29th Congress of the International Council of the Aeronautical Sciences
St. Petersburg, Russia; September 7-12, 2014

MECHANISMS OF POLLUTANT FORMATION IN THE H_2 – FUELLED COMBUSTOR OF HIGH VELOCITY AIR-BREATHING ENGINE: MODELING STUDY

L. Bezgin*, V. Kopchenov*, N. Titova*, A. Starik*
***CIAM, Russia**

Keywords: *combustion, supersonic flow, pollutant formation*

Abstract

Nowadays, a great attention is paid to the analysis of the aviation impact on the atmospheric processes. The high velocity air-breathing engine is considered today as a promising concept for hypersonic transport flight system. However, until now, there is small information about the level of possible pollutant emissions for such propulsion system. The analysis of mechanisms of pollutant NO_x formation at supersonic combustion of hydrogen in air flow is the subject of this study.

1 Introduction

For past years, a few ambitious projects were focused on the evaluations of the perspectives of hypersonic transportation system and hypersonic civil aircrafts with air-breathing engines. In Europe, the LAPCAT project has been announced [1]. One of the goals of this project is scientific and technical basic investigations addressed to the development of efficient hypersonic propulsion system for civil aircrafts. Currently, grant attention is paid to the impact of aviation on the atmosphere. These investigations have a long time history for transport and civil aircrafts with traditional air-breathing engines. The problem of pollutant formation in high velocity air-breathing engines was studied many fewer than for modern gas turbine engines. The principal peculiarity of hydrogen combustion in high velocity reacting flow is the small residence time of fuel-air mixture in combustor and high temperature in the combustion region. Moreover, the gasdynamic flow in the combustor is essentially nonuniform with the system of shocks generated due to the specific combustor shape and existence of the system of struts for fuel injection. In order to estimate the emission characteristics of such combustor, the reaction mechanism must treat both the mechanism of hydrogen-air combustion and mechanisms of NO_x and other pollutant formation. It should be noted that numerical simulation of combustion and NO_x formation was performed previously in [2] within LAPCAT project. In that work the modified version [3] of reaction mechanism [4] was implemented for describing both the combustion process and NO_x formation. One of the goals of this study is the comprehensive analysis of NO_x formation on the base of detailed reaction mechanism with high prediction ability.

2 Problem formulation and methodology

The numerical simulation was performed for the model combustor shown in Fig.1. The hydrogen was supplied tangentially through 7 pylons located at the combustor inlet. The fuel mass flow rates through all pylons were identical. The Much number and pressure of air flow at the combustor inlet were following: M_0=3.5, P_0=0.3 atm. The temperature in three considered cases was equal to T_0=1100, 1300 and 1500 K. The coefficient α of air to fuel equivalence ratio decreases from 0.89 to 0.76 at the variation of air inlet temperature from 1100 K to 1500 K.

The analysis was conducted on the basis of numerical solution of 2D Favre averaged parabolized Navier–Stokes (PNS) equations for reacting turbulent supersonic flow. The quasilaminar approach and one equation differential model for turbulent viscosity were used for the computations. The details of numerical method were presented in [5].

The applied detailed reaction mechanism includes more than 150 reversible chemical reactions with 25 species: H_2, O_2, H_2O, OH, O, H, HO_2, H_2O_2, O_3, N_2, N, NO, NO_2, NO_3, HNO, HNO_2, HNO_3, NH, NH_2, NH_3, N_2O, NNH, N_2H_2, N_2H_3, N_2H_4 and is based on the reaction mechanism of hydrogen combustion [6] and mechanism of the N-containing species formation [7, 8].

It is worth noting that the influence of boundary layer on the core of the flow in the duct is not taken into account within the applied numerical method. At the same time, the approach based on simplified PNS equations allows one applying the detailed reaction mechanisms and accurate computational grids which can reproduce properly the processes in mixing layers and formation of oblique shock waves. We believe that it is admissible to utilize the simplified PNS approach for the study of the influence of different mechanisms on NO_x formation with account for the main features of combustion process in the core of the supersonic flow.

3 Results and discussion

It is known that NO formation in hydrogen-air mixture occurs via following mechanisms [8]:

− thermal (or extended Zeldovich) mechanism which includes following reactions

$$O + N_2 = N + NO,\ N + O_2 = O + NO,$$
$$N + OH = H + NO;$$

− N_2O-mechanism in which the main reactions are

$$N_2 + O + M = N_2O + M \text{ and}$$
$$N_2O + O = NO + NO;$$

− NNH mechanism which includes reactions with elements of group N_xH_y, for example,

$$N_2 + H = NNH,\ NNH + O = NO + NH.$$

Fig. 1 shows the temperature and NO mass fraction fields for T_0=1100 K. It is seen that the complicated shock wave system in combustor exists. The static temperature behind the shock waves in the combustion region reaches 3000 K. As it follows from Fig. 1, the regions of high NO concentrations correlate strongly with high temperature zones inside the combustor.

The analysis of the rates of NO formation in the foregoing reactions was performed for all three cases with temperatures T_0=1100, 1300 and 1500 K. It was revealed that the main channel of NO formation is the thermal mechanism. The contributions of other mechanisms are essentially lower (more than two orders of magnitude).

The results of emission index calculations for cases considered are presented in Table 1. One can conclude that the emission indices for NO are higher than those for the modern commercial aircraft with gas turbine kerosene-fuelled combustor. The emission indices for other N-containing species: NO_2, N_2O, HNO, HNO_2 and HNO_3 at the combustor exit are much smaller than NO emission index.

