well reproduced. This is not only due to the fact that the deviation in formation enthalpy is less than 2% but also that the amount of aromatics, n-alcanes and iso-alcanes have been chosen appropriately.



For predictions of nitric oxides the  $NO_x$  sub mechanism of the well known GRI 3.0 [27] has been added with the exception of molecular C reactions.

The base mechanism as well as the two sub mechanisms have already extensively been validated in the past by different authors [16, 19, 26, 28]. The conjunction of all three mechanisms has been validated for ignition delay with respect to Jet A-1 fuel. Unfortunately, no test cases dealing with laminar Jet A-1 fueled flames have been found in the literature. Moss et al. [29] studied a laminar flame fueled by a kerosene surrogate consisting of 77% n-decane and 23% mesitylene which has been simulated in the past using the mentioned base and kerosene sub mechanisms. For the fuel, the kerosene surrogate composition described above [30] but also an 80% n-decane 20% benzene blend [31] have been used. Good agreement with the experimental data was found in both cases as far as temperature and soot predictions are concerned.

### **PAH chemistry**

In the course of this work the PAH model first published by Blacha et al. [13] has slightly been modified. For the sake of completeness it will be given in full detail in the following. All aromatic molecules with a molecular mass between 100 and 800 g/mol are considered PAHs (Polycyclic Aromatic Hydrocarbons). They are represented by three logarithmically scaled PAH sections with a scaling factor of two as demonstrated in Fig. 1.

The intra PAH mass distribution function is assumed to be constant in particle number density. The impact of the distribution function on mean molecular masses, stoichiometric coefficients or soot predictions has been discussed elsewhere [13, 32]. Species specific data such as H/C ratio or enthalpy values could be inter- and extrapolated from 43 reference PAHs taken from the work of Yu et al. [33]. Transport properties have been obtained using a similar procedure with data by Richter et al. [34].

PAH chemistry is divided in four sub mechanisms namely  $PAH_0$  gas phase interaction,  $C_2H_2$  condensation onto PAH, PAH collision and PAH oxidation reactions.

 $PAH_0$  gas phase interactions consider all reactions of the gas phase with the first PAH including oxidation. In the current work 19 reversible reactions have been used and are summarized in Tab. 1. Reversible reactions are used at this point in order to capture the high reversibility of PAH formation reactions. PAH growth via  $C_2H_2$  condensation follows

**TABLE 1**. PAH0 GAS PHASE INTERACTION, UNITS ARE mol,cm, s AND K.

		$k_0$	α	$T_a$
$A_1^- + C_2 H_4$	$= PAH_0 + H$	2.51E+12	0.00	3095.00
$A_1^{-} + C_3H_4$	$= PAH_0 + H$	1.00E+16	0.00	16600.00
$A_1^{-} + C_3 H_3$	$= PAH_0$	6.46E+12	0.00	0.00
$A_1^- + C_4 H_2$	$= PAH_0 + C_2H$	2.00E+11	0.00	0.00
$A_1 + C_2H$	$= PAH_0 + H$	1.00E+12	0.00	0.00
$A_1 + C_2H_3$	$= PAH_0 + H$	7.90E+11	0.00	3200.00
$A_1 + A_1^-$	$= PAH_0 + H$	1.10E+23	-2.92	7450.00
$A_1 + A_1^-$	$= PAH_0$	2.000e+26	-3.90	3180.344
$C_7H_7 + CH_2$	$= PAH_0 + H$	2.40E+14	0.00	0.00
$C_{7}H_{7} + C_{3}H_{3}$	$= PAH_0 + 2H$	6.00E+11	0.00	0.00
$C_7H_7 + C_2H_2$	$= PAH_0 + H$	3.200e+11	0.00	3522.53
$PAH_0 + H$	$= A_1^- + C_2 H_2$	2.00E+14	0.00	4882.00
$PAH_0 + O$	$= A_1^{-} + HCCC$	D 2.10E+07	2.00	950.00
$PAH_0 + O$	$= A_1^{-} + CH_3 + CC$	D 1.92E+07	1.83	110.00
$PAH_0 + O$	$= C_7 H_7 + HCCC$	D 2.00E+13	0.00	2000.00
$PAH_0 + OH$	$= A_1^- + CH_2C$	O 2.18E-04	4.50	-500.00
$PAH_0 + OH$	$= A_1 + HCCC$	<b>2</b> .44E+03	3.02	5574.00
$PAH_0 + OH$	$= C_7 H_7 + C H_2 O$	1.40E+12	0.00	0.00
$PAH_0 + OH$	$= C_7H_7 + CH_2C$	O 1.00E+13	0.00	5000.00

