CFD simulation of NO_x formation in fixed-bed biomass combustion plants

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Contents

Scope of work

- **Presentation of a 3D CFD NO_x formation model (postprocessor) including detailed reaction kinetics for biomass grate furnaces**
  - **must be applicable to engineering problems**
  - **with reasonable accuracy**
  - **with reasonable calculation time**
- **Application of the CFD NO_x postprocessor**
  - **Simulation of a pilot-scale biomass grate furnace and comparison with measurement data taken during test runs**

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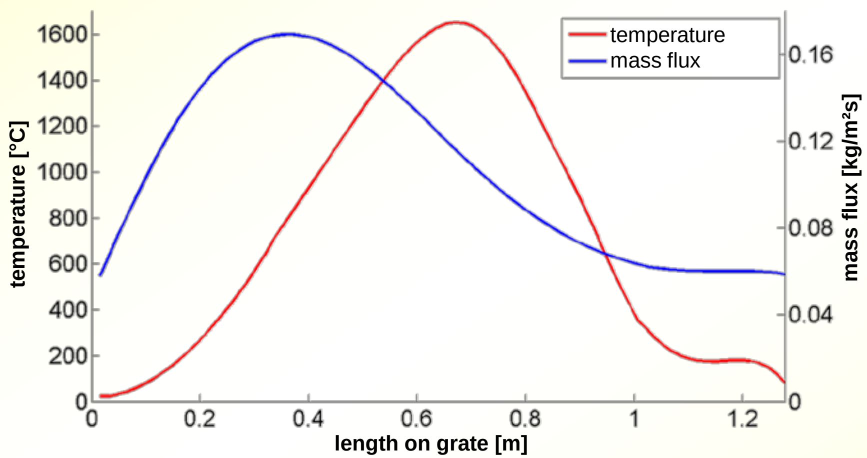
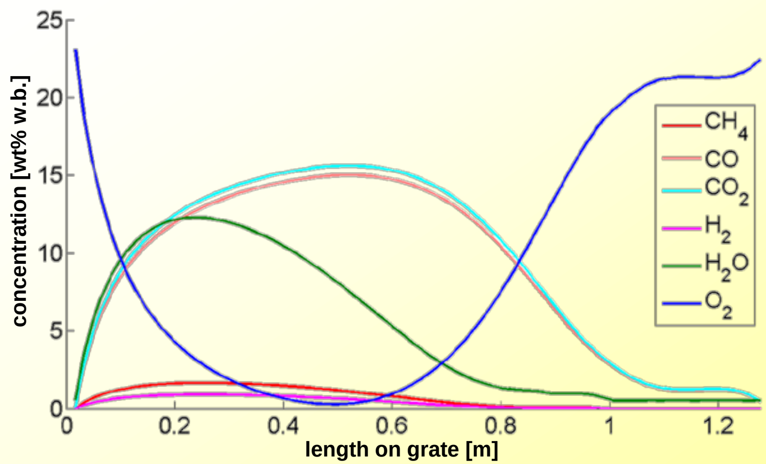
Empirical fixed bed model – basic version

- Definition of profiles for the distribution of primary air and recirculated flue gas as well as drying and thermal decomposition of the solid biomass (C, H, O) along the grate on the basis of test runs
- Definition of conversion parameters for CH_4, H_2, CO, CO_2, H_2O, and O_2 in the flue gas released based on literature data and lab-scale experiments
- Stepwise balancing of mass, species and energy





Calculated profiles of temperature, mass flux and species concentration in the flue gas along the grate for grass pellets

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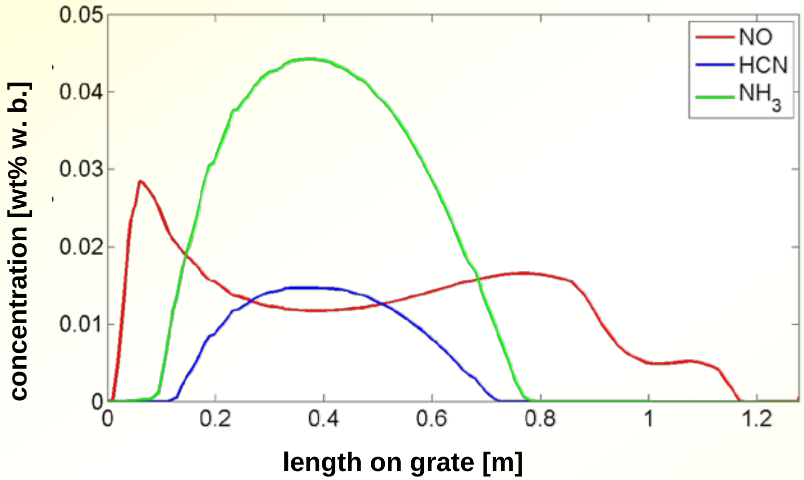
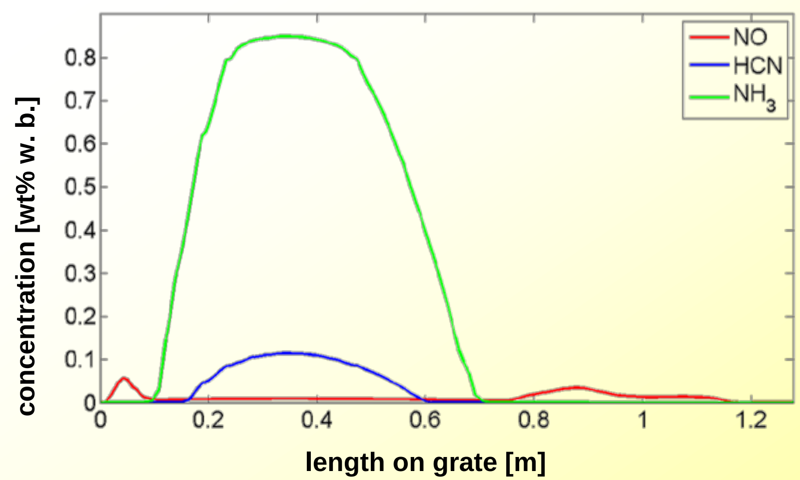
Extension of the fixed bed model – release of N species

