Institute of Combustion and Power Plant Technology
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Modelling of Mineral Transformations and Slagging in PC Flames with CFD Code AIOLOS

Conventional air flames and prospects for oxy-fuel combustion

i-Math Workshop on Mathematical Modelling of Combustion
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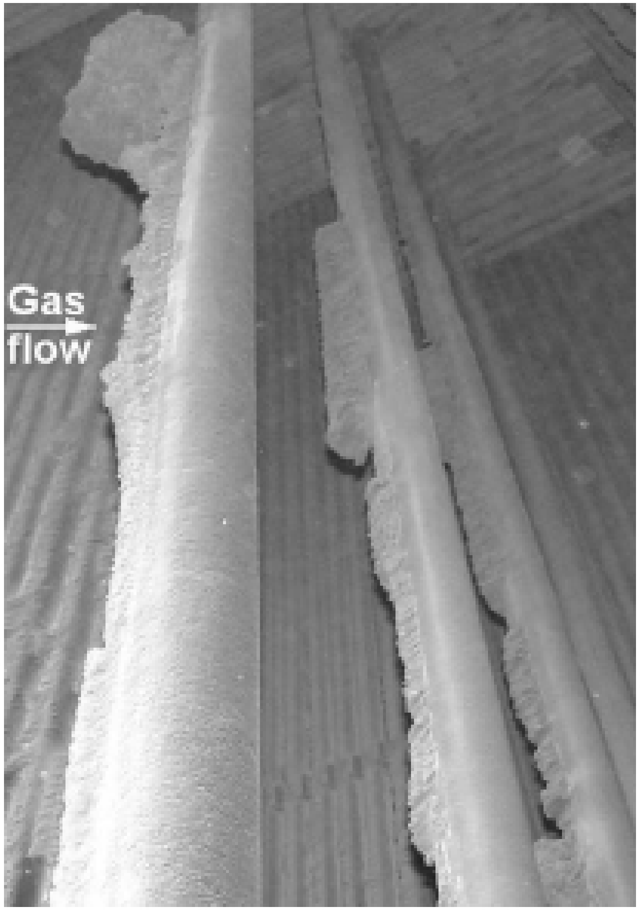
Olaf E. Lemp

Overview

- ➲ Introduction
  - ➥ CFD Code AIOLOS
- ➲ Modelling of Deposition
  - ➥ Mineral Transformation
  - ➥ Walsh´s Theory
    - ➥ Viscosity
    - ➥ Ash melting behavior
- ➲ Modelling of Oxy-fuel Combustion
  - ➥ Homogenous reactions
  - ➥ Heterogeneous reactions
  - ➥ Validation
- ➲ Summary

Motivation for Modelling Deposit Formation



Motivation for Modelling Deposit Formation

- The deposition of ash in pulverized coal flames provokes several **problems** in the functioning of power plants:
  - Due to the isolating effect of the deposition on heat tubes the **heat transfer** is significantly deteriorated.
  - The **corrosive** components of the ashes cause a lot of damage to the tube material.
  - Ash **shedding** can cause severe damage to the furnace.
- The prediction of slagging tendency has been always a big issue for power plant operators:
  - In the past mainly **slagging indices** were developed.
  - As computational power rises CFD simulations come more and more into play.
- Development of CFD software considering:
  - **Transformation** of mineral components of fuels
  - **Stickiness** of particles (and surfaces)

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Program Code

AIOLOS

Development of mathematical models and methods

3D combustion simulation for the solution of industrial problems

- Conservative Finite Volume formulation
- Modular structure
- Validation of the reliability of modeling assumptions at pilot and large scale
- Program code optimized for use of high-end super computers (Parallelisation, Vectorisation)
- Domain decomposition approach
- High level of detail (number of grid points for numerical discretisation up to 10 mio cells)

Physical Models in AIOLOS

Turbulent two-phase flow

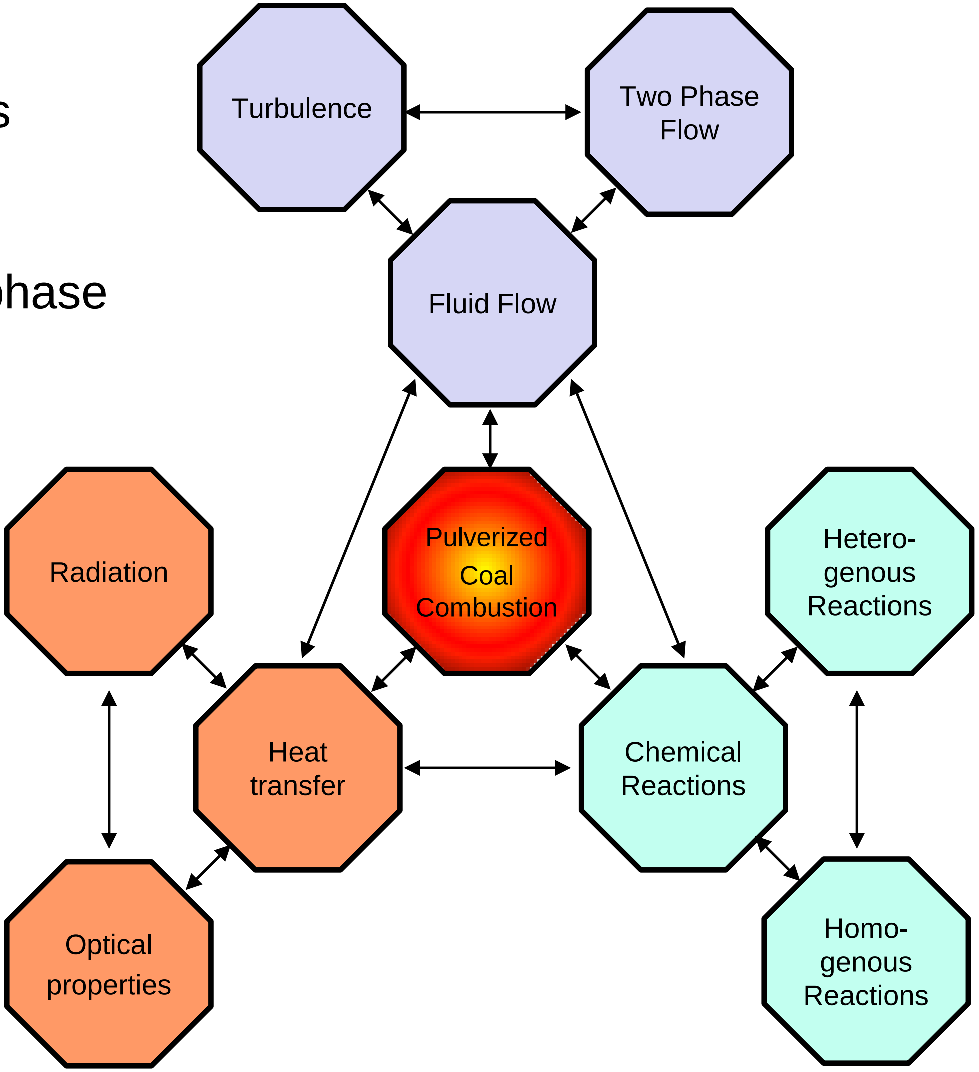
- k, ε-Model and Differential Reynolds Stress model
- Eulerian approach for the gas phase
- Lagrangian approach treating the particle phase

Radiative heat transfer

- Semi-stochastic Monte-Carlo model
- Flux method
- Discrete Ordinates Method
- Discrete Transfer model

Reaction model

- Global reaction scheme of pulverised coal combustion
- Consideration of particle size distribution
- NO_x post-processor (fuel NO, thermal NO)



Mathematical Modelling: Current Developments

- Mathematical models for heterogeneous char combustion at atmospheric and elevated pressure and under **oxy-fuel** conditions
- Modelling of **NOx** and **SOx** chemistry at oxy-fuel combustion conditions
- Numerical simulation of **deposit formation** in coal-fired utility boilers with biomass co-combustion
- Detailed **coupled simulation** of combustion and steam generation by connecting the furnace and water-steam simulation codes
- Mathematical models for fouling and slagging prediction with detailed description of mineral matter transformation and deposition mechanisms
- Investigation and optimization of **grate combustion systems for biomass** by developing a new Euler-Euler approach for 2-phase flow simulation
- Simulation of steam generation and development of process control strategies for a **solar power plant**
- Wood **pellet burner** optimization for a new decentralized electricity production system

