Evaluation of Oxy-Coal Combustion Modelling at Semi-Industrial Scale

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Overview

- Introduction
  - oxy-fuel process
  - modelling of coal combustion
- Extended chemical reaction models
  - homogeneous chemistry
  - heterogeneous chemistry
- Comparison of experiment and simulation
  - test facility and operating conditions
  - simulation results
- Conclusions & Outlook

Overview

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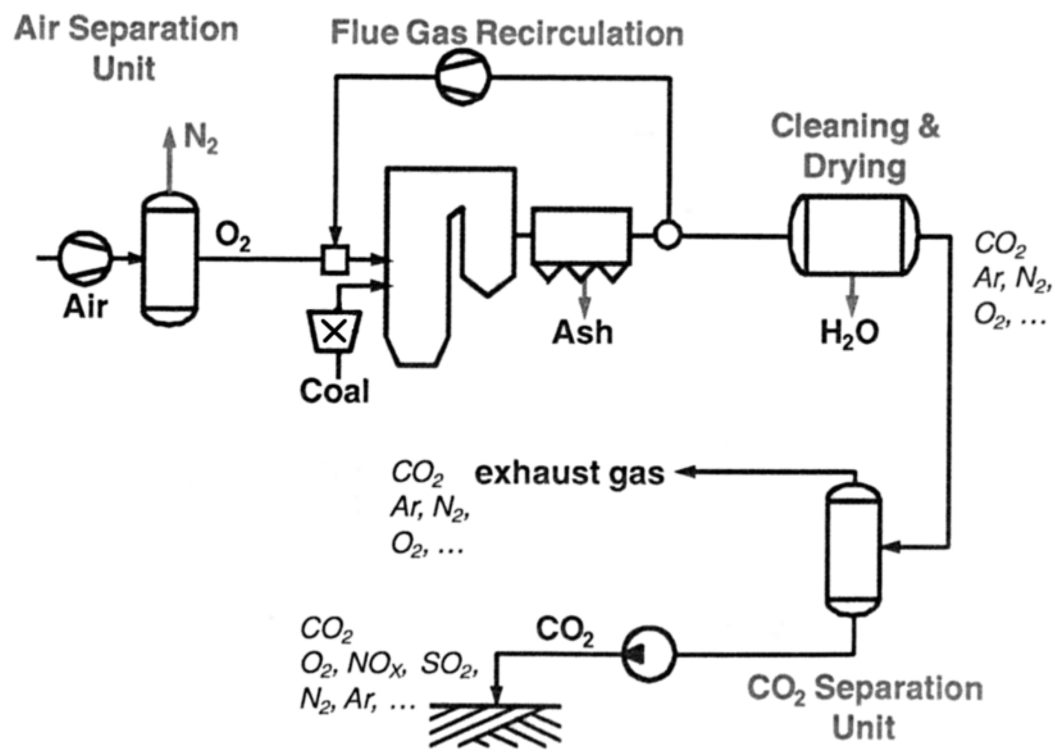
Oxy-fuel process

- Specific conditions within oxy-fuel combustion process compared to conventional operation

- modified composition of oxidizing atmosphere (mainly oxygen and recycled flue gas)
  - thermo-physical properties
  - flame characteristics
  - emission behaviour

