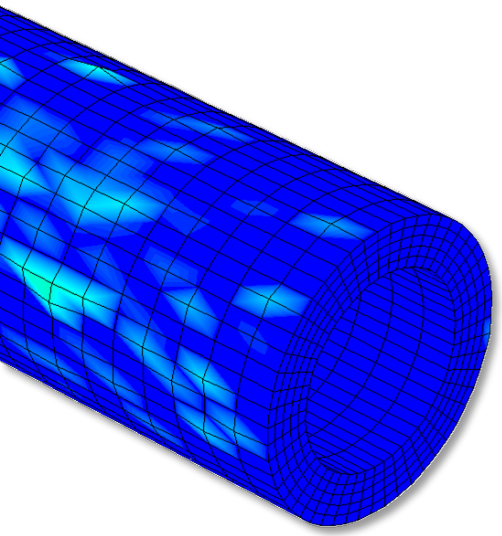
21st EUBCE 2013 - IEA CFD Workshop

CFD simulation of pulverized fuel combustion, gasification and ash deposition in entrained flow reactors



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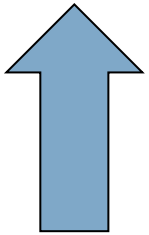
Outline

- Motivation
- **Part I: Gasification kinetics**
  - Modeling of the gasification process
  - Experimental facilities
  - Meshing
  - Solution strategy
  - Results
- **Part II: Ash deposition**
  - Deposition mechanisms
  - Experimental setup
  - Mathematical model
  - Validation
- Summary and Outlook

Motivation

Classification of gasifier types:

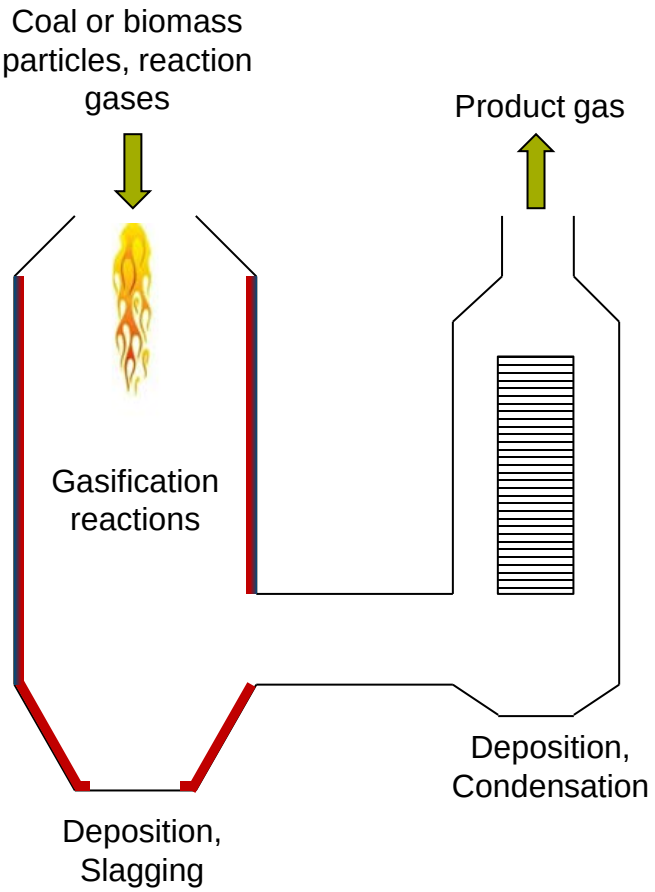
	Fixed bed	Fluidized bed	Entrained flow
Outlet temperature	425-600 ºC	900-1050 ºC	1250-1600 ºC
Oxidant demand	Low	Moderate	High
Ash conditions	Dry ash or slagging	Dry ash or agglomerating	Slagging
Size of coal feed	6-50 mm	6-10 mm	< 100 µm
Acceptability of fines	Limited	Good	Unlimited
Other characteristics	Methane, tars and oils present in syngas	Low carbon conversion	Pure syngas, high carbon conversion



Motivation

Aims and purposes of the simulation:

- Prediction of carbon conversion and product gas composition at conditions relevant to industrial scale gasifier operation (high pressures and temperatures)
- Optimization of the gasification process and the gasifier design with focus on fuel flexibility (biomass and coal)
- Prediction of ash deposition



Motivation

Why CFD?

- Calculation of complex geometries (e.g. industrial scale gasifier)
- Taking into account turbulence models and particle tracks
- Taking into account particle radiation and particle size distribution
- Implementation of particle deposition and slagging model is possible
- Visualization of the results help to better understand the gasification process

Part I

Gasification kinetics

Modeling of the gasification process

Gasification:

"A process that uses heat, pressure and steam to convert materials directly into a gas composed primarily of carbon monoxide and hydrogen."

Key steps in a gasification process:

- Drying
- Volatile release
- Homogeneous and heterogeneous reactions

Modeling of the gasification process

Heterogeneous reactions:

R1 (C oxidation): $C + 0.5O_2 = CO$

R2 (Boudouard): $C + CO_2 = 2CO$

R3 (Reforming): $C + H_2O = CO + H_2$

Homogeneous reactions:

R4 (Volatile oxidation): $C_{x_1}H_{x_2}O_{x_3}N_{x_4} + \left(\frac{x_1 - x_3}{2}\right)O_2 = x_1CO + \frac{x_2}{2}H_2 + \frac{x_4}{2}N_2$

