**K1-MET** | **Competence Center for Excellent Technologies in „Advanced Metallurgical and Environmental Process Development“**

# Success Story Area 1 Project 3

## Formation of nitrogen oxides in the Heating System of a Coke Oven

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The project investigates the formation of nitrogen oxides in the heating system of a coke plant by implementing the reaction mechanism and the combustion kinetics with the help of the CFD package FLUENT 6.3. In the latest simulations the Eddy dissipation concept was used for the species transport showing very good compliance to real plant data.

Project-Partners

## Scope

**The latest project activities focused on the modification of the simulation setup for the prediction of nitrogen oxide formation during the combustion of blast funace gas in the heating system of the coke ovens at the voestalpine in Linz. A comparison with measured off gas emissions showed that the simulations tend to overpredict the NO and CO emission loads respectively.**

## Simulation setup

**The usually implemented species transport model was the Non-premixed combustion method. This model was coupled with a mixture fraction PDF-model (for the calculation of scalars e.g. species concentrations) and a flamelet model (for the calculation of the flame surface).**
**Simulation results showed a non satisfactorily prediction of the NO emission load.**
**The results led to the assumption that the Non-premixed-PDF-flamelet concept was not suitable for the present purpose.**
**A literature survey led to the Eddy dissipation concept (EDC). This model combines species reaction kinetics with the flame turbulence by using detailed chemical reaction mechanisms.**
**The main difference between EDC and Non premixed PDF-Flamelet concept is that the EDC solves a transport equation for each species.**
**Although leading to higher computational effort this model is suitable for the calculation of the slow CO burnout and therefore we assume the EDC being the most suitable species transport model for the combustion conditions in a coke oven heating system.**
**Following Table 1 summarizes the methods and models used for the simulations.**

**Table 1: Implemented methods and models.**

| | |
|---|---|
| **Turbulence of flow** | **k-ε Model** |
| **Radiation** | **Discrete Transfer Radiation Model (DTRM)** |
| **Species transport** | **Eddy dissipation concept (EDC)** |
| **Chemical reaction mechanism** | **$CH_4$-combustion mechanism incorporating 16 species and 41 elementary reactions** |
| **NO formation** | **Thermal NO (Zeldovich-Mechanism) & Prompt NO (Fenimore-Mechanism)** |

## Illustration of the simulation results – Comparison with measured data

**Fig. 1 shows the simulated temperature distribution in the heating flue for a double stage blast furnace gas (BFG) combustion. Fig. 1 b showing the Eddy dissipation concept calculated a stronger energy release in the upstream flue leading to higher peak temperatures. Concerning the CO burnout this causes a stronger formation of OH radicals being necessary for the CO oxidation according to CO + OH → $CO_2$ + H**
**A comparison with real plant measured NO and CO emission loads (cf. Fig. 2 and Fig. 3) shows a very good compliance.**

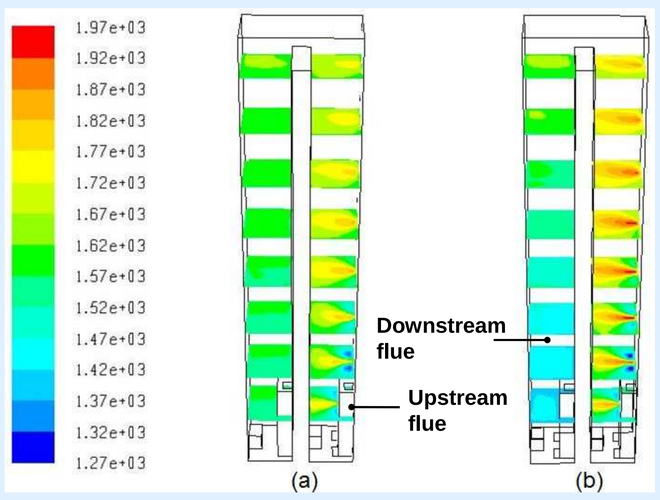


**Fig.1 Simulated temperature distribution in the heating flue.**
**(a) Non premixed PDF-flamelet concept**
**(b) Eddy dissipation concept**

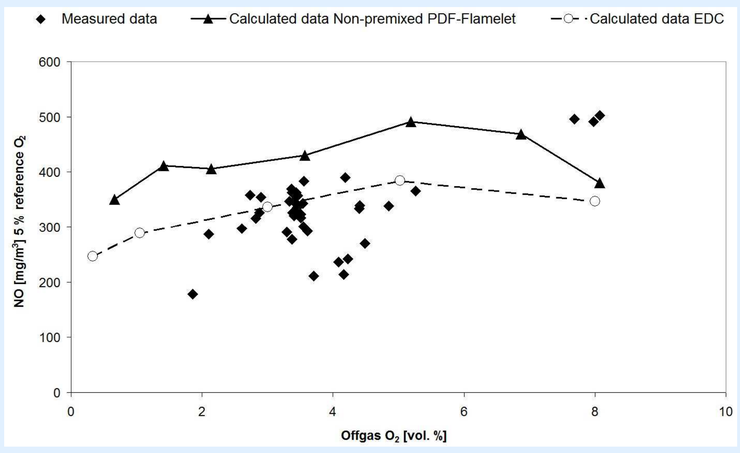


**Fig.2 Measured and simulated NO emissions for double stage combustion as a function of offgas oxygen content.**

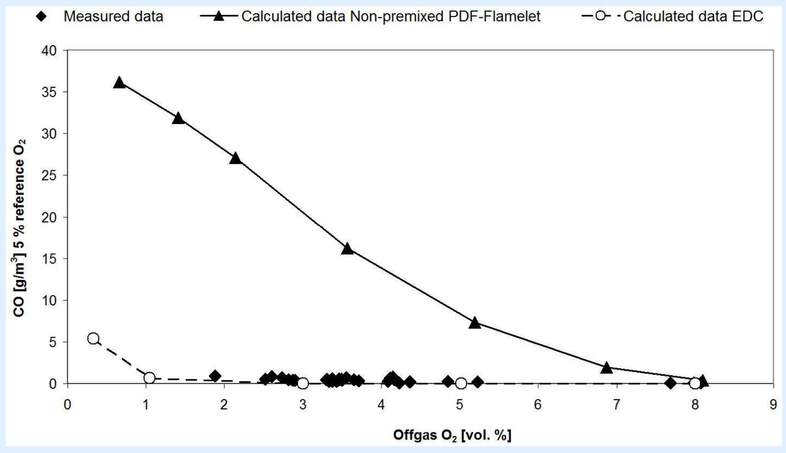


**Fig.3 Measured and simulated CO emissions for double stage combustion as a function of offgas oxygen content.**

## Conclusion

**The comparison of the EDC simulation results showed a very good compliance to real plant measured emission data. Therefore we believe that the EDC is the most suitable model for calculating the emission loads in a coke oven heating system.**

**Further project activities will focus on the sinle stage BFG combustion.**