CFD Investigation on Pollutant Production in a Cement Industrial Furnace

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Abstract: Pollutant emissions are considered as the most active factors in the acid rains production and ozone destruction process, studies and analyses of their production mechanisms may improve pollution reduction techniques and contribute to the developments of the measures and control systems.

The present work deals with a CFD modeling of the thermal NO production issued from the natural gas (NG) combustion in an industrial furnace designed for cement production. Correlation between the NO production rate and the furnace operating conditions will be achieved .The non premixed turbulent combustion of the NG/Air mixture will be analyzed by some CFD software (Gambit, CEA, and Fluent) using a finite volume approach to solve the reacting flow equations written in a Favre averaging form on an axisymetric model of the furnace. A single step chemistry will be adopted for this combustion case, the closure of the system will be ensured by a $k-\omega$ two equations model with a limited Pope correction to account for the spreading rate dynamics of the oxidant jets. Algebraic (Magnussen) model for the reaction rate is adopted, in addition, primary and co-flow jets configuration effects on the NO production are examined and correlated to the overall efficiency of the combustion process.

Key –Words: pollutant emission, thermal NO, methane, turbulent combustion, CFD simulation, Magnussen model, industrial furnace, cement production.

1 Introduction

National and international current legislations incite industrialists to optimize their processes to strongly reduce pollutants emissions; several technological approaches are available to reach this objective. Nox are the primary pollutants which closely linked to environmental problems, to limit their impact, their rejections have to be restricted. In spite of all the efforts realized during the twenty last years, the emission of such kind of primary pollutants is always very important, with regard to this issue, nitrogen oxide play an important role in main of actual environmental problems, because about 60% of the global emissions of the hazardous pollutants are believed to come from combustion processes [1], it can be envisaged to reduce significantly this way of production.

To reduce nitrogen oxides formation, several technologies approaches are available, the most important way consist in a use of an appropriate treatment of the gaseous effluents before rejection to the atmosphere, in this category, we can site the NOx reburning techniques [2], the selective and selective non catalytic reductions (SCR, SNCR) [3] and the exhaust gas recirculation (EGR) technique [4]. Among the available strategies, the EGR technique is used as one of the major methods to depress the NOx emissions by reducing the maximum temperature when diluting mixture by combustion products.

The Algerian natural gas blends are generally composed of methane and small amounts of high order hydrocarbons [5] is of interest because of its importance as likely a low cost fuel source for power generation. Methane is generally believed to be the cleanest burning hydrocarbon fuel, nevertheless, in practical systems; non optimized combustion conditions could promote undesirable by-products formation and pollutant emissions in the atmosphere. The present paper reports a numerical investigation of a non premixed turbulent Methane/Air flame developing from the industrial furnace of the cement production unit at Oued–Sly-Chlef. The CFD work, using the FLUENT commercial software was performed in order to estimate the visible flame length along the furnace axis and the NOx emission rates, in addition, secondary air and wall temperatures effects on the overall combustion efficiency are examined.

2 Configuration and operating conditions

The furnace studied is composed of a coaxial single element CH_4/Air shear injector linked to a cylindrical combustor; because of the geometrical symmetry, only a 2D axisymmetrical modeling was adopted for the present study (fig.1).

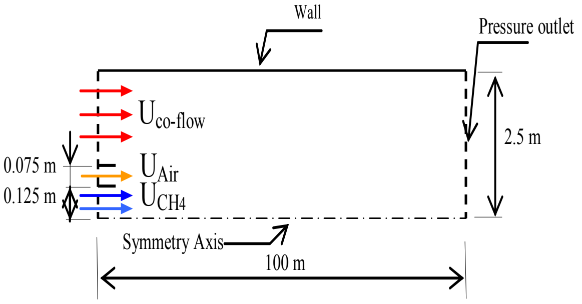

Fig.1: Geometrical modeling and boundary conditions.

The low temperature fuel jet is surrounded by a primary Air jet necessary for a diffusion flame development, in addition, the quasi laminar hot products (termed co-flow) recovered from the chamber exit are reinjected in a direction parallel to the wall. Inlet velocity type was adopted for the oxidant and fuel streams, the walls are assumed to be adiabatic (or isotherm) and a static outlet pressure condition will be assigned for the flow at the exit furnace plane. The furnace aero-thermodynamic operating conditions are described in the table below.

