RUHR-UNIVERSITÄT BOCHUM

Lehrstuhl für Energieanlagen und Energieprozesstechnik
Prof. Dr.-Ing. V. Scherer

Barracuda simulation of a CFBC test rig: comparison with experimental results

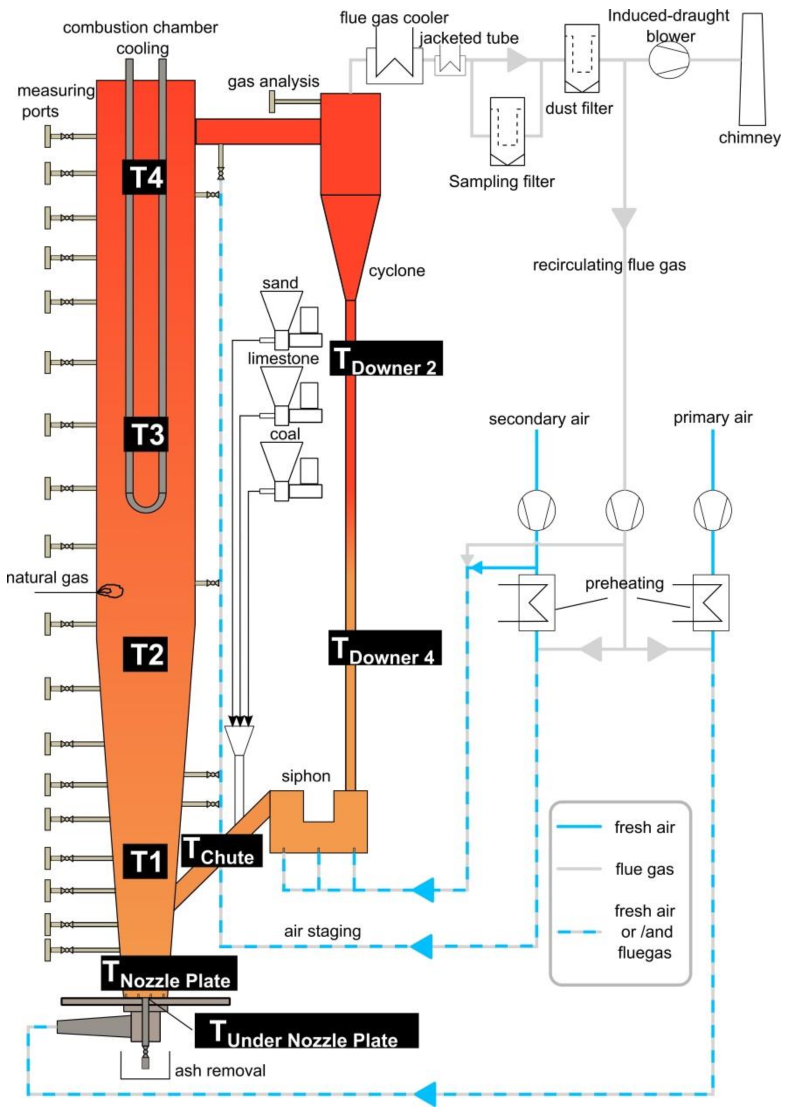
Sebastian Krusch

Department of Energy Plant Technology (LEAT)

Ruhr-University Bochum,
Germany

Introduction

- Profile Measurements of gas emissions, temperature and pressure in a 0.1 MW circulating fluidized bed combustor
- Two different bituminous coals
  - German Auguste Viktoria
  - US High Sulfur
- Global kinetic approaches from literature



Thermal capacity:	100 kW
Combustor height:	~ 5.3 m
Outer diameter:	0.7 m
Inner diameter:	0.2 - 0.3 m
Volume flow primary air:	~ 90 m_N^3/h
Volume flow Siphon air:	5 m_N^3/h
Velocity:	1.4 - 3.5 m/s
→ Residence time	~ 3 - 4 s
Max. temperature:	~ 900°C
Max. airpreheater temp.:	~ 450°C
d_{50} of bed material:	90 µm