- adjustments are required within CFD simulations

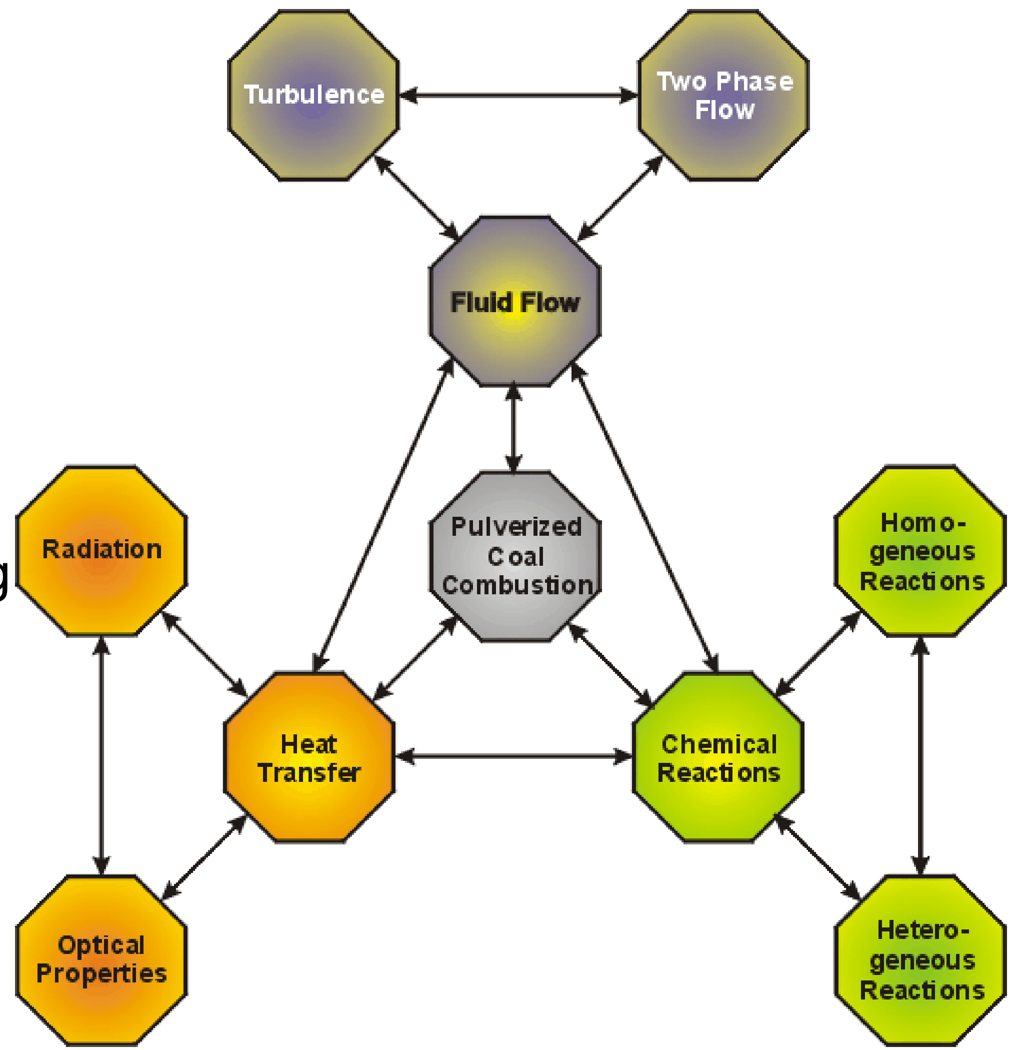


Modelling of coal combustion

» In-house developed CFD code

AIOLOS

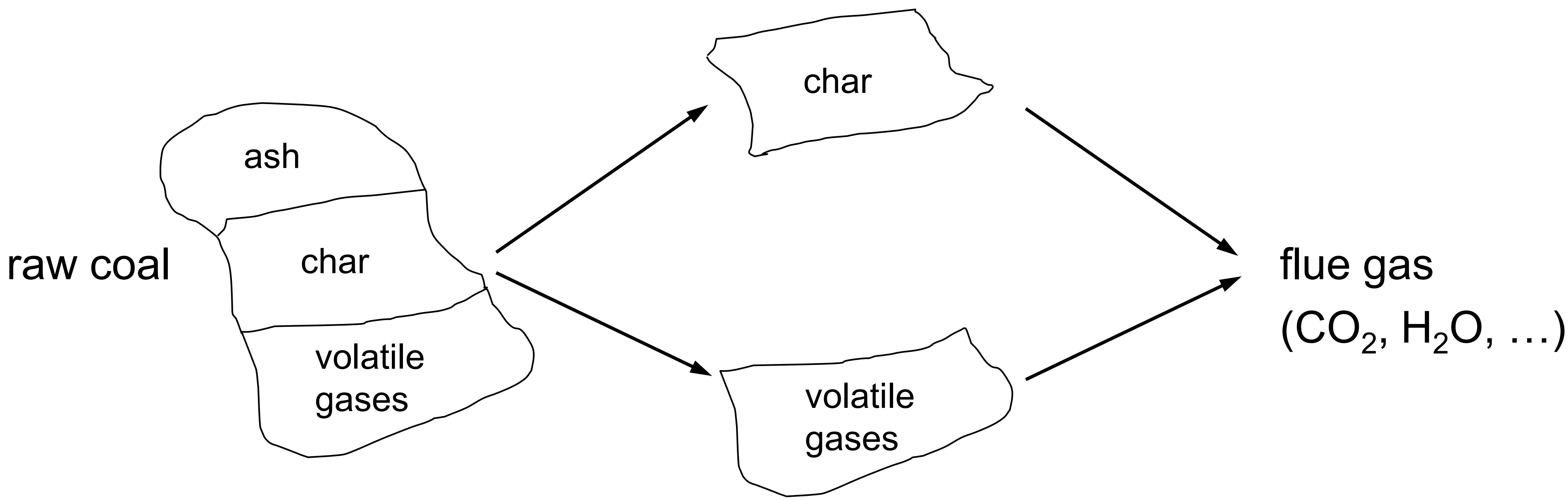
» specifically tailored for combustion simulation combining
  - » fluid flow
  - » heat transfer
  - » chemical reactions



"Evaluation of Oxy-Coal Combustion Modelling at Semi-Industrial Scale", M. Müller et al. (IFK)

Modelling of coal combustion

- Conversion process of pulverized coal combustion
  - pyrolysis: primary and secondary reactions
  - burnout of residual char
  - combustion of volatile gases



- objective of simulations:
  - prediction of flow field, temperature distribution and relevant species concentrations

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Extended chemical reaction models

» **Homogeneous chemistry (volatile combustion):**

(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 considering 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 (char burnout):**

(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)

- » gasification 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

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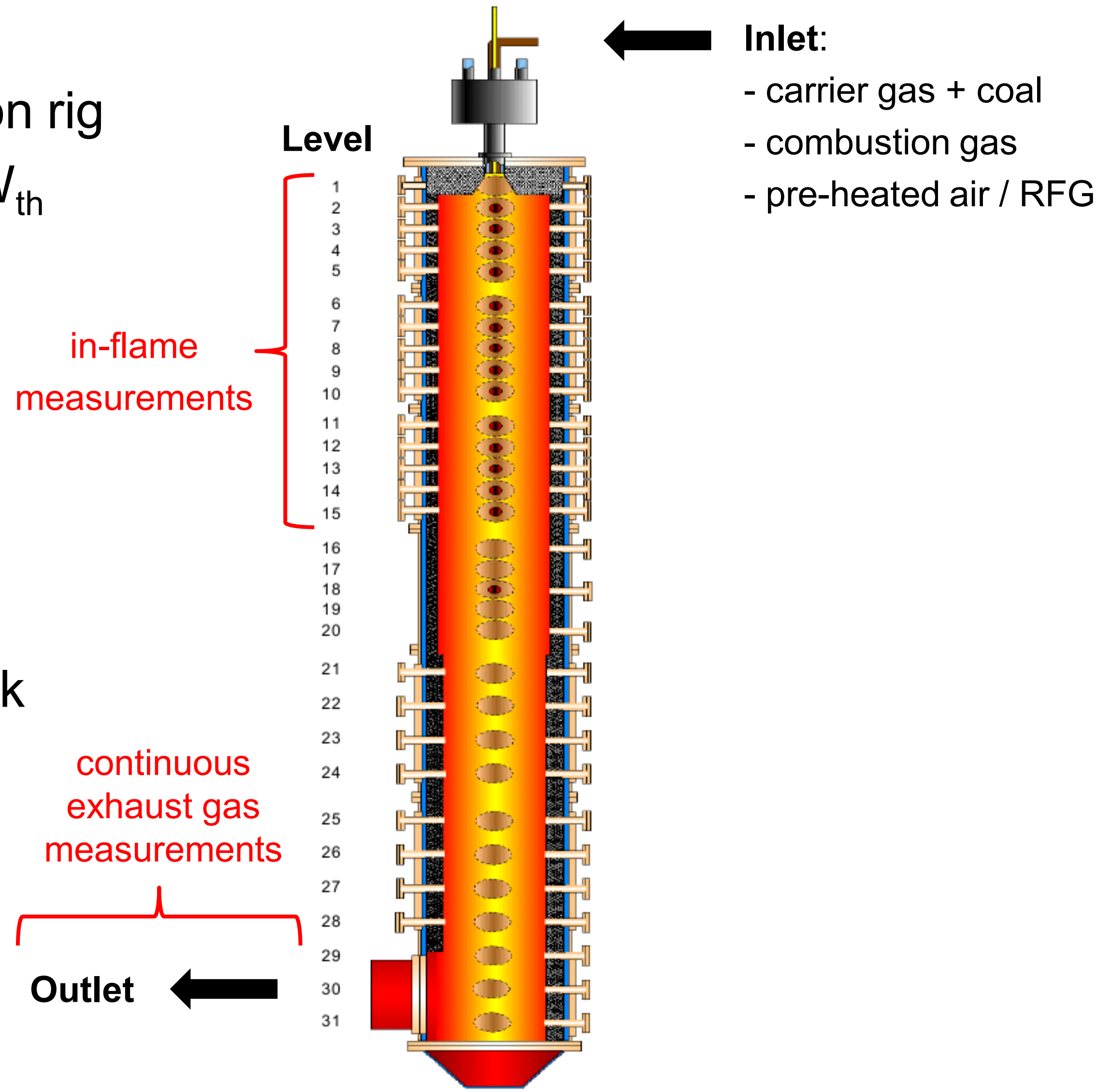
Experimental set-up