Operating Conditions	Oxidant Primary Jet (Air_1)	Co-Flow Secondary Jet (Air_2)	Fuel Jet CH_4
Temperature (K)	298.15	900	273.15
Inlet Velocity (m/s)	382.00	2.20	263.00
Inlet Turbulence Intensity (%)	10	5	10

Table.1: Furnace operating conditions.

3 Modeling turbulence and chemistry

The flame behavior depends strongly on the reacting flow turbulence, we should solve the continuity, the momentum, the energy and the species transport equations written in a Favre averaging form, the closure of the system is ensured by a standard $k-\varepsilon$ turbulence model [6] with a limited Pope correction, which describes correctly the dynamic behavior of a shearing flow downstream a coaxial single element injector [7]. The dissipation rate equation is corrected by adding an invariant term χ [8]:

$$P_{pc} = C_{\varepsilon 3}\bar{\rho}\frac{\varepsilon^2}{k}\chi \tag{1}$$

The invariant χ denote the nondimensional measure of the vortex stretching, expressed as:

$$\chi = \omega_{ij}\omega_{jl}S_{li} \tag{2}$$

where:

$$S_{li} = \frac{1}{2}\frac{k}{\varepsilon}\left[\frac{\partial \tilde{u}_l}{\partial x_i} + \frac{\partial \tilde{u}_i}{\partial x_l}\right] \tag{3}$$

$$\omega_{jl} = \frac{1}{2}\frac{k}{\varepsilon}\left[\frac{\partial \tilde{u}_j}{\partial x_l} - \frac{\partial \tilde{u}_l}{\partial x_j}\right]^2 \tag{4}$$

The Pope correction makes possible to take into account the vortex stretching effect on the jet viscosity and consequently on its spreading rate, practically, the correction is done by adjusting the $C_{2\varepsilon}$ factor in the plane jet equation so that the calculated spreading rate is equal to its maximum value.

In addition to the governing equations of the flow dynamics, one is brought to solve N convection-advection transport equations with the aim to predict the mass fraction evolution of each species in the mixture:

$$\frac{\partial}{\partial t}\left[\rho Y_n\right] + \frac{\partial}{\partial x_i}\left[\rho Y_n u_i\right] = \frac{\partial}{\partial x_i}\left[\rho D_n \frac{\partial Y_n}{\partial x_i}\right] + \dot{W}_n \tag{5}$$

The net reaction rate $\dot{W}_n$ which appears as a source term can be expressed in terms of turbulence and/or chemistry characteristics.

The stochastic models consisting in using probability density function (pdf) are mainly useful if one variable (mixture fraction for example) is considered, their extension to multivariable cases without resorting to statistical independence assumptions is particularly delicate [9], while the resolution of the pdf transport equation induces additional difficulties related to the micro-mixing modeling [10].

In the non premixed combustion cases, the algebraic approaches are mainly based on the work of Magnussen and Hjertager [11], the model suppose that the chemical reaction is fully controlled by the turbulent mixing which tends to bring back the fuel and the oxidant to the reaction zone where the large eddies occurs, chemical kinetics effects are not considered in the reaction rate calculation:

$$W_1 = \nu_i' M_i A\rho \frac{\varepsilon}{k}\left[\frac{Y_R}{\nu_R' M_R}\right]$$

$$W_2 = \nu_i' M_i A.B\rho \frac{\varepsilon}{k}\frac{\sum Y_P}{\sum_1^N \nu_j'' M_j} \tag{6}$$

$$\dot{W}_n = Min(W_1, W_2)$$

Combustion will only occur in the presence of turbulence with an intensity proportional to the large-eddy mixing time scale (k/ε).

4 Modeling pollutant formation

It is convenient to group the NOx emissions mechanisms in three major parts, thermal NO, prompt NO and fuel NO.

Thermal NO is formed everywhere where oxygen and nitrogen are present and temperature is sufficiently high, it has an exponential dependence on temperature [12] which make it very sensitive to turbulent mixing and acoustic fluctuations [13]. The prompt NO is formed in the flame by intermediate of hydrocarbon radicals, it occurs closely to the flame front and has an exponential dependence on temperature and equivalence ratio [14]; the fuel NO which consists in the oxidation of the N atoms bounded in the fuel, will not be considered here.