R5 (H_2 oxidation): $H_2 + 0.5O_2 = H_2O$

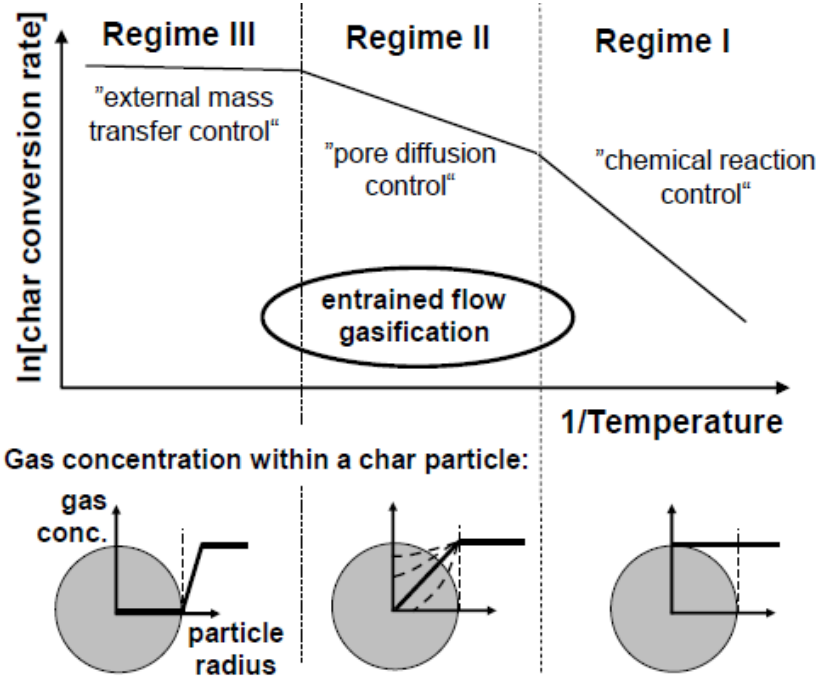
R6 (CO oxidation): $CO + 0.5O_2 = CO_2$

R7 (WGS): $CO + H_2O \leftrightarrow CO_2 + H_2$

Modeling of the gasification process

- **Regime I:** At low temperatures the intrinsic rate is slower than pore and bulk diffusion
- **Regime II:** The pore diffusion can not keep up with the chemical reaction rate at increased temperatures
- **Regime III:** At high temperatures the bulk diffusion limits the overall reaction rate

$$r = r\left(T, p_i, K_i, \ldots\right) \quad \left[\frac{g}{g \cdot s}\right]$$

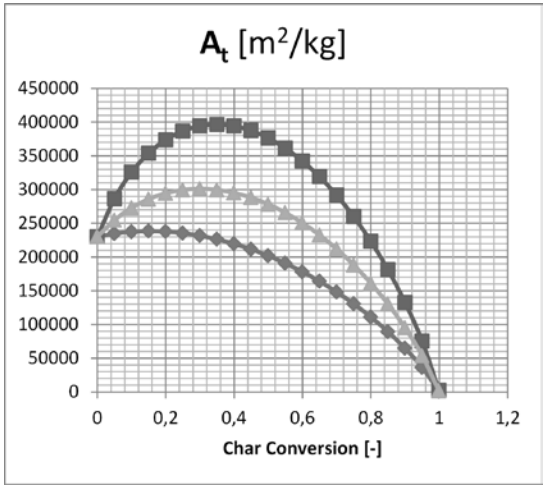


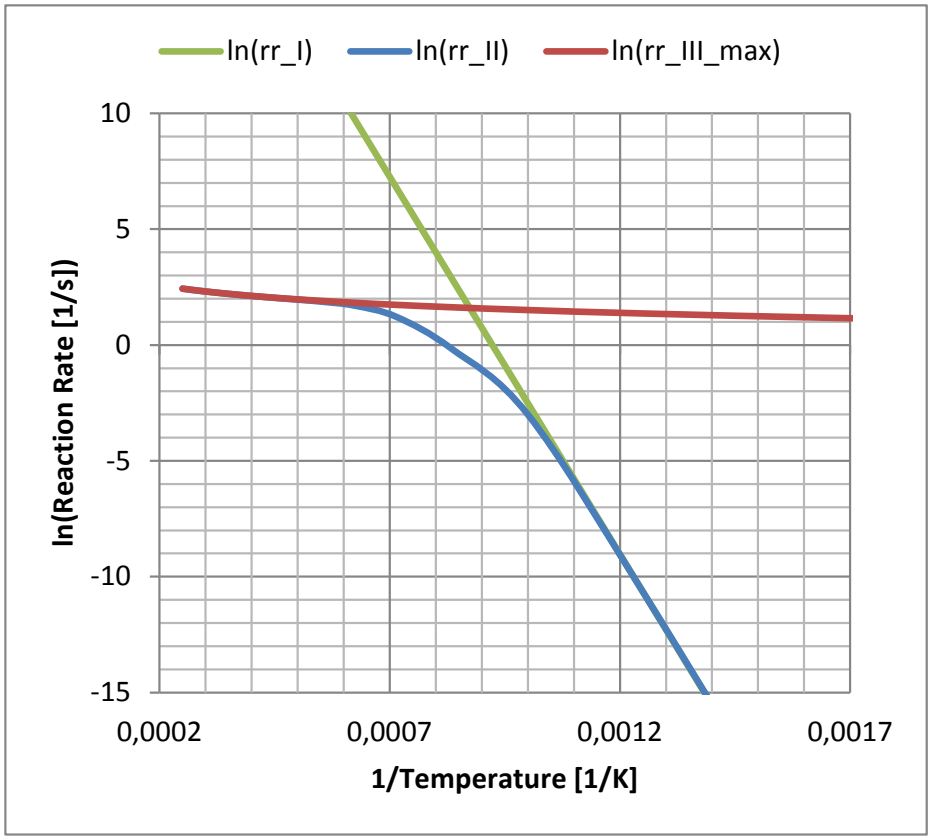
Modeling of the gasification process

$$R_{i,I} = A_t \cdot k_i \cdot p_{S,i}^n \quad , p_{S,i} = p_{bulk}$$

$$R_{i,II} = \eta_i \cdot A_t \cdot k_i \cdot p_{S,i}^n$$

$$R_{i,III} = \frac{12 \cdot N_i \cdot D_{M,i} \cdot M_i}{d_p^2 \cdot \rho_p \cdot R \cdot T_{bulk}} \cdot (p_{bulk} - \overset{0}{p_{S,i}})$$

