

Presentation of the Research-Project 'HotVeGas' and Coupling of ChemApp[®] with OpenFOAM[®]

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ABSTRACT

The scientific and technological aim of the research project HotVeGas (funded by the BMWi; project-number: 0327773B) is the investigation of the behaviour of coal and other heterogeneous feedstocks with their mineral and trace components at high temperatures and pressures under reducing conditions. The resulting data will be integrated into thermodynamic as well as CFD models. This will pave the way for the development of concepts for IGCC power plants with integrated hot gas cleaning and CCS technology.

The investigations are targeted at next generation gasification technologies (time horizon > 2020) and they are necessary in providing the basis for further process engineering developments at the right time.

Because of its inherent complexity, HotVeGas has been designed as a joint research project. It is subdivided into six parts.

In part one experimental investigations of the gasification reactions are undertaken in large-scale test facilities at industrially relevant parameters. The main aim of these experiments is the generation of data for later modelling and simulation. Experimental investigations of the ash and slag behaviour are at the core of part two. Further, the thermo-chemical and thermo-physical properties of ashes and slags and their influence on gasification are scrutinized. The focus of part three is the assembly of a database for the modelling of thermo-chemical and thermo-physical properties of ashes and slags under reducing conditions. Part four is centred on the development of CFD-models for the imaging of flows, reactions, and heat transfer during entrained-flow gasification processes. The goal of the model development is a realistic simulation of the complex interactions between solid-state and gas-phase reactions, flows, and heat transfer. Considerations about ash reactions at high temperatures and during cooling and hot gas cleaning are undertaken in part five. Finally, in part six overall process considerations round out the picture. They will define the boundary conditions for the experimental and theoretical investigations into the high-temperature reactions of gasification and hot-gas cleaning.

Tasks of the IEC

The Department of Energy Process and Chemical Engineering (IEC) is one partner in the joint research project. Its main tasks are the investigation of the influence of high pressures (50 bar) on the pyrolysis of heterogeneous feedstocks and the characterisation of real ashes and slags from several different gasification processes in terms of their chemical and mineral composition (XRF, HT-XRD), ash fusion temperatures (AFT), phase transformation heat (HT-DSC), and rheological properties (HT-viscometer). Most of the programme will be applied to complex artificial ashes and slags to enable insights into several sub-systems.

Coupling of ChemApp and openFOAM

In the course of gasifier modelling the fundamentals of the behaviour of coals and other heterogeneous reactants at high temperatures and pressures as well as strongly reducing conditions are investigated. The results will be used in CFD simulations.

One focus is the development and implementation of adapted models for gas-phase reactions into the simulation. Further, thermo-chemical calculations of the ash and slag reactions of the particles should be integrated.

OpenFOAM® (Open Field Operation and Manipulation) is a public domain software (open source) for CFD calculations. The software contains several utilities that allow pre- and post-processing tasks like data manipulation, visualisation and mesh generation.

The gas-phase reactions and the thermo-chemistry will be derived mainly from two software packages - Cantera and ChemApp®.

Cantera is mainly used for the part of the gas-phase reactions, as it provides data and solutions for the kinetics of the reactions, whereas ChemApp® is well equipped for thermo-chemical calculations especially in the field of multi-phase solution systems (e.g. slags).

The paper will give a general overview concerning the project HotVeGas. Additionally, the coupling of ChemApp® and OpenFOAM® as a special topic will be presented too.