Numerical Investigation of Reacting Flows in Gas Turbine Model Combustors

A. Fiolitakis, C. Eberle, M. Grader

published in

NIC Symposium 2018
K. Binder, M. Müller, A. Trautmann (Editors)

Forschungszentrum Jülich GmbH,
John von Neumann Institute for Computing (NIC),
Schriften des Forschungszentrums Jülich, NIC Series, Vol. 49,
ISBN 978-3-95806-285-6, pp. 397.
http://hdl.handle.net/2128/17544

Numerical Investigation of Reacting Flows in Gas Turbine Model Combustors

Andreas Fiolitakis, Christian Eberle, and Martin Grader

Institute of Combustion Technology, German Aerospace Center (DLR),
Pfaffenwaldring 38-40, 70569 Stuttgart, Germany
E-mail: {andreas.fiolitakis, christian.eberle, martin.grader}@dlr.de

The present work addresses the simulation of generic gas turbine model combustors by means of computational fluid dynamics. Two different combustors are considered: a pressurised aero-engine model combustor and an atmospheric single-nozzle flameless oxidation (FLOX) combustor. The first of these combustors serves as a validation case for soot models. Results of Large-Eddy Simulations of this combustor in conjunction with a finite rate chemistry combustion model and a comprehensive sectional soot model are presented. The second combustor serves as validation test case for a statistical approach for combustion modelling, namely a transported probability density function method. Simulation results obtained with this statistical approach are presented in this work.

1 Introduction

Although combustion is one of the oldest technologies known to mankind, its theoretical understanding is still a field of active research. This stems mainly from the fact that technical combustion occurs predominantly in turbulent flows. Hence, the understanding of combustion is closely linked with a profound understanding of turbulence. Turbulence, however, represents one of the few, still unresolved problems in physics. Although the fundamental equations describing the motion of a turbulent flow (i.e. the conservation equations for momentum, mass, and energy) are known, the solution of these equations even for simple flow configurations poses a significant challenge: turbulent flows exhibit a random nature of motion and are highly unsteady. General analytical solutions of this systems of equations do not exist. Direct numerical solutions on the other hand prove to be prohibitive for most applications. The computational cost increases drastically with the level of turbulence contained in the flow due to vast span of temporal and spatial scales, which need to be resolved.

Hence, attempts are made to solve equations for spatially filtered or statistically averaged equations. However, due to the non-linearity of the governing equations, one obtains a series of unknown correlations. This so called “closure problem” of turbulence has led to a multifold of turbulence models, which provide closures for the unknowns terms in the equations.

Turbulent combustion is even more difficult than pure fluid mechanics. For the simulation of turbulent combustion additional transport equations have to be solved in order to determine the concentration of reacting chemical components (or species). As in the case of the momentum, energy, and mass conservation equations, these species transport equations have to undergo also a filtering or averaging operation. In doing so an additional unclosed term appears in the system of equations, namely the filtered (or averaged) chemical production rate. This term is a non-linear function of temperature and composition and is, therefore, extremely difficult to model. Different “combustion models” are

available in literature to tackle this closure problem and their development is even today a field of active research. In the present work two different approaches are pursued for combustion modelling: an "assumed probability density function" closure for subgrid-scale turbulence-chemistry-interaction in the framework of large-eddy simulations, and a statistical approach termed "transported probability density function" method. Both approaches are outlined in the next section. One of the main objectives in this work is the investigation of turbulent combustion by means of these two approaches.

One reason for the pressing need for combustion research are the environmental problems connected with the use of combustion. Pollutants like carbon monoxide, nitric oxides, and soot have a negative impact on the environment and human health. Additionally, the emission of combustion products like carbon dioxide and other "greenhouse gases" influence the radiation budget of the earth, thus leading to global warming and climate change. Hence, efforts are made to reduce pollutants in the exhaust gases and the emission of greenhouse gases. This highly relevant topic is also addressed in the present work: with the help of large-eddy simulations the soot emissions in an academic, though technically relevant model combustors are analysed with the help of a sectional soot model. The objective here is to develop highly accurate methodologies for the prediction of soot emissions.

2 Methodology

In this work two different methods are used, namely large-eddy simulation (LES) and a transported probability density function method. These approaches are outlined briefly in the following.

