Methodology development for the control of NO\textsubscript{x} emissions in Aerospace Industry

G Gangisetty, A.V. Ivchenko, A. V. Thomas Jayachandran, V.Y. Sverbilov, S.S. Matveev, and I. V. Chechet

Institute of Engine and Power Plant Engineering, Samara University, Russia
gopga321@student.liu.se, fgrt@yandex.ru

Abstract. A large number of studies conducted in Russia and abroad have been devoted to the development of low NO\textsubscript{x} emission gas turbine engines for aircraft and power stations. However, the continual improvement of the environmental requirements of ICAO (International Civil Aviation Organization) forces new research to be carried out to meet the future goals of reduced emissions produced by gas turbine combustors (GTE), a better understanding of the process of formation of various pollutants is required. Both empirical and theoretical approaches will be studied in this present research work to provide the exhaust concentrations of NO\textsubscript{x} emissions. In recent years different methods are already developed for this problem, one of them is associated with a theoretical approach. It is well known that correct theoretical models are economical (help’s to avoid experimental work) and can be useful for deep examination of NO\textsubscript{x} emissions generated in the combustion chamber process. The main objective of this study is to predict NO\textsubscript{x} emissions in GTE based on the mathematical simulations and chemical kinetics approach.

To validate the simulation results, dispersion type optical system was developed in the laboratory. This system includes UV LED source ($\lambda=245-280$nm), single-pass absorption cell with length ($L=500$ mm) and spectrometer DFS-452 (spectral dispersion up to $\Delta \lambda=0.2$nm/mm) equipped photo detector MORS-1 with a detection range $\Delta \lambda=50$nm. It allowed us to measure concentrations of some matters which absorbed light in the UVC range.

1. Introduction

Due to the continuous economic growth and reduced fares, passenger traffic is expected to grow at an average annual rate of nearly 5% during the period 2001–2030 (Airbus Global Market Forecast, 2002). Civil aviation is one of the fastest developing industrial sectors. Emissions of aircraft include carbon dioxide (CO\textsubscript{2}), water vapour (H\textsubscript{2}O), nitric oxide (NO), nitrogen dioxide (NO\textsubscript{2}), carbon monoxide (CO), a variety of hydrocarbons (HC), sulphur oxides, soot and other particles [1]. The emissions of aircraft engines occur in the atmospheric regions (low stratosphere and high troposphere), which are very prudent to various perturbations, the problem of the aviation effect on atmospheric processes and climate change has come into great importance. The impact of NO\textsubscript{x} emissions from aircraft are only 1–2% of the total emissions of NO\textsubscript{x} from man-made and natural sources [2]. However, it acts as a primary source of photochemical smog and ozone in the urban air, and, more generally, in the troposphere. Furthermore, NO\textsubscript{x} participates in a chemical reactions, removing ozone from the stratosphere with the consequence of increased ultraviolet radiation reaching the Earth’s surface. In the stratosphere, above ~26km, NO\textsubscript{x} catalysis is the most important ozone loss process and an increase in NO\textsubscript{x} concentration leads to increased local ozone loss [3].

During the last three decades, the rapid growth of air traffic and the growing awareness of global climate changes, the discussion has gained an interest and numerous studies are performed on the different implications of NO\textsubscript{x} emissions from the aircraft. Therefore, civil aircraft industries also have a keen interest in ensuring that its products are environmentally acceptable. Considering the future, doubling of air traffic is expected to occur within the next few years, causing an increasing demand for new aircraft. New technologies may be developed to reduce the specific fuel consumption and the NO\textsubscript{x}.
emissions while keeping the aircraft technically safe, sound and economical. To develop the advanced new technologies, high investments are required. Therefore, it is necessary for industries to know early information on the expected impact on future aviation and required regulations. Hence, the aviation industry is interested in learning about the emissions impact on the atmosphere and in development of NOx generation models for constructors and engineers [4].

2. Theoretical Model

Currently manufactures and designers use CFD methods in the development and refinement of gas turbine engines [5-7]. The complexity of the combustion process description in the combustion chambers of GTE leads to the joint application of kinetics [8] and gas-dynamic approaches in high-end computer simulations [9]. For this purpose, scientists use Chemical Reactor Network Model (CRNM) which allows obtaining satisfactory agreement between theoretical and practical results [10-11]. For example, the CRNM [10] based on CFD simulations gives good predictions for emission NOx, CO and CnHm. It allows extending the CRNM for all kinds of combustion processes in GTE.