$$PAH_i + C_2H_2 \rightarrow c_1 PAH_i + c_2 PAH_{i+1} + c_3 H_2$$
(1)

representing a global formulation of the well-known HACA mechanism [35, 36]. The stoichiometric coefficients  $c_1 - c_3$  are solely a function of the intra PAH mass distribution function and H atom conservation. For the last PAH section this reaction leads to soot instead of PAH<sub>i+1</sub>. In the present model this mechanism is regarded irreversible due to the uncertainty of backward reaction rates but the reversible character of PAH growth is already partially captured by the PAH<sub>0</sub> gas phase interaction model mentioned above.

The PAH collision model reads

$$PAH_i + PAH_j \rightarrow c_1 PAH_i + c_2 PAH_{i+1} + c_3 H_2$$
, with  $j \le i$ . (2)

Again this reaction leads to soot instead of  $PAH_{i+1}$  in case i = 2. The Arrhenius reaction rate for this reaction is

$$k = 2.2 N_a \gamma_{i,j} \beta_{i,j} \tag{3}$$

with 2.2 being the average Van der Waals enhancement factor according to Harris et al [37] and Miller [38],  $N_a$  the Avogadro

TABLE 2. ARRHENIUS PARAMETERS OF PAH MODEL.

		$k_0$	α	$T_a$
PAH-C <sub>2</sub> H <sub>2</sub> growth		$3.98\cdot 10^7$	0.0	5100
PAH-PAH collision		$0.66 N_a k_0^*$	0.5	0
PAH-oxidation	O <sub>2</sub>	$2.0\cdot 10^6$	0.0	3800
	OH	$2.1\cdot 10^7$	0.0	2300

constant,  $\gamma_{i,j}$  the collision efficiency and  $\beta_{i,j}$  the collision frequency. For  $\gamma_{i,j}$  a constant value of 0.3 was chosen [39]. Since for PAH collisions of this test case Kn > 1 holds,  $\beta_{i,j}$  can be calculated via

$$\beta_{i,j} = \underbrace{\sqrt{\frac{\pi k_B \left(m_{PAH_i} + m_{PAH_j}\right)}{2 m_{PAH_i} m_{PAH_j}} \left(d_{PAH_i} + d_{PAH_j}\right)^2} \sqrt{T}, \quad (4)$$

leading to the Arrhenius reaction rate

$$k = \underbrace{2.2N_a \gamma_{i,j} k_0^*}_{k_0} T^{0.5}.$$
 (5)

The PAH-oxidation mechanism takes  $O_2$  and OH oxidation into account through the reactions

$$PAH_i + O_2 \rightarrow c_1 PAH_{i-1} + c_2 PAH_i + c_3 H_2 + 2 CO,$$
 (6)

$$PAH_i + OH \rightarrow c_1 PAH_{i-1} + c_2 PAH_i + c_3 H_2 + CO.$$
(7)

Again, the stoichiometric coefficients  $c_1 - c_3$  are calculated based on the intra PAH mass distribution function. For i = 0it follows that  $c_1 = 0$  because PAH<sub>0</sub> oxidation leading to molecular species has already been captured by the PAH<sub>0</sub> gas phase interaction model.

Arrhenius coefficients of the discussed PAH sub models are summarized in Tab. 2.