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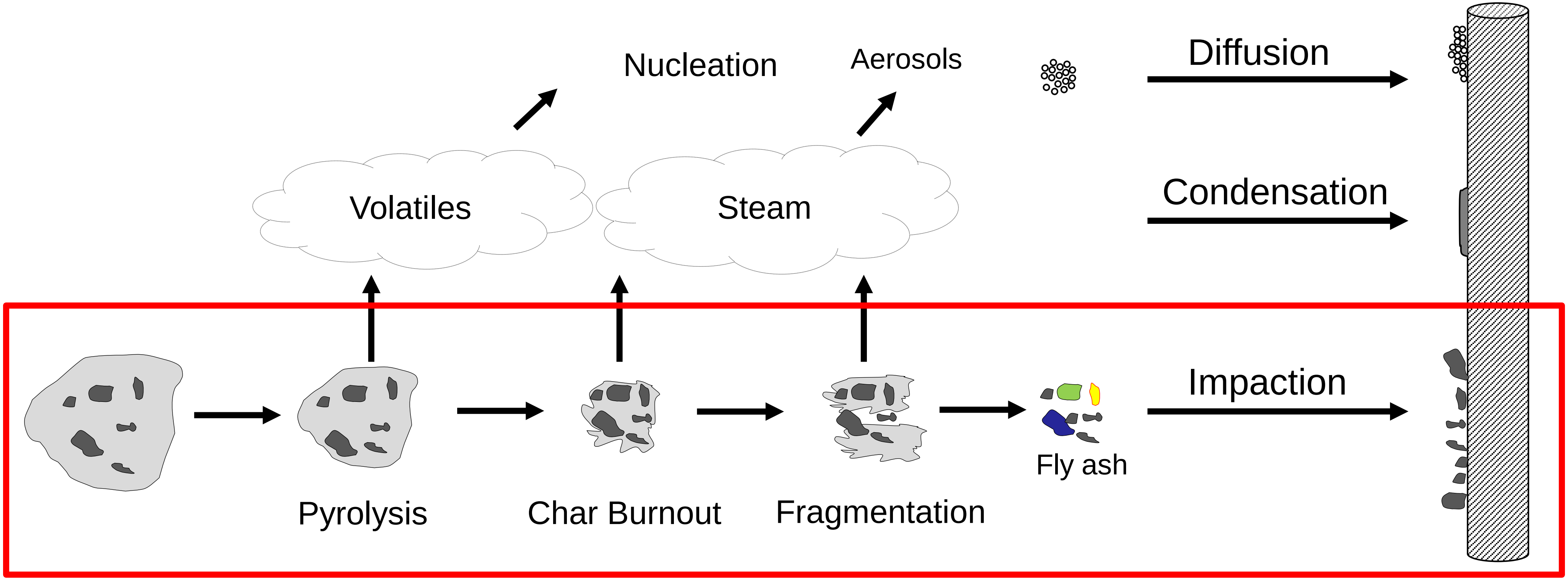
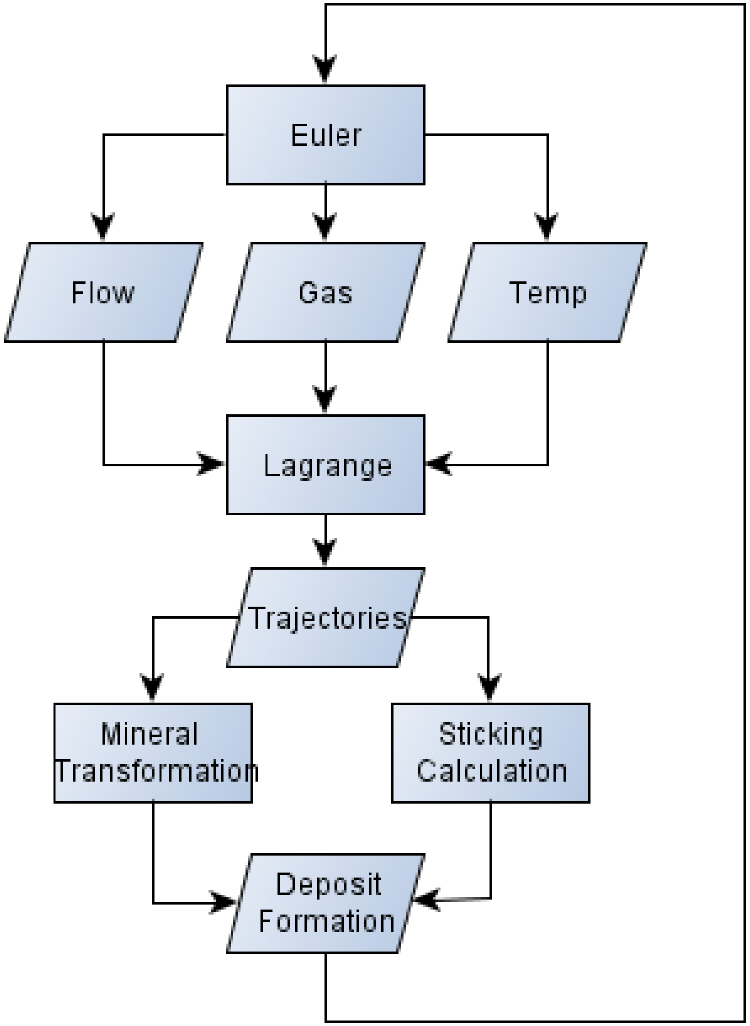
Modelling of Deposit Formation



Assumptions:

- **Full coalescence**: Each fuel particle results in one mineral particle
- Reaction is influenced by temperature of particle and surrounding fluid and the main gas concentrations
- No interaction with volatiles and char
- Only impaction is considered in this work

Flowchart – Simulation of Deposit Formation



Lagrangian Particle Tracking

Particle Tracking in AIOLOS for calculation of deposition:

- Basic Simulation with Euler description for the coal particle phase
- Stream-, temperature-, concentration field of main gas species as boundary conditions (One way coupling)
- Solving equation of motion for each time step (analytical):

$$\frac{\partial}{\partial t}(m_P \cdot u_p) = F_D + F_g \quad \Rightarrow$$

$$u_P = u_G(u_P^0 - u_G)\exp\left(-\frac{\Delta t}{\tau_P}\right) + \tau_P F_g\left[1 - \exp\left(-\frac{\Delta t}{\tau_P}\right)\right]$$

- Account for:
  - Turbulent fluctuation (Monte Carlo type approach)
  - Heat balance
  - Particle relaxation
  - 10-13 different particle size classes

Modelling of mineral matter transformation

➲ General description of mineral matter transformation:

(1) $$\nu_{1,E}E_1 + \nu_{2,E}E_2 + \cdots \leftarrow TRANSFORMATION \rightarrow \nu_{1,P}P_1 + \nu_{2,P}P_2 + \cdots$$

➲ General unsteady transform modell:

(2) $$\frac{dX}{dt} = K \cdot f(X)$$

➲ Dependency of transformation constant K (TGA/DTA analysis):

(3) $$K = f_1(\beta_t) \cdot f_2(k_0, E_A, T) \cdot f_3(p_{O_2}) \cdot f_4(p_{H_2O}) \cdot f_5(p_{CO_2})$$

➲ Mineral transformation modelling:

(4) $$f(X) = f(Physics, Chemistry)$$

Overview

Walsh´s Theory

- Walsh´s Theory for calculation of net fraction of mass deposit:

$$(1)\quad f_{STCK} = \underbrace{P_P(T_P)}_{sticking\ particles} + \underbrace{[1 - P_P(T_P)] \cdot P_S(T_S)}_{sticking\ surface} - \underbrace{k_e[1 - P_P(T_P)][1 - P_S(T_s)]}_{erosion}$$

- Sticking propensity:

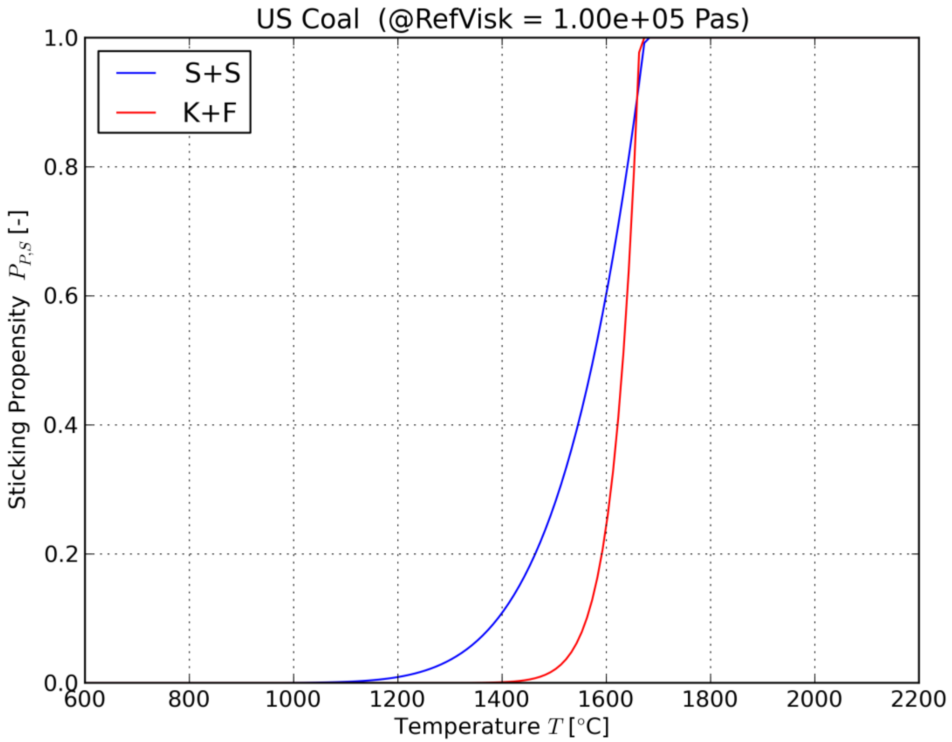
$$(2)\quad P_{P/S} = \frac{\mu_{Ref}}{\mu} \quad 0\ (non\ sticky) \dots 1\ (fully\ sticky) \rightarrow \mathrm{P} = \min\left(\frac{\mu_{Ref}}{\mu}, 1.\right)$$

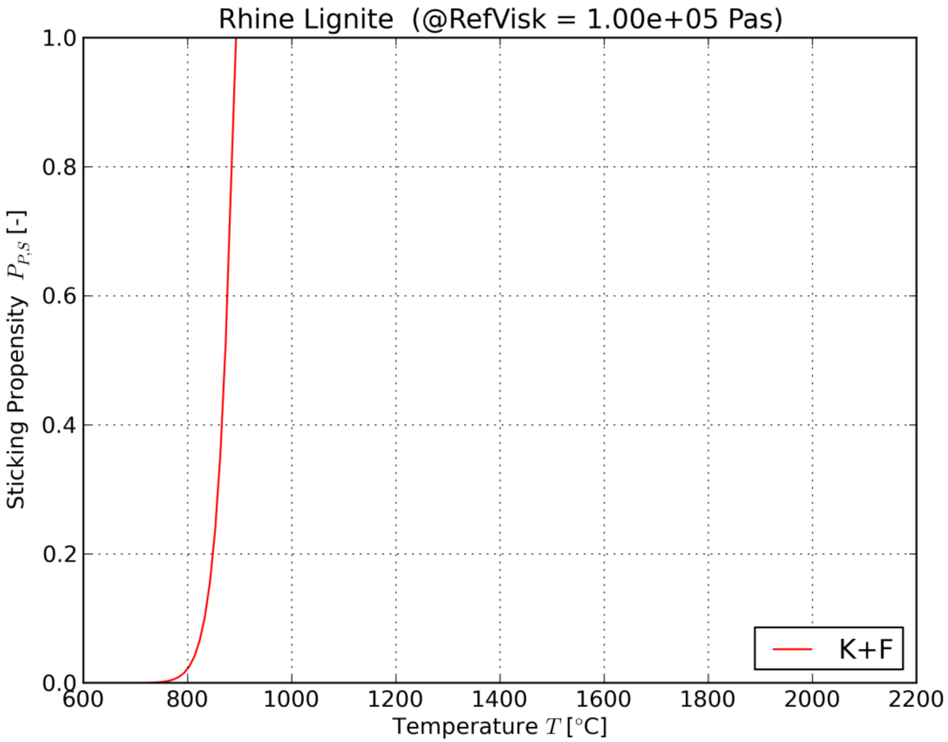
- Calculation of viscosity using empirical correlations based on „Weymanns law“

$$(3)\quad \mu = A \cdot T + \exp\left(B \cdot \frac{1000}{T}\right)$$

- Parameters A and B to be calculated with empirical correlations, e.g. Urbain, Watt+Fareday, **Kalmanovitch+Frank**, **Senior+Srinivasachar** $\dots f(CaO, Al_2O_3, Fe_2O_3, FeO, SiO_2, TiO_2, MgO, Na_2O, K_2O)$

Example Viscosity





- US Coal is a silicate rich coal
- Both coals not really known as having high slagging tendency
- Lignite has high content of CaO → S+S not applicable

