RESARCH REGARDING NO_x FORMATION IN A GAS TURBINES COMBUSTOR

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***Rezumat**: Gazele de evacuare provenite de la motoarele Diesel navale,generatoarele de abur navale şi turbinele cu gaze conţin emisii ca: oxizi de azot, oxizii de sulf, oxizi de carbon, hidrocarburi nearse şi particule mecanice. Există mai multe metode de studiere a acestor emisii, cu scopul general de a înţelege formarea acestora. Prin analiza modului de formare a emisiilor de NO_x într-o cameră de ardere a unei turbine cu gaze, putem remarca faptul că zonele de formare intensă a NO_x corespund cu zonele în care temperatura de ardere atinge valoarea maximă. Cu aceste rezultate, mai departe se poate obţine o reducere a emisiilor de NO_x dacă se realizează o metodă de reducere a temperaturilor în acele zone.*

***Cuvinte cheie**: emisii, temperatură, ardere, NO_x.*

***Abstract**: Exhaust from marine diesel engines, marine boilers and gas turbines include emissions in the form of nitrogen oxides, sulphur oxides, carbon oxides, unburned hydrocarbons and particulate matter. There are several ways of studying these emissions, with the purpose of understanding the formation of them. By analyzing the NO_x formation in the gas turbine combustor, we can see that the NO_x formation zones correspond to that high temperature zone inside the combustor. With these results, a reduction of NO_x can be obtained if we can develop solutions for the reduction of these temperatures.*

***Keywords**: emissions, temperature, combustion, NO_x.*

1. INTRODUCTION

Today using specialized software we can simulate complex mechanical, chemical, hydrodynamical and thermical processes, without been necessary to build experimental models, and with the advantage of measuring parameters in each point of the computer model.

In this paper we will present a simulation of a combustion process inside a gas turbine combustor, showing the NO_x formation zones. For this simulation we've used the ANSYS CFX software.

2. THE NO FORMATION MODEL

2.1. Thermal NO

The thermal NO mechanism is a predominant source of NO_x in gas flames at temperatures above 2000 K. The NO is formed from the combination of free radical O and N species, which are in abundance at high temperatures. The two-step mechanism, referred to as the *Zeldovich* mechanism, is thought to dominate the process:

$$O + N_2 - k_1 \rightarrow NO + N \qquad (1)$$

$$N + O_2 - k_2 \rightarrow NO + O \qquad (2)$$

In sub or near stoichiometric conditions, a third reaction may be important:

$$N + OH - k_3 \rightarrow NO + H \qquad (3)$$

When this step is included with the first two, it is referred to as the extended *Zeldovich* mechanism. [3, 6]

The rates of each of these three reactions are:

$$k_1 = \left(1.8 \cdot 10^{11}\right) \exp\left(-\frac{38370}{T}\right) \qquad (4)$$

$$k_2 = \left(6.4 \cdot 10^{9}\right) \exp\left(-\frac{3162}{T}\right) \qquad (5)$$

$$k_3 = 3.0 \cdot 10^{13} \qquad (6)$$

When multiplied by the concentrations of the reactants, they yield rates in terms of [(kmol/m^3)/s], which can be converted to a volumetric mass source term. [6]

The first step tends to be rate limiting, producing both an NO and N radical species. The N radical is assumed to be oxidized by reaction (2) in the *Zeldovich* mechanism and also by reaction (3) in the extended *Zeldovich* mechanism. Either way, these second oxidation reactions are assumed to be fast or if reaction (1) occurs, then two NO molecules will be formed. The thermal NO formation in [(kg/m^3)/s], is therefore related to the rate of reaction (1): [6]

$$S_{NO\_term} = W_{NO} \cdot k_{term} \cdot O \cdot N \quad (7)$$

$$k_{term} = 2 \cdot k_1 \quad (8)$$

Here W_{NO}, denotes the molecular mass of NO. Thus, if the molar concentrations O and N_2 of O radicals and N_2 are known, the thermal NO mechanism can be calculated.