Measurements

- 18 Measurement ports: pressure, temperature, gas probes
- Gas analysis: O_2, NO_x, CO, CO_2, N_2O, CH_4, SO_2, C_xH_y
- FTIR Measurements (31 species)
- Bedash and flyash samples
- Planned: capacity solid concentration probe, solids sampling at the downer

Solid characteristics

Fuel	d_{50}	d_{90}
	[µm]	[µm]
US High Sulfur	768	2,940
AV	642	2,482
Sand	110	190

Solid characteristics

	US High Sulfur	AV
Ultimate Analysis [wt.-%, dry]		
Carbon	72.39	79.36
Hydrogen	4.83	4.81
Nitrogen	1.52	1.85
Sulfur	2.33	1.08
Oxygen (Rest)	7.97	5.37
Proximate Analysis [wt.-%, raw]		
Ash	10.55	7.29
Volatile Matter	33.42	27.01
Fixed Carbon	52.31	62.46
Moisture	3.72	3.24
Calorific Analysis [MJ/kg, dry]		
LHV	30.5	31.2

Test conditions

Primary air	86 m_N^3/h
Siphon air	4.4 m_N^3/h
Air-ratio	1.2
Average combustor temperature (T1-T4)	850°C
Superficial gas velocity	1.4 - 3.1 m/s
Feed temperature primary air	420°C
Feed temperature siphon air	60°C

Simulation settings

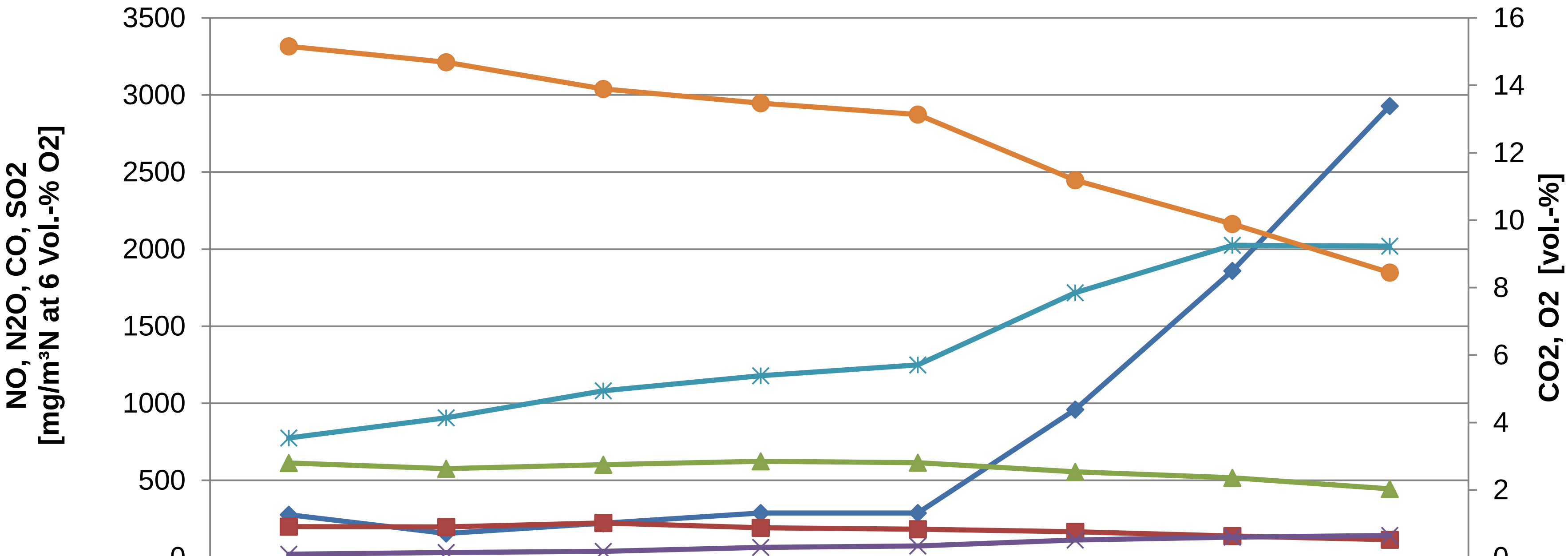
Particle to wall interaction	Normal retention coefficient e_n	0.85
	Tangential retention coefficient e_t	0.85
	Diffuse bounce D_f	2
Grid	Real cells	160,000
Drag model	Weng-Yu with EMMS	
Initial bed inventory	Quartz sand	16.5 kg
Initial number of numerical particles		3.5e+5