- The empirical fuel bed combustion model was extended in order to describe the release of N species (NO and NH_3 as well as HCN) which are relevant for the formation of fuel NO_x in biomass grate furnaces
- Conversion parameters (as a linear function of local λ) were defined for the investigated fuels based on lab-scale pot furnace (batch) reactor experiments; NH_3 showed to be the pre-dominant NO_x precursor, HCN and NO were found in lower concentrations





Example: calculated profiles of NH_3, HCN and NO concentration in the flue gas along the grate (left - fuel: corncobs; right - fuel: grass pellets)

BRUNNER Thomas, BIEDERMANN Friedrich, KANZIAN Werner, EVIC Nikola, OBERNBERGER Ingwald. 2012: Advanced biomass fuel characterisation based on tests with a specially designed lab-scale reactor. In: Proc. of the Int. Conference "Impacts of Fuel Quality on Power Production and Environment", September 2012, Puchberg, Austria, ISBN 978-3-9502992-8-1

Modelling of turbulent reactive flow – basic combustion simulation

- **Turbulence** — Realizable k-ε model
- **Gas phase combustion** — Eddy Dissipation model (A_{mag} = 0.6) / global methane 3-step mechanism (CH_4, CO, CO_2, H_2, H_2O und O_2)
- **Radiation** — Discrete Ordinates model

Modelling of NO_x formation – postprocessing mode

- Eddy Dissipation Concept (EDC)
- reduced „skeletal Kilpinen97“ reaction mechanism (28 species, 104 reactions)
- ISAT (In-Situ Adaptive Tabulation) algorithm for reaction kinetics

ZAHIROVIĆ, 2008: CFD analysis of gas phase combustion and NO_x formation in biomass packed-bed furnances, PhD Thesis
ZAHIROVIĆ et al., 2011: Validation of flow simulation and gas combustion sub-models for CFD-based prediction of NO_x formation in biomass grate furnaces. In: Combustion Theory and Modelling (2011), Vol. No. 15, Issue No. 1, pp. 61-87

Eddy Dissipation Concept (EDC)

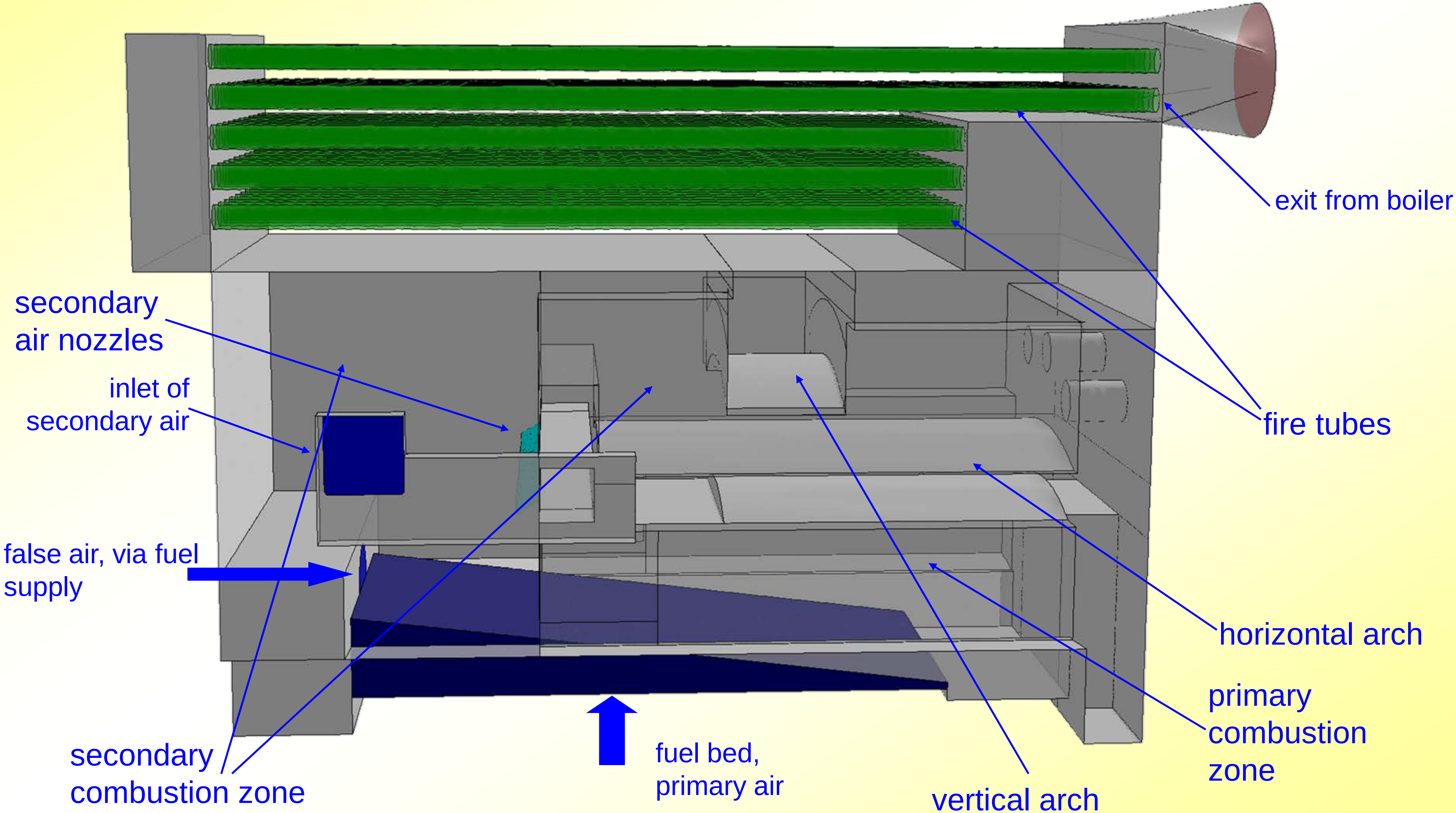
Extension of EDM; Assumption: reactions occur mainly in the smallest length scales of the turbulent energy cascade (fine structures) where turbulent energy is dissipated; fine structures are treated as ideal reactors (reactants are mixed on a molecular scale)

$$R_i = \frac{\bar{\rho}\,\gamma^2}{\tau^*\left(1-\gamma^3\right)}\left(Y_i^* - \widetilde{Y}_i\right)$$

