CFD simulation of biomass combustion plants – new developments

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IEA Bioenergy Task 32 workshop:
CFD aided design and other design tools for industrial biomass combustion plants

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Overview – fields of new CFD model developments

- Modelling of solid biomass combustion
- Gas phase reaction modelling
- Modelling of ash related processes
- Automation of CFD models

Modelling of solid biomass combustion

- State-of-the-art
  - Packed bed combustion models
    - – Empirical models and 1D-models
  - Pulverised wood combustion
    - – Lagrange models, simple kinetics for pyrolysis and char burnout
- **New developments**
  - 2D/3D packed bed combustion models
    - – Euler/ Lagrange/ Hybrid/ DEM models with particle models considering intra-particle gradients and enhanced pyrolysis and char burnout models
  - Modelling of pulverized wood combustion and co-firing
    - – Lagrange/ Hybrid models with particle models considering intra-particle gradients and enhanced pyrolysis and char burnout models
  - Fluidised bed combustion
    - – Modelling of freeboard; simple empirical models for release in the fluidised bed; Euler/ Hybrid multiphase models

Gas phase reaction modelling

- State-of-the-art
  - Simulation of gas phase combustion / CO-burnout –
    - Eddy Dissipation Model and global reaction kinetics
  - Simulation of NO_x formation
    - Postprocessor with global reaction kinetics – although for biomass combustion not applicable
- **New developments**
  - Simulation of gas phase combustion / CO burnout
    - Eddy Dissipation Concept with skeletal / reduced kinetics
  - Simulation of NO_x formation
    - Eddy Dissipation Concept with skeletal / reduced kinetics
  - Extension of gas phase models from high to low-Re flows
  - Models for mixing of gas streaks arising from packed beds
  - Reaction kinetics considering sulphur and chlorine

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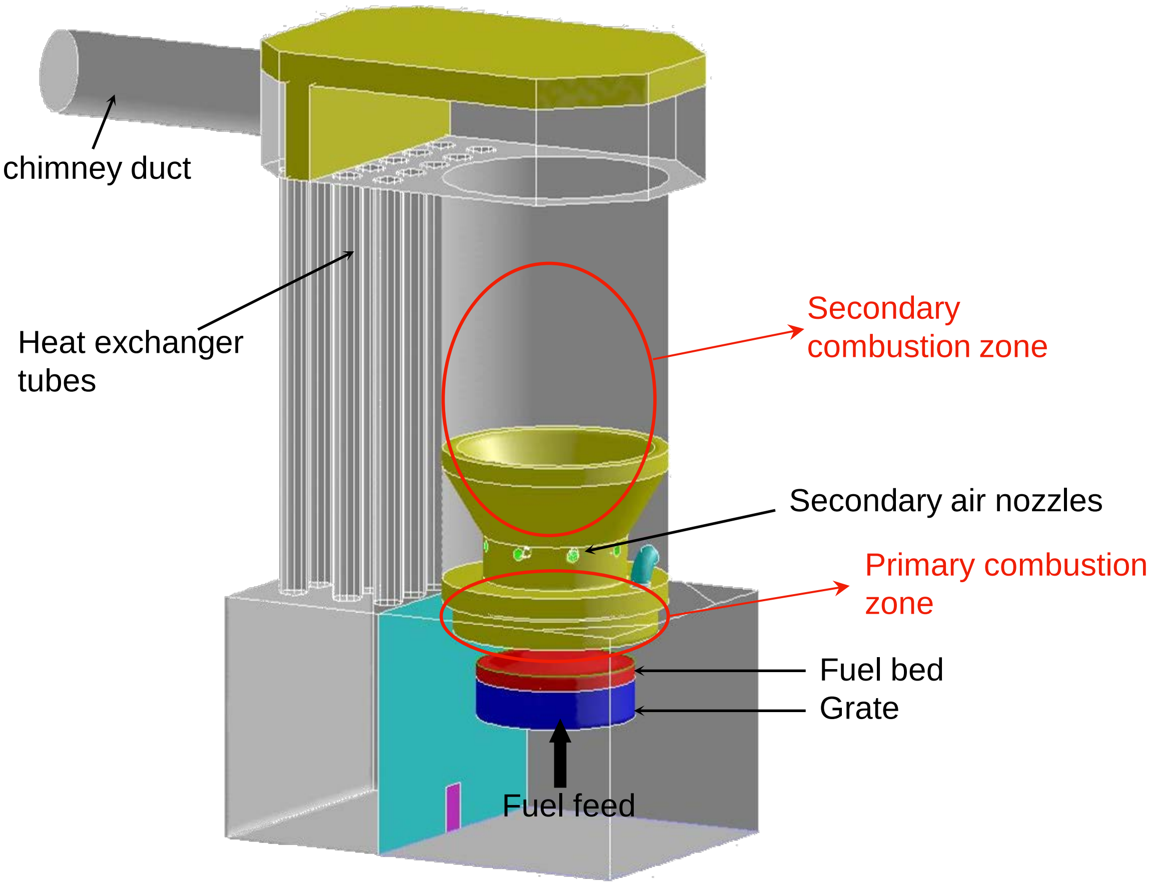
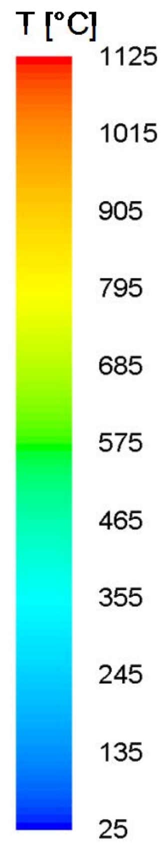
Hybrid gas phase reaction model for laminar to highly turbulent flows - overview