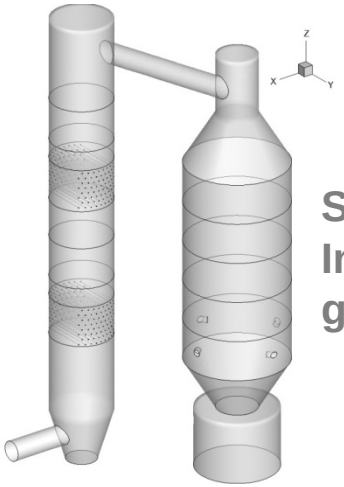




C+CO_2, p=1bar, 30% partial pressure CO_2, d_p=120µm, ρ_p=1400kg/m^3, Tortuosity = 3, At_0 = 230 m^2/g

Experimental facilities

- Atmospheric and pressurized entrained flow reactor
- Possible operation with N_2, O_2, H_2, CO_2, H_2O, Ar, CO
- Maximum temperature = 1800 ºC
- Maximum pressure = 50 bar



Simulation of Industrial scale gasifiers

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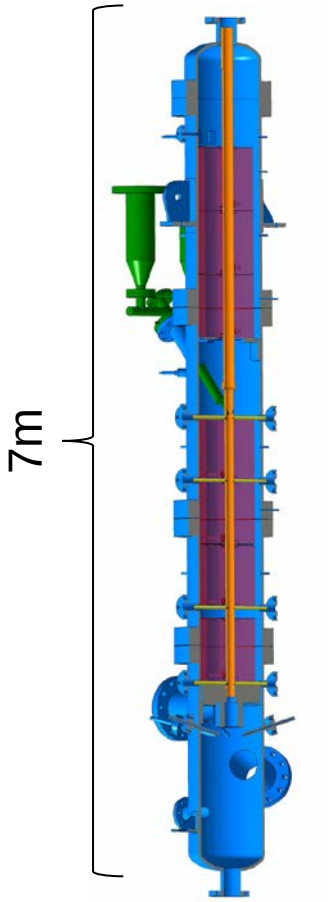
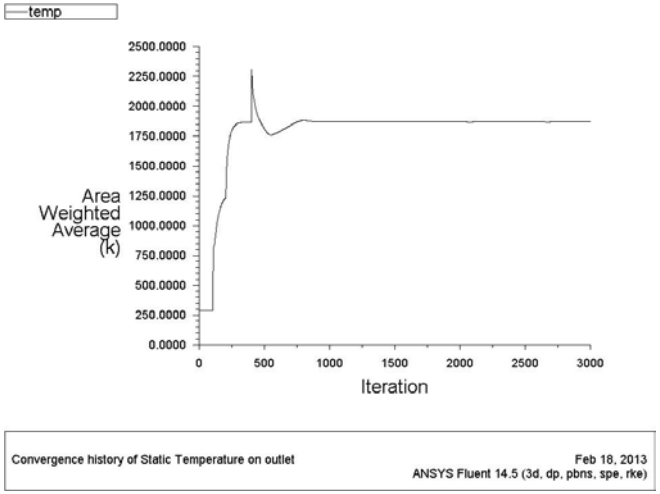
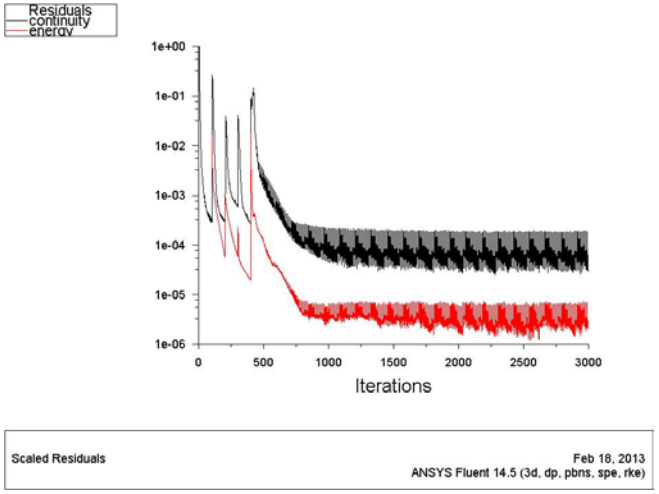


