

Fact-Function-Builder & FactOptimal in FactSage 6.3

STEPHAN PETERSEN

GTT-Technologies, Herzogenrath, Germany

ABSTRACT

Fact-Function-Builder is an add-in to the Equilib program that enables the FactSage user to calculate and display user-defined functions after each Equilib calculation.

The functions can contain expressions of thermochemical values calculated by Equilib such as compound, solution, and species activities, amounts, fractions; partial and integral thermodynamic properties; temperature, pressure, volume, etc. which can be combined using common mathematical operators.

The Fact-Function-Builder is also available from within the XML-Editor, thus functions can also be used in plotting results.

While FactSage can in principle be used to screen potential systems, for instance searching for compositions yielding a desired set of properties and a phase constitution under a given set of constraints, performing such searches “manually” for a multi-component alloy would involve thousands of grid-like calculations and would thus be extremely time-consuming.

FactOptimal extends the capability of FactSage in that area by coupling it with a Mesh Adaptive Direct Search method algorithm (MADS) developed at the *École Polytechnique* in Montréal, resulting in the ability to automate complex searches.

An introduction into both tools, as well as examples will be given.