Sticking Propensity based on ash melting behaviour

- Empirical correlations for calculation of viscosity are almost only applicable for **silicate rich** coals
- Difficulty to measure reference viscosity

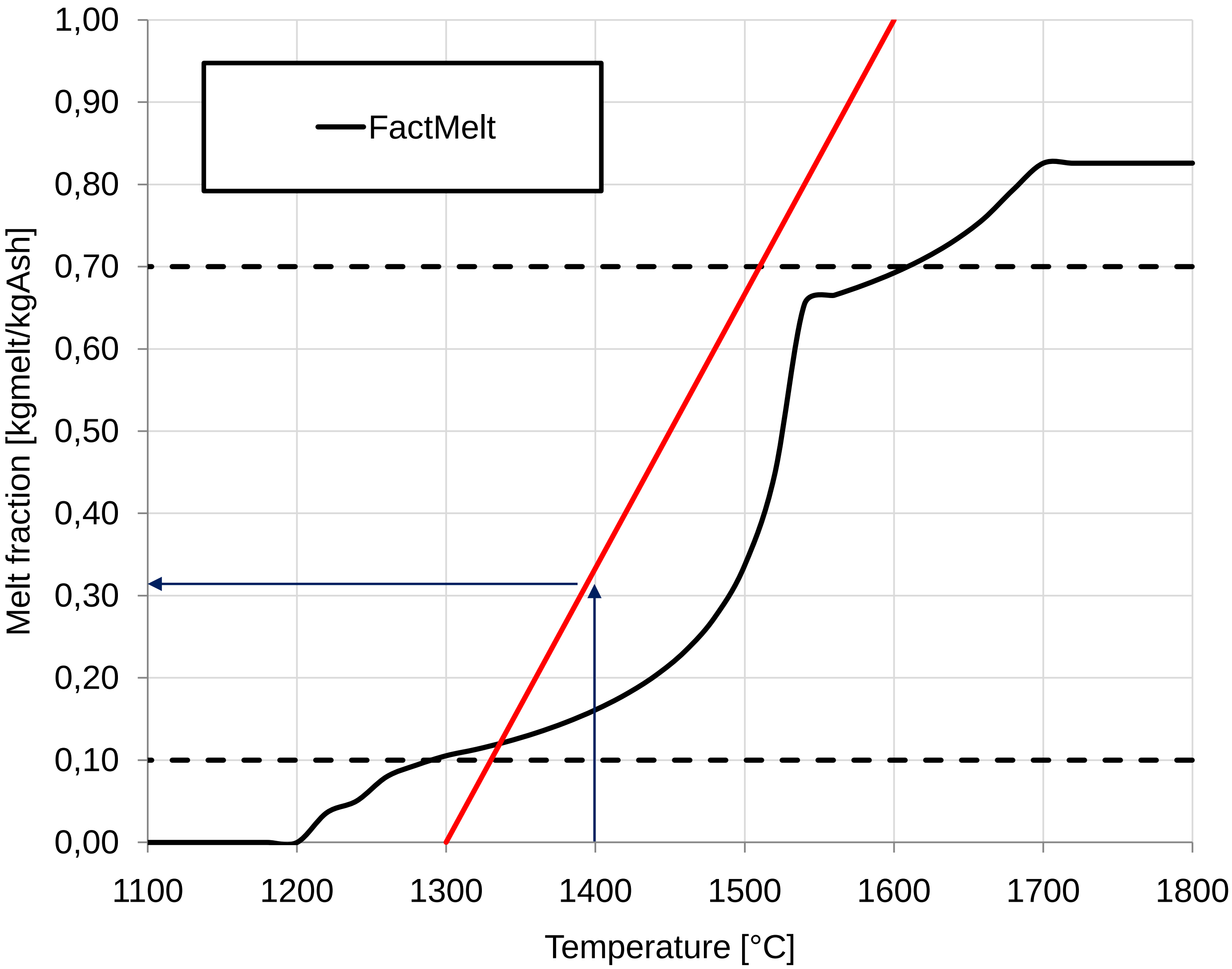
- New approach based on ash melting behavior (Danish Group)
- Software **FactSage** for calculation of thermochemical equilibrium
- Proposal **Frandsen**:

< 10% melted phase → non sticky

10% - 70% melted phase → partially sticky

> 70% melted phase → sticky

Example – US Coal



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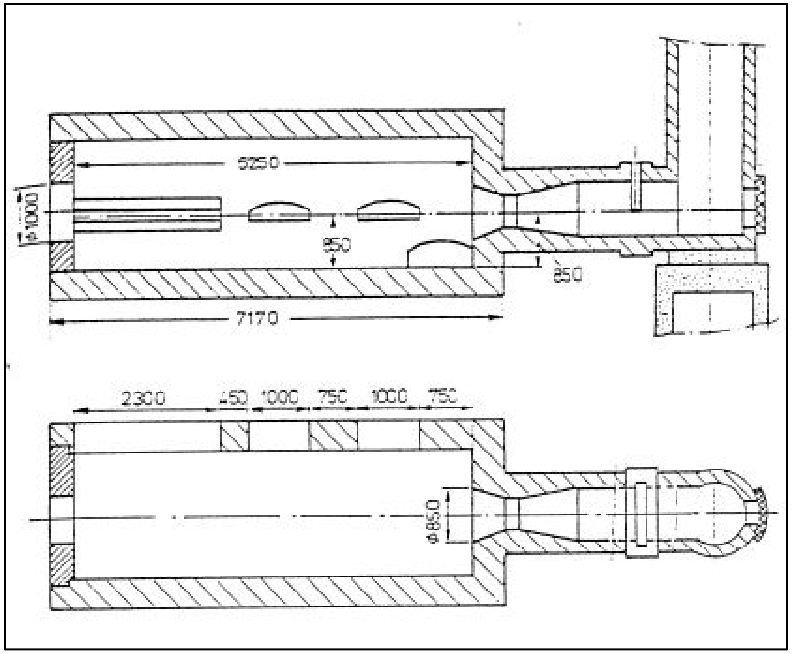
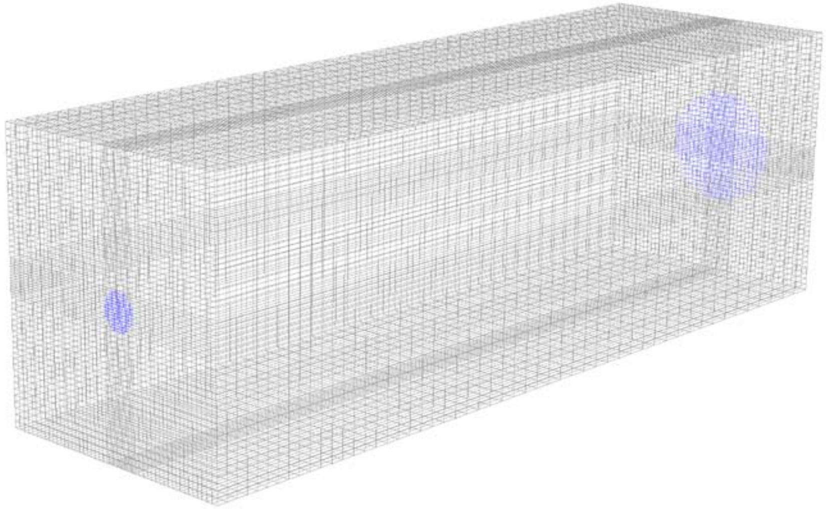
IFRF Furnace – Grid





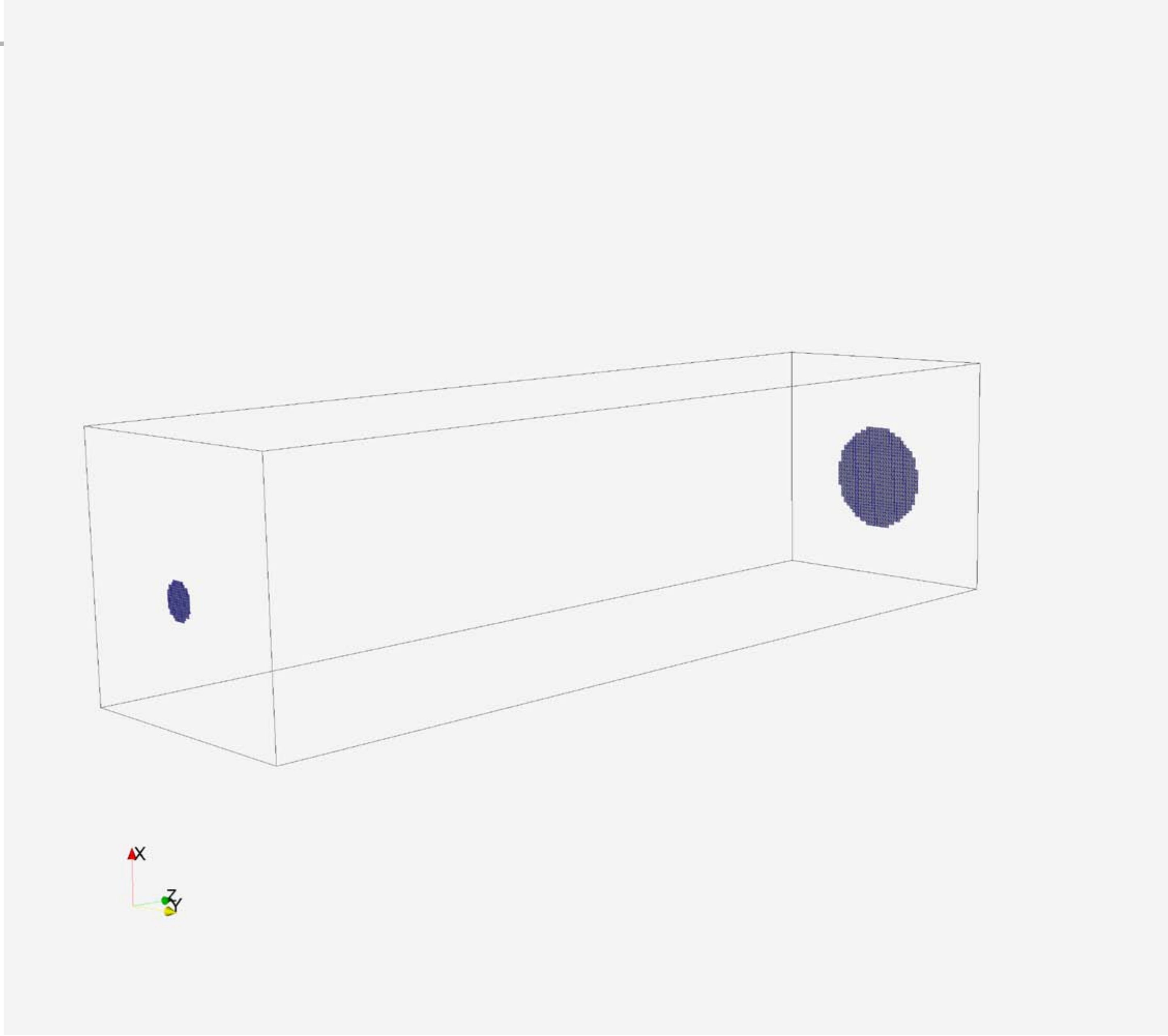
Characteristics:

