Three-dimensional modelling of circulating fluidized bed processes by a semi-empirical approach

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Introduction

- Circulating fluidized bed (CFB) processes are used for many purposes:
  - Energy production (combustion, gasification, chemical looping combustion).
  - Petrochemical processes (e.g. catalytic cracking).
  - Other chemical and metallurgical processes.
- Trends in energy production CFB processes: increasing unit sizes, new processes, improved efficiencies.
- In CFB processes, the reactions occur in a suspension formed by gas and solids $\rightarrow$ just modelling the fluid dynamics is very difficult.
- Optimal design, development, and operation of CFB processes requires comprehensive modelling tools, which can simulate the whole process:
  - Flow dynamics of gases and solids
  - Reactions
  - Attrition of solid particles
  - Heat transfer
Example CFB process: CFB boiler

1. Primary air
2. Secondary air
3. Fuel, limestone, make-up feed
4. Refractory lined lower furnace
5. Furnace walls – membrane walls
6. Internal heat transfer surfaces
7. Separator (cyclone)
8. Downcomer / return leg
9. External bubbling bed heat exchanger
10. Cross-over duct
11. Backpass with heat exchangers
12. Electrostatic precipitator (ESP)
13. Stack

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Example of process development: oxycombustion

Air-fired

Fuel → CFB boiler → Air

Oxygen-fired

Fuel → CFB boiler → Oxygen

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Example of new processes: Caoling

- Carbon dioxide capture and storage process
- \( \text{CaO} + \text{CO}_2 \leftrightarrow \text{CaCO}_3 \)
- Interconnected dual fluidised beds
- Carbonator as absorber
- Calciner as regenerator

![Diagram of CO2 capture and storage process]

- \( \text{CO}_2 \) depleted flue gas
- \( \text{CO}_2 \) rich gas to compression
- Flue gas from a combustor unit
- Oxygen from ASU and fluidizing gas
- Coal
- \( \text{CaCO}_3 \)
- Purge of ash and sintered solids

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Model approaches

- The modelling approaches of the CFB process can be categorized to:
  - Fundamentals-oriented CFD models (commercial codes, e.g. Fluent, open source codes, e.g. MFIX).
  - Practice-oriented, semi-empirical models ("in-house" models).
- The recent development of the CFD models has been fast and recently published articles present examples of modelling full scale CFB units (e.g. Zhang et al., 2010; Wang et al., 2011).
  - Simulated process times have been in the order of < 60 seconds.
- In a semi-empirical approach, fundamental balance equations (e.g. continuity of mass, energy, and species) are combined with empirical data and empirical correlations (e.g. total bed mass, solid concentration profile). This enables practical calculations, which can support the design of the processes.
- When the model has been validated based on field test measurements, it can be applied to study similar processes and cases with good accuracy.
- The range of applicability is limited by the available validation data → Importance of reliable and detailed measurements!
Semi-empirical models

- The semi-empirical models (or engineering type models) are targeted in modelling the complete process, including the reactions and heat transfer.
- The different semi-empirical models can be categorized based on dimensionality:
  - 0D-models: correlation based models for the total process.
  - 1D-models: reactor divided to vertical sections.
  - 1.5D-models (i.e. core-annulus approach).
  - 3D-models: reactor divided to control volumes in three dimensions.
- The number of feeding points and the mixing of different reactants is limited, which results to a non-homogeneous process, which can be best modelled by 3D-models.
Large furnaces - limited mixing of reactants

Łagisza CFB 460 MWe
Comprehensive 3D-models for CFB

- Despite the clear demand for comprehensive 3D-models, the number of published and actively developed models is very small:
  1) Model by Technical University Hamburg-Harburg
     - First published in 1999 (Knoebig et al., 1999).
     - Recent development: Wischnewski et al. (2010).
  2) Model by Chalmers University of Technology
     - First published in 2008 (Pallarès et al., 2008).
     - Recent development: Palonen et al. (2011).
  3) Model presented in this presentation.
     - Recent development: Myöhänen (2011).
Model frame of CFB3D

- Heat transfer to walls and internal surfaces
- Combustion, gasification & other reactions
- Inlet sources - sec. gas, fuel, limestone, sand
- Fluidization gas
- Flue gas, fly ash
- Gas, solids
- Exchange of gas / solids
- Solid-to-furnace
- Recirculation of flue gas / fly ash
- Fluidization gas