Chemical kinetic parameter

Reaction	Reaction rate
$CO+H_2O \rightarrow CO_2+H_2$	$R_1 = (-k_1 C_{CO}{}^{.5} C_{H2O}) \left[\frac{mol}{m^3 s}\right]$, [1]
$CO_2+H_2 \rightarrow CO+H_2O$	$R_2 = (-k_2 C_{H2}{}^{.5} C_{CO2}) \left[\frac{mol}{m^3 s}\right]$, [1]
$CH_4+1.5O_2 \rightarrow CO_2+2H_2O$	$R_3 = (-k_3 C_{CH4}{}^{-.3} C_{O2}{}^{1.3}) \left[\frac{mol}{m^3 s}\right]$, [2]
$2H_2+O_2 \rightarrow 2H_2O$	$R_4 = (-k_4 C_{H2}{}^{1.5} C_{O2}) \left[\frac{mol}{m^3 s}\right]$, [3]
$CO+0.5O_2 \rightarrow CO_2$	$R_5 = (-k_5 C_{CO} C_{H2O}{}^{.5} C_{O2}{}^{.25}) \left[\frac{mol}{m^3 s}\right]$, [4]
$C_2H_2+1.5O_2 \rightarrow 2CO+H_2O$	$R_6 = (-k_6 C_{O2} C_{C2H2}) \left[\frac{mol}{m^3 s}\right]$, [3]

Reaction	Reaction rate
$C+H_2O \rightarrow CO+H_2$	$R_7 = (-k_{7\_1} C_{H2O} + k_{7\_2} C_{H2} C_{CO}) \left[\frac{mol}{s}\right]$, [5]
$C+CO_2 \rightarrow 2CO$	$R_8 = (-k_{8\_1} C_{CO} + k_{8\_2} C_{CO}{}^2) \left[\frac{mol}{s}\right]$, [2]
$C+1/\varphi\ O_2 \rightarrow (2-2/\varphi)CO + (2/\varphi-1)CO_2$	$R_7 = (-k_7 C_{O2}) \left[\frac{mol}{s}\right]$, [6] $\phi = p_{O2}{}^{.21}.0076 e^{3070/T} \left[\frac{1}{kPa}\right]$, [7]