- Atm. pulverized coal combustion rig
- maximum thermal input 500 kW_{th}
- vertically fired furnace with
  - length: ~ 7.0 m
  - diameter: ~ 0.8 m

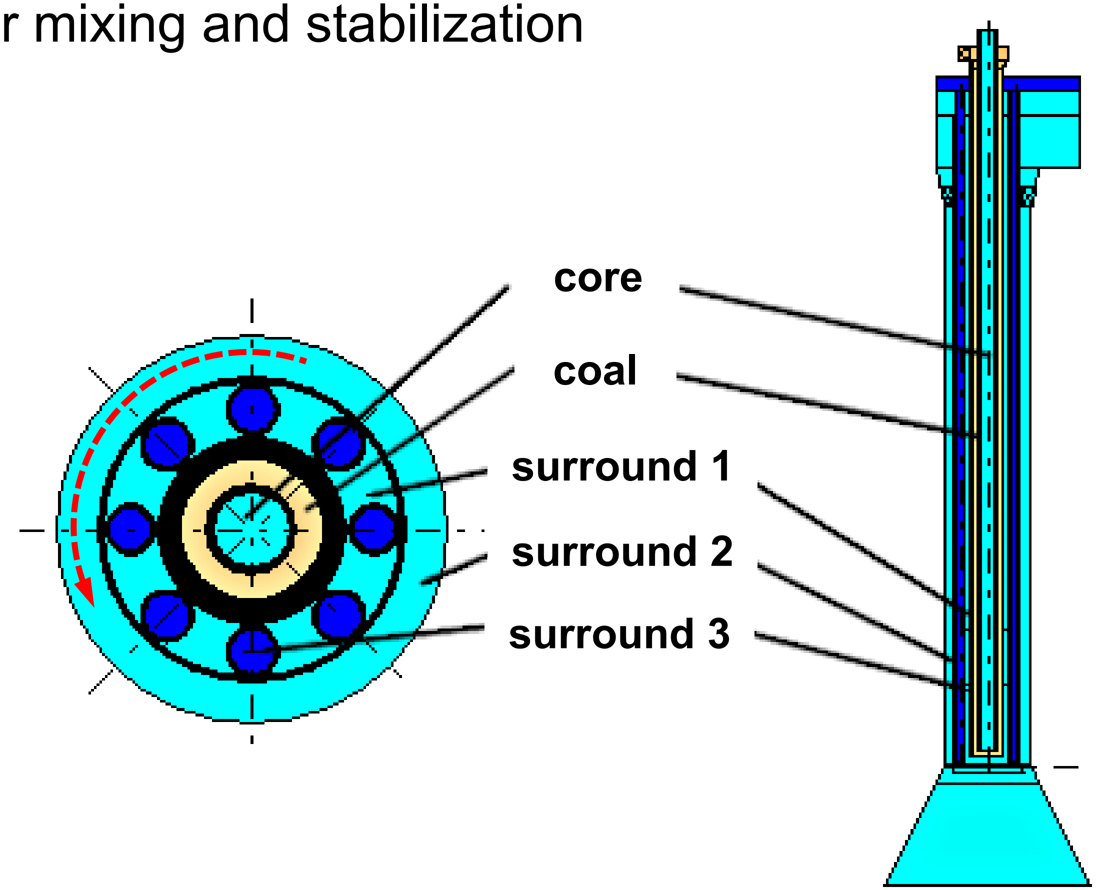
- oxy-fuel operation:
  - dry/wet flue gas recycling
  - O_2 from external storage tank



"Evaluation of Oxy-Coal Combustion Modelling at Semi-Industrial Scale", M. Müller et al. (IFK)

