Hessisches Kompetenzzentrum
für Hochleistungsrechnen

Gasification Processes with Integrated Surplus Electricity Integration for Flexible Power Generation and Production of Synthetic Fuels from Residual Materials (VERENA) II

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Clusters
Lichtenberg II Cluster Darmstadt

Software
ANSYS

Institute
Institut Energiesysteme und Energietechnik

University
Technische Universität Darmstadt

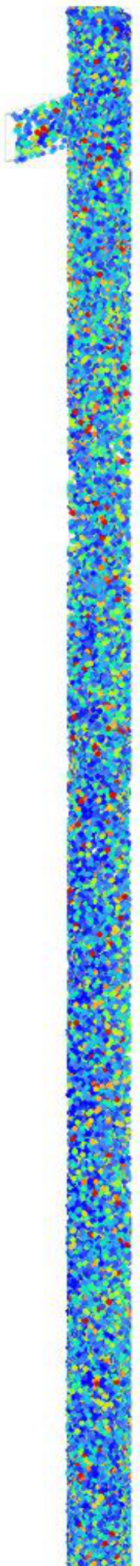

Figure 1: Left: Ilmenite oxidation degree, right: hydrogen gas fraction.

Introduction

Project VERENA aims to open new recycling paths for biogenic and municipal residues through different gasification processes. CFD simulation is used to gain a thorough understanding of the processes inside of the reactor as well as scale-up of the process from lab scale and semi-industrial scale to industrial full scale. Due to the large scale of the processes, simulation can only be conducted on a HPC in a reasonable amount of time.

Methods

The CFD model for the fluidized bed gasification is based on a 4-way coupling Euler-Lagrangian model implemented in ANSYS Fluent. Particle interactions are treated with the discrete element method (DEM). Due to the high solid loading in the fluidized bed a coarse-graining approach is used, which uses larger equivalent particles to represent many small particles thus saving computational time.
The gasification reactions are modelled using a reduced reaction network including the main homogeneous and heterogeneous reactions. Reaction kinetics for the heterogeneous reactions were determined in-house with TGA analysis, while the homogeneous reactions were modelled according to literature. For the HTW model, the reaction network was extended to account for additional reactions caused by elemental oxygen injected into the reactor. The pyrolysis model was extended to account for reaction heat while product composition was implemented according to experimental data.

Results

Simulation of DFBG gasification with waste wood pellets and wheat straw pellets have been performed and validated. A circulating fluidized bed with a core-annulus flow structure was established in the reactor. At the bottom of the reactor a dense bed with high char content formed. In this area the majority of pyrolysis and gasification reactions take place. Due to the fast release of pyrolysis gases a clear influence of the position of the fuel feeding screw can be seen.
In the simulation of the HTW gasifier, a bubbling gasification zone and a post-gasification zone with few particles are formed.

Discussion

For the DFBG simulation, the key hydrodynamic parameters pressure drop and solid circulation were predicted accurately by the model while the solid inventory was somewhat underpredicted. This due to overprediction of the particle drag. To reduce this deviation state of the art EMMS model was used for drag prediction, research on these models is still ongoing and fully accurate results cannot be expected.
Gas species at the outlet as wells as carbon conversion and oxygen carrier oxidation degree were predicted well by the

model. A high sensitivity on the gas composition is caused by the particle pyrolysis which needs to be modelled accurately. Currently, only empirical models offer a sufficient degree of accuracy.

Reactor temperature was somewhat overestimated, most likely due to the assumption of isothermal pyrolysis and inaccurate estimation of heat losses over the reactor walls.

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