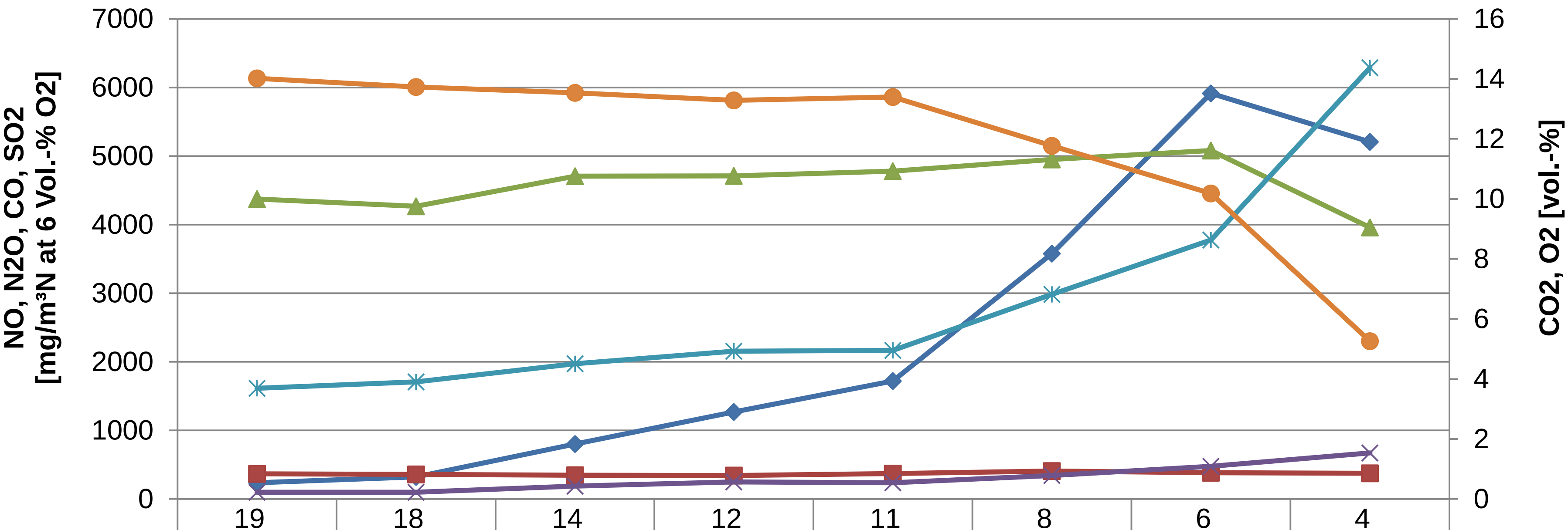
Results US



	19	18	14	12	11	8	6	4
CO*	277.0	155.3	222.0	287.7	287.7	959.0	1859.3	2929.0
N2O	199.0	198.3	224.3	193.0	182.7	165.7	138.7	115.5
SO2	612.0	576.3	602.3	623.0	613.7	555.0	516.7	444.5
NOx	20.0	31.3	38.3	65.0	75.0	112.0	131.7	141.5
O2	3.5	4.1	4.9	5.4	5.7	7.8	9.3	9.2
CO2	15.2	14.7	13.9	13.5	13.1	11.2	9.9	8.5