R_i…net production rate [kg/m^{3}s], ρ…density [kg/m^3],
τ^*…residence time in fine structure [s] = (ε, ν),
γ… volume fraction of fine structure [-] = f(k, ε, ν),
k…turbulent kinetic energy [m^2/s^2], ε...dissipation rate of k [m^2/s^3],
ν…kinematic viscosity [m^2/s],
Yi…Favre-averages (~) and fine structure- (*) mass fraction of species i [-]

- **universal application; interaction between turbulence and reaction kinetics captured; reaction kinetics can be described in detail (necessary for simulation of NO_x formation)**
- **no calibration of model parameters necessary**
- **computational time can be long depending on the reaction kinetics (which essentially determine the accuracy of the computation)**

CFD model geometry basic variant



Basic operating conditions
Grass pellets composition

Parameter	Unit	Grass pellets basic
C	[wt.% (d.b.)]	48.17
H	[wt.% (d.b.)]	6.82
O	[wt.% (d.b.)]	31.83
N	[wt.% (d.b.)]	5.77
S	[wt.% (d.b.)]	0.69
ash	[wt.% (d.b.)]	6.72
moisture	[wt.% (w.b.)]	10.81
GCV (analysed)	[MJ/kg (d.b.)]	21.20
GCV (Gaur)	[MJ/kg (d.b.)]	21.40
NCV	[MJ/kg (w.b.)]	17.30

Basic operating data

Parameter	Unit	Grass pellets basic
Adiabatic flue gas temperature	[°C]	1,361
Fuel power (related to NCV)	[kW]	432
Flue gas in combustion chamber - total	[kg/h]	949
- Flue gas release from fuel	[kg/h]	85
- Combustion air - total	[kg/h]	864
Primary air (below grate)	[kg/h]	403
Secondary air (nozzles)	[kg/h]	461
recirculated flue gas	[kg/h]	-
Primary stoichiometric ratio	[-]	0.84
Total stoichiometric air ratio	[-]	1.67
O2 fraction at combustion chamber outlet, dry	[Vol% (d.b.)]	8.4

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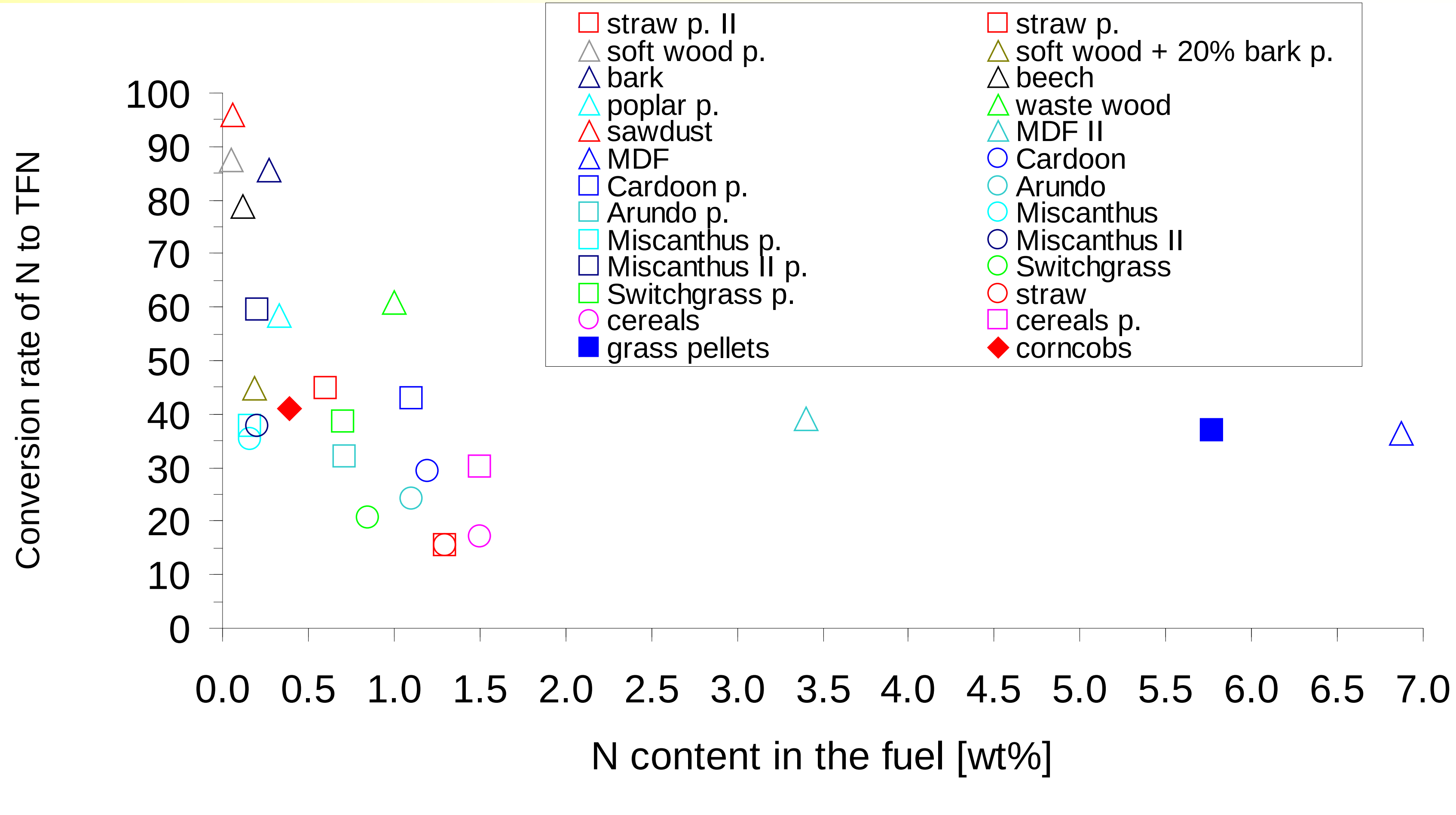
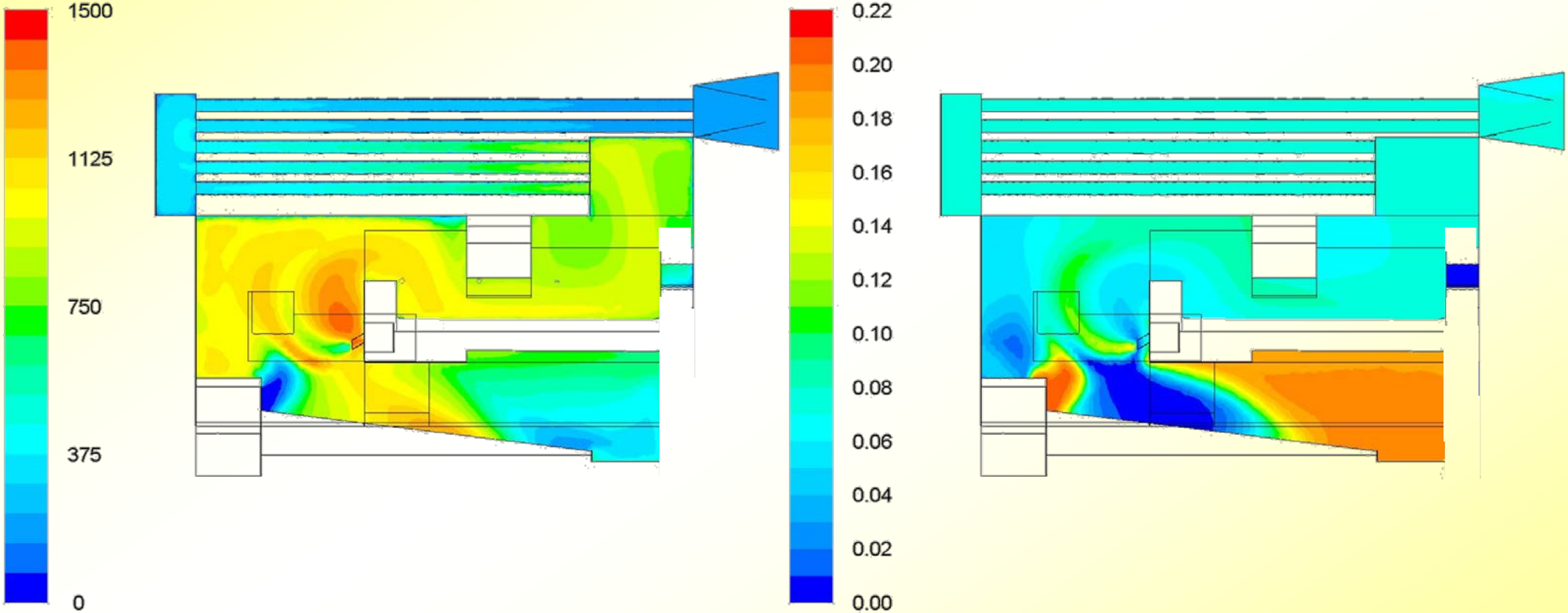
TFN-release rates for different biomass fuels