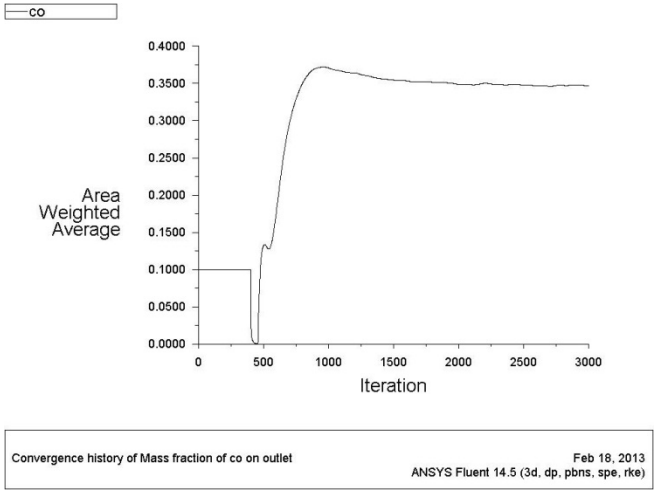
Solution strategy – Journal file

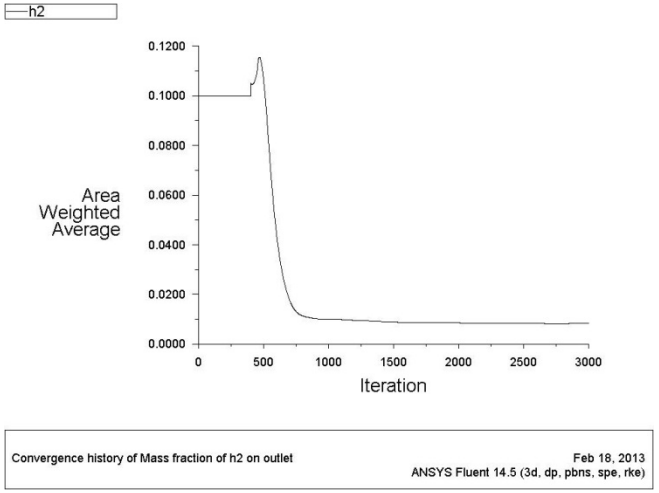
100 Iterations	• Calculation of the fluid flow with k-ε turbulence model • First order discretization
200 Iterations	• Including the energy equation and the radiation model (Discrete Ordinates)
100 Iterations	• Second order discretization
ca. 2000 Iterations	• Including species transport, reactions (FR-EDM) and particles (DPM, Lagrange) • Adjusting the under relaxation factors

