Coupling Fluid Dynamics and the Concept of Local Equilibrium

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Abstract

The computer aided design of large combustion plants by CFD (= computational fluid dynamics), is meanwhile a approved standard.

By these methods the localy distribtions of:

· Stream-velocity,
· Stream-lines,
· Temperature,
· Species of combustion and
· Retention-Time

are calculated.

For the computation of the combustion-species there are some numerical models (e.g.: the developments with LUAT Essen, LEAT Bochum, Umsicht-Oberhausen und GKS / Cutec-Schweinfurt). However only the majority components (in particular CxHy, CO, CO2, H2O, H2, N2, CO2, if necessary NO2, SO2, HCl) of pyrolysis / gasification / combusiton are computed.

For the corrosion however the minority components like the alkali/alkaline-earth/heavy metals in their various connection forms are of special importance. Almost an infinitely number of compounds can form. In principle this variety leads to three problems:

1. Limited knowledge of „product creation models "
2. Material data availability is lacking
3. Difficulties in validating.

The measurements of [Deuerling, 2005] and [Deuerling, 2006] offer at least a certain validating possibility regarding the minority components in realised plants. This will allow to evaluate product creation models concerning there usefulness. For complex systems the computation of the thermodynamic equilibrium is the most common method for the determination of the products at present. For this on the one hand robust computation programs and on the other hand numerous material data are avaible.

Therefore the results from the coupling of CFD with the equilibrium computation program ChemApp are to be presented and evaluated.

The intention is the evaluation of the comparison of local concentrations of thermodynamically computed minority components with results of radiographic analysis of certain species from a MVA.