- Jet flame
- Burner consists of two concentric tubes
- Water cooling loops

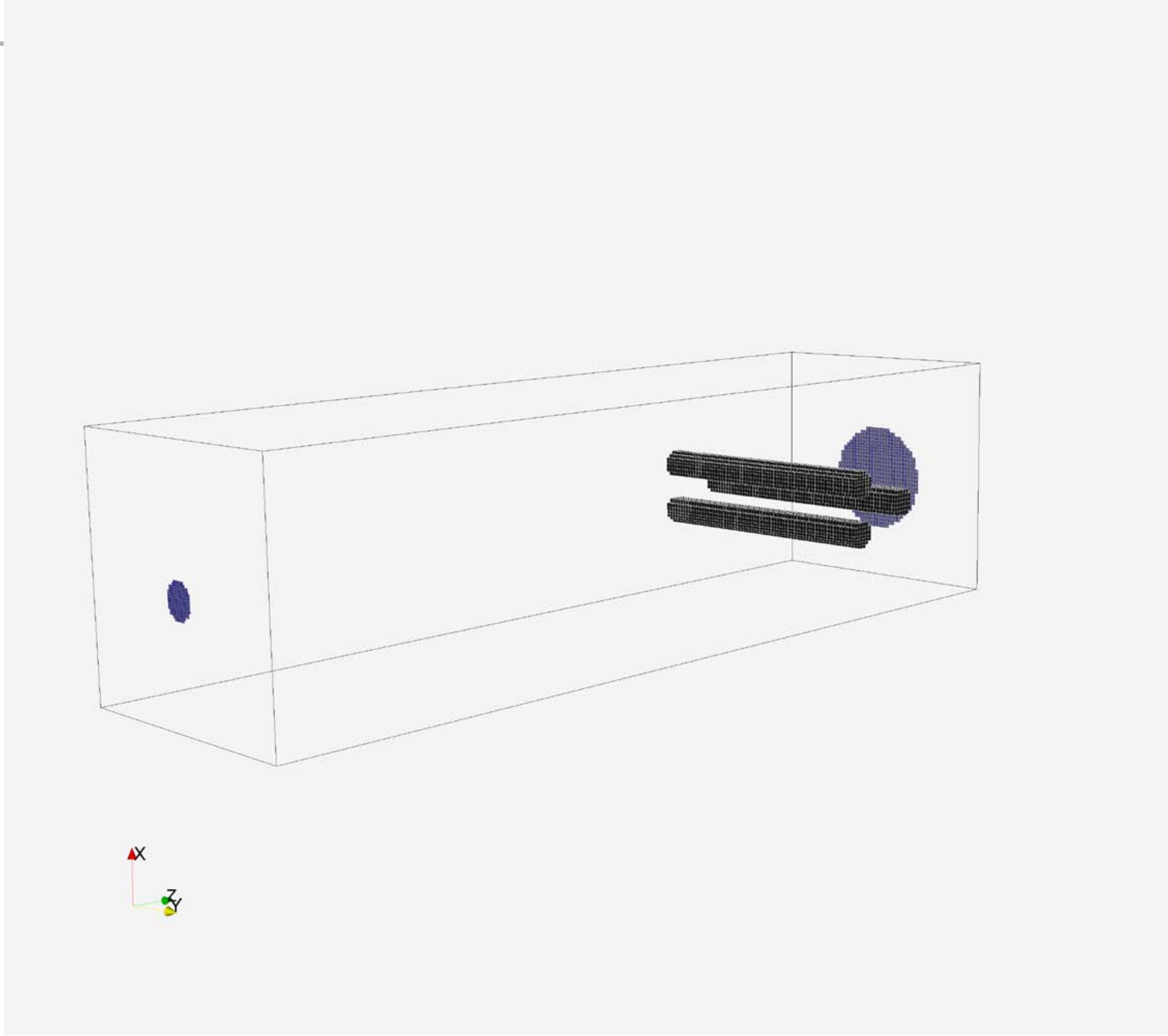
Characteristics:

- Cartesian grid
- 200 000 cells
- 100 000 iterations until convergence (24h on 4 Cores)