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



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Experimental set-up

- Burner layout:
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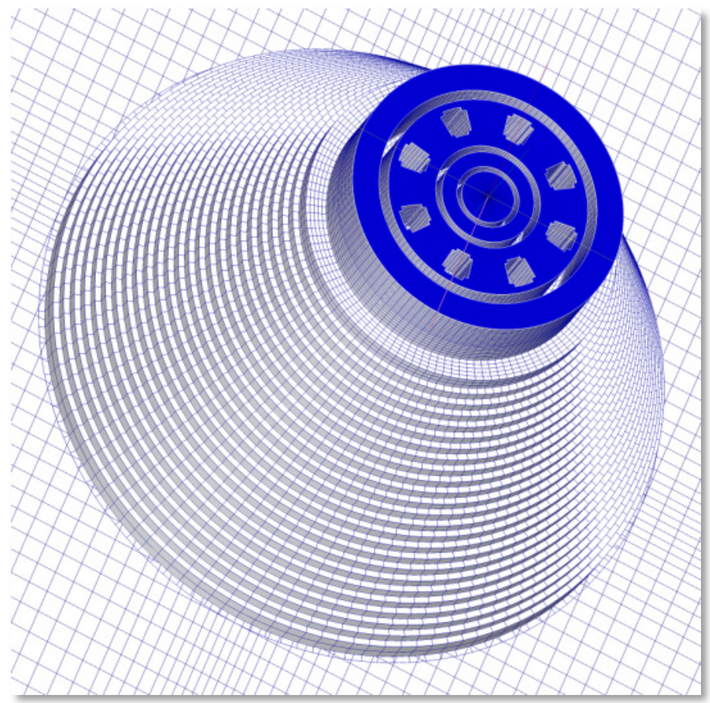
  - swirl imposed in outer annular section “**surround 2**”
  - bluff body included for mixing and stabilization

- computational mesh:
  - detailed grid with about 2.2 x 10^6 cells



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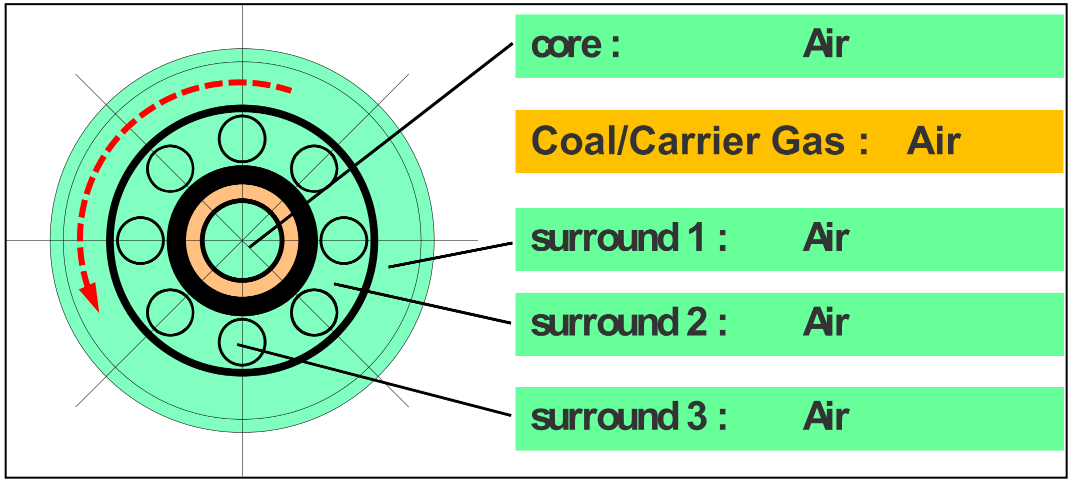
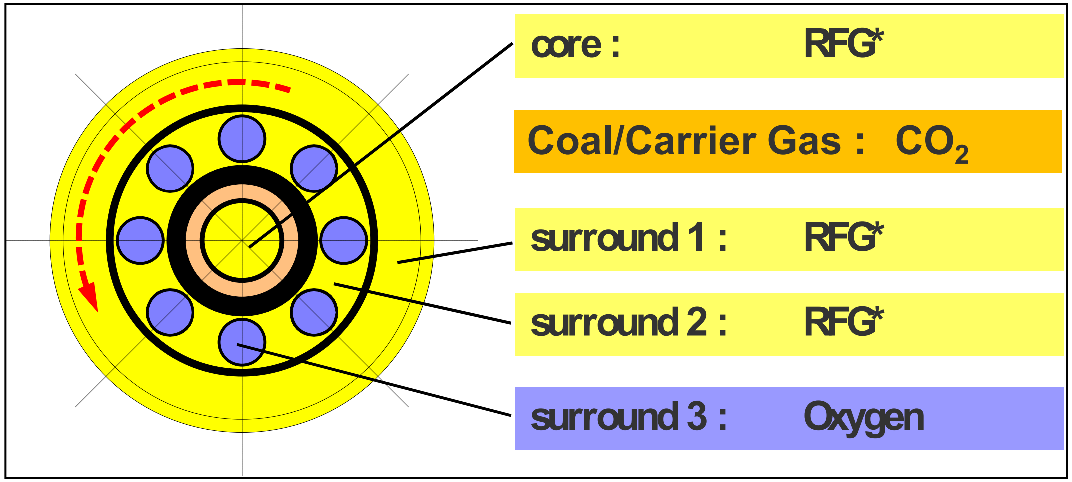
Experimental set-up

