Using ChemSheet for Practical Applications
Recent Case Studies

K.Penttilä, VTT, Helsinki

Abstract

ChemSheet, the EXCEL Add-in for thermochemical applications, is introduced showing the user interaction in the various input windows. Conceptual aspects such as the use of EXCEL functions embedded in the thermochemical calculations are highlighted. A series of very divers applications of ChemSheet is demonstrated. These cover:

Deep Impact: Asteriod Collision with Earth
(a simple way to get a first feeling)

Copper Sulfide Flash Smelting

Methane Refomer in an SOFC cell
(exhibiting kinetic inhibitions)

Scheil Solidification of a Binary Alloy

Further Applications of
Computational Thermochemistry Using ChemApp

K.Pentillä, VTT, Helsinki

Abstract

The ChemApp programming library that was used for the generation of the ChemSheet EXCEL add-in has found further application in special thermochemical modelling efforts. One result out of this work is the preparation of a generalised rotary kiln simulator which has been applied in the modelling of a cement kiln. A further case has been the link of ChemApp with the fluid-dynamics code FLUENT in the modelling of the pH neutralisation of an aqueous solution in a stirring tank. Furthermore, a dedicated code for the pulp and paper industry has been realised using the local equilibrium approach in an otherwise flowsheet like environment. The applications mentioned above will be discussed in some detail.