# Reduced NO Mechanisms Validation for a Coke Oven Gas Fed Flameless Furnace

**V.Fortunato[1], G. Mosca[2], D. Lupant[2], A.Parente[1]**

1. Service d'Aéro-Thermo-Mécanique, Université Libre de Bruxelles, Bruxelles, Belgium.
2. Faculté Polytechnique de Mons, Thermal Engineering and Combustion Unit, Mons, Belgium.

Nowadays, in the field of energy production, particular attention must be paid to improve efficiency and reducing pollutants. Flameless combustion [1] is a rather new technology that provides high efficiency in fuel consumption with low NO and soot emissions. It requires the reactants to be preheated above their self-ignition temperature and enough inert combustion products to be entrained in the reaction region, in order to dilute the flame. As a result, the temperature field is more uniform than in traditional non-premixed combustion systems, and it does not show high temperature peaks. Hence, NO formation is suppressed as well as soot formation, due to the lean conditions, low temperatures and the large $CO_2$ concentration in the exhausts recirculated. The increasing interest in flameless combustion is motivated by the large fuel flexibility, representing a promising technology for low-calorific value fuels [2], high-calorific industrial wastes as well as in presence of hydrogen [3]. Recently several studies showed also the compatibility of such regime with biogas [4-6].

As far as the pollutants are concerned, the very low NO production and the specific formation routes make the NO prediction very challenging. Galletti et al. [7] recently investigated two reduced kinetic models for the quick evaluation of NO emissions from MILD combustion of $H_2$-enriched fuels through post-processing of Computational Fluid Dynamics simulations.

The present work aims at validating those reduced NO formation routes in a flameless furnace fed with Coke Oven Gas.

The system under investigation is a 30 kW furnace, equipped with a ceramic fiber heat-insulating layer. It has a square internal section of 0.35 m x 0.35 m and it is 1 m high. Two fuel injectors, with a 4.5 mm diameter and an 11° tilt angle from the vertical axis, are symmetrically located around the air nozzle, whose exit diameter is 24.8 mm. Combustion air, supplied by a compressor, can be preheated at three different levels (670 K, 870 K and 1070 K) by an electrical preheater. The fuel is Coke Oven Gas (2% $N_2$, 1.5% $CO_2$, 28.5% $CH_4$, 62% $H_2$ and 6% CO).

Calculations were run using Ansys16 package.

Due to the symmetry of the geometry just one quarter of the furnace was modeled. The grid consists in 760k cells. Standard k-ε and Discrete Ordinate coupled with WSGG domain based were considered to model turbulence and radiative heat transfer respectively. Turbulence-chemistry interactions were taken into account using the Eddy Dissipation Concept coupled with the KEE58 kinetic mechanism. Numerical calculations were run for all the three levels of air preheating. Those calculations were then post processed to calculate NO emissions.

The calculations were run considering the new reduced mechanism reported by Galletti et al. [7]. Those models were derived from a Rate Of Production Analysis carried out with two different detailed kinetic schemes POLIMI [8] and Glarborg [9] kinetic schemes. The resulting reduced mechanism incorporates thermal, $N_2O$, NNH as well as $HNO/NO_2$ intermediate routes.

Despite the high level of preheating of the inlet air, since flameless regime is achieved in the furnace there are no peaks of temperature. For the three cases, outlet temperatures are 1351 K, 1393 K and 1430 K respectively.

Results for the NO calculations are reported in Table 1, and are also compared with the ones obtained considering the default parameters implemented in Ansys16.
It can be noticed that the new reduced mechanisms provides values for the NO emissions in better agreement with the experimental data than the ones obtained with the default parameters.

| | NO emissions [ppm dry] | | |
|---|---|---|---|
| **Air Inlet Temperature [K]** | Exp | New Mechanism | Ansys 16 |
| 670 | 9.5 | 5.5 | 15.2 |
| 870 | 11.7 | 8.7 | 23.9 |
| 1070 | 13.9 | 15.7 | 33.9 |

Table 1: NO emissions for three different levels of air preheating, obtained with different mechanisms.

In order to better evaluate those results the error metric normalized with respect to the measured value was evaluated, which is defined as:

$$\left|\frac{\bar{E}}{\bar{Y}_e}\right| = \left|\frac{Y_m - \bar{Y}_e}{\bar{Y}_e}\right| \quad (1)$$

where $\bar{Y}_e$ and $Y_m$ are the mean measurement and the predicted value of variable $Y$.
Values of the relative validation metric are reported in Table 2.

| | Relative metric | |
|---|---|---|
| **Air Inlet Temperature [K]** | New Mechanism | Ansys16 |
| 670 | 0.43 | 0.59 |
| 870 | 0.25 | 1.04 |
| 1070 | 0.14 | 1.44 |

Table 2: Relative validation metric on the NO emissions evaluations, obtained with different mechanisms.

In the first case ($T_{air}$ = 670 K) the deviation from the experimental value is similar. For the other two cases, the new mechanism gives a much lower deviation than the one obtained with the default mechanisms.

**References**


1 Wünning J.A., Wünning J.G., Flameless oxidation to reduce thermal no-formation Prog. Energy Combust. Sci. 23 (1997) 81–94.
2 Choi G.M., Katsuki M., Advanced low $NO_x$ combustion using highly preheated air, Energy Convers. Manage. 42 (2001) 639–652.
3 Sabia P., de Joannon M., Fierro S., Tregrossi A., Cavaliere A., Hydrogen-enriched methane mild combustion in a well stirred reactor, Exp. Therm. Fluid Sci. 31 (2007) 469-475.
4 Colorado A.F., Herrera B.A., Amell A.A., Performance of a Flameless combustion furnace using biogas and natural gas, Bioresour. Technol. 101 (2010) 2443-2449.
5 Hosseini S.E., Bagheri G., Wahlid M.A., Numerical investigation of biogas flameless combustion, Energy Convers. Manage. 81 (2014) 41-50.
6 Chen S., Zheng C., Counterflow diffusion flame of hydrogen-enriched biogas under MILD oxy-fuel condition, Int. J. Hydrogen Energy 36 (2011) 15403–15413.
7 Galletti C., Ferrarotti M., Parente A., Tognotti L., Reduced NO formation models for CFD simulations of MILD combustion, Int. J. Hydrogen Energy 40 (2015) 4884–4897.
8 Ranzi E, Sogaro A, Gaffuri P, Pennati G, Faravelli T. Wide range modeling study of methane oxidation. Combust Sci Technol 96 (1994) 279-325.

9 Glarborg P, Alzueta MU, Dam-Johansen K, Miller JA. Kinetic modeling of hydrocarbon/nitric oxide interactions in a flow reactor. Combust Flame 115 (1998) 1-27.