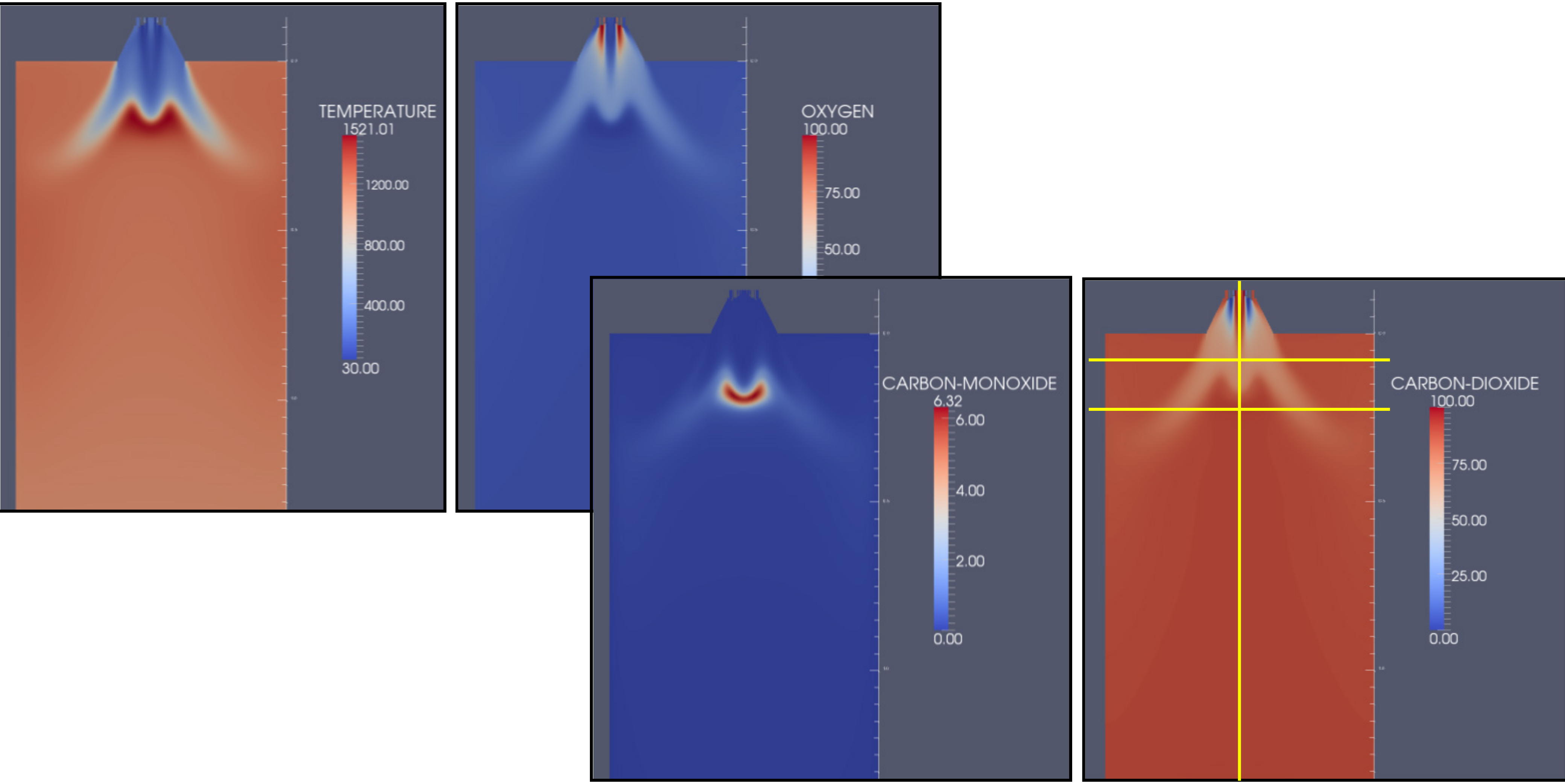
- Operational conditions:
  - oxy-fuel and air case
  - fuel: hard coal Pittsburgh #1
  - thermal input: ~ 280 kW_{th}
- oxy-fuel test case:
  - direct injection of O_2
  - wet flue gas recycling
  - total O_2 level: ~ 32 %
  - recycling rate: ~ 75 %





Evaluation

» Oxy-fuel test case – simulation results



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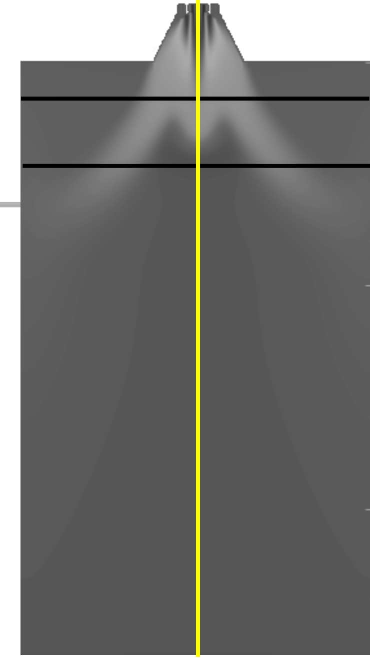
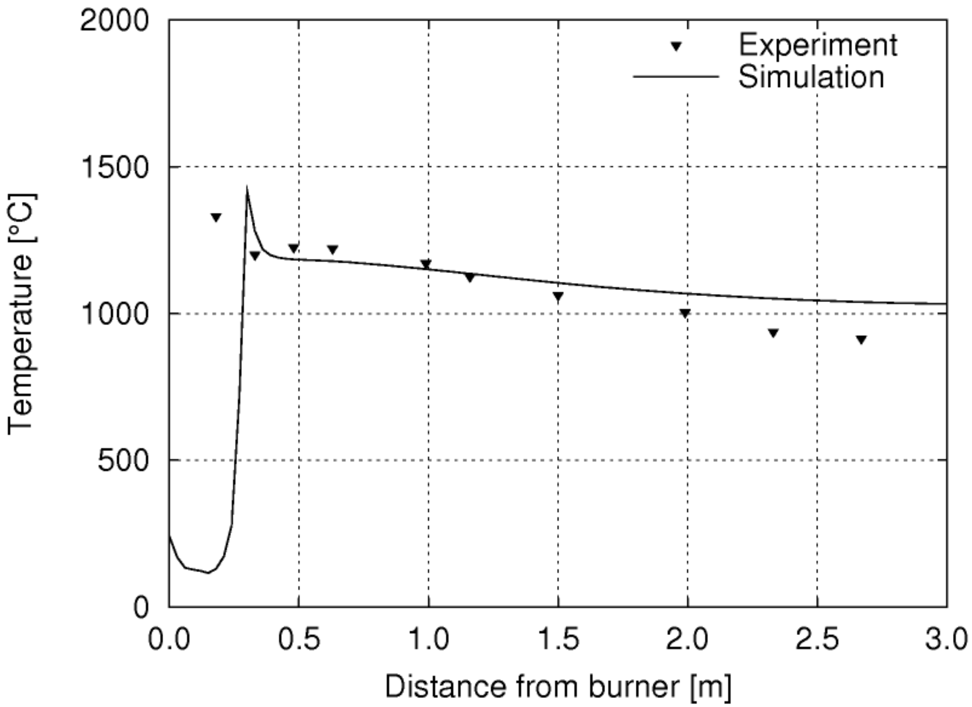
Evaluation