Average gas concentration profile for US

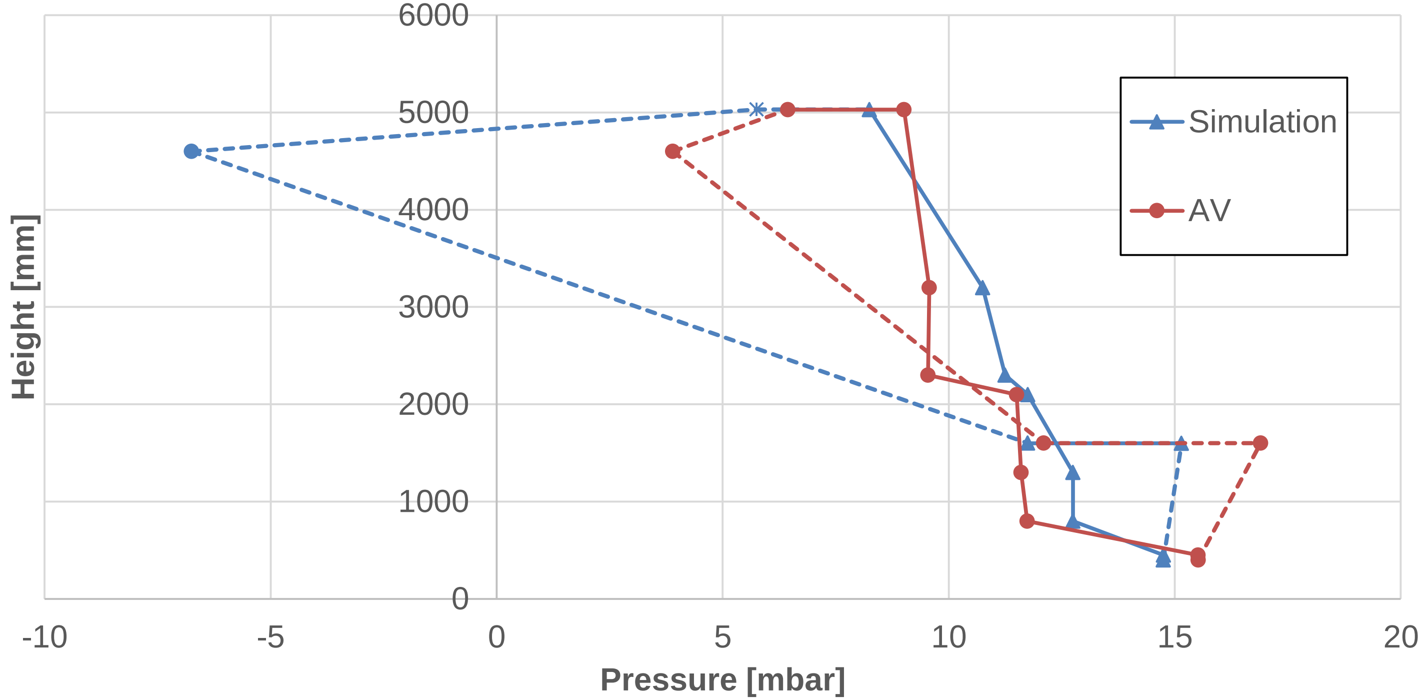
Results AV



	19	18	14	12	11	8	6	4
CO*	237	322.2	804.1	1271.5	1722.5	3576.1	5914.4	5205.7
N2O	367	360.4	346.4	341.4	371.2	408.3	382.6	374.7
SO2	4374	4267.3	4705.6	4710.1	4778.4	4950.3	5080.9	3959.5
NOx	98	101.1	186.8	250.8	237.5	341.8	476.1	671.5
O2	3.7	3.9	4.5	4.9	5.0	6.8	8.6	14.4
CO2	14.0	13.7	13.5	13.3	13.4	11.8	10.2	5.3

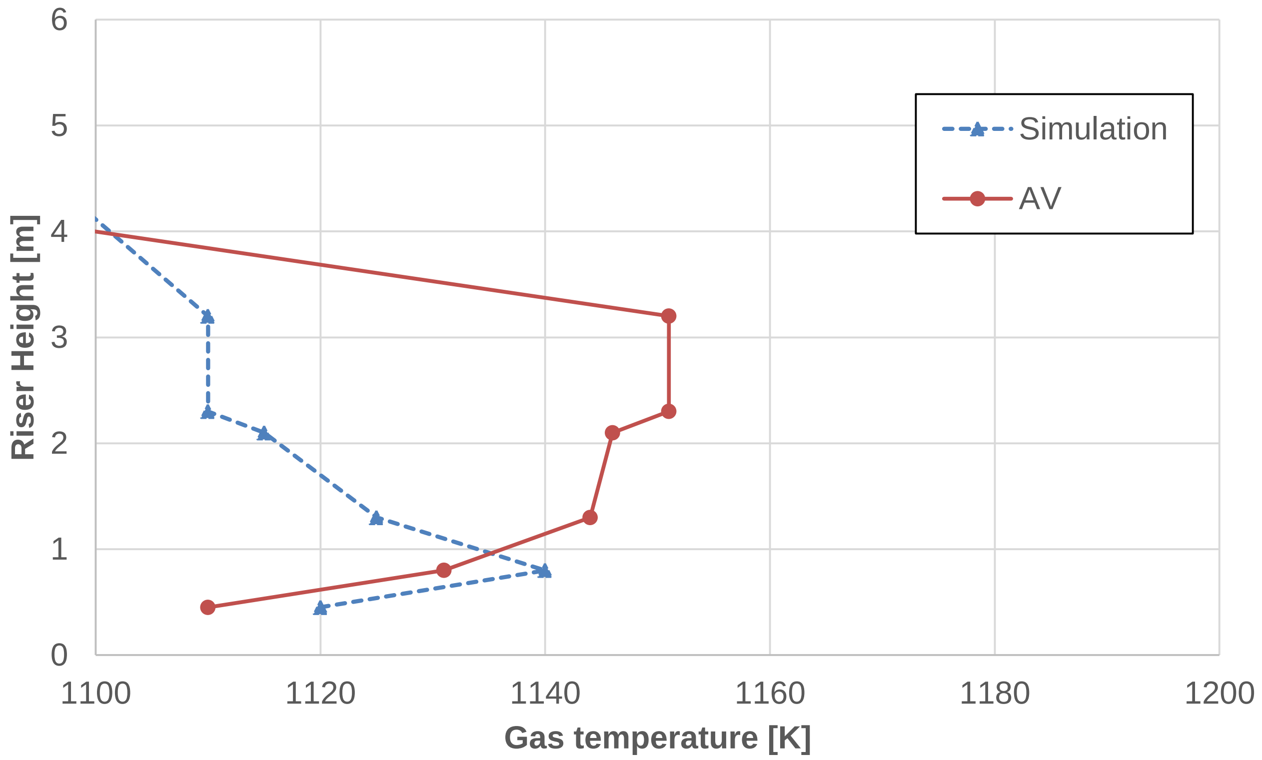
Average gas concentration profile for AV