explanation: all data taken from reactor experiments with lab-scale pot furnace;
TFN … mass of all N-moles contained in NO, NH_3, NO_2, HCN und N_2O, released from the fuel bed

Results of basic analysis – temperatures and O_2 concentrations



Iso-surfaces of temperatures [°C] (left) and O_2 concentrations [m³ O_2/ m³ wet flue gas] (right) in the symmetry plane of the combustion chamber and the boiler

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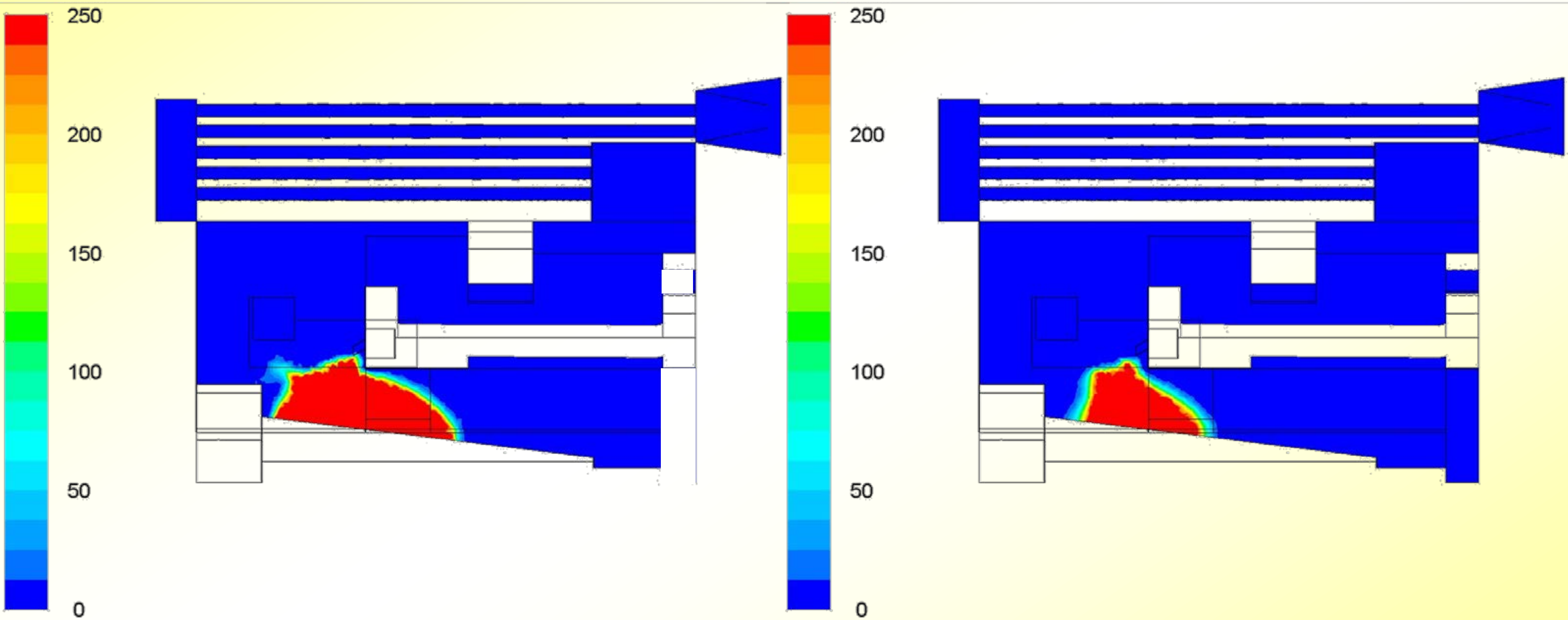
Results of basic analysis – NH_3 and HCN concentrations