#### Soot chemistry

All species heavier than the last PAH section are considered soot which is represented by soot mass fraction  $Y_s$  and soot number density  $N_s$ . The thermodynamic data of soot has been determined according to the work of Blacha et al. [13] using the same mass specific enthalpy as  $C_2H_2$  in order not to alter flame temperature. In the turbulent test case, thermophoresis and molecular diffusion are neglected for soot. Heat radiation from soot is captured with the assumption of an optically thin medium according to Di Domenico [39]. Neglecting heat absorption only heat loss is accounted for minimizing the computational effort. The calculation of the heat sink follows

$$\dot{q} = 4 \cdot \sigma_S \cdot \rho \cdot \alpha_{soot} \cdot Y_{soot} \tag{8}$$

where  $\sigma_S$  is the Stefan Boltzmann constant and

$$\alpha_{soot} = \frac{441 \frac{1}{Km}}{\rho_{soot}} \cdot T^5.$$
<sup>(9)</sup>

Since Eqn. (8) is strongly nonlinear in temperature space, heat radiation has been averaged using the temperature PDF in analogy to reaction rate averaging mentioned in [39]

$$\overline{\dot{q}} = 4 \cdot \sigma_S \cdot \overline{\rho} \cdot \overline{T} \cdot \overline{\left(\frac{\alpha_{soot}}{T}\right)} \cdot \overline{Y_{soot}}$$
(10)

with

$$\overline{\left(\frac{\alpha_{soot}}{T}\right)} = \int \frac{\alpha_{soot}}{\hat{T}} P(\hat{T}) d\hat{T}$$
(11)

where  $\overline{\left(\frac{\alpha_{\beta}}{T}\right)}$  has been calculated and tabulated in preprocessing as a function of mean temperature  $\overline{T}$  and temperature fluctuation

$$T_f = \frac{\sqrt{\sigma_T}}{\overline{T}}.$$
 (12)

The soot model considers collisions with PAH molecules,  $C_2H_2$  growth, oxidation, and coagulation (soot formation has already been accounted for in PAH chemistry) and has been taken from the work of Di Domenico [39]. In order to obtain a more general formulation all reactions have been transformed in Arrhenius like formulation.

$$S_r = k_0 T^{\alpha} \exp\left(\frac{-T_a}{T}\right) N_s^{O'_{N_s,r}} \prod_{\beta=0}^{N_{sp}} C_{\beta}^{O'_{\beta,r}}.$$
 (13)

Solely the soot PAH collision model needs extra considerations since it cannot directly be transformed because the corresponding source term reads

TABLE 3. SUMMARY OF CHEMICAL MECHANISM.

	species	reactions
base mechanism	43	304
kerosene sub mechanism	16	68
NO <sub>x</sub> sub mechanism	17	103
soot and PAH model	5	75
total	81	550

$$S_r = const. \cdot \underbrace{\left(d_{\text{PAH}_k} + d_s\right)^2 \cdot \sqrt{\frac{1}{m_s} + \frac{1}{m_{\text{PAH}_k}}}}_{(I)} \cdot T^{0.5} \cdot \left(c_{\text{PAH}_k} N_s\right).$$
(14)

with

$$d_s = \sqrt[3]{\frac{6\rho Y_s}{\pi \rho_s N_s}},\tag{15}$$

$$m_s = \frac{\rho Y_s}{N_s}.$$
 (16)

However the term in Eqn. (14) marked with (I) can be resolved assuming

$$\sqrt{\frac{1}{m_s} + \frac{1}{m_{\text{PAH}_k}}} \approx \sqrt{\frac{1}{m_s}} + \sqrt{\frac{1}{m_{\text{PAH}_k}}}.$$
 (17)

and Eqn. (14) can be transformed into a sum of six Arrhenius reaction rates. The maximum error of the assumption made in Eqn. (17) is 41% in case  $m_s = m_{\text{PAH}_k}$ . Since in most cases  $m_s >> m_{\text{PAH}_k}$ , this error is negligible.

The resulting overall mechanism consists of 81 species, 475 elementary and 75 global reactions as shown in Tab. 3.

#### **TEST CASE DESCRIPTION**

The considered test case concerns the combustion chamber of a Rolls-Royce Deutschland lean burn development combustor [40] at cruise conditions. The combustion chamber is an annular combustor, of which only one sector has been modeled using periodic boundary conditions to reduce the computational effort. Each sector contains a lean burn multi passage injector leading main air to the combustion chamber, while cooling air is supplied at the walls by thin slots or effusion holes. The effusion holes are not resolved during the simulation but modeled by thin inflow slots. The fuel is a Jet A-1 kerosene spray which, for the simulation, is represented by the kerosene surrogate mentioned above. It enters the combustion chamber either in the main combustion zone or through a pilot nozzle. For ignition usually the pilot takes 100% of the fuel in order to stabilize the flame. For cruise conditions though the aim is to achieve a pilot/main ratio as low as possible, since in the main region the mixing is much more efficient leading to less pollutants such as soot. Therefore most fuel is injected through the main injector during the current test case.