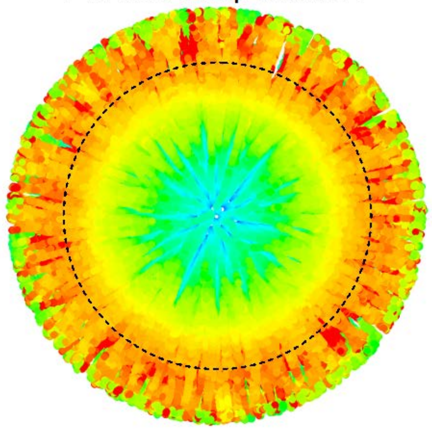
- Reduced reaction kinetics (Kilpinen 97-skeletal)
- ISAT (in-situ adaptive tabulation) algorithm for run-time tabulation of the reaction kinetics (reduction of CPU time)
- Calculation of reaction rate with Finite Rate Kinetics (FRK) and Eddy Dissipation Concept (EDC)
- Evaluation of the flow regime based on the local turbulent Reynolds Number
- Effective reaction rate is calculated with both reaction rates weighted with a weight function W as a function of the turbulent Reynolds Number with a sharp increase from 0 to 1 at Re = 64:
  - $R_{eff} = R_{EDC} * W + R_{FRK} (1-W)$
  - Re >> 64: $R_{eff} = R_{EDC}$
  - Re << 64: $R_{eff} = R_{FRK}$

Hybrid gas phase reactions model for laminar to highly turbulent flows – example: test of the model for a 20 kW underfeed stoker furnace (1)