Results – Stability and convergence

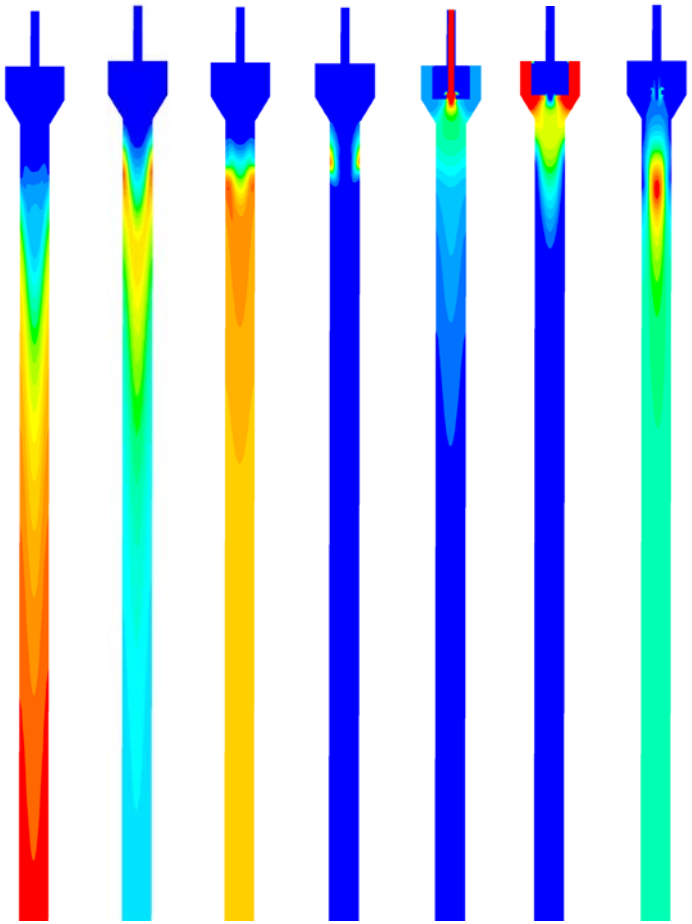


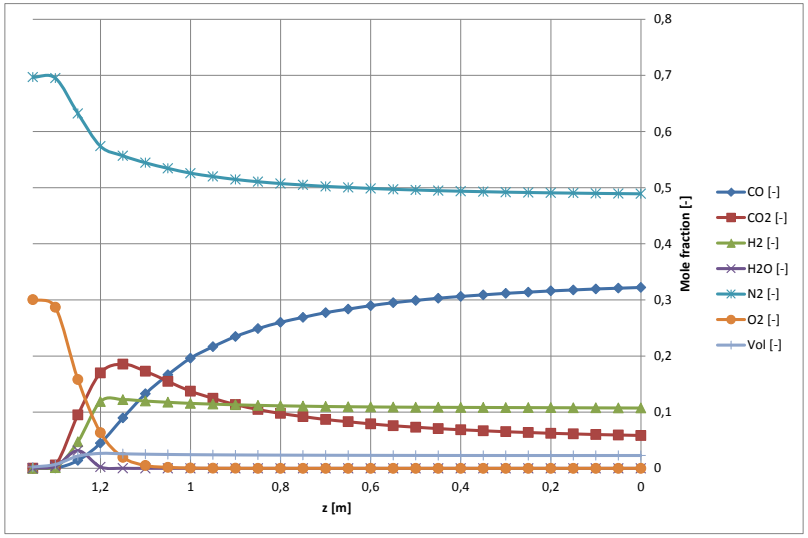


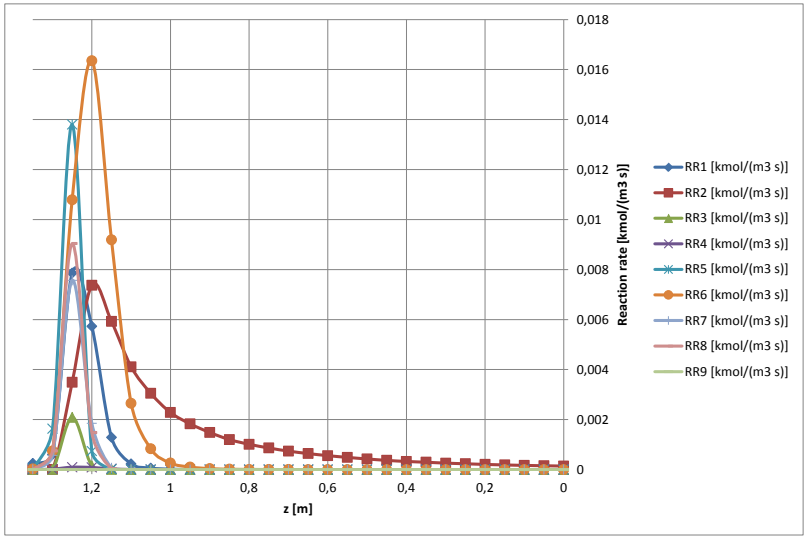




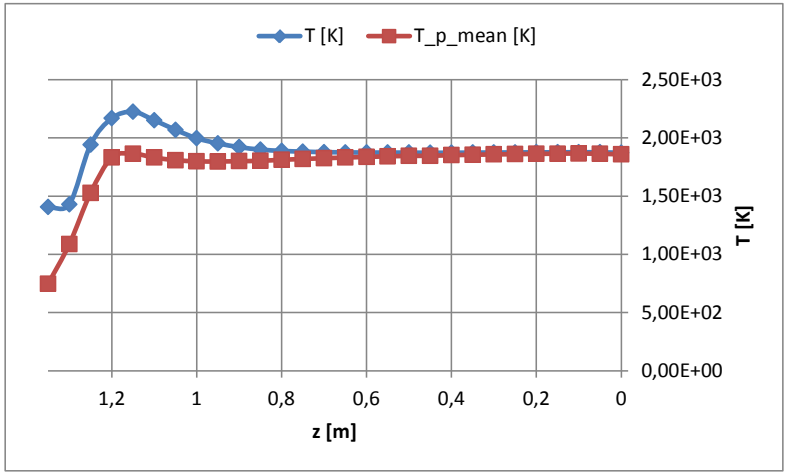
Results – Gas composition

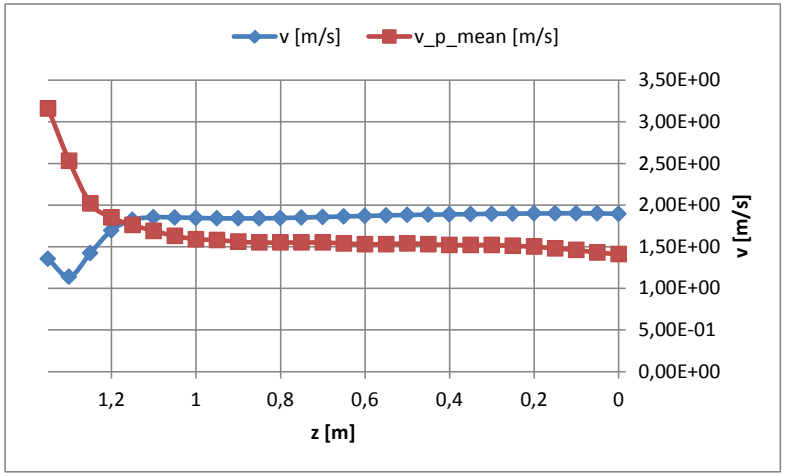


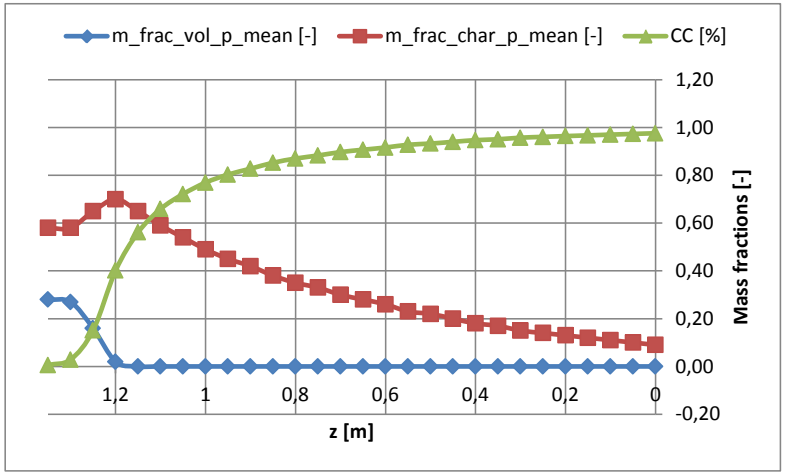


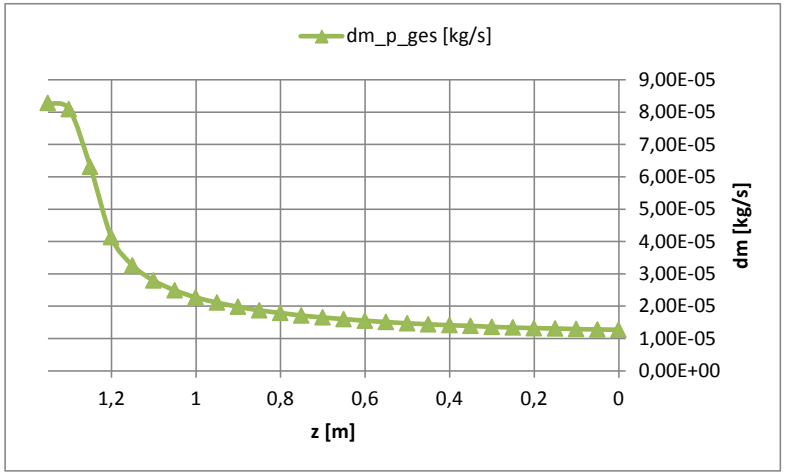


Results – Mean values







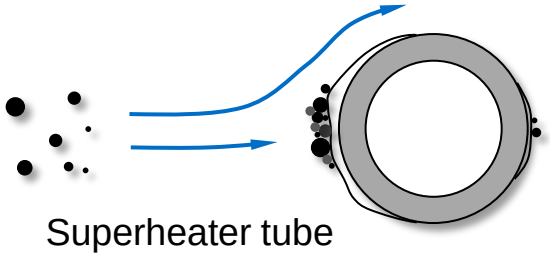


Part II

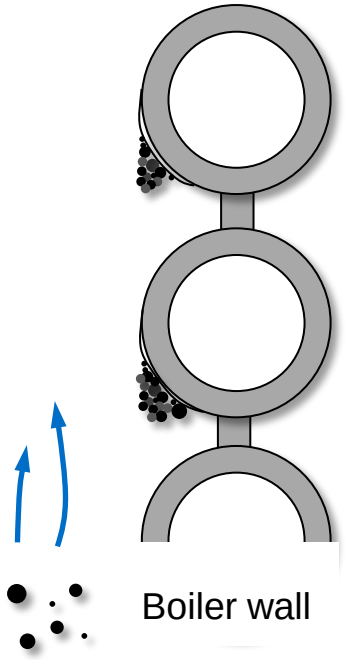
Ash deposition

Deposition mechanisms

- **Mechanisms building depositions:**
  - Inertial impaction
  - Condensation
  - Thermophoresis
  - Chemical reactions (heterogeneous reactions with deposits)