No temperature measurements have been performed but since the combustion process is very close to completion, a good guess for the average temperature in the exit plane is the equilibrium temperature. Furthermore probe measurements have been performed at the exit of the combustion chamber for the CO and NO<sub>x</sub> index [41] which can be calculated via

$$EI_{CO} = \frac{\dot{m}_{CO} \cdot 1000g/kg}{\dot{m}_{fuel}},$$
(18)

$$EI_{NO_{x}} = \frac{(\dot{m}_{NO} * 1.533 + \dot{m}_{NO_{2}}) \cdot 1000g/kg}{\dot{m}_{fuel}}.$$
 (19)

Based on Eqn. (19) CO and NO<sub>x</sub> mass fractions can be derived

$$Y_{\rm CO} = \frac{\mathrm{EI}_{\rm CO} \cdot \dot{m}_{fuel}}{\dot{m} \cdot 1000g/kg},\tag{20}$$

$$Y_{\rm NO_x} = \frac{\rm EI_{\rm NO_x} \cdot \dot{m}_{fuel}}{\dot{m} \cdot 1000g/kg}$$
(21)

where

$$Y_{\rm NO_x} = Y_{\rm NO} * 1.533 + Y_{\rm NO_2}.$$
 (22)

The soot volume fractions have not been measured directly but smoke numbers have been determined at the combustion chamber exit. Empirical transformation tables to soot volume fraction exist but it should be kept in mind that using this technique measurement uncertainties are relatively high.

The computational grid consists of three million polyhedrons namely tetrahedrons, hexahedrons and pyramids. Calculations were parallelized on 128 Intel Xeon processors and took approximately one month for this test case.

TABLE 4. NORMALIZATION VARIABLES.

variable	normalized with
temperature, T	equilibrium temperature
soot volume fraction, $fv$	measured $fv$
CO mass fraction, $Y_{CO}$	measured $Y_{\rm CO}$
$NO_x$ mass fraction, $Y_{NO_x}$	measured $Y_{\rm NO_x}$
NO mass fraction, $Y_{\rm NO}$	measured $Y_{\rm NO_x}$
NO <sub>2</sub> mass fraction, $Y_{NO_2}$	measured $Y_{\rm NO_x}$

#### RESULTS

For reasons of confidentiality the results are presented in normalized formulation. The choice of normalization base is summarized in Tab. 4

**TABLE 5**.
 SIMULATED NORMALIZED VALUES AT THE EXIT.

Т	$Y_{\rm CO}$	$Y_{\rm NO_x}$	fv
1.015	0.7	2.7	0.3

A summary of the simulated values at the exit plane - where measurements were taken - can be found in Tab. 5. The prediction of the averaged soot volume fraction being less than a factor of 4 below the measured values can be considered good. On the one hand smoke number measurements imply high uncertainties when they are related to soot volume fraction. On the other hand a deviation in the prediction of soot volume fraction in the range of an order is nothing exceptional for complex 3D combustion chambers. One reason for this deviation range is due to the high simplification level of soot related reactions in current models as in reality soot involves thousands of different species and pathways which are still far from being completely understood. Furthermore soot also strongly depends on the flow field and gas phase species such as hydrogen, acetylene or aromatics. Because of the high complexity of a real scale combustor, no measurements have been performed neither for the flow field nor concerning selected species leaving few room for interpretations in this context. Likewise it is possible that the unsteady fluctuations inside the combustor are not just small scale turbulence effects but large scale phenomena affecting the whole flow field. In this case unsteady methods such as URANS instead of stationary RANS would give much more reliable results. Moreover, two equation turbulence models are limited in their applicability in particular when applied to complex 3D configurations. Here LES simulations are much more accurate. However, stationary RANS equations have been solved instead in favor of the computational efficiency. Whereas for the current test case URANS simulations would increase the effort by approximately a factor 5, the applicability of LES simulations is still beyond all question. Furthermore turbulence chemistry interactions are modeled by a simple but very cost efficient APDF approach. Certainly, both species PDF and temperature PDF can be modeled much more accurately using transported PDF methods, but again the additional computational cost of such methods would be prohibitive.

