Slag Modelling Based on Coal Ash Compositions

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ABSTRACT

At the institute for Energy Systems, methodologies for the project *HotVeGas* (high temperature gasification and flue gas cleaning) are developed to lay an essential foundation for future high efficient processes of gasification for producing and providing synthetic fuels.

Mathematical simulations are performed to describe the processes of the inorganic ash-particles that derive from gasification. Since the heat transfer efficiency of the reactor is reduced by the deposition of these particles and therefore the whole reaction efficiency, it is essential to find models and perform numerical simulations to mimic the particles to get a better understanding of how the reactor geometry should be designed to reach higher efficiencies.

In the gasification process the deposition at the reactor walls melts at high temperatures and flows as a slag driven by gravity. Due to the wall with lower temperatures and since the temperature distribution over the thickness of the deposition is to be assumed as linear, there is a part of the deposition next to the wall that remains solid.

To get better insight into these processes, simulations have to be performed that mimic the behaviour of slag with suitable models and physical parameters like viscosity, density, heat capacity, heat conductivity etc. The physical parameters are based on the coal ash composition and the viscosity is computed with an empirical formula which is valid within a specific range.

Since the slag is only Newtonian with temperatures high enough so it is completely liquid, the model doesn't work with lower temperatures when the slag begins to solidify. Therefore a critical value has to be introduced to delimit Newtonian behaviour that is the critical viscosity temperature, also based on the composition of the coal ash. Below this value another model is used that takes the volume fraction of the solids of the partly crystallized slag into account. FactSage delivers the results of the volume fraction of solids within a specific temperature range and this modifies the viscosity of the slag.

For the simulation method of the slag flow, a relatively new approach has been used, the *Smoothed Particle Hydrodynamics* (SPH). This approach takes place in a Lagrangian frame that discretizes the domain with interpolation points. At these points the slag quantities are computed influenced by their neighbouring particles. In comparison to a Eulerian frame, the free surface of the slag can be computed without effort and another advantage is the possibility to model large deformation and even break ups of the slag.

Based on the deposition location and the deposition rate the slag flow is computed non-steady to deliver the final deposition in the reactor after shut down. With these results the geometry of the reactor can be modified to minimize the negative effects of slagging.