Iso-surfaces of NH_3 concentrations [ppmv w.b.] (left) and HCN concentrations [ppmv w.b.] (right) in the symmetry plane of the combustion chamber and the boiler

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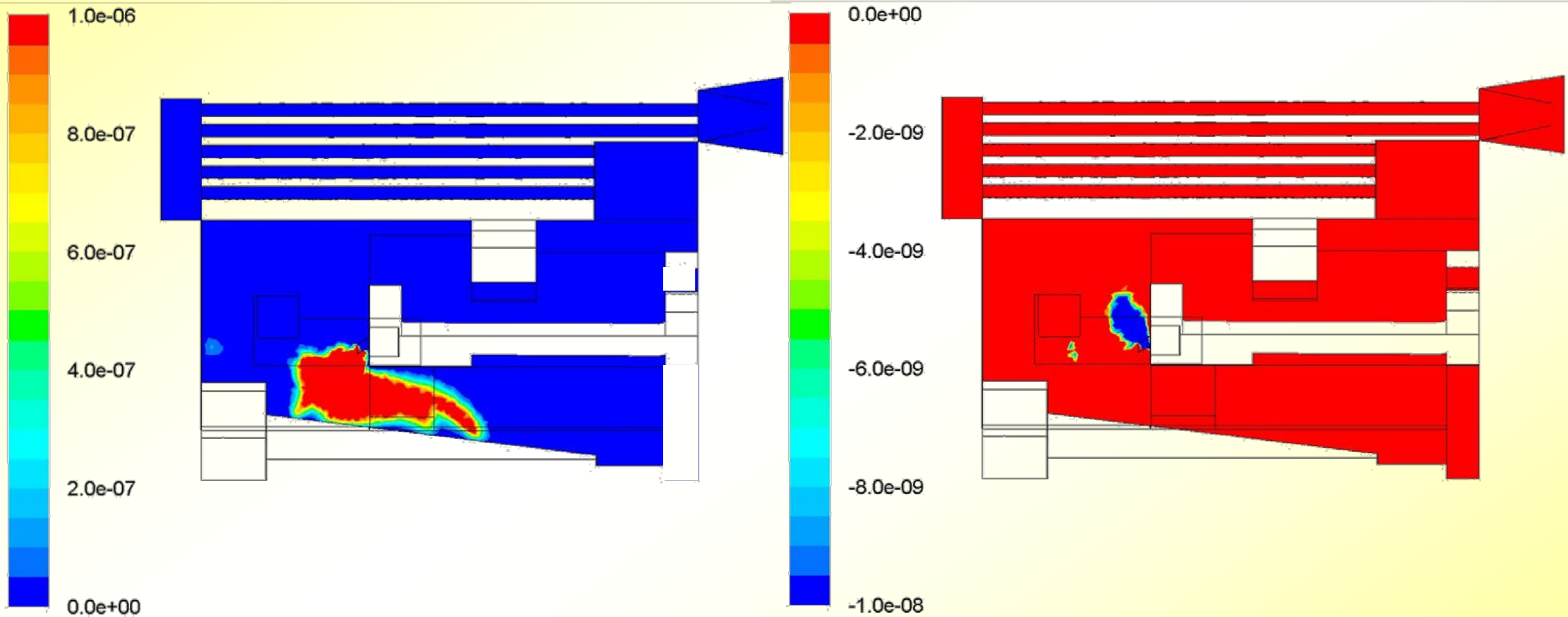
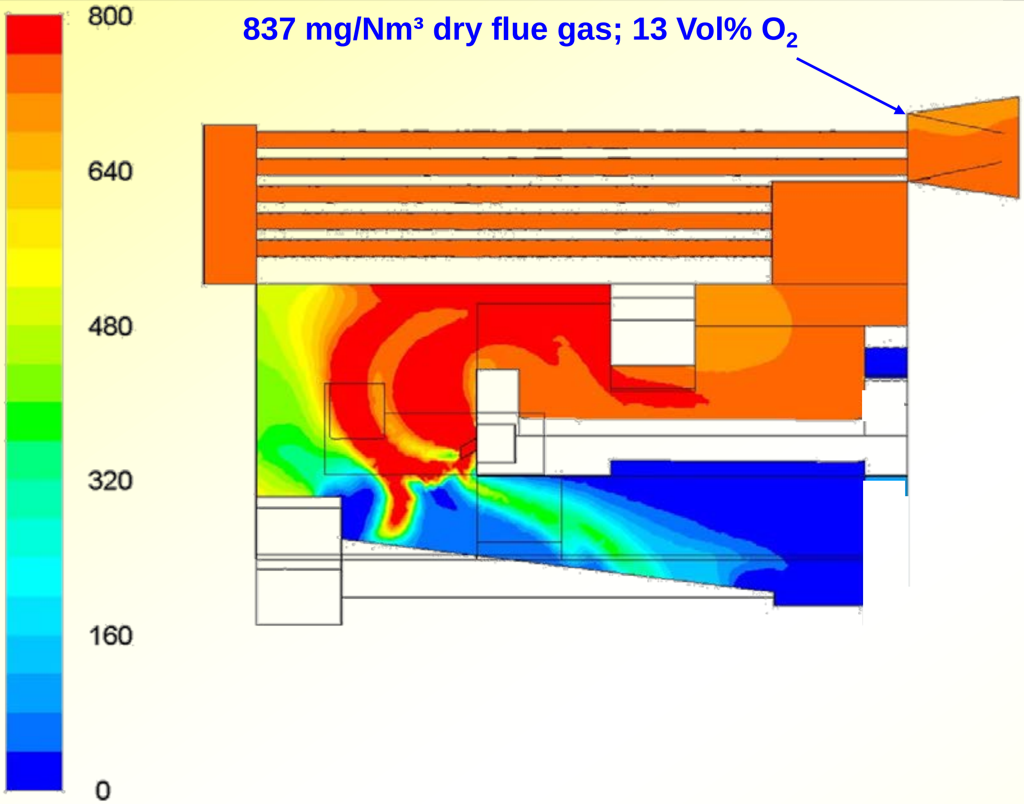
Results of basic analysis – rates of formation of N_2 from NO and of NO from N_2