CO levels are by a factor of 1.5 lower whereas  $NO_x$  levels are by a factor of 2.7 higher than the measurements. The deviations from the experimental values may be explained by uncertainties in the flow field due to turbulence modeling but also turbulence chemistry interactions may play an important role as mentioned above. In addition, it has already been found in the past that the GRI 3.0  $NO_x$  sub mechanism may overpredict NO levels by a factor two in the case of partially premixed flames and that there is a general need for further refinement and validation of detailed  $NO_x$  mechanisms [28]. Keeping in mind the high uncertainty of probe measurements at the exit plane and the general uncertainty of NO predictions, the simulated CO and  $NO_x$  values are in good agreement with the experimental data.

The averaged normalized temperature is slightly larger than the equilibrium temperature revealing that boundary conditions are not completely consistent with the experiment. In particular wall temperatures have never been measured during the experiment and might have been overestimated leading in turn to extra heat flux into the combustor. However the deviation of no more than 2% is considered to be very small although exit temperatures slightly below the equilibrium temperature should be expected.

Figure 2 shows the temperature distribution in the combustion chamber. A complex flame structure can be observed with peak temperatures 1.5 times higher than at equilibrium. Respecting that the equilibrium temperature has been calculated based on the overall lean combustion including oxidation air, this does not surprise, because in the flame zone fuel to air ratios close to stoichiometry appear. The high efficiency of the wall cooling in the first half of the combustor is also visible. In these regions a cold air layer protects the combustor walls from hot gases of the flame. Fig. 8 illustrates that in the exit plane of the combustor there is a non-uniform temperature distribution as it was found before by [40]. Although this finding indicates insufficient mixing, it needs to be kept in mind that optimal mixing in a full scale 3D combustion chamber is not a trivial task but in deed one of the main research objectives in the field of combustor development.

Figures 3 and 4 show the regions where soot can be found. As expected high soot concentrations are found in rich regions where the spray condenses to gas phase. Along the center plane



**FIGURE 2**. CONTOUR SLICES AND ISOSURFACE AT 1.4 OF NORMALIZED TEMPERATURE.



**FIGURE 3**. CONTOUR SLICES AND ISOSURFACE AT 1000 OF NORMALIZED SOOT VOLUME FRACTION. THE PURPLE SUR-FACE INDICATES AN ISOSURFACE ON N-DECANE (RICH REA-GIONS).



**FIGURE 4**. ISOSURFACE OF NORMALIZED SOOT VOLUME FRACTION AT 1 AND CONTOUR SLICES OF TEMPERATURE.



**FIGURE 5**. CONTOUR SLICES AND ISOSURFACE AT 30 OF NORMALIZED CO MASS FRACTION.



**FIGURE 6**. CONTOUR SLICES OF NORMALIZED NO MASS FRACTION.



**FIGURE 7**. CONTOUR SLICES AND ISOSURFACE AT 0.2 OF NORMALIZED NO<sub>2</sub> MASS FRACTION.



**FIGURE 8**. CONTOUR OF NORMALIZED TEMPERATURE IN EXIT PLANE.



**FIGURE 9**. CONTOUR OF NORMALIZED SOOT VOLUME FRACTION IN EXIT PLANE.



**FIGURE 10**. CONTOUR OF NORMALIZED CO MASS FRAC-TION IN EXIT PLANE.



**FIGURE 11**. CONTOUR OF NORMALIZED NO<sub>x</sub> MASS FRACTION IN EXIT PLANE.

it seems that no soot reaches the exit of the combustion chamber but that it is completely oxidized. However Fig. 4 demonstrates that there are pathways where soot oxidation is nearly frozen. Since these pathways are in cold regions close to the wall and soot oxidation rates are strongly temperature dependent it is very probable that the wall cooling air layer is responsible for the constraint of soot oxidation.