» **Oxy-fuel** test case – comparison

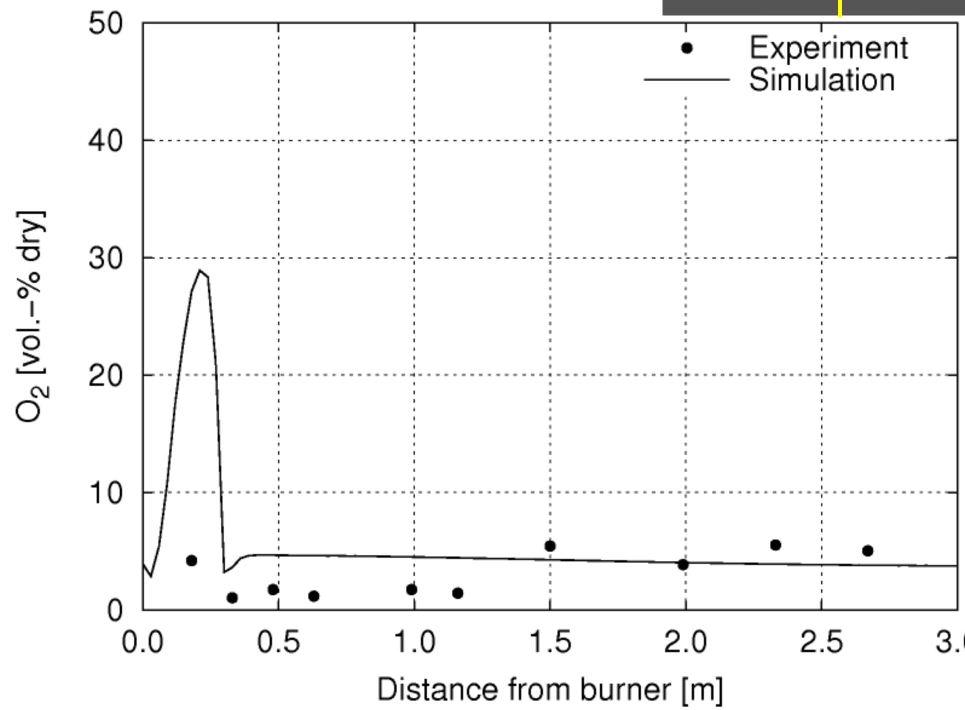
» **axial** plots on furnace centerline



» gas temperature:



O_2 concentration:



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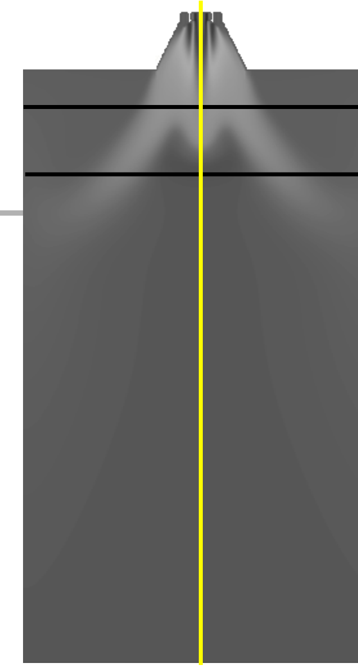
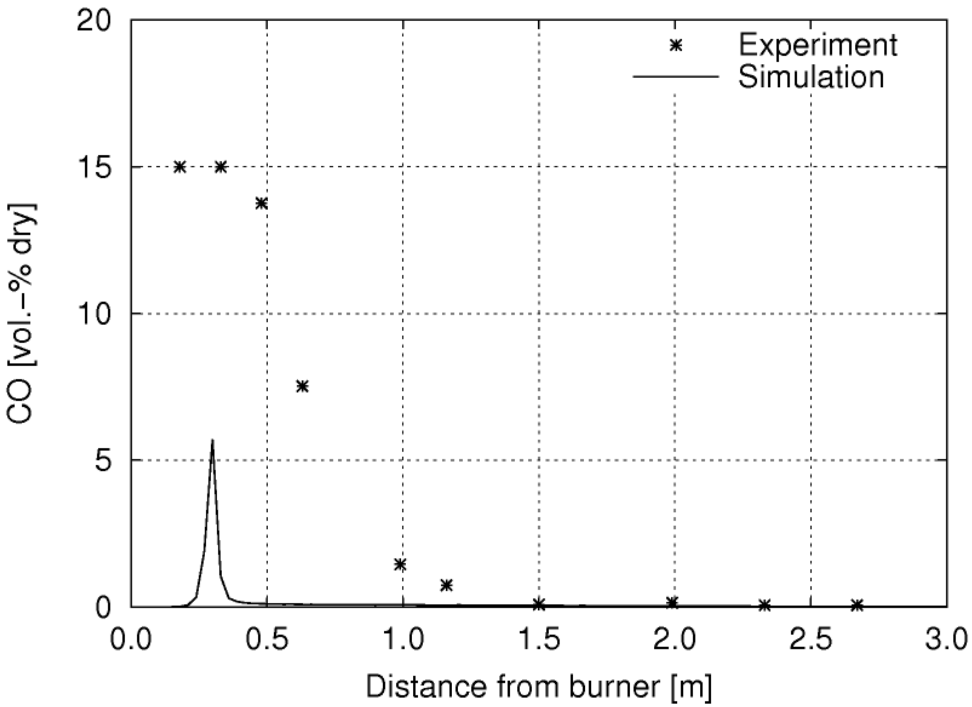
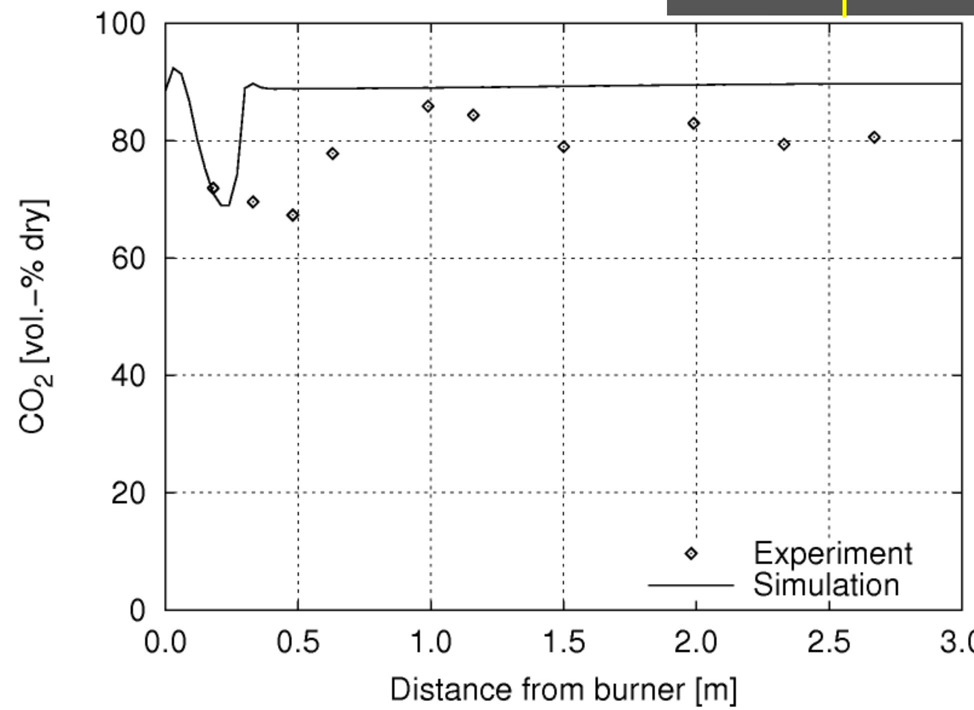