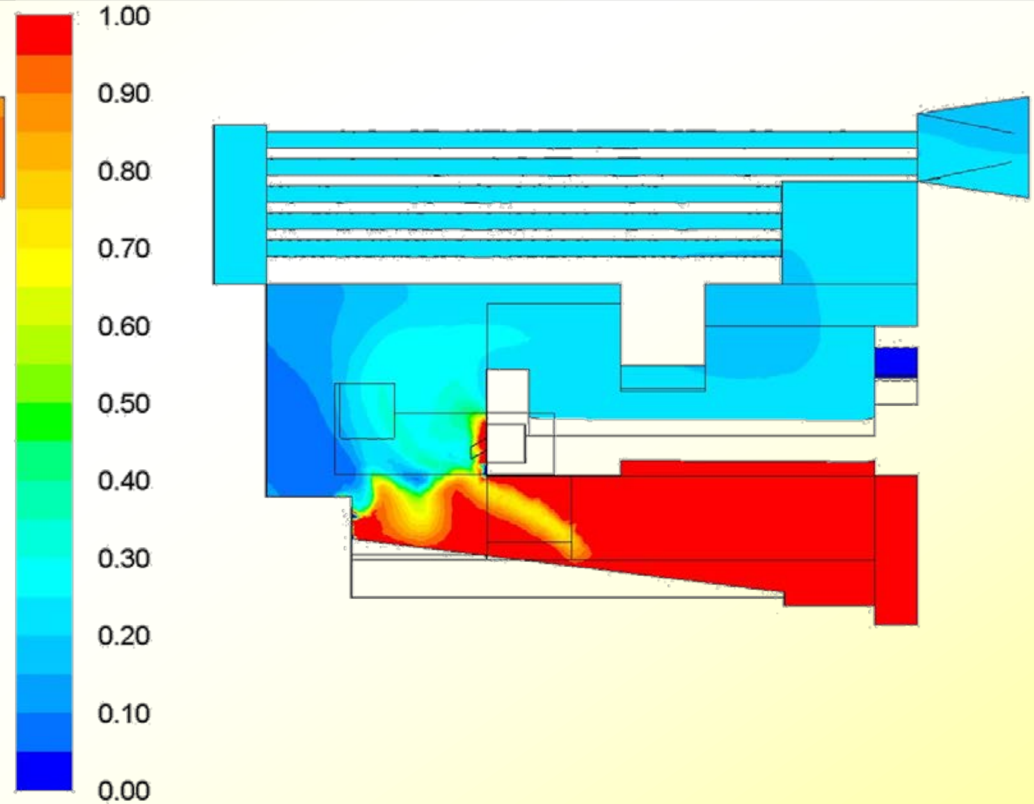
Iso-surfaces of the reaction rates [kmol/(m^3*s)] of the reaction N + NO → N_2 + O for the reduction to N_2 (left) and of the reaction N + NO ← N_2 + O for the formation of NO from N_2 (right) in the symmetry plane of the combustion chamber and the boiler

Results of basic analysis – NO_x concentrations and TFN/TFN_{in} ratio



Iso-surfaces of NO_x concentrations [ppmv w. b.] in the symmetry plane of the combustion chamber and the boiler

explanations: NO_x concentrations as sum of NO, NO_2 and N_2O concentrations, all in [ppmv w. b.]



Iso-surfaces of local TFN/TFN_{in} ratios in the symmetry plane of the combustion chamber and the boiler

explanation: all data taken from reactor experiments with lab-scale pot furnace;
TFN … mass of all N-moles contained in NO, NH_3, NO_2, HCN und N_2O, released from the fuel bed

Results of basic analysis – Evaluation

Evaluation of basic analysis:

- Small primary combustion zone (small flue gas residence time for reduction)
- thermal NO_x (high local flue gas temperatures)

Measures taken for optimization:

- new position of secondary air nozzles
- flue gas recirculation (temperature control)

Basic and optimized operating conditions
Grass pellets composition

Parameter	Unit	Grass pellets basic	Grass pellets optimised
C	[wt.% (d.b.)]	48.17	49.23
H	[wt.% (d.b.)]	6.82	6.53
O	[wt.% (d.b.)]	31.83	30.41
N	[wt.% (d.b.)]	5.77	5.47
S	[wt.% (d.b.)]	0.69	0.65
ash	[wt.% (d.b.)]	6.72	6.80
moisture	[wt.% (w.b.)]	10.81	11.18
GCV (analysed)	[MJ/kg (d.b.)]	21.20	21.20
GCV (Gaur)	[MJ/kg (d.b.)]	21.40	21.46
NCV	[MJ/kg (w.b.)]	17.30	17.28

Basic and optimized operating data

Parameter	Unit	Grass pellets basic	Grass pellets optimised
Adiabatic flue gas temperature	[°C]	1,361	1,042
Fuel power (related to NCV)	[kW]	432	370
Flue gas in combustion chamber - total	[kg/h]	949	1,126
- Flue gas release from fuel	[kg/h]	85	72
- Combustion air - total	[kg/h]	864	753
Primary air (below grate)	[kg/h]	403	362
Secondary air (nozzles)	[kg/h]	461	391
recirculated flue gas	[kg/h]	-	301
Primary stoichiometric ratio	[-]	0.84	0.79
Total stoichiometric air ratio	[-]	1.67	1.64
effective stoichiometric ratio on grate(1)	[-]		0.91
effective stoichiometric ratio on grate(2)	[-]		1.03
ratio of recirculated flue gas below grate	[-]	-	0.52
flue gas recirculation ratio	[-]	-	0.27
O2 fraction at combustion chamber outlet, dry	[Vol% (d.b.)]	8.4	8.3