Results AV



Pressure profile

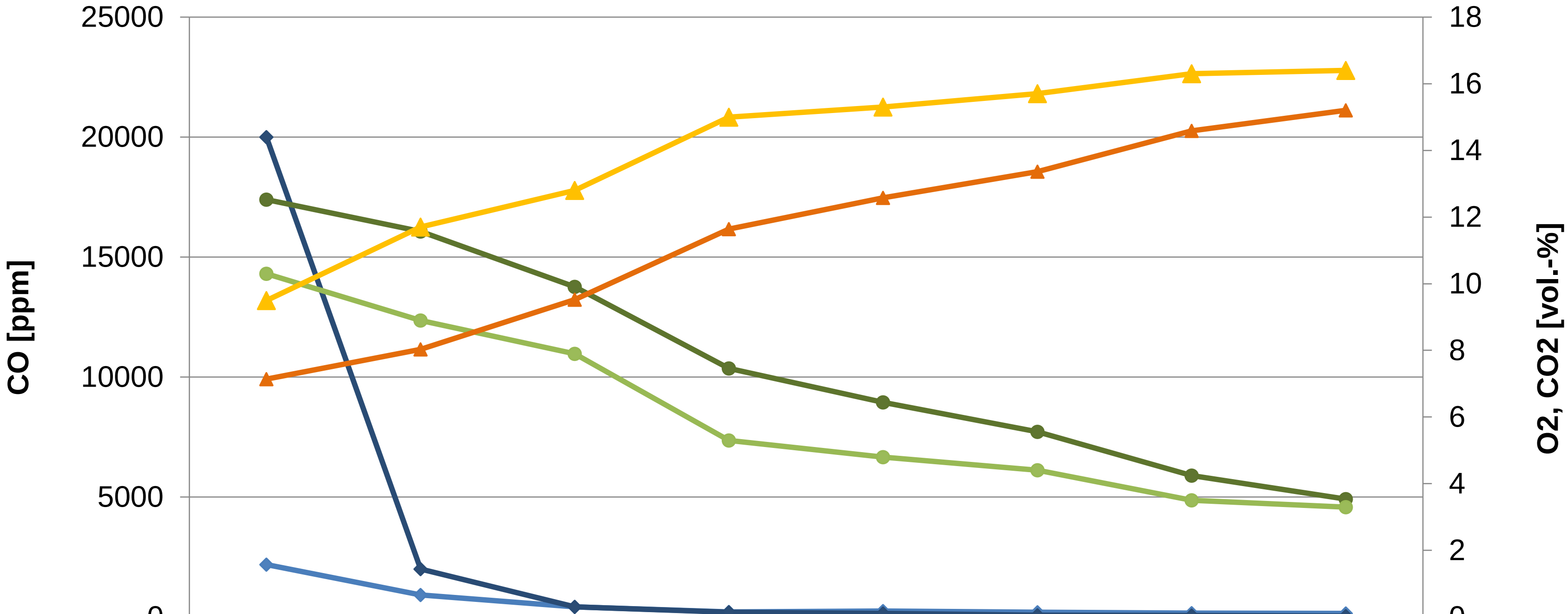
Results AV



Temperature profile

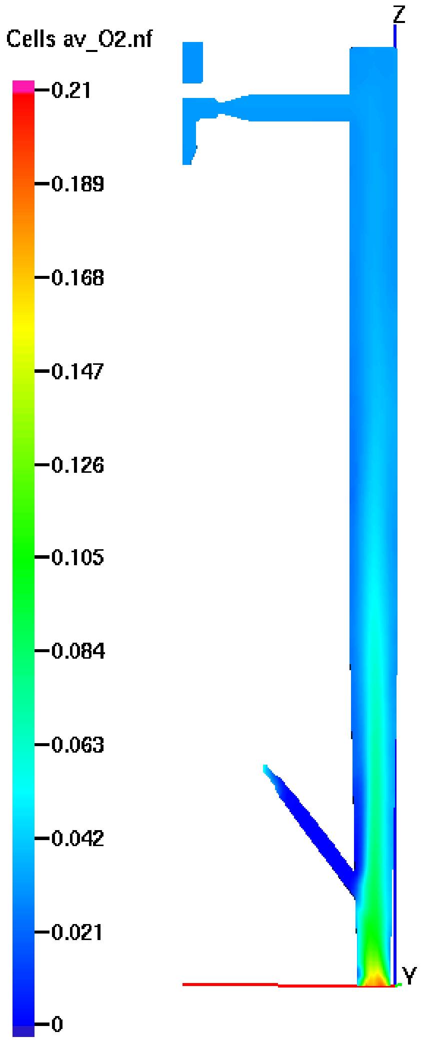
Results

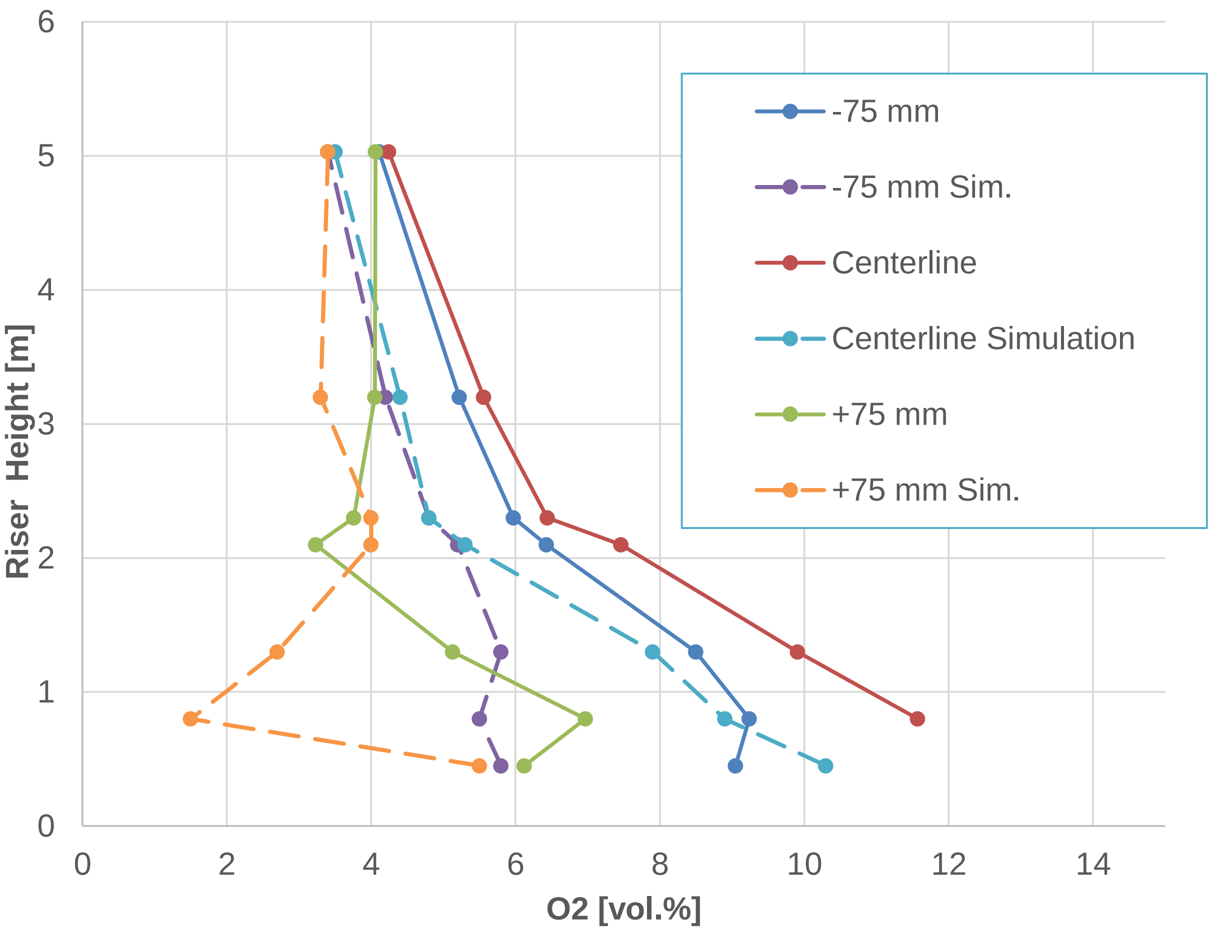
Middle



	4	6	8	11	12	14	18	Endpoint
CO	2184	924	422	217	244	202	160	156
CO_Sim.	20000	2000	420	200	150	70	60	40
O2	12.5	11.6	9.9	7.5	6.4	5.6	4.2	3.5
O2_Sim.	10.3	8.9	7.9	5.3	4.8	4.4	3.5	3.3
CO2	7.1	8.0	9.5	11.6	12.6	13.4	14.6	15.2
CO2_Sim.	9.5	11.7	12.8	15	15.3	15.7	16.3	16.4

Results


Cells av_O2.nf
0.21
0.189
0.168
0.147
0.126
0.105
0.084
0.063
0.042
0.021
0
Z
Y


Riser Height [m]
O2 [vol.%]
0
1
2
3
4
5
6
0
2
4
6
8
10
12
14
-75 mm
-75 mm Sim.
Centerline
Centerline Simulation
+75 mm
+75 mm Sim.

Summary and outlook

- Quantitative good fit