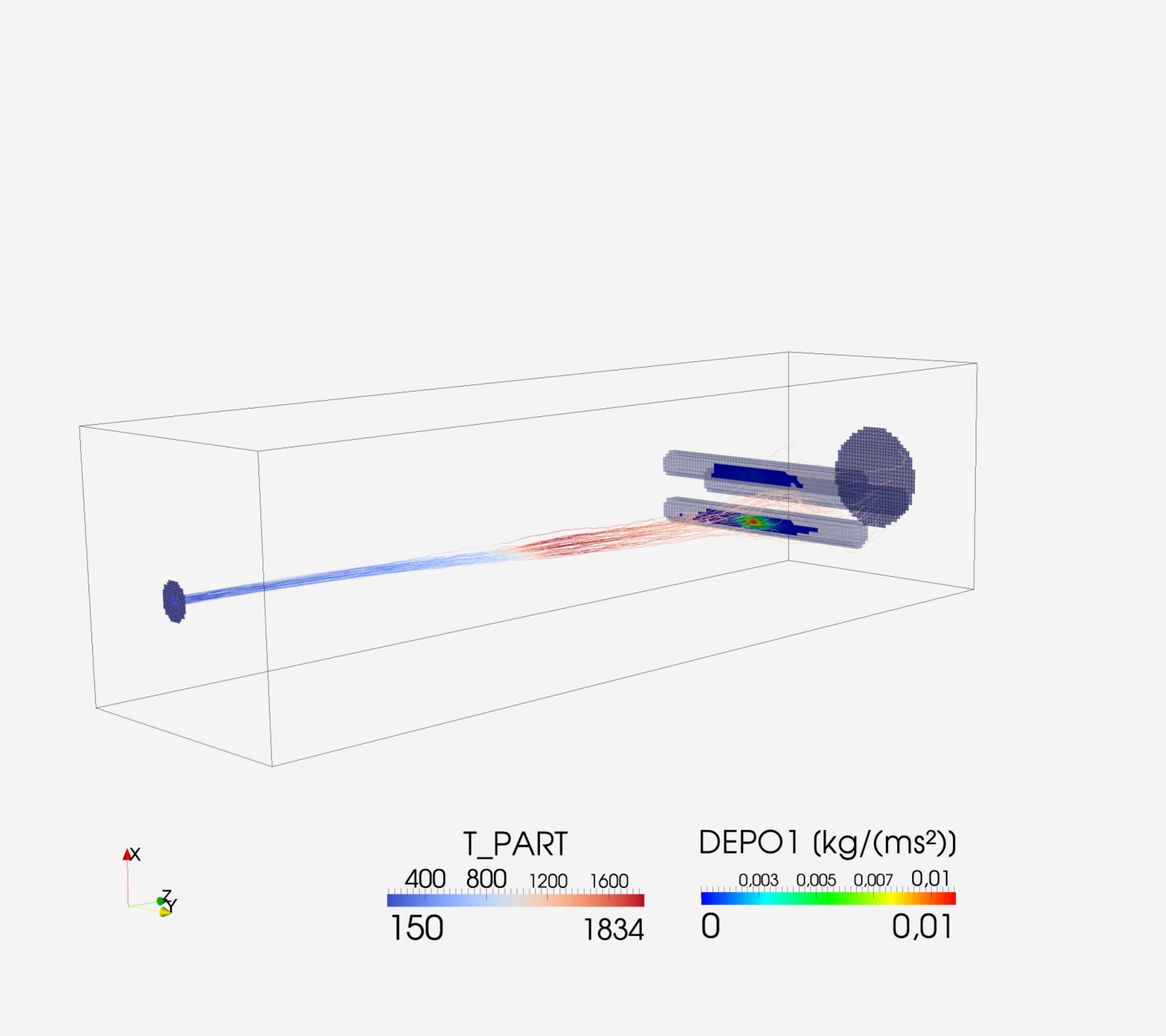
Testcase – Modified IFRF Furnace



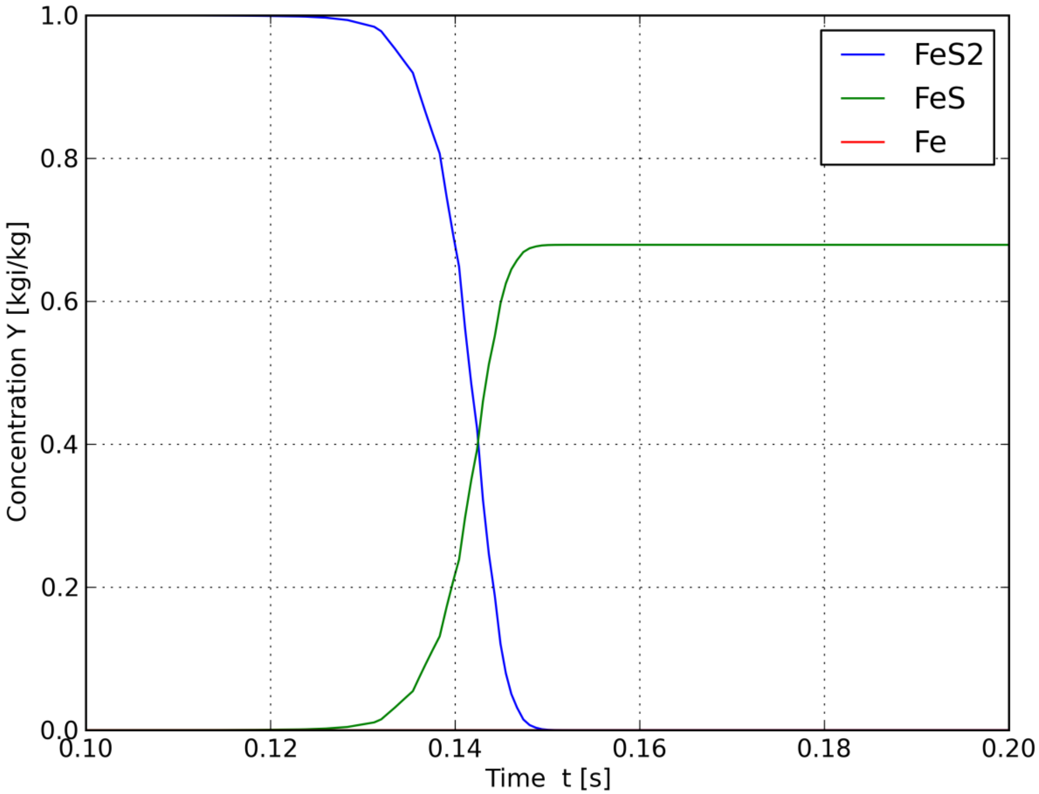
Testcase – Modified IFRF Furnace



Testcase – Modified IFRF Furnace



Mineral Transformation - Pyrite



$$FeS_2[s] \rightarrow FeS[s] + S_2[g] \qquad (1)$$

$$FeS[s] \rightarrow Fe[s] + 0.5\ S_2[g] \qquad (2)$$

$$3(FeS_2) + 8\ O_2 \rightarrow Fe_3O_4 + 6\ SO_2 \qquad (3)$$

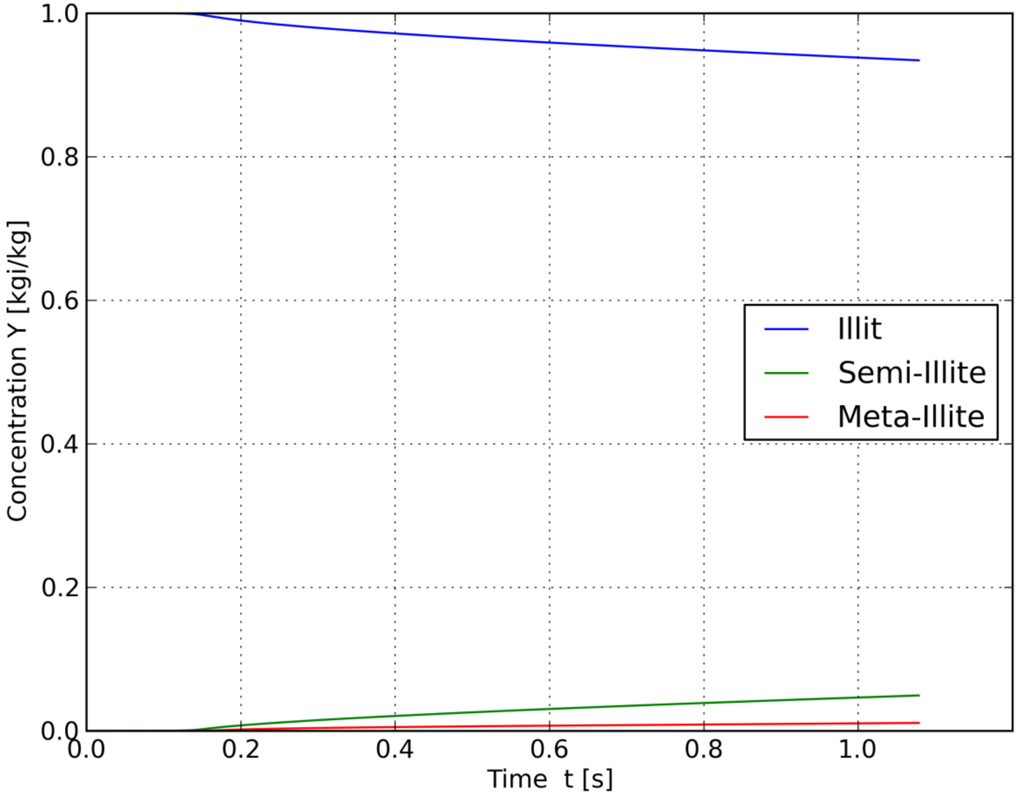
$$FeS + O_2 \rightarrow Fe_3O_4 + SO_2 \qquad (4)$$

$$Fe_3O_4 + 0.25\ O_2 \rightarrow 1.5\ Fe_2O_3 \qquad (5)$$

$$Fe + 0.66\ O_2 \rightarrow 0.33\ Fe_3O_4 \qquad (6)$$

- Particle less than 1.5s in the furnace
- Predominant reactions are (1) and (2)
- Reactions (3) – (6) are pretty slow as oxygen used mainly for char combustion
- In large scale furnaces reaction (5) takes place in the deposition

Mineral Transformation - Illite



(1) $(K, H_3O)Al_2[OH]_2[AlSi_3O_{10}] \rightarrow semimetaillite + 1.53\ H_2O$

(2) $semimetaillite \rightarrow metaillite + 0.97\ H_2O$

- ➲ Dehydroxilation
- ➲ Slow reaction
- ➲ At temperatures higher than 1500 K mullite is build (missing kinetic)

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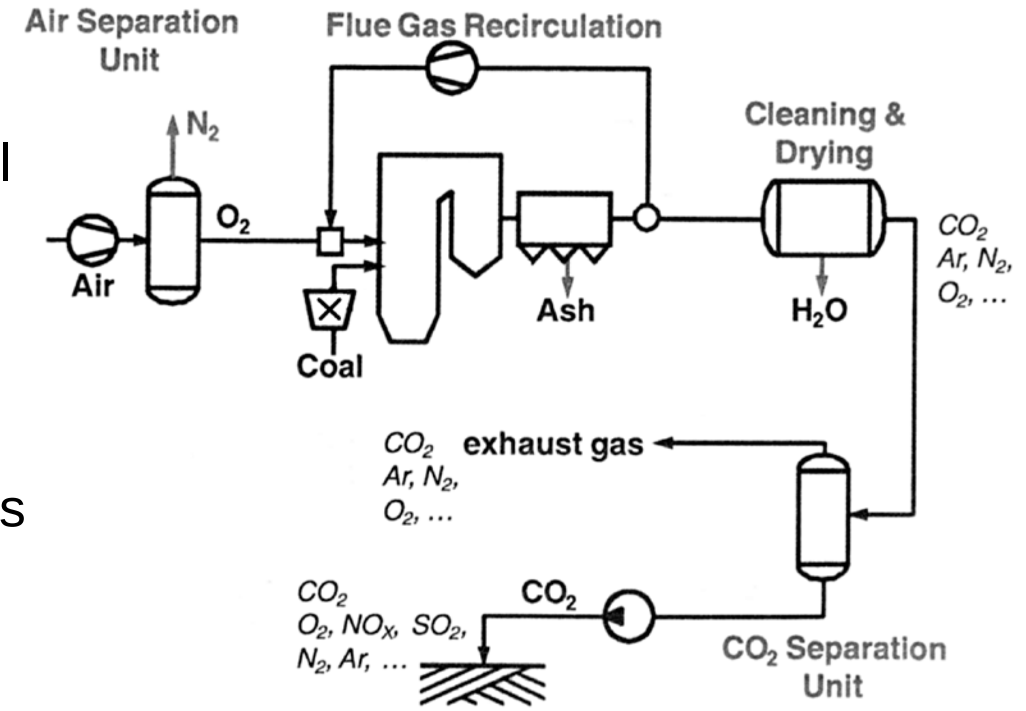
Oxy-fuel Process

- Oxy-fuel combustion process causes compared to conventional operation specific conditions

- The modified composition of oxidizing atmosphere (mainly oxygen and recycled flue gas) has effect on:
    - thermo-physical properties
    - flame characteristics
    - emission behavior

- Adjustments for various sub-models within simulations are required



Extended chemical reaction models

➲ Homogeneous chemistry:

(1) $C_nH_m + n/2\,O_2 \rightarrow n\,CO + m/2\,H_2$

(2) $C_nH_m + n\,H_2O \rightarrow n\,CO + (m/2 + n)\,H_2$

(3) $H_2 + ½\,O_2 \leftrightarrow H_2O$

(4) $CO + H_2O \leftrightarrow CO_2 + H_2$

- implementation of additional reactions and assuming equilibrium reactions enables accounting for chemical effects of specifically high O_2 and CO_2 levels in the oxidizing atmosphere during oxy-fuel combustion

- including reverse reaction of (3) is particularly required for correct prediction of local flame temperatures since equilibrium is shifted towards educts in high temperature flames

Extended chemical reaction models

➲ Heterogeneous chemistry:

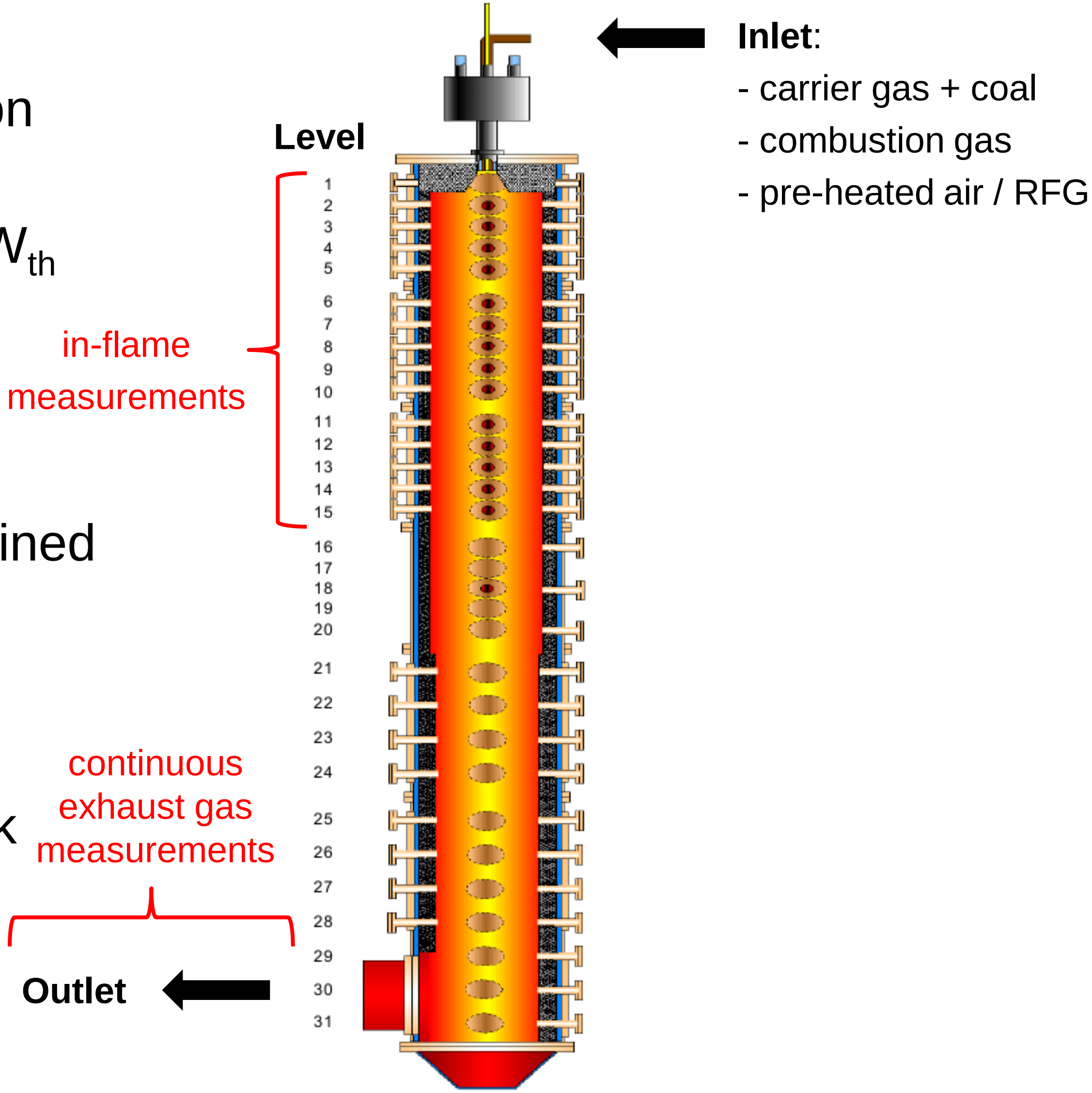
(1)	$C + ½\, O_2 \rightarrow CO$	(char oxidation)
(2)	$C + CO_2 \rightarrow 2\, CO$	(Boudouard reaction)
(3)	$C + H_2O \rightarrow CO + H_2$	(water-gas-shift reaction)