2.1 Large-Eddy Simulation for Soot Prediction

The basic concept of large-eddy simulation (LES) is to resolve the large, energy containing scales of a turbulent flow whereas the small scales are modelled. The advantage of this approach lies in the fact, that any macroscopic motion is properly resolved. At the same time any unresolved part is of "universal nature" which facilitates the modelling of these quantities. In this work the "wall adapting local eddy viscosity" (WALE[11]) is used to model the subgrid-scale stress tensor. Subgrid-scale source terms of thermochemical quantities are closed by an "assumed probability density function" (APDF) model[8]. It accounts for the influence of subgrid-scale temperature and composition fluctuations. The mathematical shape of the probability density function is assumed in this approach and it is parameterised by subgrid-scale variance of temperature and the trace of the species covariance matrix. An important aspect in this simulation is the inclusion of soot. Kinetic models are necessary which can reproduce the relevant processes of soot formation: starting from the gas phase species, large poly-aromatic molecules are formed which grow further in size and form in the end soot particles. This chemical process is not fully understood yet and has, therefore, to be modelled. To this end a sectional model[4] is used here. To model gas phase chemistry a detailed reaction mechanism is necessary. This increases the size of the simulation drastically: A total of 81 equations have to be solved for this problem, i.e. 16 times more equations than for a non-reacting flow. However, only such an extensive modelling provides reliable results.

2.2 Transported Probability Density Function Method

In contrast to LES, where the large scales of the turbulent flow are resolved, the approach in the transported probability density function (TPDF) method is entirely different. The idea behind this approach is to regard the turbulent flow as a random process. In a given point in physical space and time quantities like velocity, density, composition, temperature, and pressure are random variables. The distribution of these random variables is described statistically by their joint probability density function (PDF). The idea behind the TPDF method is to determine this PDF through the solution of a PDF transport equation. For chemically reacting flows a PDF transport equation was initially proposed by Dopazo and O'Brien[1,2] and Pope[12]. The tremendous advantage of such an approach lies in the fact, that the chemical production rate, which is difficult to model in averaged or filtered equations, appears in closed form. Therefore, this methodology is in particular attractive for the modelling of turbulent combustion.

In the present work only thermochemical quantities are considered in the PDF. The flow velocities and turbulence time and length scales are provided by solving the conservation equations for mass and momentum together with turbulence model equations. These are solved by a finite volume method (for details refer to Sec. 2.3). The PDF transport equation is treated, however, differently. This equation has a very high dimensionality. Not only does this equation include changes of the PDF in physical space and time, but also in the thermochemical space. Hence, a Monte-Carlo methods is employed here as proposed by Pope[13]. In this Monte-Carlo method different samples or "stochastic particles" are simulated. These particles change their thermochemical composition and their position in physical space due different physical and chemical processes. Like in an experiment, these samples are then used to compute statistical quantities like expectations. Details on the method used in the present work are provided by Fiolitakis *et al.*[5,6].

2.3 THETA Code

For the simulations in this project the DLR in-house code THETA (**T**urbulent **H**eatrelease **E**xtension of the **TA**U code) is used. It is a low Mach-number extension of the DLR TAU code. THETA utilises unstructured meshes and is thus well suited for the numerical investigation of complex geometries. The numerical details are given in the following list:

- Time discretisation: First-order and second-order
- First, second, and fourth order spatial discretisation schemes
- Krylov space solvers
- Multigrid methods
- Incompressible and compressible pressure correction methods
- Lagrangian Monte-Carlo method for the solution of the TPDF model equation
- Implicit treatment of chemical source term with analytical Jacobian matrix

The code provides a variety of different turbulence and combustion models. This includes:

- WALE-LES model
- Scale-Adaptive Simulation (SAS) model
- Various two-equation turbulence models for RANS (Reynolds Averaged Navier Stokes) simulations
- Detailed soot and soot precursor models (sectional approach)
- Models for turbulent combustion:
  - TPDF method for the joint-thermochemical PDF
  - Finite Rate Chemistry (FRC)
  - FRC with assumed-PDF model in temperature and composition
  - Steady Flamelet-PDF model
  - Eddy Dissipation Model (EDM)

The scalability of the THETA code on JURECA is shown in Fig. 1 for the finite volume solver and the Monte-Carlo method. The speed up shown here is normalised to 192 cores for the finite volume method and to 96 cores for the Monte-Carlo method. The finite volume method, which is used for the simulations described in Sec. 3.1 shows an excellent scalability up 1536 cores. For the Monte-Carlo method, the speed up is not as good beyond 384 physical cores. This is due to the parallelisation strategy of the Monte-Carlo method. A pure particle partitioning has been used for the simulations presented in this work. This means, that each parallel processes gets a fraction of the particles residing in a cell of the computational mesh. Hence, on each parallel process the entire computational mesh is present. In situations, where the mesh size is large, this strategy results in a large communication overhead which has a negative impact on the parallel performance. To compute, for example, the average of the particle data in a cell, the partial sums of each cell must be exchanged for all cells of the computational mesh. This so called "All-to-all" communication is very expensive in terms of communication time and affects, therefore, the parallel performance of the Monte-Carlo method. A solution to this problem is to introduce a domain decomposition of the Monte-Carlo method which is future work.