Carbon monoxide values are displayed in Fig. 5. The extreme ratio of peak and exit CO levels illustrates the efficient degradation of this pollutant. As expected also CO is mainly formed in rich regions. Moreover Figs. 9 and 10 reveal that there is a strong correlation between CO and soot. One reason for this correlation is certainly that being formed in similar regions both CO and soot follow similar spacial pathways except for the influence of diffusion. Therefore also CO oxidation rates are probably constrained by the wall cooling air layer. On the other hand the soot oxidation mechanism which can generally be described via

$$\operatorname{soot} + \operatorname{O}_2 \to \operatorname{soot} + 2\operatorname{CO},$$
 (23)

$$\operatorname{soot} + \operatorname{OH} \to \operatorname{soot} + \operatorname{CO}$$
 (24)

is also a source of CO. However in both cases it is the wall cooling air layer leading to elevated CO levels in the exit plane. A comparison with Fig. 8 reinforce this finding, because CO levels peak where temperature levels are low.

The distributions of NO and NO<sub>2</sub> in Figs. 6 and 7 respectively demonstrate that the main contributor to nitric oxides is NO which shows very high concentrations in the flame zone degrading slowly to the end of the combustor. NO<sub>2</sub> in turn is only found in smaller quantities preferably at lower temperatures. To the end of the combustor it can therefore mainly be found near the walls. Figures 8 and 11 reveal furthermore that there is a strong correlation between temperature and NO<sub>x</sub> levels. This is mainly due to the fact that the dominating nitric oxide NO requires high temperatures for its formation and that it degrades in colder regions.

# CONCLUSIONS

Pollutants and temperature distributions have successfully been modeled for a full scale turbine engine combustor. Soot, CO and NO<sub>x</sub> predictions are in good agreement with experimental data and show important insight in the formation and decomposition of these pollutants. In particular soot and CO seem to be strongly effected by wall cooling air layers which constrain oxidation whereas on hotter pathways they are completely oxidized before the end of the combustor. Nitric oxide emissions are clearly dominated by NO at concentrations approximately an order higher than NO<sub>2</sub>. Towards the end of the combustor CO and soot emissions being linked to cold gas regions and NO being linked to hot gas regions are all a function of mixing efficiency. Consequently, in order to further reduce emission levels high emphasis on the improvement of mixing efficiency should be taken. In particular, the influence of cooling air forming cold channels, where combustion is nearly frozen, should be taken into account.

The agreement between simulation and experimental measurements is very promising. However, the computational effort for a single test case is still beyond the limit of practical applications and needs further optimization in the future.

#### ACKNOWLEDGMENT

Thanks go to R. Eggels and Rolls Royce Deutschland for offering the experimental data of the test case.

# NOMENCLATURE

с	stoichiometric coefficients
С	concentration, $mole/m^3$
d	diametre, m
EI <sub>CO</sub>	CO index
EI <sub>NOx</sub>	$NO_x$ index
fv	soot volume fraction
k	Arrhenius reaction rate
$k_0$	constant of Arrhenius reaction rate
m	mass, <i>kg</i>
'n	mass flow, $kg/s$
$N_s$	soot number density
Nsp	number of species
O'	reaction order of educt
Р	probability density function
ġ	heat flux, $W/m^3$
$S_r$	source term of reaction r
Т	temperature, K
$T_{f}$	temperature fluctuation
$T_a$	activation temperature, K
Y	mass fraction
$Y_s$	soot mass fraction
α	exponent of Arrhenius reaction rate
$\alpha_{soot}$	soot radiation coefficient, $K^4m^2/kg$
β	collision frequency
γ	collision efficiency
ρ	density, $kg/m^3$
$\sigma_T$	temperature variance, $K^2$

- REFERENCES
- [1] Barfknecht, T. R., 1983. "Toxicology of soot". *Progress in Energy and Combustion Science*, **9**(3), pp. 199–237.