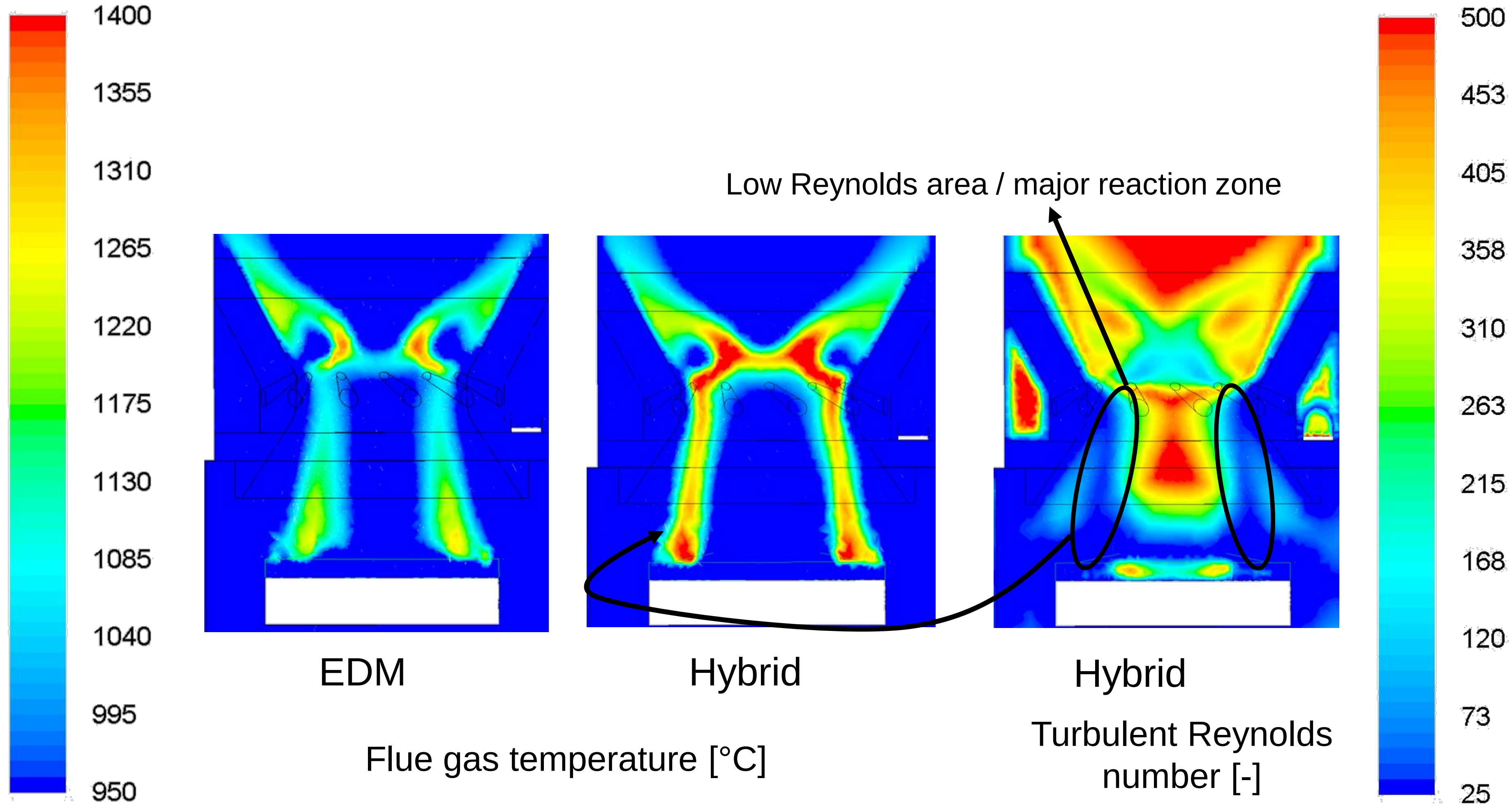
Particle temperatures



Visual observation

<u>Operating data:</u> Biomass fuel: softwood pellets;
Moisture content= 8.1 wt.% (wet base); λ_{total}= 1.58; λ_{prim}= 0. 64, no flue gas recirculation

Hybrid gas phase reactions model for laminar to highly turbulent flows – example: test of the model for a 20 kW underfeed stoker furnace (2)



Iso-surfaces in a vertical cross-section through the furnace (up to the upper edge of the refractory lining)

Modelling of ash related processes

- State-of-the-art
  - Estimation of fly ash deposition, material erosion and precipitation rates
    - Simulation of particle trajectories as well as particle impaction rates at furnace and boilers walls
    - Correlation of the results with flue gas and wall temperatures as well as flue gas velocities

- **New developments – models for grate furnaces and pulverised fuel furnaces**
  - Models for release of ash forming elements
  - Models for condensation of ash vapours on boiler walls
  - Models for deposition of coarse fly ash particles
  - Models of formation and deposition of fine particles
  - Erosion models
  - Models for corrosion (based on empirical correlations; based on detailed modelling of transport and chemical processes in the deposit and corrosion layer)

Fine particle and ash deposit formation model – overview (1)

- Empirical fixed bed release model for major combustion species, ash vapours and coarse fly ash particles from the grate
- CFD simulation of turbulent reactive flow
- Condensation of ash vapors

transport equations of the elements
N, C, H, O, K, Na, S, Cl

→ equilibrium calculation* →

220 gas species
382 solid/liquid phases

ISAT- tabulation

→

ash forming vapours considered
KCl $(KCl)_2$
K_2SO_4; K_2CO_3
NaCl $(NaCl)_2$
Na_2SO_4