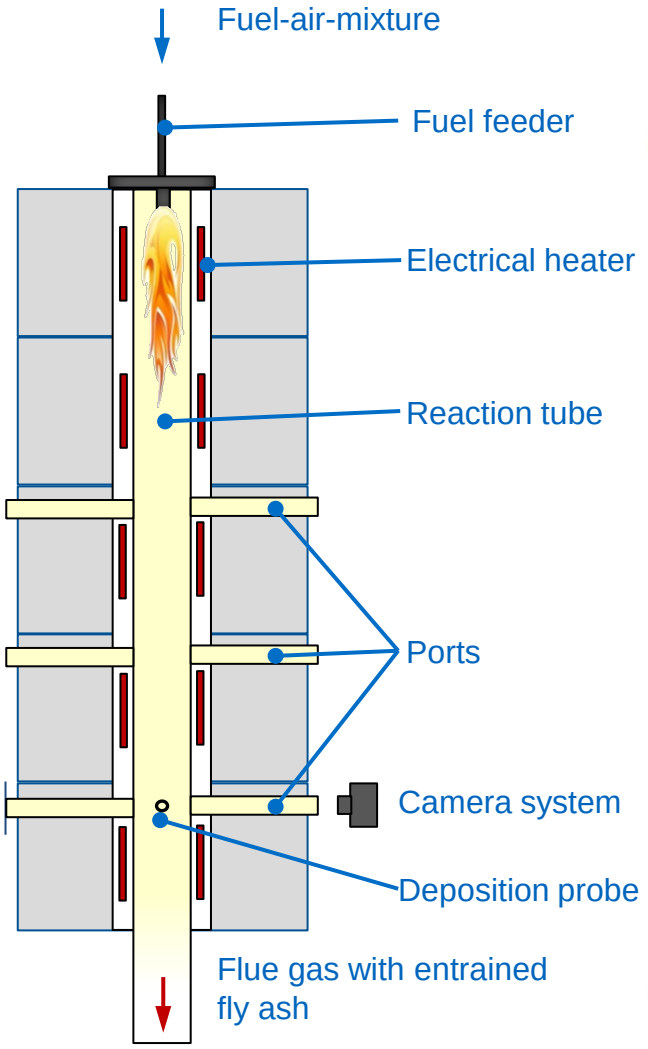
- **Mechanisms removing depositions:**
  - Erosion (by sharp unmolten particles impacting with high mass and velocity)
  - Shedding (by gravity and weak strength)
  - Shedding (by thermally or mechanically induced stresses)
  - Melting and drip off

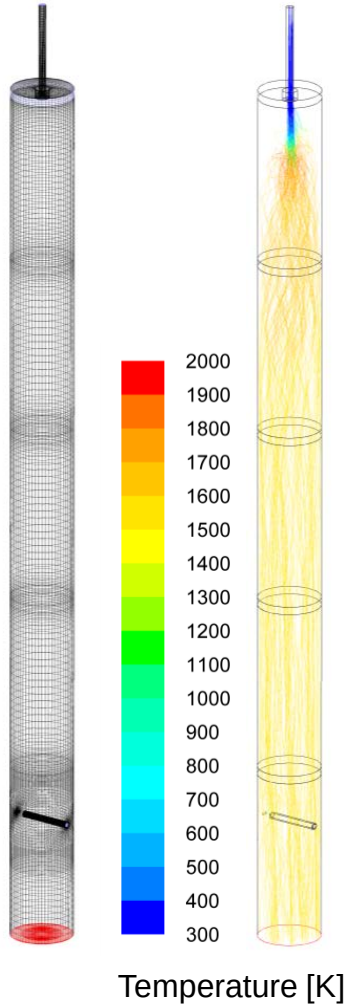


Experimental setup

- **Entrained flow reactor**
  - Electrically heated (up to 50 kW_{el})
  - Fuels up to 2 kg/h (or 15 kW_{th})

- **Investigations on different solid fuels under varying conditions:**
  - Temperatures (up to 1600 °C)
  - Air-fuel ratio (oxidizing or reducing)
  - Fuels (bit. coal, lignite, biomass)
  - (Oxidation medium)



