Using SimuSage for the Modelling of Diverse Processes in Energy Conversion

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Abstract

At the conversion of solid feedstock via combustion or gasification, also the mineral content of the feedstock is converted. Problems like slagging, fouling, corrosion and other process issues are linked to the mineral conversion.
Due to a lack of kinetic data, the thermo chemical modelling is a powerful tool to estimate the behaviour of ashes and slag.
At the Institute of Energy Process and Chemical Engineering SimuSage™ is used for modelling the slagging and fouling behaviour in pulverized coal-fired boilers.
Further, a model has been set up to describe the behaviour of alkali metals and their compounds in the British Gas – Lurgi gasification (BGL).
The first approach was done in close cooperation with RWE. A model made of isothermal equilibrium stages describes the different combustion and steam generator zones. The model was adjusted by XRD analysis of process samples (ash/slag deposits) and 7 different coals. To take kinetic inhibitions into account, the coal ash was divided into a reactive and an inert fraction. From the validated model, different classification numbers were developed. In connection with the model, these classification numbers allow the estimation of the slagging and fouling behaviour for different mixtures of the investigated coals.
Another combustion model is currently under development. It describes the co-combustion of hard coal and biomass. First, the stage model described previously is adapted for the currently combustion of different hard coal mixtures. In the second step, the influence of the biomass on slagging or fouling will be estimated. To keep the alkali-charge for the combustion chamber at a low level, the biomass will be pyrolysed and only the gaseous pyrolysis products enter the combustion chamber. The approximate pyrolysis gas composition, especially K-, Na-, S- and Cl- containing species, is determined in laboratory tests and in a 5 MW test facility. After implementing the pyrolysis gas into the model, the slagging and fouling behaviour will be estimated with the help of the previously described characterisation numbers.
Another approach is the description of the behaviour of alkali metals and other volatile ash-components in the BGL-gasification. The BGL-gasification is based on the classical Lurgi - fixed bed gasification. Similar to a blast furnace, a mixture of pelletised municipal solid waste, industrial waste and coal are fed from the top. The gasification agent, a mixture of oxygen and steam, enters the reactor from the bottom. The product gas (H2, CO, CH4) leave the reactor at the top and the slag is tapped at the bottom. Due to the counter current flow and the temperature distribution, volatile ash components evaporate in the lower part end condensate at the upper part. That results in the accumulation of Na-, K-, Pb- and Zn-compounds. The condensing material builds up a deposit at the raw gas outlet, which influences the gasifier performance.
On the base of process samples, the BGL-gasifier was modelled with two isothermal equilibrium stages, where one stage describes the volatilisation and the other the condensation of the volatile ash components. With the help of the model, the accumulation of Na and K can be described. Furthermore it provides information about phase separations in the slag bath and Pb- and Zn accumulation.