A preliminary thermochemical work using the CEA [15] code on the CH_4/Air flame under the ECDE furnace operating points (inlet mixture ratio fluctuations) shows a dominance of the CO_2, H_2O and NO species over other products, in addition, since we focus on the thermal and not the chemical effects of the combustion process, only the extended Zeldovitch mechanism [16] with the governing reactions:

$$O + N_2 \rightarrow N + NO$$

$$N + O_2 \rightarrow O + NO$$

will be considered in the present study. The calculation of the net production rate of the NO is achieved by assuming a partial equilibrium approach for O radicals [17] resulting from the third-body reaction:

$$O_2 + M \rightarrow O + O + M$$

We also focuses on what seems to be centre of many modern furnace designers, it's finding a trade-off between the NOx emissions and the combustion efficiency, we thus pay attention on the control of the temperature distribution at the exit plane of the furnace by defining an overall temperature distribution factor (OTDF), expressed as:

$$OTDF = \frac{T_{exit}^{\max} - \langle T \rangle_{inlet}}{\langle T \rangle_{exit} - \langle T \rangle_{inlet}} \tag{7}$$

The combustion regime is considered as ideal if the radial static temperature profile at the furnace exit is uniform, consequently, the overall temperature distribution factor (OTDF) which is indirectly a measure of the combustion efficiency, reach the value unity (OTDF =1) in this ideal case.

5 Results and discussions

The first step in carrying out the CFD simulation is to set up the geometric mesh using a commercial preprocessor Gambit [18] to create the required mesh, this last was developed by implementing throughout the entire axisymmetrical domain a quadrilateral elements scheme while keeping the element size at 0.08, hence, a structured mesh containing 38750 quadrilateral elements was retained for the simulation, several numerical tests on finer grids revealed a relative error not exceeding 5% on the axial temperature field (fig.2).

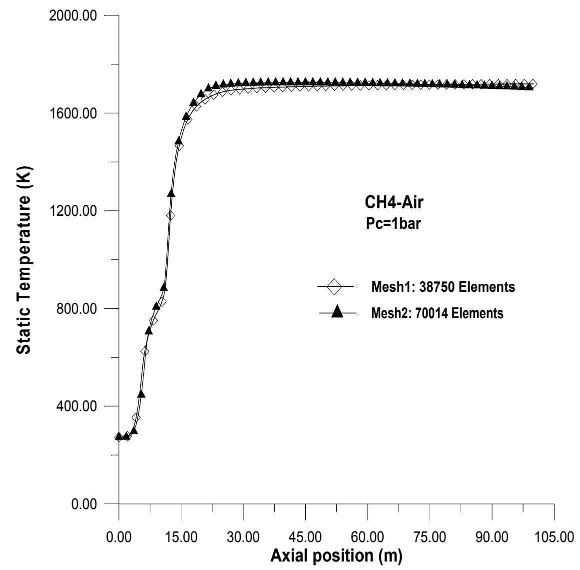

Fig.2: Furnace axial temperature for various meshes.

The thermochemistry analysis of the CH_4/Air mixture under atmospheric pressure shows that the adiabatic flame temperature (close to 2200 K) is reached for a mixture ratio $o/f = 18$ with a standard air composition (21% O_2, 79% N_2), whereas an important decrease is noted (fig.3) when the oxygen dilution is reduced to 9%, this agrees quite well with the non premixed methane/air flames characteristics [19], in addition, mixture viscosity and thermal conductivity were calculated using appropriate mixing rules [20] with an interpolation technique [21].

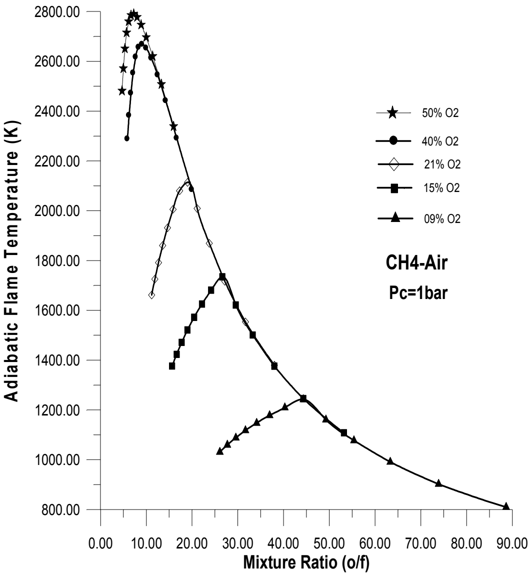

Fig.3: Adiabatic flame temperature for various oxygen dilutions.