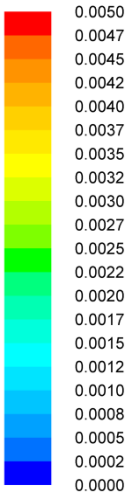


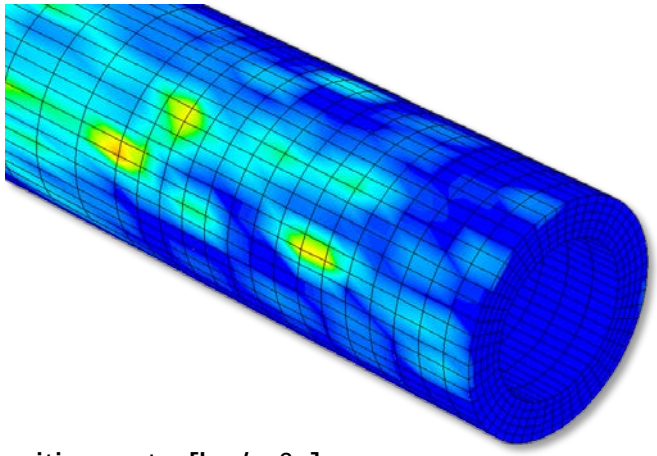
Mathematical model – deposition growth

200 flow iterations until stationary

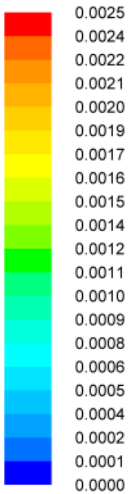
- Calculation of stationary deposition rates (sticking criterion based on TGA/DTA measurements)
- ⇩
- Calculation of deposit layer thickness dx for each cell
- ⇩
- Identification of cell nodes
- ⇩
- Grid modification for each cell node and adjacent cells
- ⇩
- Adjust thermal conductivity of underlying cell
- ⇩
- Iteration of fluid flow until new stationary solution with changed deposition rate and surface temperatures

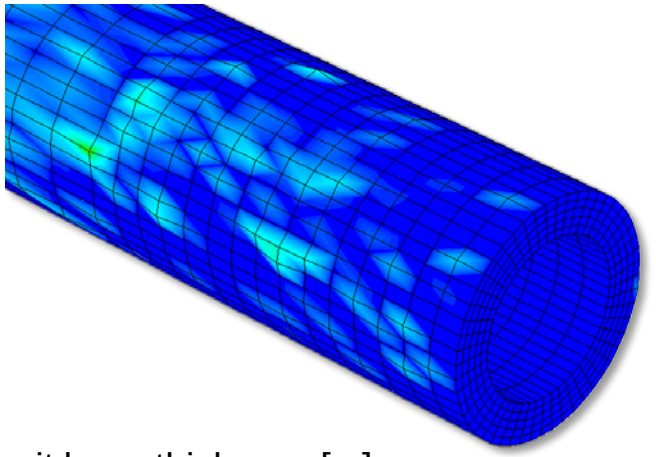
$$dx = \frac{\phi_{dep} \cdot t}{\rho_{solid} \cdot (1 - \varepsilon)}$$





Deposition rate [kg/m²s]

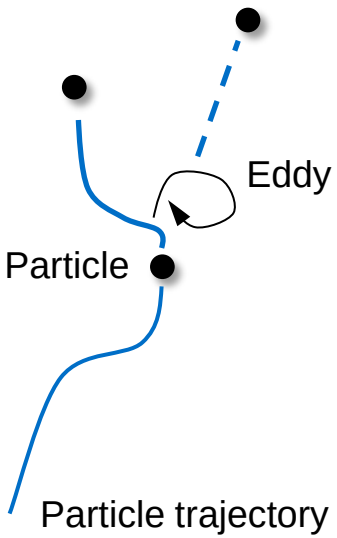




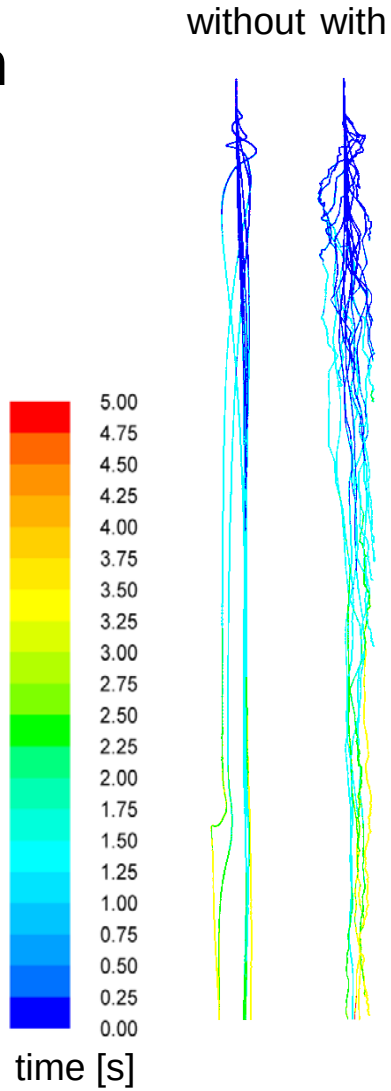
Deposit layer thickness [m]

Mathematical model – Turbulent Dispersion

Particle trajectory is calculated by including an instantaneous value of the flow velocity (RANS-equations).

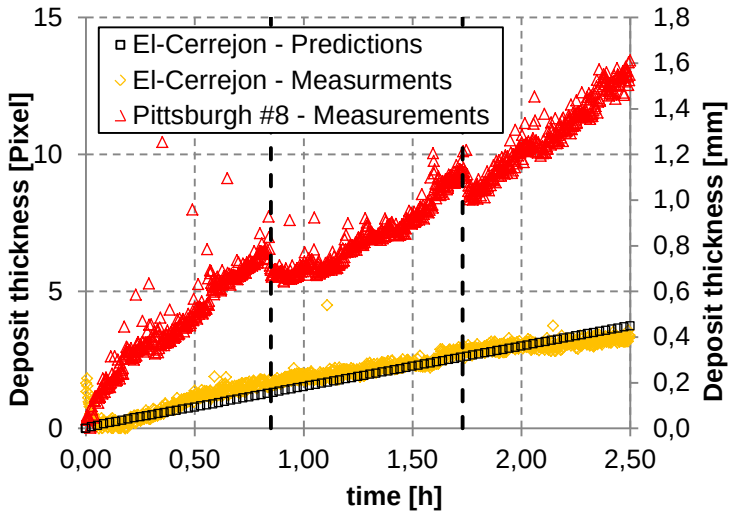


- Turbulent kinetic energy is used to calculate statistical particle trajectory
- Strong influence on particle tracks
- There are two different models available in literature: Cloud Model, Discrete Random Walk Model

