Equations-Of-State Models in ChemApp/ChemSheet, a Fluent-KilnSimu Link and a Metallurgical Process Simulation Tool Based On SimuSage

STEPHAN PETERSEN¹, KARRI PENTTILÄ²

¹GTT-Technologies, Herzogenrath, Germany ²VTT Technical Research Center of Finland, Espoo, Finland

Abstract

Using the concept of "user defined models", support for various types of equations-of-state and activity coefficient models has been added to *ChemApp* and thus also *ChemSheet*, allowing for the utilization of a large variety of thermodynamic data for organic systems (VTT Process Chemistry).

KilnSimu, a program to simulate a variety of production processes involving rotary kilns, has been linked to *Fluent*[®] in order to improve simulation results by taking into account a 3D model of the kiln space (VTT Process Chemistry, Process Flow Ltd Oy).

SimuSage was used to create a recipe-based process model in order to flexibly and dynamically simulate processes that can be described by consisting of a single reactor space which receives its input from multiple feed and recycle streams, thus providing the user with an interactive process model consisting of a user-defined sequence of basic treatment steps (GTT-Technologies).