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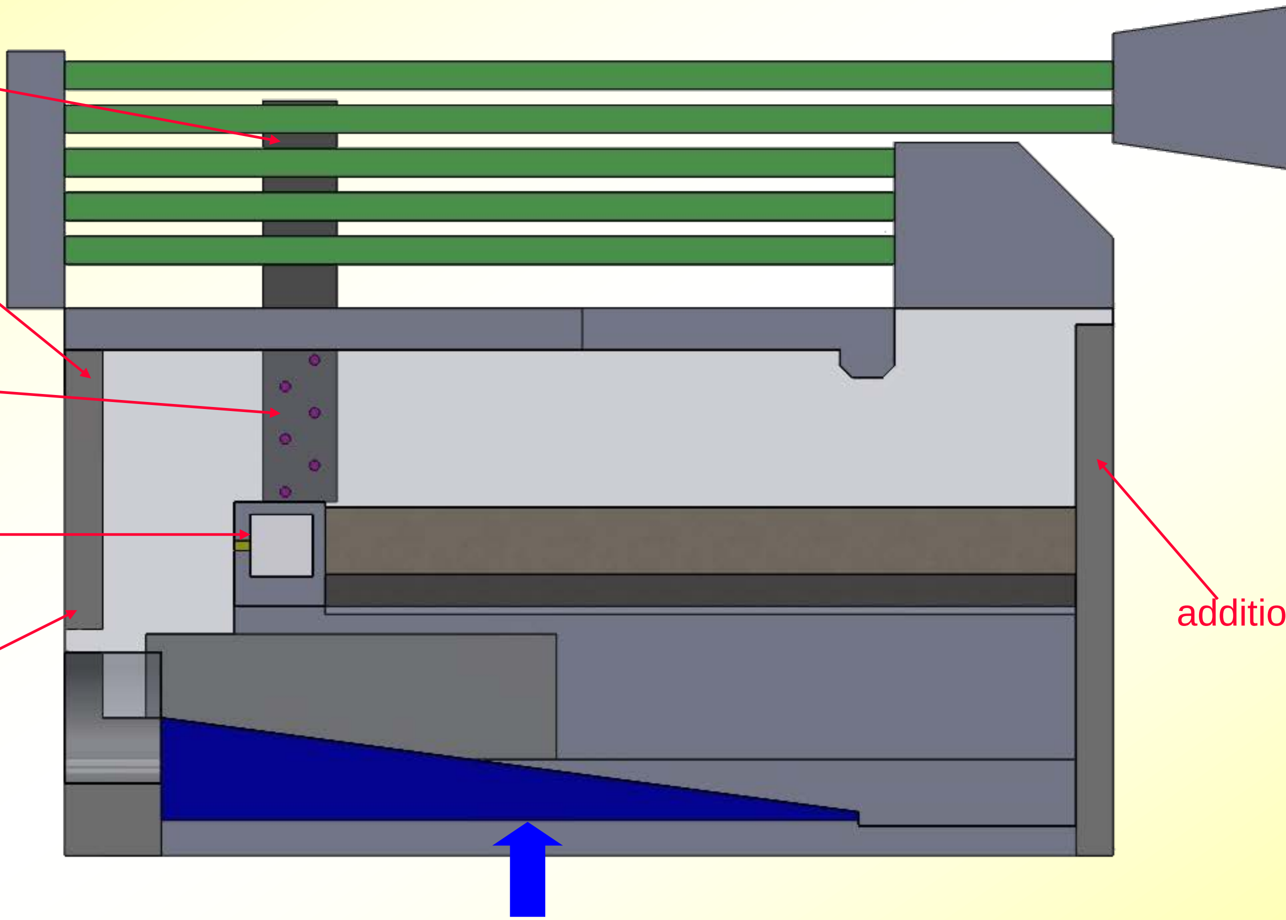
CFD model geometry
optimised variant



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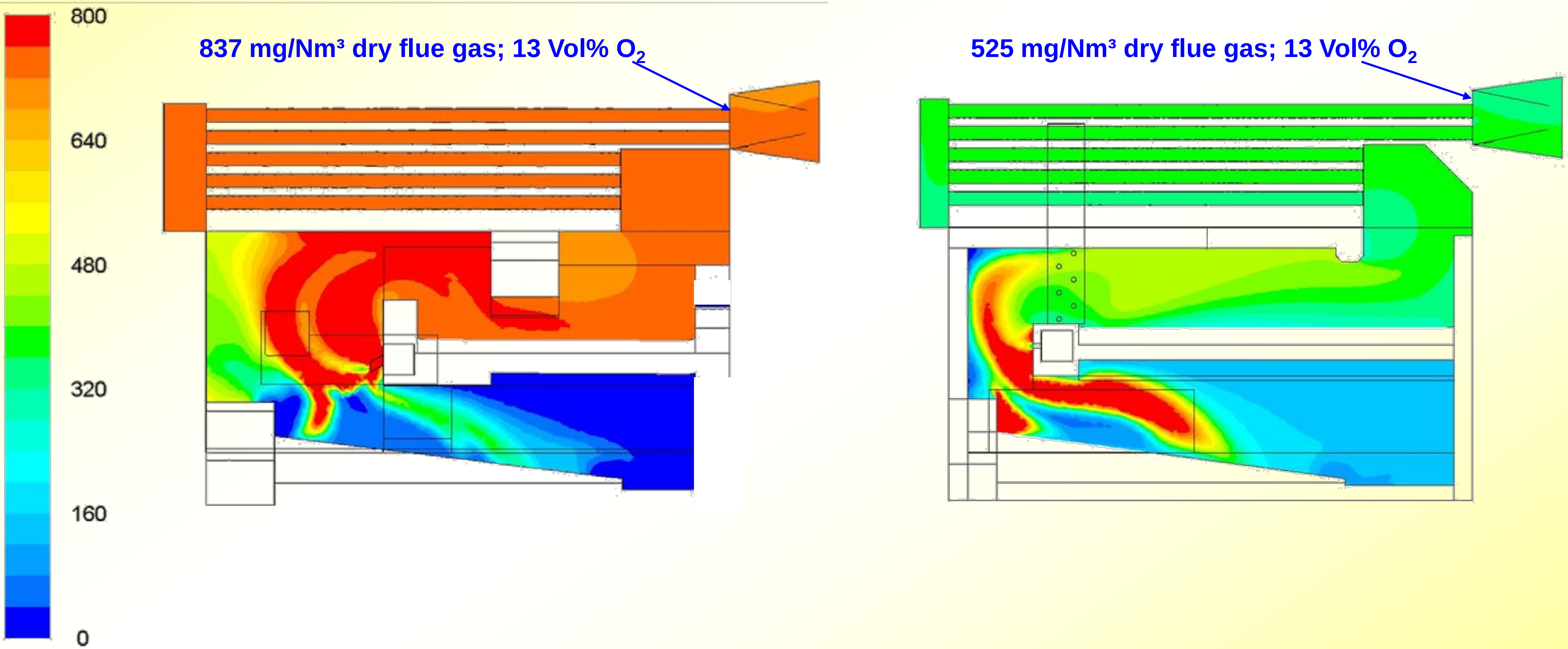
Results of optimization – NO_x concentrations