- ➥ reactions (2) and (3) may have major impact in **O_2-lean regions** due to higher partial pressures of CO_2 and H_2O compared to conventional air-firing
- ➥ at ambient pressure and typical combustion temperatures the reactions (2) and (3) may be considered **irreversible** since the equilibrium is shifted towards the product side

Experimental set-up

- Atm. pulverized fuel combustion rig
- maximum thermal input 500 kW_{th}
- vertically fired furnace with
  - length: ~ 7.0 m
  - diameter: ~ 0.8 m
  - water-cooled and refractory lined

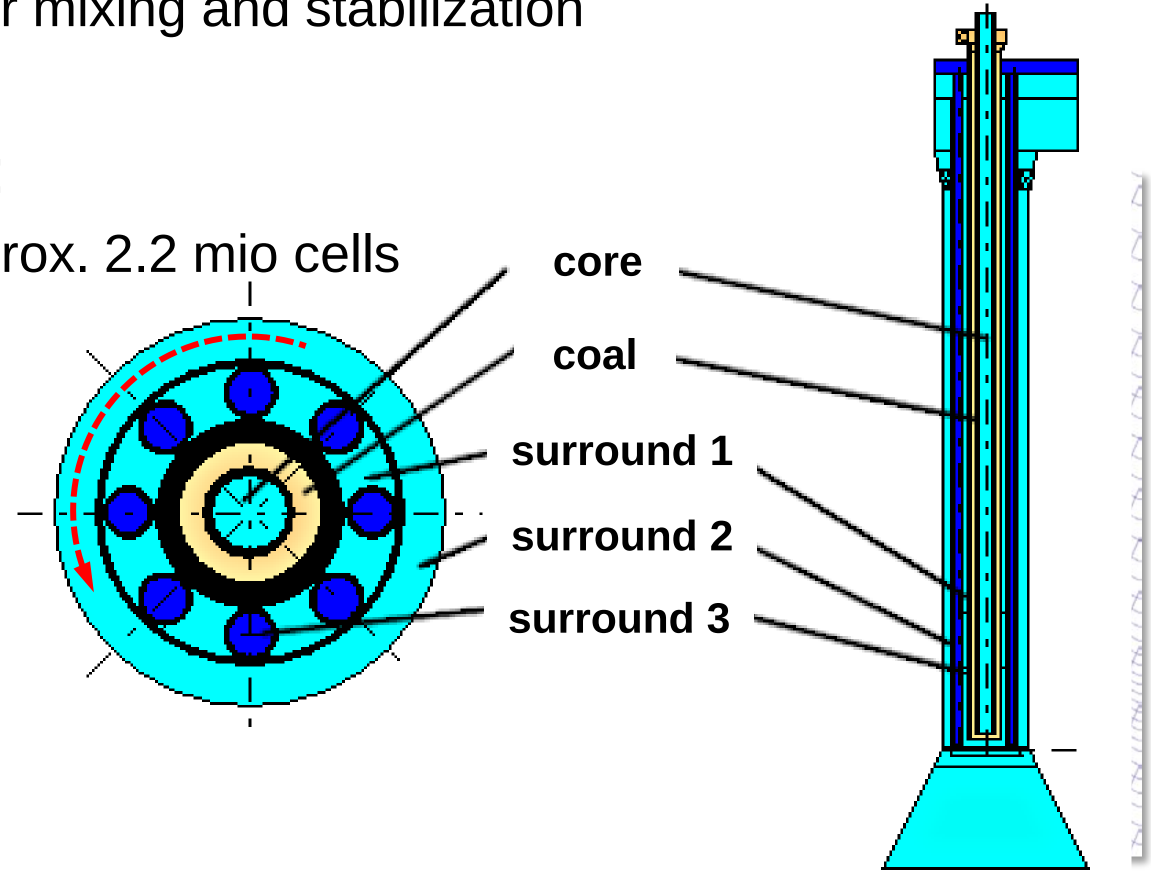
- oxy-fuel operation:
  - flue gas recycling
  - O_2 from external storage tank



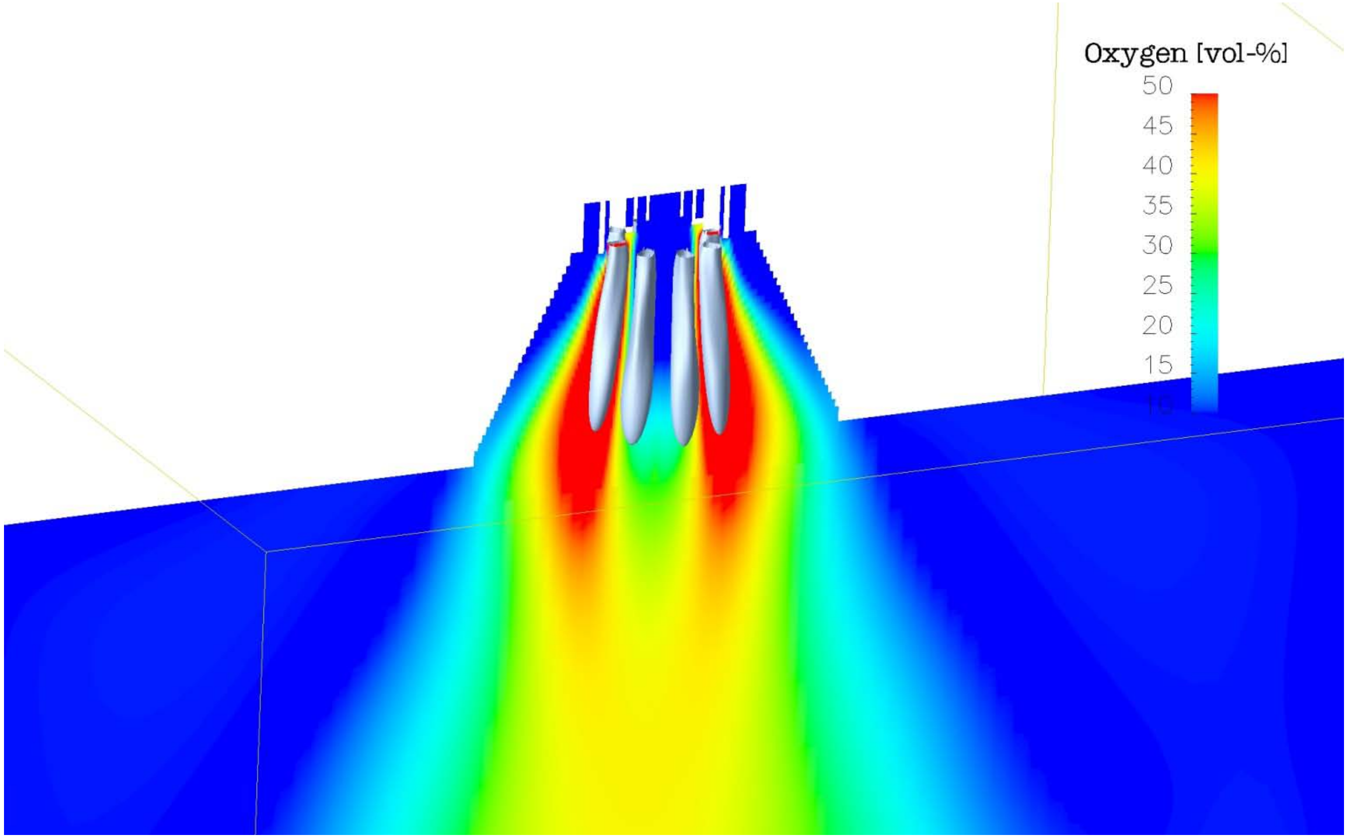
Experimental set-up

- Burner layout:
  - four oxidizer inlets → highly flexible operation
  - swirl imposed in outer annular section “surround 2”
  - bluff body included for mixing and stabilization