In ANSYS, when we build the simulation model, if we use the laminar flamelet burning model (LFB), almost always the O radical concentration can be taken without further assumptions from the solution since the model predicts it directly. [6]

If we use the Eddy Dissipation model (EDM) and/or the Finite Rate Chemistry model (FRC), O radical concentrations usually are not known directly but must be derived from other quantities. Here, the O radical concentration is estimated from the molecular oxygen dissociation:

$$\frac{1}{2}O_2 \Leftrightarrow O \quad (9)$$

And by substitution between (7) and (9) the effective source term for NO will be like:

$$O = 12567\left[kmol^{\frac{1}{2}} \cdot m^{-\frac{3}{2}} \cdot K^{\frac{1}{2}}\right] \cdot T^{-\frac{1}{2}} \exp\left(-31096 \cdot \frac{K}{T}\right) \cdot O_2^{\frac{1}{2}} \quad (10)$$

$$S_{NO\_term\_O2} = W_{NO} \cdot k_{term\_O2} \cdot O^{\frac{1}{2}} \cdot N_2 \quad (11)$$

$$k_{term\_O2} = 4.5241 \cdot 10^{15}\left[\frac{m^{\frac{3}{2}} \cdot kmol^{-\frac{1}{2}} \cdot K^{\frac{1}{2}}}{s}\right] \cdot T^{-\frac{1}{2}} \exp\left(69466 \cdot \frac{K}{T}\right) \quad (12)$$

2.2. Prompt NO

At temperatures lower than 2000 K, hydrocarbon flames tend to have an NO concentration that is too high to be explained with the *Zeldovich* mechanisms. Hydrocarbon radicals can react with molecular nitrogen to form HCN, which may be oxidized to NO under lean flame conditions. [6]

$$CH + N2 = HCN + N \quad (13)$$

$$HCN + O_2 = NO + ... \quad (14)$$

In this situation the source term is:

$$S_{NO\_prompt} = W_{NO} \cdot k_{prompt} \cdot O^{\frac{1}{2}} \cdot N_2 \cdot Fuel \cdot \left(\frac{W}{\rho}\right)^{\frac{3}{2}} \quad (15)$$

$$k_{prompt} = A_{prompt} \exp\left(-\frac{T_{A\_prompt}}{T}\right) \quad (16)$$

Where W_{NO} and W denote molar mass of NO and the mean molar mass of the mixture. The Arrhenius coefficients A_{prompt} and T_{A_prompt} depend on the fuel. Usually the following values are used: [6]

- Methane fuel:

$$A_{prompt} = 6.4 \cdot 10^6\left[\frac{1}{s}\right] \quad (17)$$

$$T_{A\_prompt} = 36510[K] \quad (18)$$

- Acetylene fuel:

$$A_{prompt} = 1.2 \cdot 10^6 \left[\frac{1}{s}\right] \quad (19)$$

$$T_{A\_prompt} = 30215[K] \quad (20)$$

There are also other formation mechanisms, but I will only resume to these two.

3. GAS TURBINE COMBUSTOR

The combustion chamber has the difficult task of burning large quantities of fuel, supplied through the fuel spray nozzles, with extensive volumes of air, supplied by the compressor, and releasing the heat in such a manner that the air is expanded and accelerated to give a smooth stream of uniformly heated gas at all conditions required by the turbine. This task must be accomplished with the minimum loss in pressure and with the maximum heat release for the limited space available. [5]

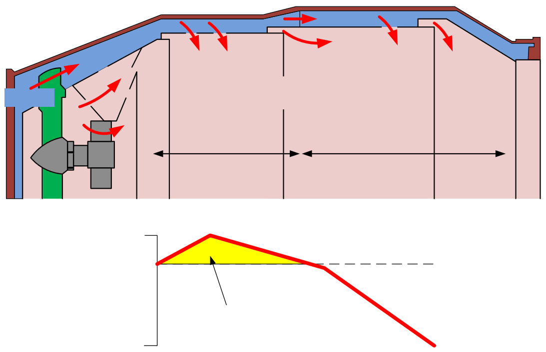

Fig. 1. Air distribution in the flame tube

The temperature of the gases released by combustion is about 1800 to 2000 deg. C., which is far too hot for entry to the nozzle guide vanes of the turbine. The air not used for combustion, which amounts to about 60 per cent of the total airflow, is therefore introduced progressively into the flame tube. Approximately a third of this is used to lower the gas temperature in the dilution zone before it enters the turbine and the remainder is used for cooling the walls of the flame tube. [8]

4. THE FLAME TUBE CONSTRUCTION

The 2D model with the fluid inlet and outlet zone is shown in fig. 2. The 3D model build in ANSYS is presented in fig. 3.