- [2] Jensen, E., and Toon, O., 1996. "The potential impact of soot particles from aircraft exhaust on cirrus clouds". *Nucleation and Atmospheric Aerosols*, pp. 848–851.
- [3] Petzold, A., Ström, J., Schröder, F., and Kärcher, B., 1999. "Carbonaceous aerosol in jet engine exhaust: emission characteristics and implications for heterogeneous chemical reactions". *Atmospheric Research*, 33(17), pp. 2689– 2698.
- [4] Mauzerall, D., Sultan, B., Kim, N., and Bradford, D. F., 2005. "NOx emissions from large point sources: variability in ozone production, resulting health damages and economic costs". *Atmospheric Environment*, 39(16), May, pp. 2851–2866.
- [5] Lee, C., 1975. "Estimates of luminous flame radiation from fires". *Combustion and Flame*, **24**, pp. 239–244.
- [6] Lefebvre, A., 1969. "Radiation from flames in gas turbines and rocket engines". *International Symposium on Combustion*, 12(1), pp. 1247–1253.
- [7] Nakamura, M., Koda, S., and Akita, K., 1982. "Sooting behavior and radiation in methanol/benzene/air diffusion flames". *International Symposium on Combustion*, 19(1), pp. 1395–1401.
- [8] Kennedy, I., 1997. "Models of soot formation and oxidation". *Prog. Energy Combust. Sci.*, 23, pp. 95–132.
- [9] Naydenova, M., 2007. "Soot formation modeling during hydrocarbon pyrolysis and oxidation behind shock waves". PhD thesis, Rupertus Carola University of Heidelberg, June.
- [10] Kronholm, D., 2000. "Molecular weight growth pathways in fuel-rich combustion". PhD thesis, Massachusetts Institute of Technology, June.
- [11] D'Anna, A., and Kent, J., 2008. "A model of particulate and species formation applied to laminar, nonpremixed flames for three aliphatic-hydrocarbon fuels". *Combustion and Flame*, 152, pp. 573–587.
- [12] Richter, H., Granata, S., Green, W., and Howard, J., 2005.
   "Detailed modeling of PAH and soot formation in a laminar premixed benzene/oxygen/argon low-pressure flame". *Proceedings of the Combustion Institute*, 30, pp. 1397–1405.
- [13] Blacha, T., Domenico, M. D., Gerlinger, P., and Aigner, M., 2010. "Soot modeling in partially premixed C<sub>2</sub>H<sub>4</sub>/air flames". AIAA paper 2010-1516, 48th AIAA Aerospace Sciences Meeting and Exhibit, January.
- [14] Wen, Z., Yun, S., Thomson, M., and Lightstone, M., 2003.
   "Modeling soot formation in turbulent kerosene/air jet diffusion flames". *Combustion and Flame*, *135*, pp. 323–340.
- [15] El-Asrag, H., Lu, T., Law, C., and Menon, S., 2007. "Simulation of soot in turbulent premixed flames". *Combustion and Flame*.
- [16] Blacha, T., Domenico, M. D., Köhler, M., Gerlinger, P., and Aigner, M., 2011. "Soot modeling in a turbulent unconfined C<sub>2</sub>H<sub>4</sub>/air jet flame". AIAA paper 2011-0114, 49th AIAA

Aerospace Sciences Meeting and Exhibit, January.