- Computational mesh:
  - detailed grid with approx. 2.2 mio cells



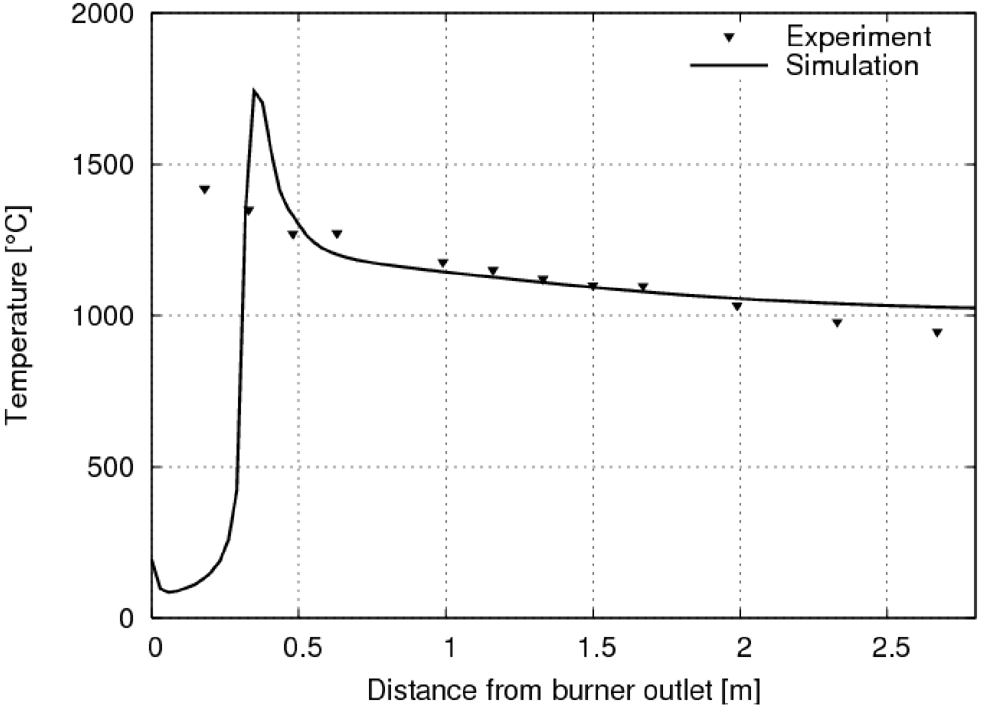
Modelling of Oxy-fuel Combustion



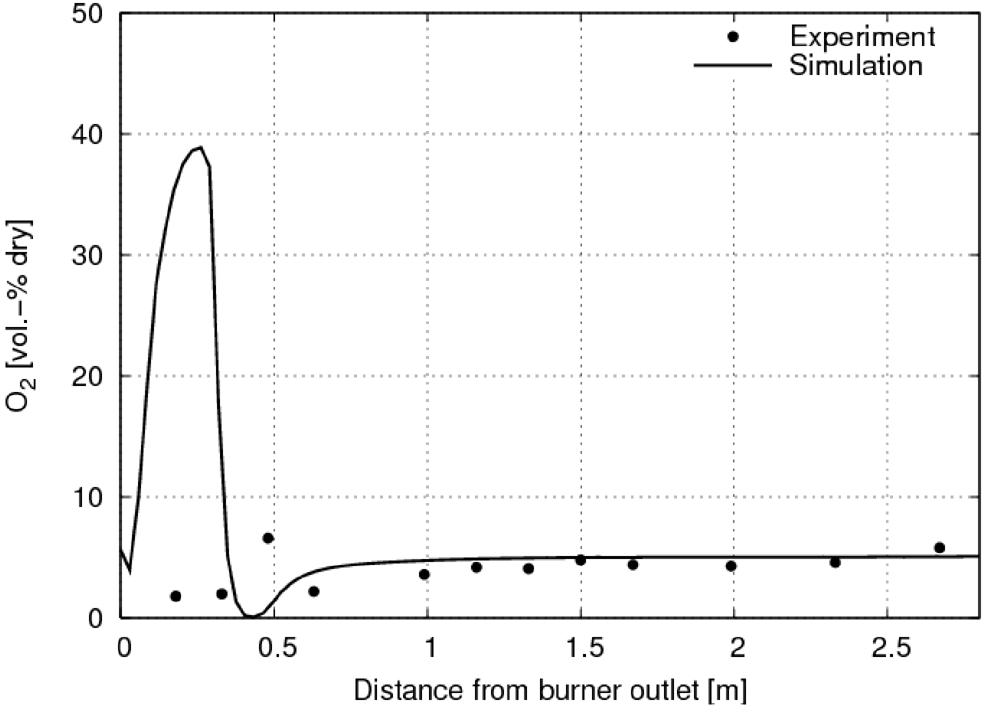
Comparison of experiment and simulation

- Oxy-fuel test case
  - **axial** plots on furnace centerline

gas temperature



O_2 concentration



Comparison of experiment and simulation

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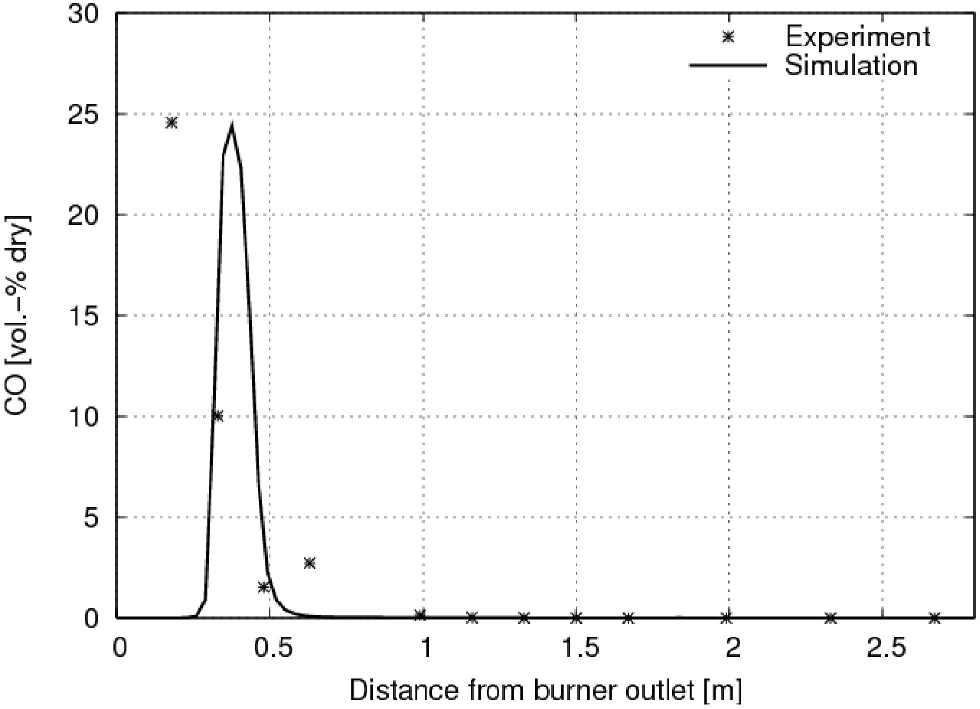
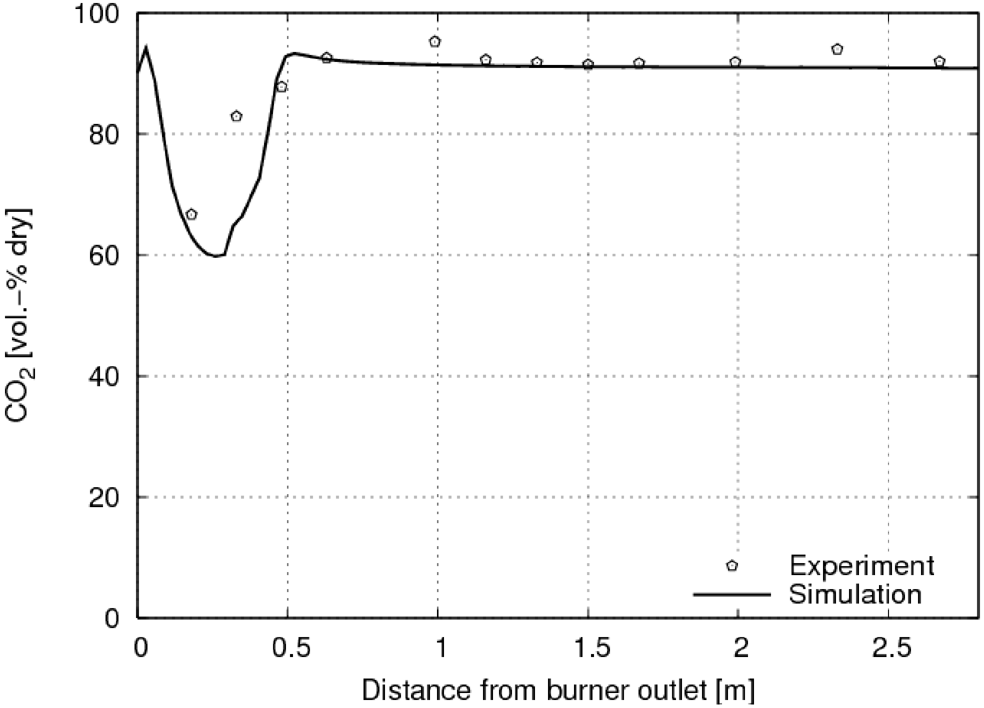
CO concentration

