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
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 $Re = 64$:

$$R_{eff} = R_{EDC} \cdot W + R_{FRK} \cdot (1-W)$$

- $Re >> 64$: $R_{eff} = R_{EDC}$
- $Re << 64$: $R_{eff} = R_{FRK}$
Hybrid gas phase reactions model for laminar to highly turbulent flows – example: test of the model for a 20 kW underfeed stoker furnace (1)

Operating data: Biomass fuel: softwood pellets;
Moisture content = 8.1 wt.% (wet base); $\lambda_{\text{total}} = 1.58$; $\lambda_{\text{prim}} = 0.64$, 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)
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

* Formation of sulphates based on kinetic approach (Christensen):

$$\text{SO}_2 + 0.5 \text{O}_2 \rightarrow \text{SO}_3$$
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
Simulation results regarding aerosol formation in a 70 kW\textsubscript{th} fixed-bed pellet boiler: left) total particle concentrations [mg/Nm\textsuperscript{3}]; middle) fine particles formed by nucleation/condensation of KCl [mg/Nm\textsuperscript{3}]; right) fine particles formed by nucleation/condensation of K\textsubscript{2}SO\textsubscript{4} [mg/Nm\textsuperscript{3}]

Simulation of fine particle and deposit formation – example: simulation of fine particle formation in a 70 kW pellet boiler
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 MWth thermal oil boiler; fuel: wood dust and wood chips
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
Thank you for your attention

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