Thermochemical calculation of solid fuels with SimuSage

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Solid fuels like hard coal or lignites differ widely in chemical and mineralogical composition. It is mandatory for stable boiler performance to identify critical minerals and chemical compositions in coals or biomasses in advance. To minimize physical measurements and to support this data, thermochemical calculations basing on coal analysis can be used. Here, combustion parameters play an important role and have to be included into the calculation to verify a satisfying correlation between calculation and reality. Within project *VerSi* (*Prediction of Deposit Formation via Thermochemical Modelling and CFD-Modelling – Basic Experiments and Thermochemical Modelling*) GTT-Technologies and Forschunsgzentrum Jülich GmbH (IEK-2) created a thermochemical model using the software *SimuSage*. It is based on the thermochemical database *GTOx* including all main elements in coal, biomass and their ashes. Furthermore, the model is designed to simulate a lignite boiler, but can also be modified to simulate hard coal boilers.

This model uses mass streams which can be variably subdivided into sub-streams. For this, different coal and air streams with variable ratios are used. In total 25 reactors are calculating the mineral compositions including gas and liquid phases at different temperature steps. Also, additional phase splitters include the possibility to separate output streams like liquid and gaseous phases. Depending on hot gas recycling, programmed loops are used to find the equilibrium composition of the affected reactors. In addition, coarse particles can partially or completely be separated from the residual mass stream to consider different kinetic reaction rates.
Five hard coals and five lignites have been calculated and the results have been compared to ash fusion data and X-ray diffraction analysis to verify their reliability. In total, good agreement has been obtained concerning X-ray diffraction data. Moreover, the correlation of the amount of slag phase with ash fusion test results was possible. In addition, it was possible to identify critical amounts of coarse quartz particles.