- » **axial** plots on furnace centerline
- » CO concentration:



CO_2 concentration:



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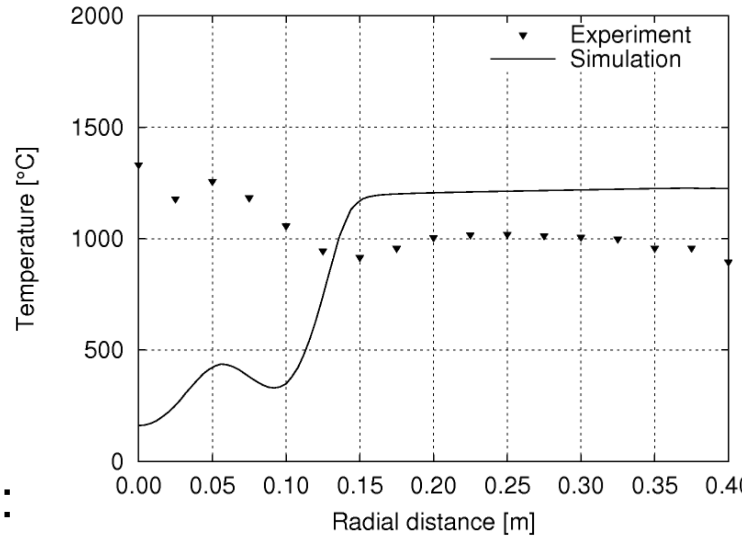
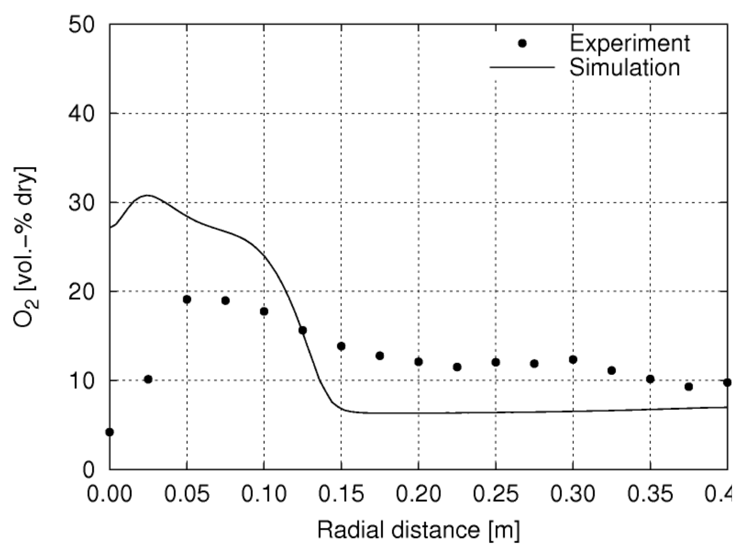
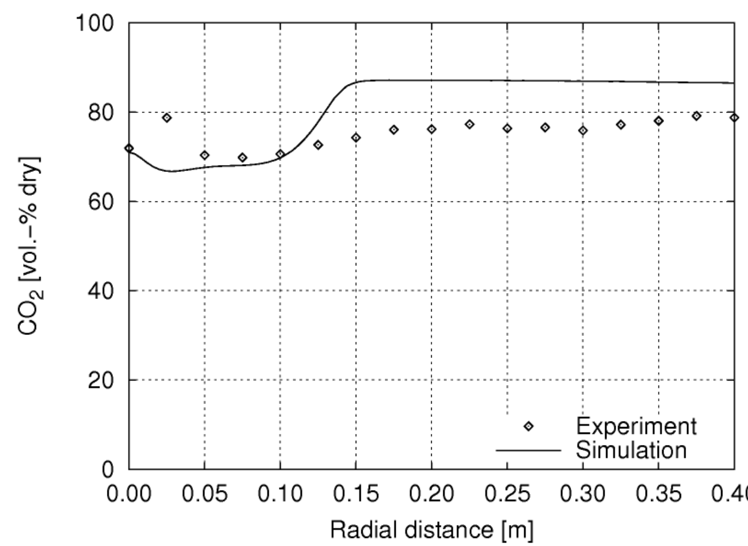
Evaluation

- **Oxy-fuel** test case – comparison
  - **radial** plots at 0.18 m below the burner (level 2)