* **Formation of sulphates based on kinetic approach** (Christensen):
$SO_2 + 0.5\ O_2 \rightarrow SO_3$

Fine particle and ash deposit formation model – overview (2)

- Fine particle formation and deposition
  - Nucleation due to super-saturation of ash compounds
  - Condensation of ash vapours on the surface of existing aerosol particles
  - Deposition mechanisms: thermophoresis and diffusion (Fick´s law)

- Deposition model of coarse fly ash particles
  - Viscosity approach for silica particles and melting approach for salt particles as well as the condensation layer
- Erosion of deposits by coarse fly ash particles
  - Ductile and brittle erosion
- Modelling of the time-dependent formation of the deposit layer and its influence on heat transfer

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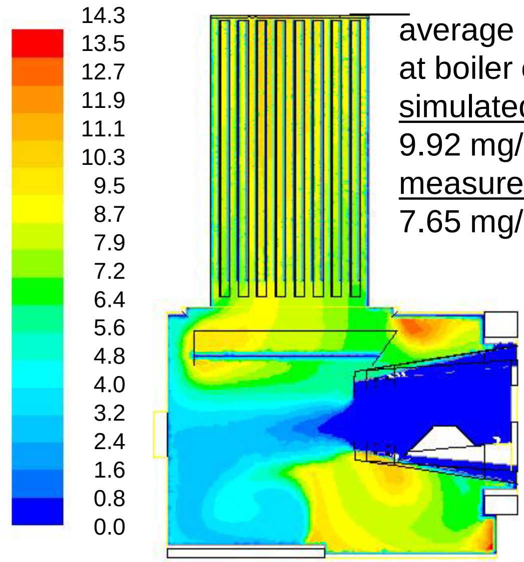
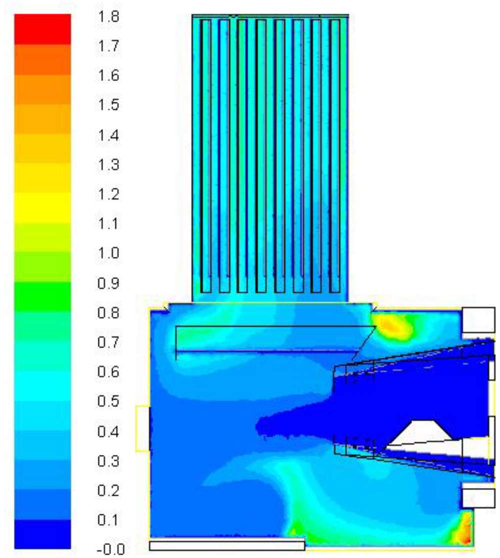
Simulation of fine particle and deposit formation – example: simulation of fine particle formation in a 70 kW pellet boiler

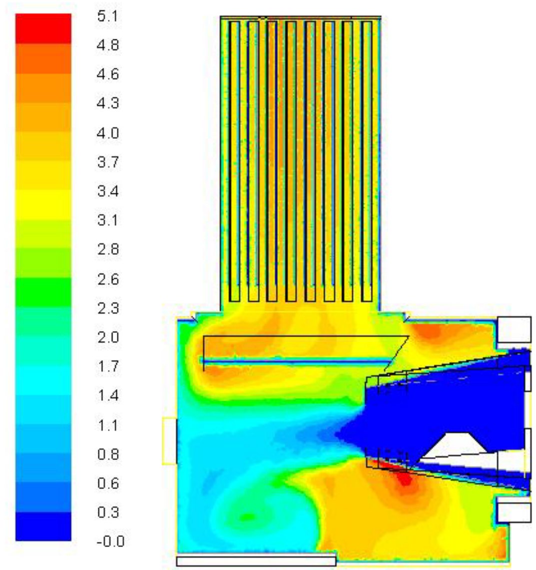


average concentration at boiler outlet:
simulated:
9.92 mg/Nm³
measured:
7.65 mg/Nm³