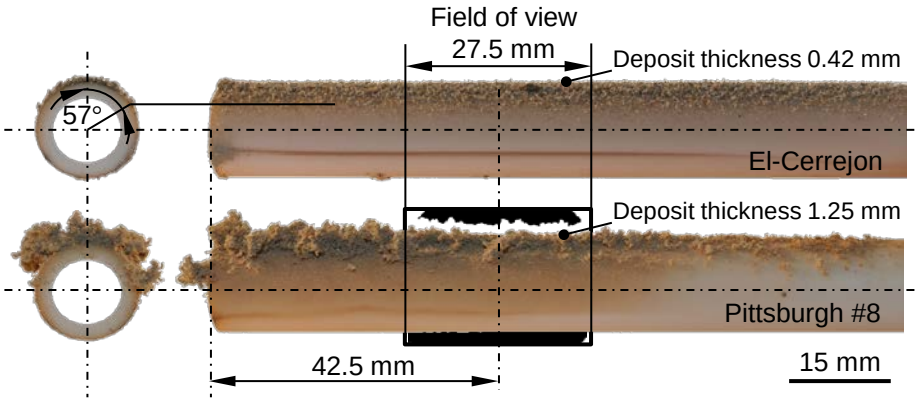


Comparison of experimental results and predictions

Deposition rates [mm/h]:

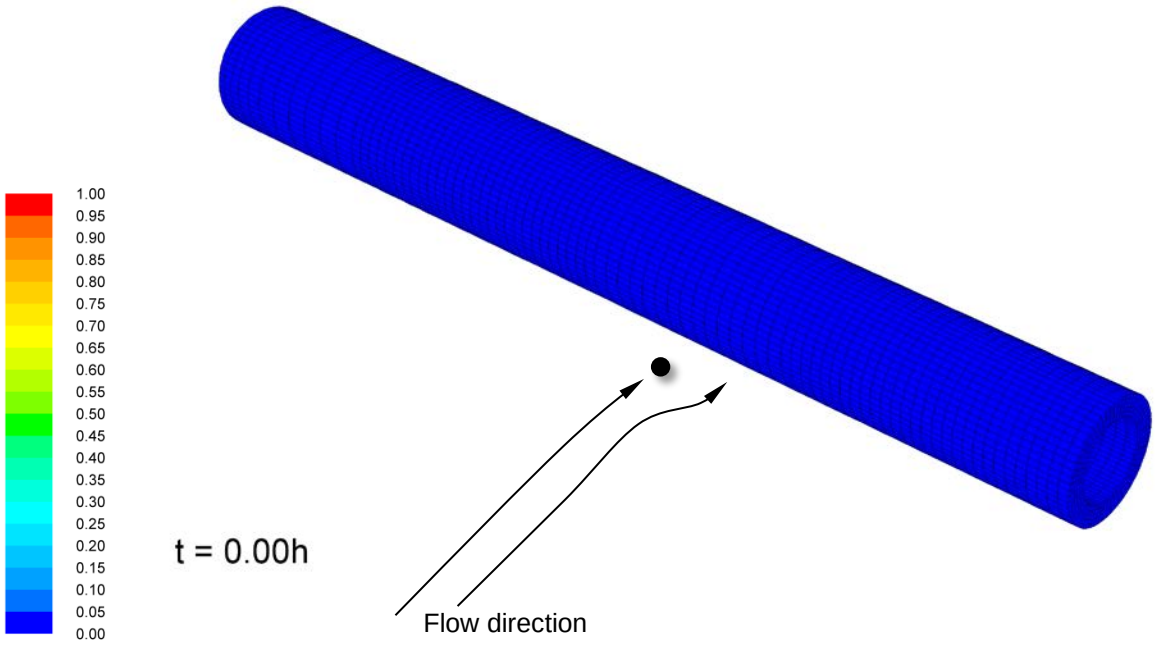


Deposition photographs:

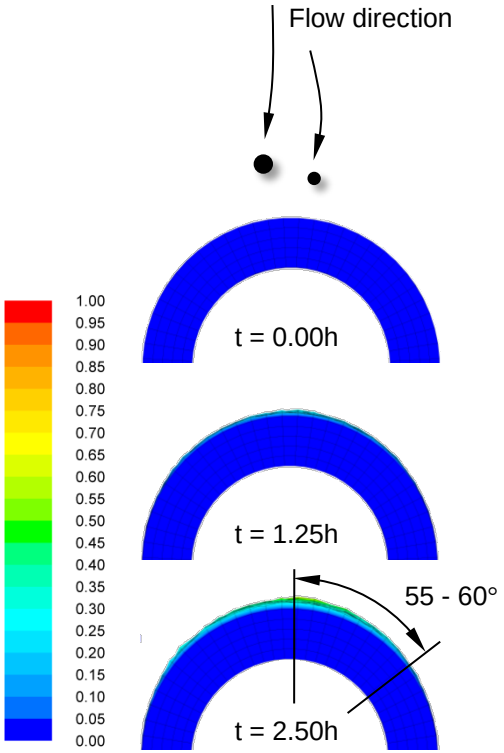


Comparison of experimental results and predictions

Prediction of deposit growth over time:



Deposit layer thickness [mm]



Deposit layer thickness [mm]

Summary

- Prediction of char conversion, gas composition and ash deposition
- Detailed modeling of heterogeneous reaction rates by means of a User Defined Function (DEFINE_PR_RATE), including several sub-models
- Good convergence by applying a journal-file-based solution strategy
- Mathematical model is able to capture deposition process and growth
- Particle diameter and deposit porosity are crucial parameters

Outlook

- Intrinsic reaction rates are needed as input parameters for each biomass or coal, in order to validate the CFD model with the lab-scale gasifiers at the Institute
- Further development of the particle reaction model:
  - More detailed devolatilization approach
  - Temperature-dependent d/ρ evolution (burning mode)
  - Detailed kinetics of WGS reaction kinetics by means of a UDF
- Particle diameter and density evolution (fragmentation, condensation)
- Validation for different parameters (temperature and air-fuel ratio), fuels

Thank you for your attention!