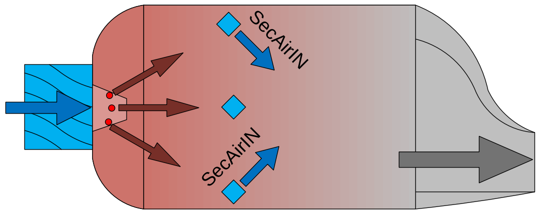

Fig. 2 Inlet and outlet zones

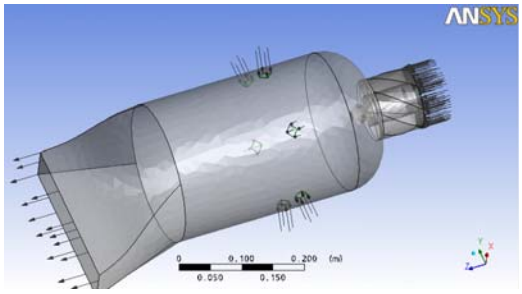

Fig.3 3D model in ANSYS

5. RESULTS OF SIMULATION

5.1. Temperature variance

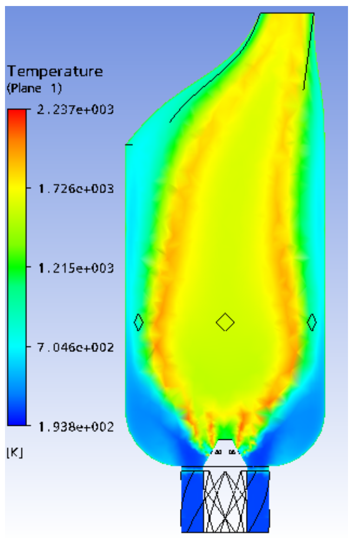

Fig. 4Temperature variance

Values of temperature Table 1

Parameter	FuelIN	AirIN	SecAirIN	GasOUT
T[K]	389	300	407	1286

Cooling

5.2. O_2 concentration

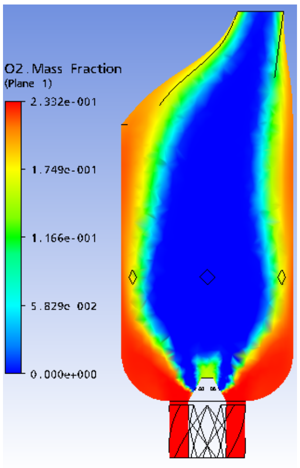

Fig. 5 Concentration of O_2

Values of O_2 Table 2

Parameters	FuelIN	AirIN	SecAirIN	GasOUT
C_{O2}	0.0005	0.23292	0.22643	0.1238

5.3. N_2 and NO concentration

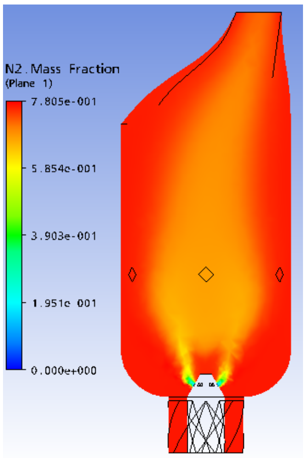

Fig. 6 Concentration of N_2

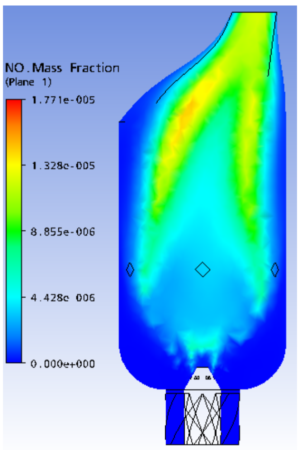

Fig. 7 Concentration of NO

Values of N_2 and NO Table 3

Parameters	FuelIN	AirIN	SecAirIN	GasOUT
C_{N2}	0.046	0.767	0.768	0.751
C_{NO}	$9.7 \cdot 10^{-9}$	$3.8 \cdot 10^{-18}$	$6.3 \cdot 10^{-8}$	$5.8 \cdot 10^{-6}$

6. CONCLUSIONS

Analyzing the graphical results obtained with the program, we can observe that the highest values of NO correspond to the regions where the temperature exceeds 2000 K. This is caused by the thermal mechanism of NO_x formation, which is the main source for the NO_x emissions.

In the last twenty years several technologies where developed to reduce this temperature and finally to reduce NO_x emissions. Some of these technological solutions are:

- Water injection;
- Steam injection;
- Dry combustor with high excess air factor. [7]

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