2.1 Chemical Reactor Network Model

Our reactor model is based on the CFD calculations performed in a three-component fuel mixture with kerosene in the real prototype of the combustion chamber. According to the results of 3D modeling, different zones were identified. They are presented by the PSR and Plug Flow reactors to describe the flow section at the exit of the combustion chamber. In this work, the volumes of the reactors were determined on the basis of the calculated areas with an equivalence ratio’s are shown in the Fig. 1 and the calculated (ø) values are presented in Table 1.

| Zones | Equivalence Ratio (ø) |
|-------|------------------------|
| 1     | 1.81 – ∞               |
| 2     | 1.11 – 1.78            |
| 3     | 0.83 – 1.09            |
| 4     | 0.55 – 0.82            |
| 5     | 0.00 – 0.55            |

In the CRNM, selected areas were represented by ideal mixing reactors (Fig. 2), where the evolution of an instantaneous mixing was simulated under given conditions (volume, residence time, pressure and temperature). All data for the reactor were given from the CFD calculations. In zone 1, the temperature is maintained constant and it is equal to the bulk temperature. In other reactors, the temperature is calculated.
on the basis of temperature equations, and the composition of mixtures entering into the reactor. The reactor is represented by a PFR flow reactor that simulates chemical processes in a stream.

Figure 2. Schematic representation of the CRNM. (1-5 areas are defined in Fig.1)

The first reactor zone has the volume of 6.2% of the combustion chamber and this area represents the main burning area. Zone 2 has 8% of volume of the combustion chamber - this is the burning zone behind the burner plate near the walls of the closed gas cylinder and the next for the reverse current zone. Zone 3 has 10.3% of volume of the combustion chamber with high temperature characteristics. Zone 4 has 16.8% of the volume of the combustion chamber - the area between the first and second row of mixing holes. Zone 5 has 58.7% of volume of the combustion chamber, including 1.2% of the near wall-layer components. This zone includes near-wall layers and the area behind the second row of cooling holes, including the exit of the combustion chamber. Simulation of the near-wall layer considered simultaneously in the main flow calculation, in order to determine the concentrations of individual components formed at high temperatures in the combustion zone. In this model, we used the kinetic mechanism JetSurf [12] with the formation of nitrogen oxides by means of GRI 3.0 [13]. The dependence of the output parameters (temperature and velocity) from the initial reactor temperature is obtained and it can be seen in Fig.3

This model is in good agreement with the CFD calculation for a three-component fuel mixture with kersone surrogate (72.7% n-decane, 18.2% benzene, 9.1% n-hexane [14]) by temperature fields and air distribution along the length of the tube. The results were obtained at the initial temperature 1425 K and the flow velocity 102 m/s. This model was verified by the output concentrations of individual components such as CO, CO₂ and H₂O.

Figure 3. The dependence of the output parameters in accordance with temperature in the initial reactor.
3. Experimental Setup

For the validation of simulation results, we use the set of experimental equipment for the initiation and investigation of the combustion processes. According to [15], our experimental setup includes burning test bench with system for recording of gas-dynamic and thermodynamic parameters as well as optical systems for combustion product detection. In this work, we use combustion unit presented in Fig.4. This unit consists of the following main elements: a diffuser (1); combustion chamber bodies (3); burner (4); flame tube bodies (5). The diffuser is designed to reduce the flow rate to the desired value. The case is the main power element on which all the details are fixed: connecting flanges, spark plug, and burner. The body is made up of stainless steel with a thickness of 4 mm. The walls of the housing are interconnected by laser welding. Threaded holes are provided for connecting the flanges and installing the nozzle and spark plugs. With one of the frontal parts of the case, a seat is provided in an optically transparent quartz glass. When installing quartz glass is placed in a niche and pressed through the gasket flange 9. By using sets of clamping frames and set of probes, gas sampling was carried out. For detection of gas composition we used NDUV gas analyzer GMS800 which allowed to check NOx emission. Additionally, for NOx detection we have used the multispectral experimental setup presented in Fig.5. This system allows us to record absorption in the UV range (245-275 nm) and obtain a concentration of some gas components by using Lambert-Beer Law for different wavelengths [16].

The experimental setup in Fig.5 includes two sources of gas mixtures. The first of them was used for NOx feeding. It has water tank 1 for the NOx displacement of water in the gas sampling probe 3 with taps 2, 4. The second source may be used both for ozone generation by means of 6-8 unit and for zero air feeding of the supply line 5. The optical system, including UV LED 11, quartz lenses 12, 14, single-pass optical cell (L=500 mm) 13, beam splitter 15, spectrograph DFS-452 18 and photodetector MORS-1 was used for absorption recording. In this system the spectroscopic data was processed by computer system 20-22.