Separator(s) - separation eff.
- Heat transfer
- Reactions

External heat exchangers - heat transfer
- Reactions

Solids

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Concentration field of total solids

- The concentration field of total solids is defined by empirical equations.
- The parameters for vertical distribution are fitted based on measured pressure profiles.
- In horizontal direction, the solid concentration is assumed flat, except for a denser wall layer, which is solved as superimposed over the main furnace model. The volume fraction of solids at wall layer is determined as a function of the local average volume fraction of solids across the cross-section of the furnace.
Solution of velocity fields and mixing

- The net solid velocity field is solved by potential flow approach taking account for the different sources (e.g. circulating mass flow from return legs) and sinks (e.g. sinks due to reactions).
- The net gas flow field is solved by combining a continuity equation and a simplified momentum equation.
- The different mixing processes are modelled by dispersion.
  - E.g. continuity equation for gaseous species:

\[ \int_A w_r \rho_g v_g \cdot dA - \int_A \varepsilon_g \rho_g D_g \nabla w_r \cdot dA = \int_{v'} \phi^{'''}_r dV + \int_{v'} R^{'''}_r dV \]

Convection    Dispersion    Sources    Reactions

Potential field and velocity field of solids

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Particle size fractions and comminution of solids

- Solid materials (combustible fuel, ash, sand, limestone) are divided into six particle size fractions (population balance approach).
- Comminution of solids is simulated by a rate model, in which the mass change is proportional to the mass.
- Agglomeration of particles can be simulated as well, but normally the particle size is decreasing (mechanical wear, temperature shocks and effects of chemical reactions).
Combustion model

Devolatilization

Char combustion

Example modelling results from bottom of a furnace

Char gasification

Gas combustion reactions
- CO + 0.5O₂ → CO₂
- H₂ + 0.5O₂ → H₂O
- CH₄ + 2O₂ → CO₂ + 2H₂O
- C₂H₄ + 3O₂ → 2CO₂ + 2H₂O
- H₂S + 1.5O₂ → H₂O + SO₂

Shift conversion
- CO + H₂O ↔ CO₂ + H₂

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Mixing of fuel

- The mixing of reacting fuel (char, volatiles, moisture) can be simulated by two alternative methods:
  - Target-dispersion model (old method, requires empirical knowledge of the target profile to which the fuel is mixing by dispersion).
  - Convection model (new method, momentum balance solved for fuel).
- The new method is better suited for reactive and elutriative fuels, such as many biofuels.

Illustration of differences in small scale:
Sorbent model for calcitic limestone

Modelled sulphur dioxide profile in oxygen-fired combustion

CaCO₃ → Calcination → CO₂
CaSO₄ → Sulphation → +SO₂+½O₂
CaCO₃ → Carbonation → +CO₂
CaO → Desulphation → SO₂+CO₂
CaO → Direct sulphation → CO₂
CaO → +CO
Validation case: air-fired 235 MWe CFB burning lignite

Uneven fuel feed distribution

Modelled vs. measured profiles

Heat flux  Oxygen  CO

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Calculation example: Compostilla 300 MWe

- A planned circulating fluidized bed boiler for flexible operation with air-fired and oxygen-fired combustion.
- The limestone reactions are different in oxygen-fired conditions due to high partial pressures of CO$_2$ and SO$_2$.
Gasifier study

- Thermal capacity: 50 MWth
- Air-blown, atmospheric gasification
- Fuel: wood based biomass
  - 49.8% volatiles, 9.0% char
  - 40.0% moisture, 1.2% ash
- Sorbent: calcitic limestone
- Geometry approximated by hexahedral control volumes, mesh size 41200 cells
- The 3D modelling can be applied to study the progress of reactions along the furnace height and to support optimal design.
3D-modelling of a pilot calcinator for CaOling

Calcination process:
\[ \text{CaCO}_3 \rightarrow \text{CaO} + \text{CO}_2 \]
Discussion and summary

- The development of the CFB processes requires valid modelling tools, which can be used to optimize the design and operations.
- The application of the currently available CFD models is still limited.
- Only a few comprehensive process models exist, which can model large circulating fluidized bed reactors three-dimensionally.
- The presented model has been successfully applied for studying different CFB processes.
- The development of the model is a continuous process: the different sub-models can be always improved as more knowledge is achieved.
References


