Use of ChemSheet and KilnSimu for Material and Energy Saving Processes

PERTTI KOUKKARI, RISTO PAJARRE

VTT Process Chemistry, Espoo, Finland

ABSTRACT

The adaptation of the systematic computational approach has created a completely new way to treat multicomponent and multi-phase problems in thermochemistry. The new software and algorithms allow for material and energy saving solutions in several industrial applications and give new openings in applied science.

ChemSheet and KilnSimu have provided a modelling platform for several industrial applications for improving the resource intensity of both high temperature systems and processes at ambient conditions.

Recovery of zinc from electric arc furnace dusts has been modelled by both ChemSheet and Kilnsimu and the modelling has supported the development of awarded Best Available technology for the Waelz Zn-recovery kilns.

A novel ChemSheet application is currently being developed for the selective treatment of acidic mine waters to reduce their environmental impact.

The introduction of immaterial constraints into the thermodynamic multicomponent models has enabled the simulation of a number of new kinds of processes. A recent example of the usage of immaterial constraints in ChemSheet for the simulation of para-equilibria applicable in e.g. solidification problems will be shortly described