grass pellets basic geometry basic operating conditions	grass pellets optimized geometry optimized operating conditions



Iso-surfaces of NO_x concentrations [ppmv w. b.] in the symmetry plane of the combustion chamber and the boiler

explanations: NO_x concentrations as sum of NO, NO_2 and N_2O concentrations, all in [ppmv w. b.]

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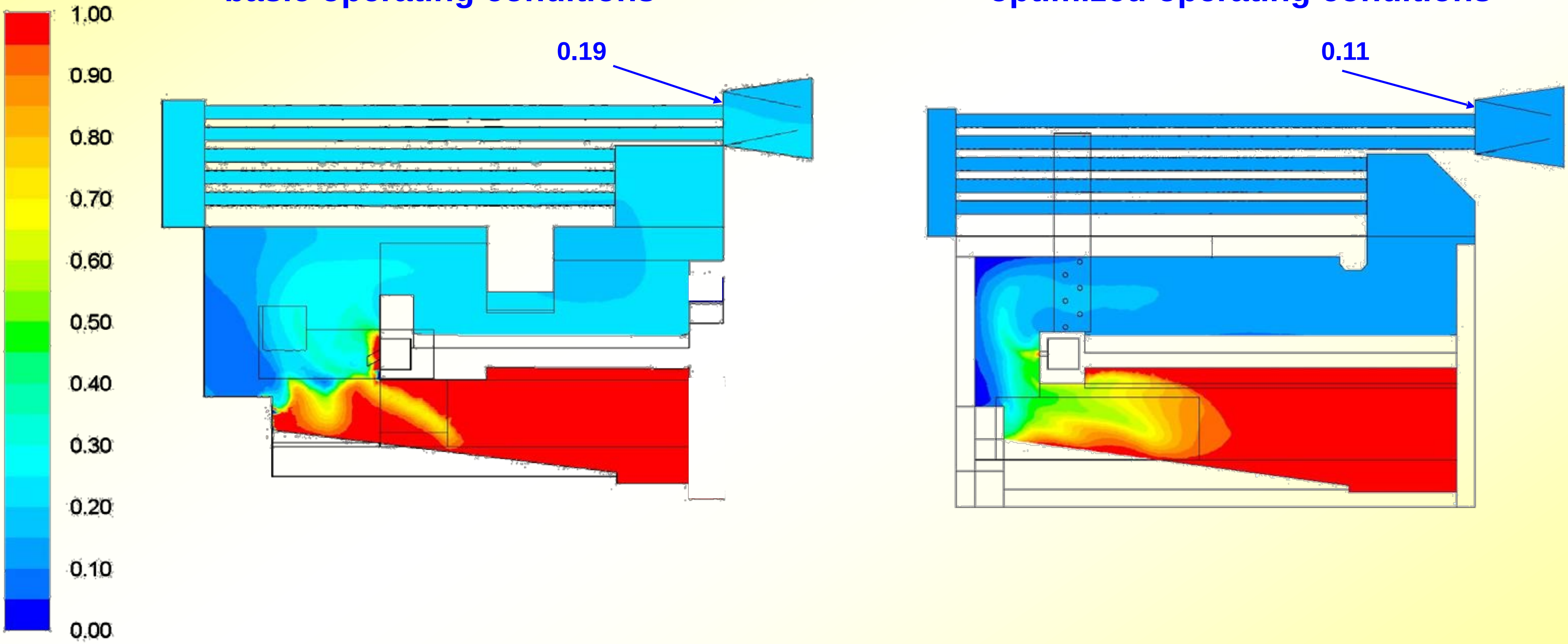
Results of optimization – TFN/TFN$_{in}$ ratios

grass pellets
basic geometry
basic operating conditions

grass pellets
optimized geometry
optimized operating conditions



Iso-surfaces of local TFN/TFN$_{in}$ ratios in the symmetry plane of the combustion chamber and the boiler

explanation: TFN … mass of all N-moles contained in NO, NH_3, NO_2, HCN und N_2O, released from the fuel bed

Results of optimization – measurement compared to simulation results

	Unit	Grass pellets optimised
simulated NO_x-emissions (calculated as NO_2) at the boiler exit	mg NO_x/Nm³ dry fuel gas; 13 Vol.% O2	525
measured NO_x-emissions	mg NO_x/Nm³ dry fuel gas; 13 Vol.% O2	572

Summary and conclusions

- 3D simulations of biomass grate furnaces with the CFD NO_x post-processor including detailed chemistry have been performed.
- Detailed information of NO_x formation and reduction in grate combustion plants as well as a relevant influencing parameters can be gained.
- Good qualitative and semi-qualitative agreement of simulation results with measurements achieved for different biomass fuels.
- The NO_x postprocessor for biomass grate furnaces is a powerful tool for the design and optimisation of furnace geometries and process control in order to optimize NO_x reduction by primary measures.

Thank you for your attention

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