- [17] Lignell, D., Chen, J., Smith, P., Lu, T., and Law, C., 2008. "The effect of flame structure on soot formation and transport in turbulent nonpremixed flames using direct numerical simulation". *Combustion and Flame*, **151**, pp. 316–333.
- [18] Howard, J., 2010. Kinetic models and data used in calculations. On the WWW. URL http:// web.mit.edu/anish/www/MITcomb.html.
- [19] Blacha, T., Domenico, M. D., Slavinskaya, N., Gerlinger, P., and Aigner, M., 2011. "Modeling of soot size distributions in partially premixed C<sub>2</sub>H<sub>4</sub>/air flames". AIAA paper 2011-0414, 49th AIAA Aerospace Sciences Meeting and Exhibit, January.
- [20] Le Clercq, P., Domenico, M. D., Rachner, M., Ivanova, E., and Aigner, M., 2010. "Impact of fischer-tropsch fuels on aero-engine combustion performance". *AIAA-2010-0613*, 48th AIAA Aerospace Science Meeting, January.
- [21] Blümcke, E., Brandt, M., Eickhoff, H., and Hassa, C., 1993.
   "Particle dispersion in highly swirling, turbulent flows". *Particle & Particle Systems Characterization*, 10, pp. 182–190.
- [22] Menter, F., 1994. "Two-equation eddy-viscosity turbulence models for engineering applications". *AIAA Journal*, 32(8), August.
- [23] Gerlinger, P., 2006. Numerische Verbrennungssimulation, Effiziente numerische Simulation turbulenter Verbrennung, 1<sup>st</sup> ed. Springer.
- [24] Girimaji, S., 1991. "A simple recipe for modeling reactionrates in flows with turbulent-combustion". AIAA-91-1792, 22nd Fluid Dynamics, Plasma Dynamics and Lasers Conference.
- [25] Girimaji, S., 1991. "Assumed beta-pdf model for turbulent mixing: Validation and extension to multiple scalar mixing". *Combustion, Science and Technology*, 78, pp. 177– 196.
- [26] Slavinskaya, N., 2008. "Skeletal mechanism for kerosene combustion with pah production". AIAA paper 2008-0992, 46th AIAA Aerospace Sciences Meeting and Exhibit, January.
- [27] Smith, G., Golden, D., Frenklach, M., Moriarty, N., Eiteneer, B., Goldenberg, M., Bowman, C., Hanson, R., Song, S., Gardiner, W., Lissianski, and Qin, Z., 1999. Homepage of gri3.0. On the WWW. URL http://www.me.berkeley.edu/gri\_mech.
- [28] Barlow, R., Karpetis, A., Frank, J., and Chen, J., 2001. "Scalar profiles and no formation in laminar opposed-flow partially premixed methane/air flames". *Combustion and Flame*, 127, pp. 2102–2118.
- [29] Moss, J., and Aksit, I., 2007. "Modelling soot formation in a laminar diffusion flame burning a surrogate kerosene fuel". *Proceedings of the Combustion Institute*, 31, pp. 3139–3146.

- [30] Blacha, T. "Entwicklung eines Rußmodells mit sektionalem Ansatz für die Anwendung in laminaren und turbulenten Flammen". PhD thesis, Universität Stuttgart, Germany (to be published).
- [31] Di Domenico, M., Gerlinger, P., and Aigner, M., 2010. "Development and validation of a new soot formation model for gas turbine combustor simulations". *Combustion and Flame*, 157, pp. 246–258.
- [32] Pope, C., and Howard, J., 1997. "Simultaneous particle and molecule modeling (spamm): An approach for combining sectional aerosol equations and elementary gas-phase reactions". *Aerosol Science and Technology*, 27, pp. 73–94.
- [33] Yu, J., Sumathi, R., and Green, W., 2004. "Accurate and efficient method for predicting thermochemistry of polycyclic aromatic hydrocarbons – bond-centered group additivity". *JACS, ISSN 0002-786*, *126*, pp. 12685–12700.
- [34] Richter, H., and Howard, J., 2009. Kinetics models and data used in calculations. On the WWW. URL http://web.mit.edu/anish/www/MITcomb.html.
- [35] Frenklach, M., Clarya, D., Gardiner, W., Stein, J., and Stein, S., 1985. "Detailed kinetic modeling of soot formation in shock-tube pyrolysis of acetylene". *International Symposium on Combustion*, 20(1), pp. 887–901.
- [36] Frenklach, M., and Wang, H., 1990. "Detailed modeling of soot particle nucleation and growth". *International Symposium on Combustion*, 23, pp. 1559–1566.
- [37] Harris, S., and Kennedy, I., 1988. "The coagulation of soot particles with van der waals forces". *Combustion Science and Technology*, **59**, pp. 443–454.
- [38] Miller, J., 1991. "The kinetics of polynuclear aromatic hydrocarbon agglomeration in flames". *International Symposium on Combustion*, **23**(1), pp. 91–98.
- [39] Di Domenico, M., 2008. "Numerical simulations of soot formation in turbulent flows". PhD thesis, Universität Stuttgart, Germany.
- [40] Lazik, W., Doerr, T., Bake, S., Bank, R., and Rackwitz, L., 2008. "Development of lean-burn low-nox combustion technology at rolls-royce deutschland". *Proceedings* of the ASME Turbo Expo 2008, Power for Land, Sea and Air, GT2008-51115, June.
- [41] Eggels, R., 2010., April. Email correspondance between R. Eggels and T. Blacha.