The multispectral experimental setup operates in three stages. At the first stage, zero air come through optical cell. In this moment photodetector records initial light intensity I0. If it is necessary, spectral correction of the spectrograph and photodetector is carried out by using a line spectrum of spectroscopic lamp 16. At the second stage, light-absorbing gas comes into the optical cell and photodetector records the signal associated with absorption I. In this case, taps 4,9,10 provide encapsulating of single-pass optical cell 13. In practice, it means that concentration of mixture component doesn’t change during the measurement time interval because of gas diffusion. By using values I0 and I, we determine the absorption coefficient and concentration according to [17]. At the third stage, taps 4,9,10 are open and absorption gas is replaced from optical cell.

Thus, burning test bench, NDUV gas analyzer GMS800 and multispectral experimental setup are able to provide a comparison of simulation and experimental results.

Figure 4. The Combustion chamber compartment: 1 - diffuser; 2 - flange; 3- outer casing of a combustion chamber; 4 - burner; 5 - flame tube; 6 – tube installation; 7 - ceramic paper pads; 8 - quartz glass; 9 - clamping flange; 10 - window frame.
Figure 5. The multispectral experimental setup for NO\textsubscript{x} optical detection in the gas mixture.

1 - water tank; 2,4,9,10 – taps; 3- gas sampling probe; 5- supply line; 6 - flow meters set; 7 - ozonator; 8 high-voltage power source 11- UV LED (FWHM - 12nm); 12,14,17 – quartz lenses; 13-single-pass optical cell; 15- beam splitter; 16- spectroscopic lamp; 18- spectrograph DFS-452 (\(\lambda=180-1100\text{nm}\); spectral dispersion-1.6 nm/mm); 19- photodetector MORS-1 (\(\Delta\lambda=50\text{ nm}\); spectrum resolution- 0.015nm); 20-USB cable; 21-computer; 22-monitor.

4. Results and Discussions:

According to the traditional approach, the data obtained from mathematical model should be compared with experimental results or information from literature. It provides the model validity and reliability of computational results. In this work, we compared the results obtained by means of CRNM (see section 2) with experimental data of spectral optical method (see section 3).

It is well known that multispectral absorption methods are widely used for the quantitative analyses of chemical substances and the identification of their traces in the air on a par with chromatography method [18]. Possibilities of absorption spectroscopy with LED allows to detect chemical compounds in a gas medium with accuracy in absorption less than 0.1% and provides a concentration measurement with accuracy around 1-5% [19]. In this connection, the multispectral absorption setup becomes an important part of the combustion product monitoring system to provide the detection of component in the light-absorbing gas mixture.

For the recording emission of NO\textsubscript{2} in combustion processes, we have used NDUV gas analyzer GMS800 and the multispectral experimental setup discussed in section 3. GMS800 was used as the primary measuring tool. At the same time, we used the multispectral experimental setup for additional observation and measurement of gas mixture absorption.
In our case, the experimental work consists of two stages. In the first stage we checked our spectral equipment and in the second stage we determined the concentration of combustion products.

In the first stage of investigation, NDUV gas analyzer GMS800 was calibrated by using reference gas mixtures. At the same time, the multispectral experimental setup was tested by using ozone-air mixture. In this case, the initial light intensity ($I_0$) and the light signal associated with ozone absorption ($I$) were accumulated during system stability period (20s) at the spectrum exposition 200ms for both signals. The system stability was estimated in real condition by means procedure described in [20]. The obtained Allan’s diagram of our multispectral experimental setup is presented in Fig.6.

The minimum of Allan’s variance (see Fig.6) allows us to estimate the dynamic range of the setup. If multispectral experimental setup with single-pass optical cell length of 0.5 m is able to distinguish light intensities $I_0$ and $I$ with an accuracy of 0.3%, it will detect minimum absorption coefficient around 0.006 m$^{-1}$, while maximum absorption coefficient will be around 9.2 m$^{-1}$ at dark noise level of 0.006$I_0$. In order to check up performance characteristics of the multispectral experimental setup (Fig.5), the ozone-air mixture was input in single pass optical cell. The light intensity ($I_0$) and the transmitted light intensity ($I$) were accumulated during system stability period (20s) at the spectrum exposition 200ms for both signals. The system stability was estimated in real condition by means procedure described in [20]. The obtained Allan’s diagram of our multispectral experimental setup is presented in Fig.6.