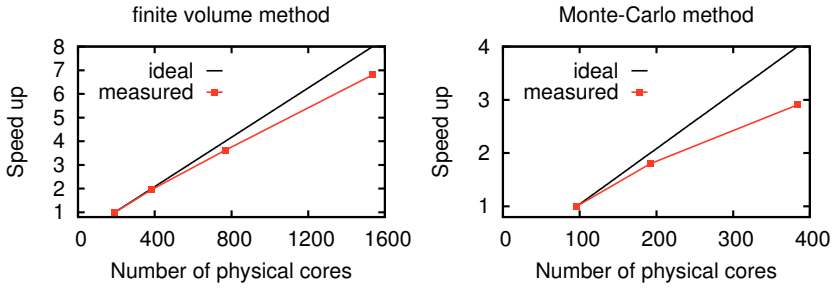

Figure 1. Scalability of the finite volume and Monte-Carlo method in THETA on JURECA.

3 Simulations

3.1 LES of Soot Formation in Aero-Engine Model Combustor

LES has been used here in conjunction with a finite rate chemistry combustion model, an assumed PDF closure for the subgrid-scale chemical source terms, and a sectional soot model, in order to investigate the formation of soot in an aero-engine model combustor. The computational model of the injection system of this burner is shown in Fig. 2. Primary air at ambient temperature is supplied through two co-swirling air flows which can be controlled separately. Gaseous fuel (ethylene) is injected between these air flows through 60 straight channels. The fuel channels form a concentric ring and mimic the atomising lip for spray combustion in aero-engine combustors. Due to the swirling motion of the air flows, a compact swirl flame is established here, which is stabilised by inner and outer recirculation zones. In addition, the injection of secondary air further downstream is possible. In this way the secondary air injection in aero engines, which is used to oxidise the soot formed in the fuel rich primary zone, is imitated in this experiment. On this burner different operating points ("OP") were investigated. Starting from a reference operating point "OP5" with secondary air injection, this secondary air injection is first deactivated and the effect on soot is studied. This operating point without secondary air injection is termed "OP4". In a further variation, the fuel mass flow rate is increased compared to operating point "OP5" but the secondary air injection remains active. This operating point is termed "OP9".

Computational results for the three operating points are summarised together with experimental data in Fig. 3. Comparing first "OP4" to the reference point "OP5" it is found experimentally, that the amount of soot increases drastically. The soot fills up the entire space in the combustion chamber since no secondary air is available for its oxidation. Com-

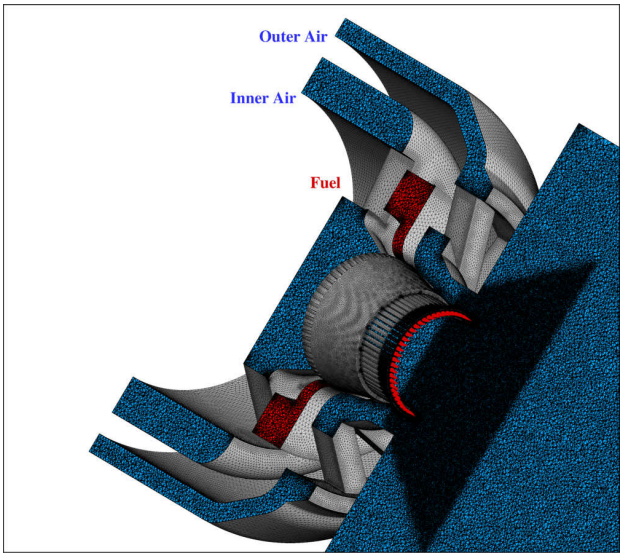

Figure 2. The aero-engine model combustor (reproduced from Eberle *et al.*[3]). Detailed view of injection system.

