Coupling of Thermodynamic Equilibrium Libraries with a Multidimensional CFD Solver - Application and Potential

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Abstract

When local effects are relevant and convective transport is relevant for processes to be designed, CFD-tools like FLUENT are utilized for simulation. If species transport is important, quite often the kinetic transport processes are not known sufficiently or a partial equilibrium can be assumed. In such situations sophisticated equilibrium solvers like ChemApp can be used to provide local partial equilibrium.

The key for using sophisticated equilibrium solvers like ChemApp within real CFD applications is efficiency, since the partial equilibrium needs to be estimated repeatedly in every grid cell. Using In-Situ Adaptive Tabulation we show that this is possible for biomass fly-ash and flue-gas deposition in the heat exchanger section of a biomass furnace as one example.

In this application the equilibrium between different phases (gaseous, solid and/or liquid) needs to be evaluated within each finite volume cell to predict gas condensation rates and for each particle-wall interaction on the surfaces of the underlying numerical mesh to determine the behaviour of fly-ash particles with a given composition when colliding with a wall. We present a complex example where both processes are coupled within one simulation.