The simulation was first based on a process that required a convergent cold flow baseline prior to the activation of the reactions, the cold flow is particularly interesting because it separates the effect of turbulent mixing from combustion, such that one can validate the turbulence model, hence, the maximum half jet was obtained for a $C_{2\varepsilon}$ constant model equal to 1.90 accordingly to the Pope correction, moreover, the jet spreading improves the turbulent mixing and consequently, the fresh mixture quality.

Because of the highly non linear character of the reaction rate appearing as a source term in the species transport equation (eqn.5), the solution can be numerically difficult and very sensitive to chemistry unknowns, to reach a stable converging solution on the reacting flow calculation, it's useful to proceed in a two step procedure where the cold flow solution provide a starting solution of the combustion system.

Since the combustion is fully controlled by the turbulent mixing, the flame seems to be concentrated at the region located at the top side of the furnace (fig.4) where the oxygen is trapped; consequently, brick damage occurs often in this region due to tremendous heat fluxes [22], moreover, the visible flame length (about 20 meters) estimated from the axial temperature distribution (fig.5) is quite similar to the furnace process data [23], however, an overestimation of 200 K is noted on the peak value of the temperature when using a one step chemistry.

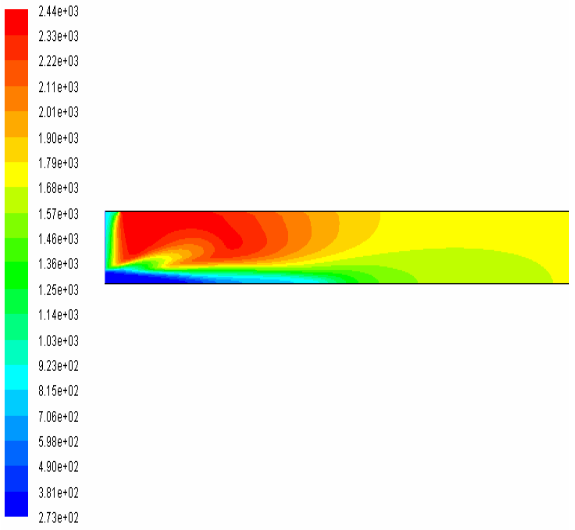

Fig.4: Contour of the static temperature.

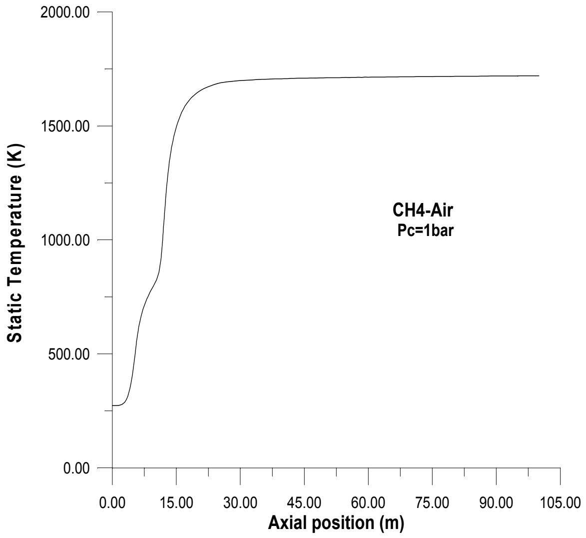

Fig.5: Axial static temperature.

Because of the important amount of the gas products rejected to the atmosphere, it is of great importance to have a prediction of the nitrogen oxide rate at the furnace exit area, hence, the exit radial profile (fig.6) of the mean NO present a peak value of 1400 ppm at the furnace centerline which is quite similar to the density averaged value measured by the axial sensor [23].

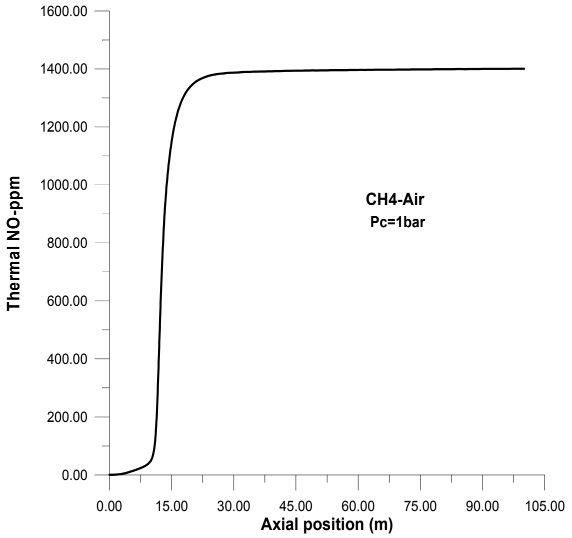

Fig.6: Axial NO profile.