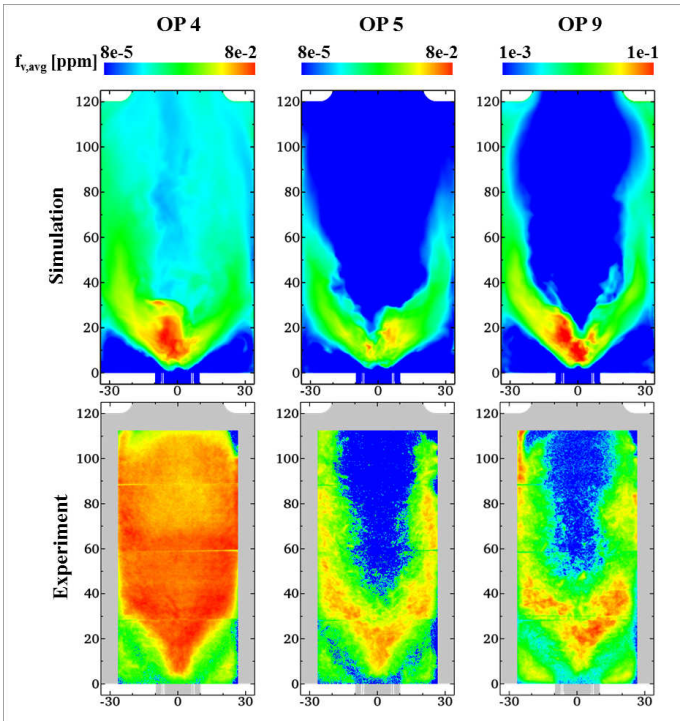

Figure 3. Predicted (reproduced from Grader *et al.*[9]) and measured (Geigle *et al.*[7]) time-averaged soot volume fractions in turbulent swirl flames at different operating conditions.

paring on the other the side soot distributions of "OP5" to "OP9" shows however hardly any difference in the shape of the soot structures. However, the maximum amount of soot found in the structures increases in "OP9" due to the richer combustion conditions.

These trends, though easy to understand qualitatively, are extremely difficult to predict quantitatively by means of LES. The simulation results given in Fig. 3 demonstrate that the present methodology (i.e. sectional soot model with finite rate chemistry combustion model and LES) is capable to predict the trends quantitatively. The volumetric soot distribution in "OP4" as well as the increase of soot emissions in "OP9" are accurately reproduced by the model.

3.2 TPDF Simulation of Confined Jet Flame

In the present work the TPDF method is used for the simulation of a confined jet flame which has essential features of a "flameless oxidation" (FLOX) burner. One half of the burner is shown together with stochastic particles of the Monte-Carlo method and computed streamlines of the flow in Fig. 4. The combustion chamber is hexahedral and has a single nozzle on its bottom. Here, a mixture of air and methane is injected as a turbulent jet into the combustion chamber. Due to the high momentum of the jet a recirculation zone is formed which transports exhaust gases back to the injection nozzle, where they mix with

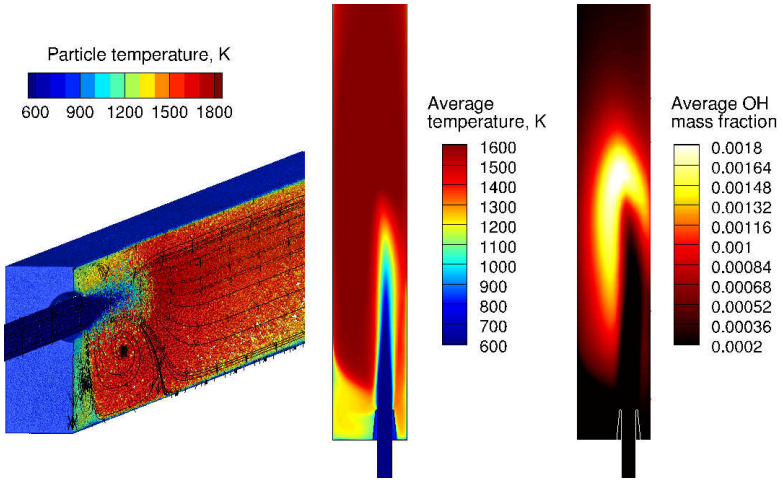

Figure 4. Results of TPDF simulation.

the reactants and help thus ignite the mixture and stabilise the flame. Additionally, the re-circulated exhaust gases serve as a diluent which helps to avoid temperature peaks and thus to reduce emissions of nitric oxides. Such a combustion process is frequently encountered in FLOX burners.