For comparison, we also performed the calculations of NO emission with modified Jachimowski mechanism [3], that was used in the computations [2]. Obtained values of NO emission index are also shown in Table 1. One can see that for the case with temperature T_0=1100 K, the values of emission indices for NO predicted with the use of reaction mechanism [3] and detailed mechanism [6-8] practically coincide. The emission index for NO_2, calculated by using the mechanism [3] is two times lower than that predicted by detailed mechanism. With the rise of T_0, the values of emission indices predicted by reaction mechanism [3] are essentially lower than those for detailed reaction mechanism. For the case with temperature T_0=1500 K, $EI(NO)$ and $EI(NO_2)$ predicted with the model [3] are, respectively, three and five times lower in comparison with values calculated with detailed mechanism.

4 Conclusion

The analysis of NO_x formation for supersonic combustion regime in hydrogen-fueled combustor was performed with account for turbulent mixing and gasdynamic flow structure. The applied detailed reaction mechanism treats both the submechanism of hydrogen-air combustion and the principal mechanisms of *NO* formation. It is shown that at the conditions considered the thermal mechanism is responsible for *NO* formation. The emission indices of NO_2 and N_2O are essentially lower (by a factor of 10^4) than that for *NO*.

References

[1] Steelant J. LAPCAT: a technical feasibility study on sustained hypersonic flight. *ISABE*, Paper 2007-1205, 2007.

[2] Kindler M., Gerlinger P., Aigner M. Numerical investigations of NO_x-formation in scramjet combustors using wall and strut injectors. *AIAA*, Paper 2011-405, 2011.

[3] Wilson G., MacCormack R. Modeling supersonic combustion using a fully implicit numerical method. *AIAA Journal*, Vol.30, No. 4, pp 1008-1015, 1992.

[4] Jachimowski C.J. An analytical study of the hydrogen - air mechanism with application to scramjet combustion. *NASA*, TP-2791, 1988.

[5] Bezgin L.V., Ganzhelo A.N., Gouskov O.V., Kopchenov V.I. Some numerical investigation results of shock-induced combustion. *AIAA,* Paper 1998-1513, 1998.

[6] Starik A.M., Titova N.S., Sharipov A.S. Kinetic mechanism of H_2-O_2 ignition promoted by singlet oxygen $O_2(a^1\Delta_g)$. *Deflagrative and detonative combustion.* Eds. Roy G.D. and Frolov S.M. Moscow: Torus Press, pp 19-42, 2010.

[7] Dautov N.G., Starik, A.M. On the problem of choosing a kinetic scheme for the homogeneous reaction of methane with air. *Kinetics and Catalysis*, Vol.38, No.2, pp 185-208, 1997.

[8] Kuleshov P.S., Starik A.M., Titova N.S. Kinetics of oxidation and combustion of methane and propane. *Nonequilibrium physico-chemical processes in gaseous flows and novel combustion concepts.* Ed. Starik A.M. Moscow: Torus Press, pp 53-87, 2011 (in Russia).

Table 1. Emission indices at the exit cross-section of model combustor for different values of air flow temperature at the combustor entrance

	EI g/(kg H_2)		
Species	T_0=1100 K	T_0=1300 K	T_0=1500 K
α	0.89	0.82	0.76
Detailed reaction mechanism [6-8]			
NO	27.6	43.2	32.3
NO_2	1.1×10^{-3}	1.5×10^{-3}	1.1×10^{-3}
N_2O	5.1×10^{-3}	3.6×10^{-3}	3.2×10^{-3}
HNO	2.3×10^{-3}	3.4×10^{-3}	2.5×10^{-3}
HNO_2	3.6×10^{-3}	4.6×10^{-3}	3.1×10^{-3}
HNO_3	7.8×10^{-9}	8.8×10^{-9}	5.4×10^{-9}
Reaction mechanism [3]			
NO	26.3	20.3	12.8
NO_2	0.48×10^{-3}	0.34×10^{-3}	0.19×10^{-3}
HNO	5.6×10^{-3}	4.6×10^{-3}	3.2×10^{-3}

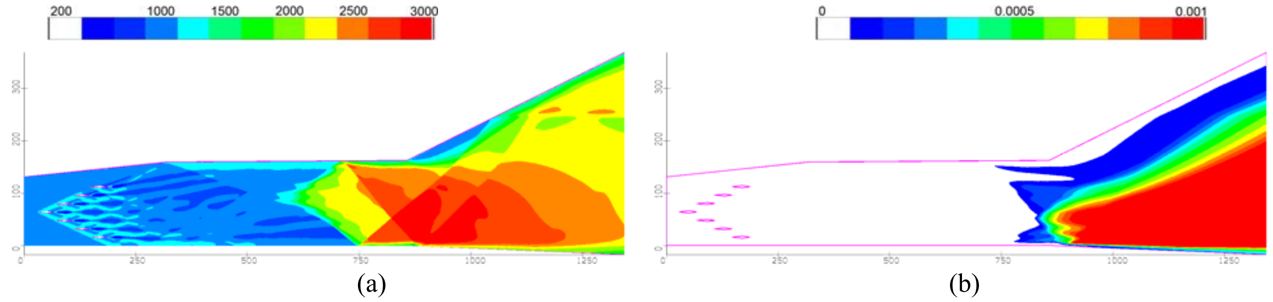

Fig. 1. Static temperature (a) and *NO* mass fraction (b) fields for model combustor in the case T_0=1100 K

Contact Author Email Address

mailto: kop@ciam.ru
Valery Kopchenov
Leonid Bezgin

Copyright Statement