It is obvious that the gas products temperature tend to decrease from its exit value when the flow is reinjected at the furnace inlet because of the heat transfer between the ducts and the ambient air, for that reason, several simulations were carried out for various co-flow temperature and shows that the overall temperature distribution factor (OTDF) and the exit NOppm rate presents a contradictory behavior (fig. 7) which express a compromise between an efficient and a safe-clean combustion.

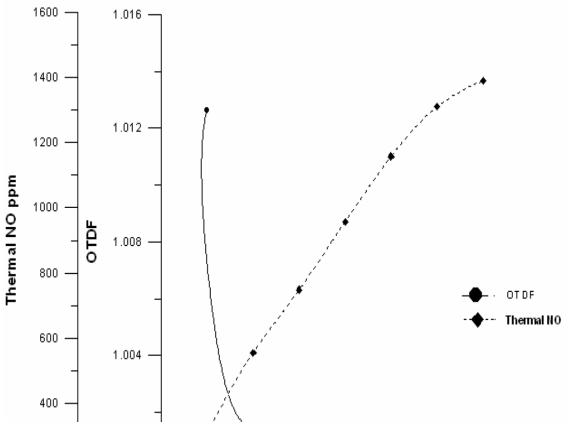

Fig.7: Co-Flow temperature effect on OTDF and NO rate.

If the hot products are cooled at 600 K, it is possible, when the adiabacity of the furnace walls is ensured, to reduce the exit NO rate until 900 ppm (fig.7) while keeping an acceptable OTDF value, in addition, a parametric analyses shows that an exit NO rate lower than 250 ppm can be reached if the inner sides of the furnace walls could be maintained at a fixed temperature of 600 K, however, these processes requires additional and probably, high cost hardware (coolers, exchangers, regulators, sensors….) and consequently, represents a technological challenge for furnace designers.

6 Conclusion

Rejections of NOx pollutants issued from combustion processes are strongly restricted; industrialists have to include the environmental parameters to their production politics. A better understanding of the dynamic behavior of the CH_4/Air systems may allow a better control of NOx emissions, in this context; several methods are available and are more or less implemental in an industrial site. For the implementation of such methods, it is necessary to act on fuel / air injection parameters in the aim to obtain the desired combustion efficiency and pollution level, however, such operations often affect the cement quality and induce production break-off, hence, it have to be simulated before.

A CFD work was performed in order to study the flow field and predict the NO rate produced by a Methane/Air non premixed flame occurring in a burner of an industrial furnace designed for cement production.

In this work, we focus on the burner non premixed flame simulated with one step chemistry, we pay attention to the flame length at given mixture ratio and concentrate on the control of exit temperature distribution in addition to the Zeldovitch-NO production rate and its relation with the combustion efficiency.

The simulation shows that the visible flame length depending strongly on the flow turbulence characteristics was well predicted, while the temperature field was slightly overestimated because of the complete combustion chemistry model, moreover, combustion under current operating conditions, presents an acceptable level of NO emission which can be reduced by adding cooling equipments for the reinjected back flow and the furnace walls.

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Symbol	Designation
A	Constant of the Magnussen model
B	Constant of the Magnussen model
$C_{\varepsilon 2}, C_{\varepsilon 3}$	Turbulence model constants
CEA	Chemical Equilibrium and Applications
CFD	Computational Fluid Dynamics
ECDE	Entreprise des Ciments et Dérivées
EGR	Exhaust Gas Recirculation
OTDF	Overall Temperature Distribution Factor
D_n	Diffusion coefficient for a species "n"
k	Turbulent kinetic energy
M_i	Molecular weight of a species "i"
N	Species total number in the mixture
o/f	Mixture ratio
P	Production rate of k
S_{ij}	Rate of strain tensor
T	Temperature
$\widetilde{u}_i, \overline{u}_i$	Averaged values (Favre and Reynolds) of the i th component of the velocity vector
$\dot{W}$	Reaction rate of a species
x_i	Position vector
Y_k	Mass fraction of the species
Greek symbols	
ε	Dissipation rate of k
χ	Vortex stretching invariant
ν	Stoichiometric coefficient
ω_{ij}	Rotation tensor
$\overline{\rho}$	Averaged (Reynolds) density
Subscripts	
P	Product
Pc	Pope correction
R	Reactant