sum of fine particles formed



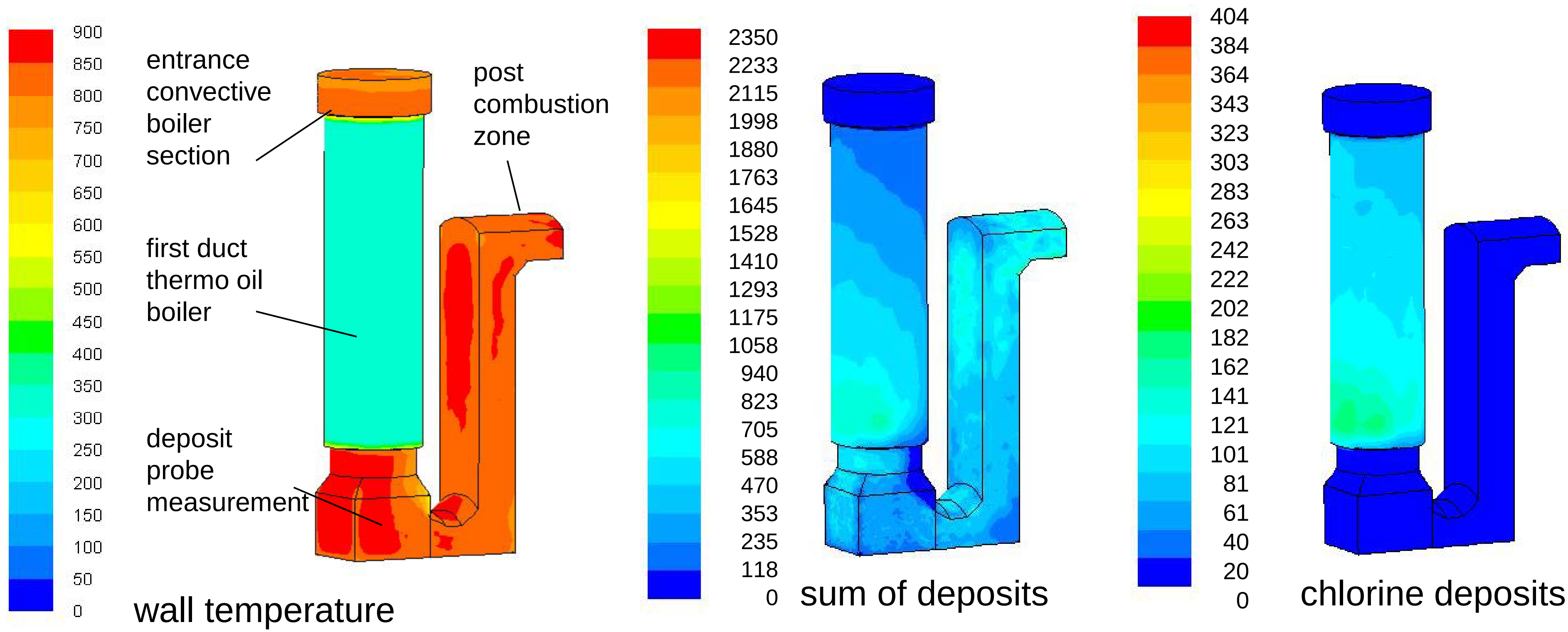
$KCl + (KCl)_2$



K_2SO_4

Simulation results regarding aerosol formation in a 70 kW_{th} fixed-bed pellet boiler: left) total particle concentrations [mg/Nm³]; middle) fine particles formed by nucleation/condensation of KCl [mg/Nm³]; right) fine particles formed by nucleation/condensation of K_2SO_4 [mg/Nm³]

Simulation of fine particle and deposit formation – example: simulation of deposit formation in a 10 MW thermal oil boiler



Wall temperature [°C] (left), **total deposit mass flux** caused by condensation and fine particle precipitation **[mg/m²h]** (middle) and **deposit mass flux of chlorine [mg/m²h]** caused by condensation and fine particle precipitation (right) simulated for the post combustion chamber and the radiative section of a 10 MW_{th} thermal oil boiler; fuel: wood dust and wood chips process & particle engineering TU Graz BIOENERGIESYSTEME GmbH bioenergy2020+

Automation of CFD-simulations

- State-of-the-art
  - Manual performance of furnace development and optimisation
    - – Performance of case studies with manually defined variations

- **New developments**
  - Parameterisation and automation of geometry and mesh definition (e.g. for secondary air nozzles)
  - Automatic performance of case study and data evaluation
  - Link of CFD simulations with optimisation tools

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Thank you for your attention

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