- Better kinetic data for qualitative better fit
- Sulfur and nitrogen models have to be implemented
- Kinetic data of AV coal are measured
  (TG, bubbling bed)
- Volatile content is analyzed by GC
- Solid fraction measurements with capacity probe will follow

Thank you for your attention

Literature

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[4] Lyon, R. K., Hardy, J. E., Von Holt, W., Oxidation kinetics of wet CO in trace concentrations (1985). Combustion and flame, 61(1), Pages 79-86.
[5] Syamlal, M., Bissett, L. A., METC gasifier advanced simulation (MGAS) model (No. DOE/METC--92/4108) (1992). USDOE Morgantown Energy Technology Center, WV (United States).
[6] Gungor, A., Eskin, N., Two-dimensional coal combustion modeling of CFB (2008), International Journal of Thermal Sciences, Volume 47, Issue 2, Pages 157-174.
[7] Tognotti, L., Longwell, J. P., & Sarofim, A. F., The products of the high temperature oxidation of a single char particle in an electrodynamic balance (1991). In Symposium (International) on Combustion, Vol. 23, No. 1, Pages 1207-121

FTIR Species

Ethyne
Ethene
Acetaldehyde
Ethane
Ethanol
Prophet
Propene
Propane
n-butane
Butenine
Furan
1,3-butadiene
Isobutene
Benzene
Toluene
Methane
Methyl alcohol
Carbon monoxide
Carbon dioxide
Carbonyl sulfide
Carbon disulphide
Hydrogen sulphide
Hydrogen chloride
Hydrogen cyanide
Hydrogen fluoride
Nitrous oxide
Ammonia
Nitric oxide
Nitrogen dioxide
Sulphur dioxide
Water
Acetic acid
Formaldehyde
Formic acid