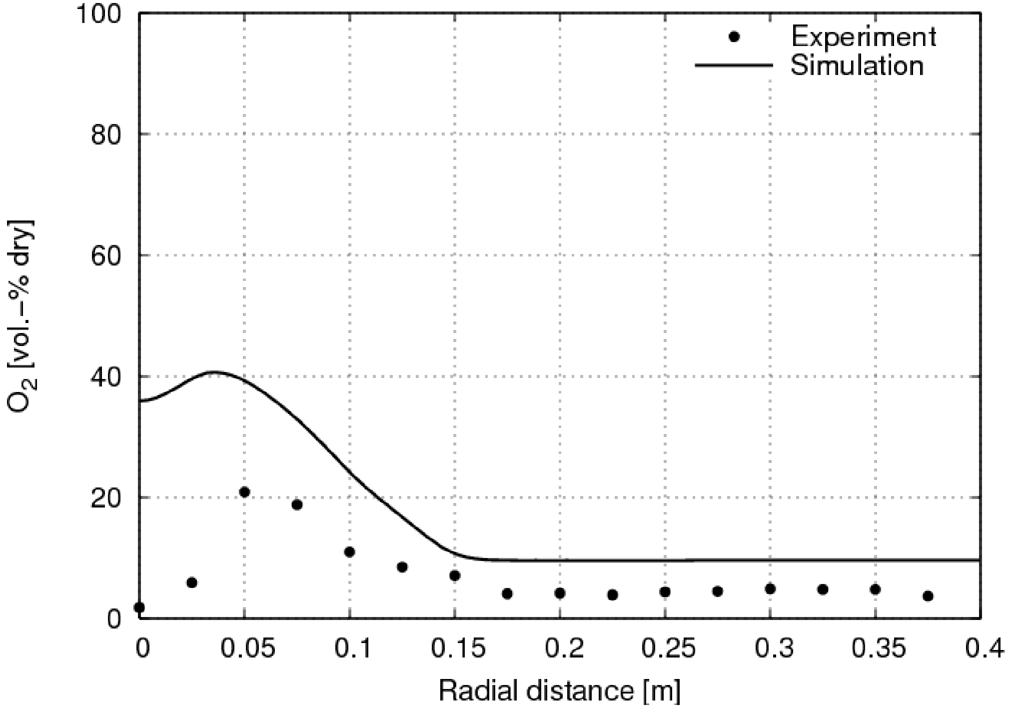


CO$_2$ concentration

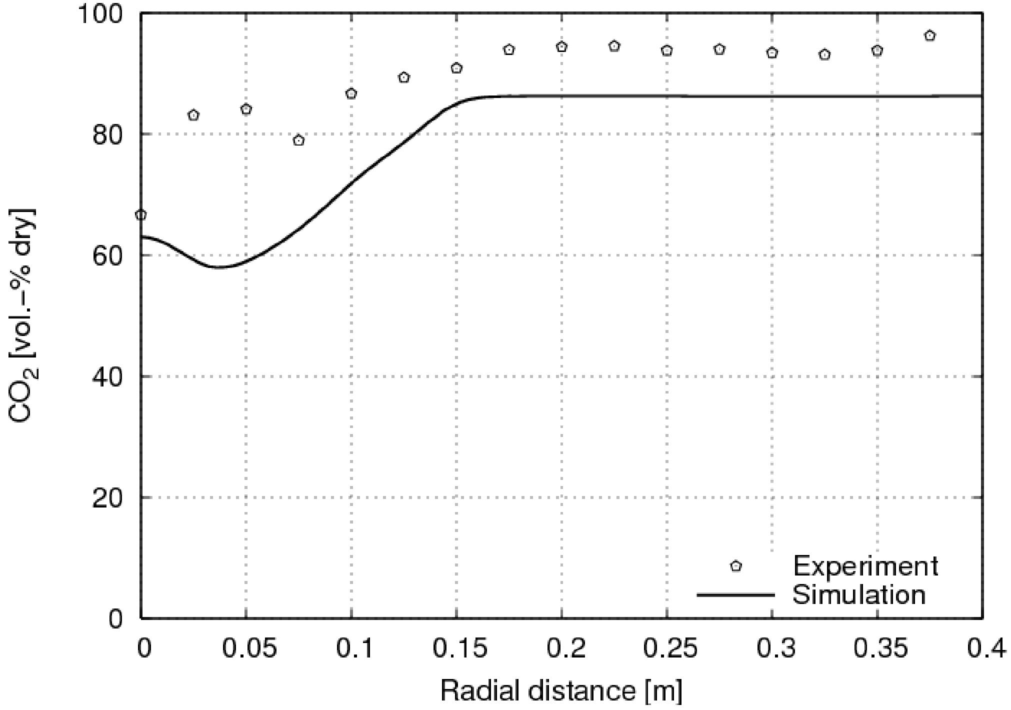


Comparison of experiment and simulation

- Oxy-fuel test case
  - » **radial** plots at 0.16 m below the burner (level 2)



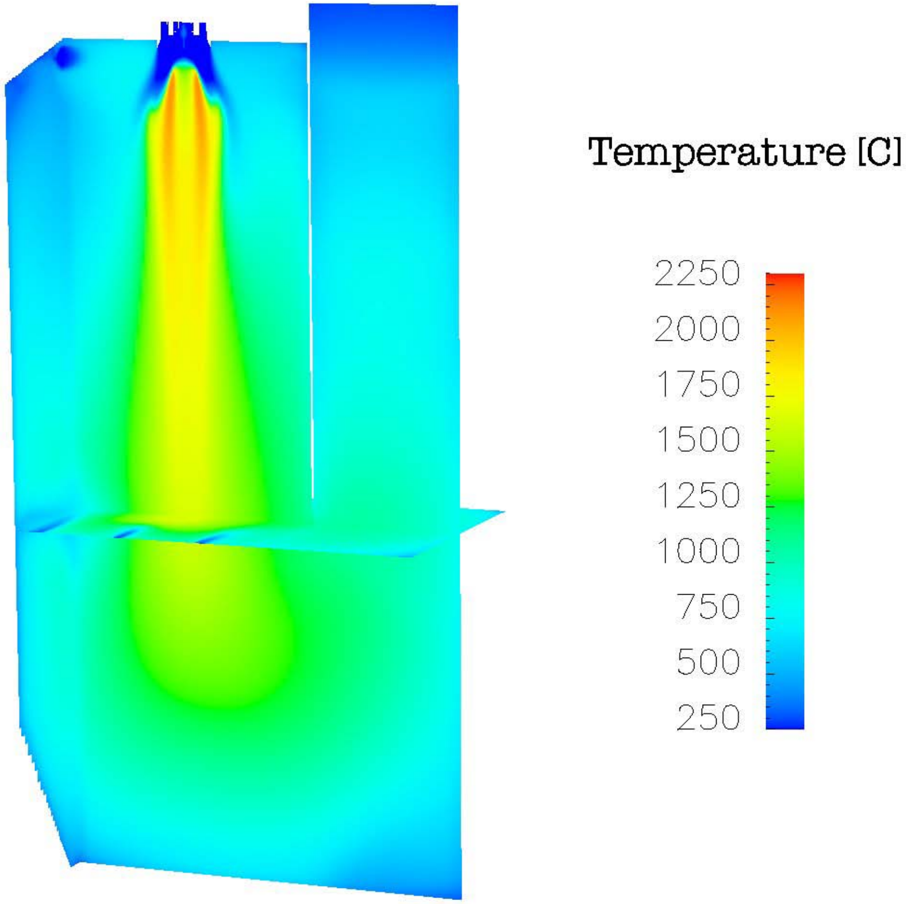
O_2 concentration

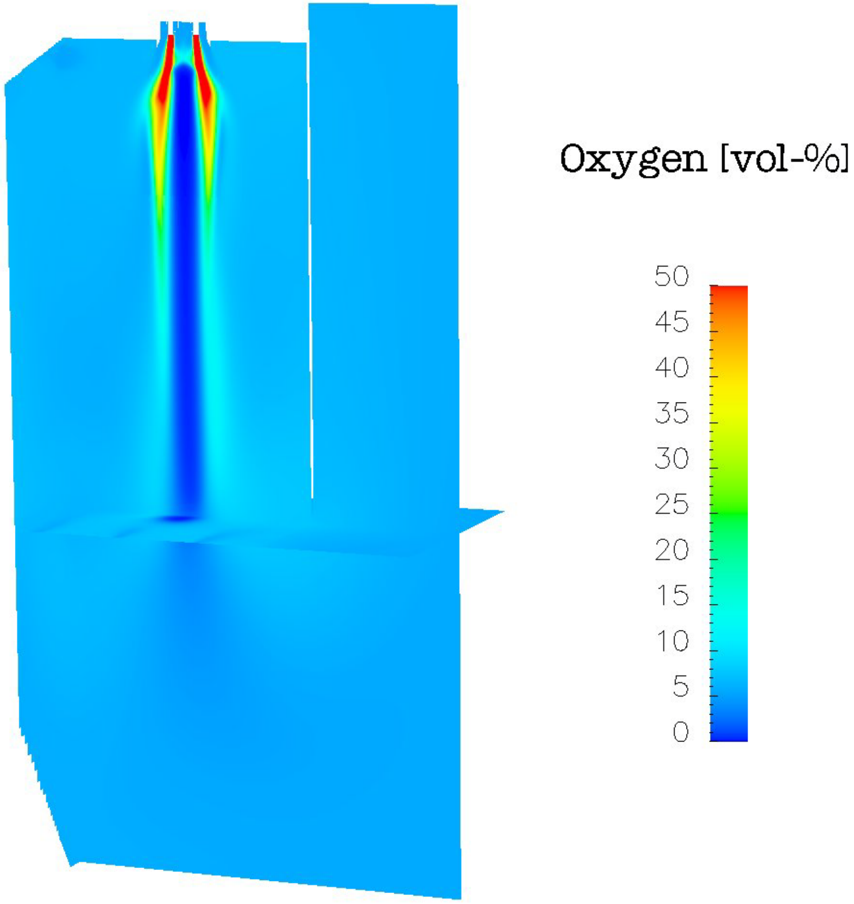


CO_2 concentration

Modelling of Oxy-fuel Combustion

- Simulation of Oxy-fuel combustion pilot plant „Schwarze Pumpe“ (30 MW)





Summary and Outlook

- General description of mineral matter transformation has been implemented in CFD code AIOLOS
- Two approaches for prediction of stickiness have been introduced → enables to simulate the deposit build-up at furnace walls
- Oxy-fuel combustion modelling in AIOLOS

- Rise of computational power will be used to combine the simulation of various single phenomena into one approach
- Improvement of stickiness criteria and validation have to be carried on (Project TU Munich)
- Effect of oxy-fuel atmosphere on mineral matter transformation has to be investigated and implemented (running projects at IFK)

References (1)

- **Schnell**, U.: Numerical Modelling of Solid Fuel Combustion Processes Using Advanced CFD-Based Simulation Tools. PCFD 1 (2001) No. 4, 208-218
- **Walsh**, P.M.; Sarofim, A.F. und Beer, J.M.: Fouling of Convection Heat Exchangers by Lignitic Coal Ash. Energy & Fuels, 6-709 , 1992
- **Michel**, J.-B., Payne, R.: Detailed measurement of long pulverized coal flames for the characterization of pollutant formation, Research Report, IFRF, Ijmuiden, 1980.
- **Leiser, S. : Numerical Simulation of Oxy-fuel Combustion, Dissertation**
- **Müller, M.: Advanced modeling of pulverized coal combustion under oxy-fuel conditions, Clearwater, 2010.**
- **A. Kather and G. Scheffknecht: „The oxycoal process with cryogenic oxygen supply“, Naturwissenschaften, vol. 96, pp 993-1010, 2009.**
- Stefan **Richter**, Numerische Simulation der Flugaschedeposition on kohlestaubgefeuerten Dampferzeugern. Stuttgart, 2002.
- **Urbain**, G. et al.: Viscosity of silicate melts, Trans. J. Br. Ceram. Soc. 80 (1981), pp. 139 – 141
- **Browning**. et al.: An empirical Method for the Prediction of coal Ash Slag Viscosity, Energy & Fuel 17 (2003), pp. 731 – 737
- **Watt**, J.D.; Fereday, F.: The flow properties of slags formed from the ashes of British coals: Part 1, J. Inst. Fuel 42 (1969), pp. 99 – 103

References (2)

- **Bozic**, O.: „Numerische Simulation der Mineralumwandlung in Kohlenstaubfeuerungen“, TU Braunschweig, 2003.
- **Tomeczek**, J. : „Kinetics of mineral matter transformation during coal combustion“, Fuel 81, pp 1251-1258, 2002.
- M. **Frank** D.P. **Kalmanovitch**, "An Effective Model of Viscosity for Ash Deposition Phenomena," in *Proc. of the EF Conference*, Santa Barbara, CA, 1989.
- F.J. Frandsen, K. Dam-Johansen S. **Vargas**, "Rheological properties of high-temperature melts of coal ashes and other silicates," *Progress in Energy and Combustion Science*, vol. 27, no. 237-429, 2001.
- S. **Srinivasachar** C.L. **Senior**, "Viscosity of Ash Particles in Combustion Systems for Prediction of Particle Sticking," *Energy and Fuels*, pp. 9-277, 1995.
- **Tanaka**, H: „Thermal analysis and kinetics of solid state reactions“, Thermochimica Acta, 267:29-44, 1995.

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And thank you for your attention!