The change of optical signals from $I_0$ to $I$ allowed us to determine the spectral absorption coefficient distribution (see Fig.7) according to Lambert-Beer Law [16]. In Fig.8, the experimental curve (1) has maxima at $\lambda=255$ nm. The curve shape corresponds to the Hartley band [21,22]. By using experimental data and cross sections of O$_3$ for the photons absorption process [23], Ozone concentration was determined for absorption at $\lambda=250$ nm. This value was around $C_{O_3} = 0.4195$ g/m$^3$ ($\approx$342 ppm). We have checked the value via inverse calculation of absorption coefficient for different wavelength (with different ozone cross sections). The obtained result is presented by dots in Fig.8. The maximum concentration deviation between experimental data and calculated results was 2.7%. So, this experiment proves that our multispectral experimental setup may be used for UV absorption detection with excellent accuracy.

In the second stage of investigation, the NO$_x$ emission at the outlet of the model combustion chamber (see Fig.4) was experimentally determined by using the NDUV gas analyzer GMS800. While multispectral experimental setup recorded absorption of samples after the combustion process under standard temperature. The results of the experiments were compared with the results of calculations by using CRNM obtained under $T=623K$ at the inlet of the combustion chamber unit. The resulting uncertainty of CRNM was around 25%. The obtained results of experimental and calculated values of NO$_x$ in terms of NO$_2$ are presented in Table 2.

According to Table 2, the NO$_x$ content was detected by NDUV gas analyser GMS800 at the level 62 ppm. The multispectral experimental setup also recorded absorption (see Fig.9a). However, a behavior of absorption coefficient (see Fig.9b) in the spectral range (248-268 nm) needs to be explained.

On the one hand, the absorption coefficient curve may be explained by multispectral absorption of NO$_x$ and SO$_2$. It was confirmed by measurement of GMS800 which detected the presence of SO$_2$ with concentration around 12-18 ppm. On the other hand, it may be caused by low temperature conversion NO$_2$ into N$_2$O$_4$ [24]. This possibility was confirmed by simulation of absorption coefficient for NO$_x$/SO$_2$ mixtures.
Figure 9. Optical signal changing (a) and spectral absorption coefficient distribution (b) under replacement of air in optical cell by a gas mixture of combustion products. 1- Emission band of UV LED. 2 - The transmitted light intensity during absorption process.

Table 2. Comparison between theoretical values and experimental data

| Method                  | NOx ppm |
|-------------------------|---------|
| Chemical Reactor network| 72±18   |
| Model                   | 62±6.2  |

Thus, the results of simulation by means of CRNM and experimental results have satisfactory agreement, therefore these methods may be used for GTE – development.

5. Conclusions

1. For a description of combustion processes of complex fuel mixtures in GTE the reactor net model based on CFD simulation is developed. The model may be used for consideration of NOx emission in different areas of the combustion chamber. It may be useful for improvement of GTE in the future.

2. The multispectral experimental setup for detection NOx by UV absorption was developed and tested for ozone-air and combustion product mixture. For single-pass optical cell with length L=0.5 m, the setup had a dynamic range of absorption coefficient from 0.006 to 9.2 m\(^{-1}\). While concentration measurements of single-component absorption had accuracy less than 2.7%. The setup may be used for concentration measurement of gas mixture components under multi-component absorption.

3. The model prediction of NOx emission under T=623K at the inlet of the combustion chamber unit was confirmed by experimental results obtained with accuracy around 10%. CRNM-uncertainty has value around 25%.

6. References

[1] M. Gauss1, I. S. A. Isaksen1, D. S. Lee2, and O. A. Søvde1, 2006 ‘’Impact of aircraft NOx emissions on the atmosphere - tradeoffs to reduce the impact. ‘’Atmospheric Chemistry & Physics.

[2] A.M. Starik, Gaseous and Particulate Emissions with Jet Engine Exhaust and Atmospheric Pollution, Central Institute of Aviation Motors.

[3] S. Amabile and L. Cutrone and F.Battista, Analysis of a low-emission combustion strategy for a high performance trans-atmospheric aircraft engine, 46th AIAA/ASME/SAE/ASEE, Joint Propulsion Conference & Exhibit 25 - 28 July 2010.

[4] U Schumann, The Impact of Nitrogen Oxides Emissions From Aircraft Upon Atmospheric Flight Altitudes – Results From The AERONOX Project, Atmospheric Environment Vol.31, No-12, pp. 1723,1733, 1997.
[5] Orlov, M.Y.Matveev, S.S. Numerical simulation of an influence of a compressor and a turbine on characteristics of a combustion chamber of small-sizes gas turbine engine. *Life Science Journal* 11(11), 119 pp. 650-654, 2014.