The stochastic particles shown in Fig. 4 represent "virtual samples" of the turbulent flow in this burner. To each of them an individual thermochemical state is assigned. As an example, the particles shown in Fig. 4 are coloured with their individual temperature. The distribution of these particle properties models essentially the distribution in the real flow. With the help of the particle data averages can be computed as shown in Fig. 4 for the hydroxyl (OH) mass fraction or temperature. Due to the fact, that the effect of chemical reactions appears closed in this method (cf. Sec. 2), the approach is well suited for kinetically controlled effects like flame lift-off, which is typical for flames in gas turbine. This effect can be successfully reproduced as Fig. 4 shows: the OH distribution (which is a marker for the reaction zone) is clearly detached from the nozzle, which indicates a lifted flame. This behaviour has also been observed experimentally[10].

4 Summary

In the present work CFD simulations using the DLR in-house code THETA are presented for two different combustion systems, namely a generic aero-engine model combustor and a single-nozzle FLOX combustor. These are simulated with different model approaches available in THETA. LES is used in conjuction with a sectional soot model, an assumed PDF closure for the subgrid-scale chemical source terms, and a finite rate chemistry combustion model in order to study soot formation in the aero-engine model combustor. A TPDF method on the other side is used to study the combustion in a FLOX burner. It is demonstrated that both models can reproduce the relevant effects in each of the combustion systems accurately. The scalability of the THETA code is also analysed here. An excellent

scalability was found for the finite volume solver in THETA. The scalability of the Monte-Carlo method in THETA is sufficient for the simulation presented but needs to be revised for larger problems. Future work will therefore focus on improving the scalability of this particular solver.

Acknowledgements

The authors gratefully acknowledge the computing time granted by the John von Neumann Institute for Computing (NIC) and provided on the supercomputer JURECA at Jülich Supercomputing Centre (JSC).

References

1. C. Dopazo and E. E. O'Brien, *An Approach to the Autoignition of a Turbulent Mixture*, Acta Astronautica **1**, 1239–1266, 1974.
2. C. Dopazo and E. E. O'Brien, *Statistical Treatment of Non-Isothermal Chemical Reactions in Turbulence*, Combustion Science and Technology **13**, 99–122, 1976.
3. C. Eberle, P. Gerlinger, K. P. Geigle, and M. Aigner, *Numerical Investigation of Transient Soot Evolution Processes in an Aero-Engine Model Combustor*, Combustion Science and Technology **187**, 1841–1866, 2015.
4. C. Eberle, P. Gerlinger, and M. Aigner, *A Sectional PAH Model with Reversible PAH Chemistry for CFD Soot Simulations*, Combustion and Flame **179**, 63–73, 2017.
5. A. Fiolitakis, P. R. Ess, P. Gerlinger, and M. Aigner, *Development and Application of a Transported Probability Density Function Method on Unstructured Three-Dimensional Grids for the Prediction of Nitric Oxides*, Journal of Engineering for Gas Turbines and Power **136**, 031506-01–031506-10, 2013.
6. A. Fiolitakis, P. R. Ess, P. Gerlinger, and M. Aigner, *Modeling of Heat Transfer and Differential Diffusion in Transported PDF Methods*, Combustion and Flame **161**, 2107–2119, 2014.
7. K. P. Geigle, R. Hadef, and W. Meier, *Soot Formation and Flame Characterization of an Aero-Engine Model Combustor Burning Ethylene at Elevated Pressure*, Journal of Engineering for Gas Turbines and Power **136**, 021505-1–021505-7, 2014.
8. P. Gerlinger, B. Noll, and M. Aigner, *Assumed PDF Modeling and PDF Structure Investigation using Finite-Rate Chemistry*, Progress in Computational Fluid Dynamics **5**, 334–344, 2005.
9. M. Grader, C. Eberle, P. Gerlinger, and M. Aigner, *LES of a Pressurized, Sooting Aero-Engine Model Combustor at Different Equivalence Ratios with a Sectional Approach for PAHs and Soot*, submitted to Proceedings of ASME Turbo Expo 2018.
10. O. Lammel, M. Stöhr, P. Kutne, C. Dem, W. Meier, and M. Aigner, *Experimental Analysis of Confined Jet Flames by Laser Measurement Techniques*, Journal of Engineering for Gas Turbines and Power **134**, 041506-1–041506-9, 2012.
11. F. Nicoud and F. Ducros, *Subgrid-scale Stress Modelling Based on the Square of the Velocity Gradient Tensor*, Flow, Turbulence and Combustion **62**, 183–200, 1999.
12. S. B. Pope, *The Probability Approach to the Modelling of Turbulent Reacting Flows*, Combustion and Flame **27**, 299–312, 1976.
13. S. B. Pope, *PDF Methods for Turbulent Reactive Flows*, Progress in Energy and Combustion Science **11**, 119–192, 1985.