## THERMODYNAMIC MODELLING: FROM THERMODYNAMIC DATABASE TO INDUSTRIAL PROCESS SIMULATION

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Since second half of the 20th century industrial-strength numerical methods of mathematic optimization emerged. Access to these methods led to computer-aided minimization of Gibbs energy, which gave birth to computational thermodynamics, the large part of which were gathered under the umbrella of the scientific field and society named Calculations of Phase Diagrams and Thermochemistry (Calphad).

The Calphad method is based on the basic idea of finding Gibbs energies as parametric regression models which are optimized using experimental and theoretical data with particular emphasis on a comprehensive critical evaluation of the data. This allows obtaining thermodynamic functions which are then used for carrying calculations of practical application use. In other words, thermodynamic modeling creates a bridge between experimental fundamental research and the application of its principles and data to practical problems.

However, in practice, the reactions occurring in real industrial processes are extremely complex. Therefore, the particular skill of materials scientists lies in their ability to decompose complex chemical processes into simpler reactions accessible to traditional thermodynamic analysis. Today, the active integration of computing resources and information technology into production processes makes these issues particularly relevant.

This report is devoted to main features of constructing thermodynamic models in the field of science and technology and differences between models developed by scientists and models in demand in practical calculations.

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