Three-dimensional modelling of steam-oxygen gasification in a circulating fluidized bed

Kari Myöhänen, Lappeenranta University of Technology
Matti Koski
Jouni Ritvanen, Lappeenranta University of Technology
Timo Hyppänen, Lappeenranta University of Technology
Juha Palonen, et al.

Available at: https://works.bepress.com/kari_myohanen/14/
Three-Dimensional Modelling of Steam-Oxygen Gasification in a Circulating Fluidized Bed

Presented by: Kari Myöhänen
Co-authors: M. Koski, J. Ritvanen, T. Hyppänen, J. Palonen, K. Häkkinen, S. Kokki

a Lappeenranta University of Technology
b Oilon Oy
c Foster Wheeler Energia Oy
Introduction

- Gasification = thermal conversion of solid or liquid fuel into a gaseous mixture.
- Gasification reactions occur at high temperature and at restricted amount of oxygen, which prevents complete incineration of combustible matter. This results to a product gas, which contains high amounts of combustible gases: carbon monoxide, hydrogen, methane, and other hydrocarbons.
- The product gas can be utilized for energy production or it can be further converted to liquid fuels.
- In a CFB gasifier, the reactions occur in a circulating fluidized bed.
  - Fuel: solid fuel, e.g. biomass.
  - Gasifier agent: air, steam, oxygen.
- Utilization of gasification technology for energy production is growing rapidly and new concepts are constantly developed.
- The development requires support from reliable and effective modelling tools.
Main reaction paths

Evaporation

Inert

Devolatilization

Char gasification

C + H₂O → CO + H₂
C + CO₂ → 2CO

Char combustion

+O₂

CO, CO₂
H₂O
SO₂
NO, N₂O

Main gas combustion reactions

CO + 0.5O₂ → CO₂
H₂ + 0.5O₂ → H₂O
CH₄ + ½O₂ → CO + 2H₂
C₂H₄ + O₂ → 2CO + 2H₂
CₓHᵧ + ½xO₂ → xCO + ½yxH₂
H₂S + 1.5O₂ → H₂O + SO₂

Shift conversion

CO + H₂O ↔ CO₂ + H₂

Other gasification reactions

CH₄ + H₂O ↔ CO + 3H₂
C₂H₄ + 2H₂O ↔ 2CO + 4H₂
CH₄ + CO₂ ↔ 2CO + 2H₂

In addition:

Limestone reactions
(CaCO₃, CaO, CaSO₄, CaS)

Nitrogen chemistry
(HCN, NH₃, NO, N₂O)

Tar chemistry (complex CₓHᵧ)

Lappeenranta University of Technology
Air-blown vs. steam/oxygen-blown gasification

Air-blown

Fuel → Gasifier

Product gas

Air

Steam/oxygen-blown

Fuel → Gasifier

Product gas

Steam

Oxygen

CO
H2
CxHy
CO2
H2O
N2
Other

Lappeenranta University of Technology
Synthesis gas plant producing bioliquids

[Source: VTT, Technical Research Centre of Finland]
Three-dimensional model for CFB furnaces

Control volume method

- Heat transfer to walls and internal surfaces
- Combustion, gasification & other reactions
- Inlet sources: sec. gas, fuel, limestone, sand
- Fluidization gas

Separators
- Separation eff.
- Heat transfer
- Reactions

Gas, solids
- Exchange of gas / solids
  - Solids
  - Gas
- External heat exchangers
  - Heat transfer
  - Reactions

Solids to furnace

Fluidization gas

Flue gas, fly ash
- Recirculation of flue gas / fly ash
- Bottom ash

Lappeenranta University of Technology
Model capabilities

- Applied to CFB combustion and gasification processes and to calcium looping processes.
- Flow dynamics of gas and solids.
  - Semi-empirical submodels.
- Combustion and gasification of fuel.
  - Drying, devolatilization, char combustion, water-gas and Boudouard reactions.
- Comminution of solids.
- Homogeneous combustion and gasification reactions.
- Heat transfer within bed and to surfaces.
- Sorbent reactions and sulfur capture.
- Post-solver for NO\textsubscript{x} emissions.
- Solid material types:
  - fuel, sand, sorbent (unlimited number of each)
    - combustible fuel = char+volatiles+moisture
    - inert ash handled separately
    - sorbent = CaCO\textsubscript{3}+CaO+CaSO\textsubscript{4}+CaS+inert
- Gas components:
  - O\textsubscript{2}, CO\textsubscript{2}, H\textsubscript{2}O, SO\textsubscript{2}, CO, H\textsubscript{2}, CH\textsubscript{4}, C\textsubscript{2}H\textsubscript{4}, C\textsubscript{g}, H\textsubscript{2}S, NO, N\textsubscript{2}O, HCN, NH\textsubscript{3}, Ar, N\textsubscript{2}
Calculation case: 12 MWth gasifier

NSE Biofuels Oy Ltd.
Demonstration plant
Stora Enso mill, Varkaus, Finland

Reactor modelled three-dimensionally
Mesh size 8800 hexahedral cells

Secondary gases (oxygen, steam, nitrogen)
Fuel (wood based biomass)
Sorbent (calcitic limestone)
Make-up sand

Fluidization gas (oxygen & steam)
Evaporation, devolatilization, char combustion
=> total heat from reactions and temperature profile
Combustion of char vs. gasification reactions

CO from combustion of char

Boudouard reaction

Water-gas reaction

Shift conversion

C + ½O₂ → CO

C + CO₂ → 2CO

C + H₂O → CO + H₂

CO + H₂O ↔ CO₂ + H₂

Lappeenranta University of Technology
Gas concentration profiles

Oxygen

Carbon dioxide

Water vapour

Carbon monoxide

Hydrogen

Lappeenranta University of Technology
Average profiles and comparison to measurements

Moist gas composition (vol-%, wet)

Dry gas composition (vol-%, dry)

O2
CO2
H2O
CO
H2
CH4
N2

Measured
Modelled

*) N2 share high in pilot due to purge systems.
Large scale case: 320 MWth pressurized gasifier
Discussion and summary

- The development of the CFB gasification processes requires valid modelling tools, which can be used to support the design and to optimize operations.
- Modelling of main gasification reactions have been implemented to a semi-empirical three-dimensional model, which has been originally developed for modelling CFB combustors.
- A case of 12 MWth steam/oxygen-blown was modelled and the calculated results were in good agreement with the measurements.
- The validation of the model continues and the model is already used to support development of large scale units.