  - gas temperature:
  - O_2 and CO_2 concentration:





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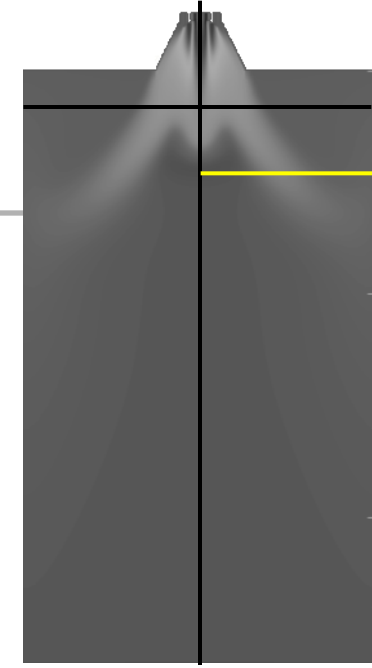
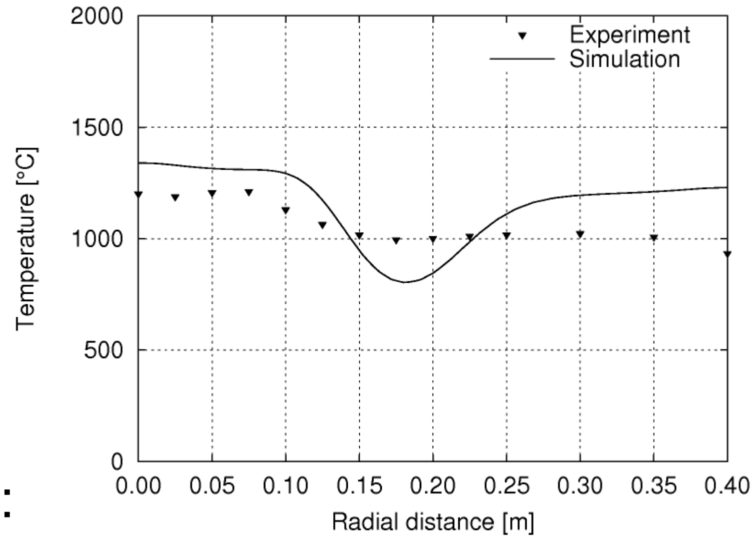
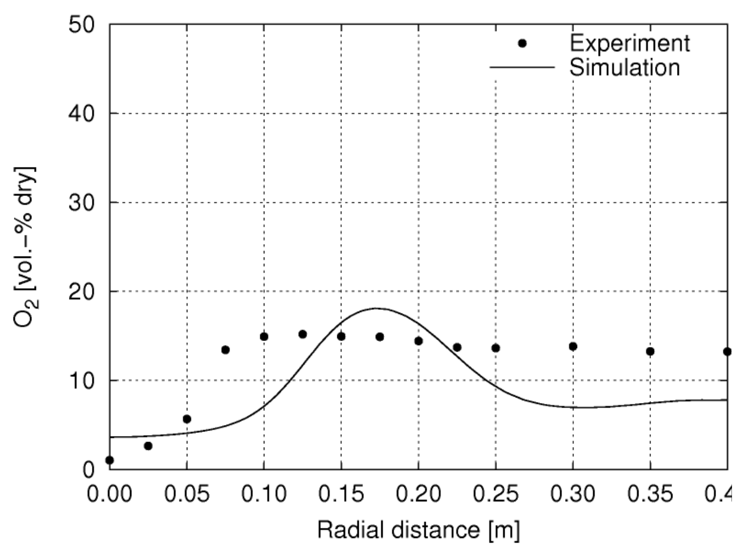
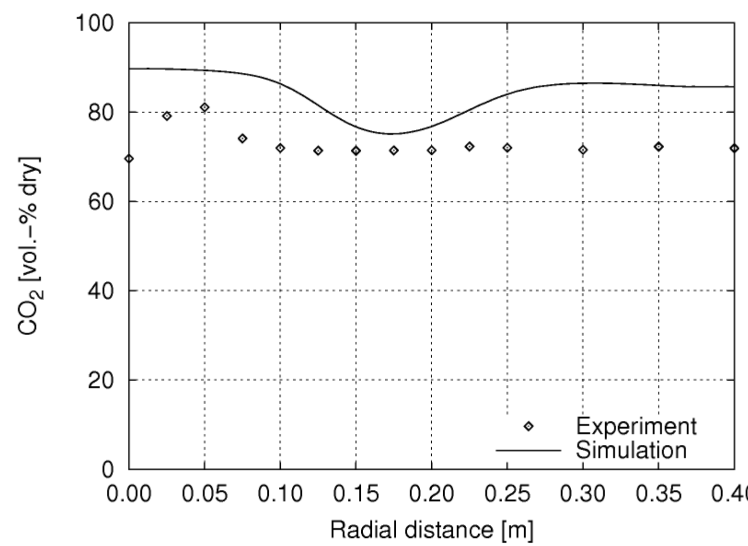


- **Oxy-fuel** test case – comparison
  - **radial** plots at 0.33 m below the burner (level 3)
  - gas temperature:
  - O_2 and CO_2 concentration:







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Conclusions & Outlook

- **Evaluation** of extended chemical reaction models against experiments at IFK's 500 kW_{th} test facility
  - oxy-fuel case
  - air-fired case

- fundamental trends agree in both operation modes

  → improved reaction mechanisms work fine

- deviations are identified in near burner zone
  - simulations predict ignition too late
  - temperature, CO levels too low and delayed O_2 consumption

  → flow field and mixing behaviour of particular burner design ???

Conclusions & Outlook

Next steps:

- extensions regarding emission behaviour at oxy-fuel combustion conditions
  - nitrogen chemistry (NO_x)
  - sulphur chemistry (SO_x)

- further validation against various facilities required
  - 20 kW_{th} once through furnace (IFK)
  - 500 kW_{th} test rig (IFK) operated with staged flame
  - 30 MW_{th} oxy-fuel pilot plant at Schwarze Pumpe

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VATTENFALL

Thank you for your attention!