[6] Orlov, M.Y., Matveev, S.S., Makarov, N.S., Zubrilin, I.A. Numerical modeling problems of operating process of combustion chamber of GTE and solution approaches. *Journal of Engineering and Applied Sciences* 9 (12), pp. 2894-2899, 2014.

[7] Zubrilin, R.A, Matveev, S.S., Zubrilin, I.A., Matveev, S.G. Gaseous fuel flame stabilization in a modular swirled burner. ASME Turbo Expo 4B-2016, GT2016-57441, 2016.

[8] Zubrilin, I.A., Matveev, S.S., Matveev, S.G., Idrisov, D.V. Measurements & Experimental Database Review for Laminar Flame Speed Premixed Cl4/Air Flames, IOP: Materials Science & Engineering 302(1), 012078, pp. 1-6, 2018.

[9] Development of Reactor Models of Diffusion Combustion Chamber for Comparative Analysis of Detailed and Reduced Kinetic Schemes of Combustion of Hydrocarbon Fuels / V.M. Zhkrov et al. // Combustion, Explosion & Shock Waves, 2009- Vol. 45, No. 2, P. 126-133.

[10] Impact of Operating Regime on Aviation Engine Emissions: Modeling Study / A.M. Starik et al // Journal of Propulsion and Power - 2013. - Vol. 29, No.3, - P.709-717.

[11] Application of reactor net models for the simulation of gas-turbine combustor emissions / A.M. Starik et al // Int. J. Sustainable Aviation – 2014. - Vol. 1, No. 1, pp 43-57.

[12] https://web.stanford.edu/group/haiwanglab/JetSurF/JetSurF2.0/Index.html

[13] http://combustion.berkeley.edu/gri-mech/version30/text30.html

[14] Strelkova, M. I., Kirillov, I. A., Potapkin, B. V., Safonov, A. A., Sukhanov, L. P., Umanskiy iy S. Ya. Deminsky, M. A., Dean, A. J., Varatharajan, B. and Tentner, A. M. (2008). Detailed and Reduced Mechanisms of Jet a Combustion at High Temperatures’, *Combustion Science and Technology*, 180: 10, 1788-1802.

[15] Matveev, S.S., Chechet, I.V., Semeniikhin, A.S., Abrashkin, V.Y., Lukachev, S.V., Matveev, S.G. Experimental Study of the Combustion of Kerosene and Binary Surrogate in the Model Combustion Chamber. *Journal of Combustion*, Volume 2017, Article ID 3963075.

[16] Brock J.R. A note on the Beer-Lambert law\ Anal. Chim. Acta 27.(1962) -P.95-97.

[17] UV Spectroscopy, Techniques, instrumentation and data handling // Eds. Clark, B.J., Frost, T., Russell, M. A.-New-York: Springer, 1993.

[18] Laser monitoring of the atmosphere/ Edited by E.D. Hinkley - Berlin -Heidelberg-New-York: Springer, Verlag, 1976.

[19] Stepanov E.V. LED spectroscopy and analysis of biomarker-molecules – Moscow, Fizmatlit Publisher, 2009–416p. [In Russian].

[20] Measurement of ozone concentration in the atmosphere by the absorption of the LED radiation/ I.V. Nikolaev, V.N. Ochkin., et al// Bulletin lebedev physics institute (2013) - i2. P 36-41.

[21] Rothman L.S. The evolution and impact of the HITRAN molecular spectroscopic database// Quantitative Spectroscopy and Radiative Transfer (2010) - V.111, i.11- P.1567.

[22] Keller-Rudek, H., Moortgat, G. K., Sander, R. & Srensen, R.: The MPI-Mainz UV/VIS Spectral atlas of gaseous molecules of atmospheric interest/Earth Syst. Sci. Data, (2013) - i5. P.365-373.

[23] DeMore W.B. and Raper O. Hartley band extinction coefficients of ozone in the gas phase and in liquid nitrogen, carbon monoxide, argon // J. Phys. Chem. (1964) V.68 - P.412-414.

[24] Extinction Coefficients of NO₂ & N₂O₅/A.M.Bass et al.// Journal of research of the National Bureau of Standards – A. Physics and Chemistry (1976), V.80A, No.2. – P.143-166

Acknowledgments
The Ministry of education and science of the Russian Federation in the framework for implementation of the Program for increasing the competitiveness of Samara University among the world leading scientific and educational centres for 2013-2020 years supported this work.