Integrated computational materials engineering, CALPHAD and Hans Leo Lukas

Integrated Computational Materials Engineering (ICME) has become one of the new hot topics in materials science and engineering in recent years, and numerous worldwide conferences and symposia have been dedicated to this topic. The goal of ICME is to enhance and accelerate materials and process development by linking computation and experiment. Although ICME has been practiced, at least in part, on a variety of materials and processes at numerous locations for a number of years, it gained attention as a discipline after the National Research Council of the National Academies of the United States [1] published its recent report. In this report the CALPHAD method is identified as a fundamental ICME tool.

The CALPHAD method was originally developed by Kaufman for calculations of phase equilibria [2] using mathematical models with adjustable parameters to describe the Gibbs energies of the phases in a system. The approach taken by the CALPHAD method has since been extended to modeling of diffusion mobilities, molar volumes and many other phase specific properties. One strength of the CALPHAD method is the efficient treatment of multicomponent systems, providing much needed data for the development of commercial materials which frequently consist of six or more components. Another strength of the CALPHAD method is that it can be readily coupled with mechanical and mesoscale property models and process simulations.

The two key elements of the CALPHAD method are software tools and databases. Today’s state-of-the-art computational thermodynamics would not have been possible without the contributions of Hans Leo Lukas, who retired 15 years ago from the Max-Planck-Institut für Metallforschung in Stuttgart, Germany. In 1977 Lukas published his seminal paper, “Optimization of Phase Diagrams by a Least Squares Method Using Simultaneously Different Types of Data” [3]. This paper had significant impact on how the model parameters of the analytical phase descriptions were obtained by demonstrating that, instead of a trial and error method, a Gaussian least squares method can be used. In addition to publication of the paper, Lukas wrote the programs BINGSS and TERGSS for thermodynamic optimization of the analytical description of binary and ternary systems and the programs PMLFKT and TERFKT for the calculation of phase diagram and thermochemical properties of these systems. Lukas distributed his programs freely and thereby laid the foundation for the development of high quality thermodynamic databases. Later the suite of “Lukas Programs”, as these programs came to be known in the CALPHAD community, was expanded with programs for quaternary systems (QUAGSS and QUAFKT) and a program for general phase equilibria calculations (PMLFKT). Unlike the other programs, PMLFKT [4] could be used on any arbitrary number of components due to the generality of the algorithms employed. The general nature of the program made it straightforward to implement new models and to couple the code with solidification calculations [5], paving the way for implementation of the CALPHAD approach into casting simulation and property modeling software.

Hans Leo Lukas also taught the community how to perform quality thermodynamic optimizations (or thermodynamic assessments) of systems. One important element of a thermodynamic optimization is the proper choice of thermodynamic models. For example, crystal structure and the site occupations should be used to guide the selection of the model and decisions on constraints or potential simplifications in the description of ordered phases. Another important element is the critical evaluation of the experimental data. Lukas always emphasized the importance of using the originally measured data since they are free of accumulated errors, errors in data conversion or errors in interpretation. The other important issue is the critical evaluation of data to determine the appropriate weights to give the data considered in the optimization. For example, if the range of congruent melting temperatures reported for a phase is greater than the experimental errors associated with the individual measurements, a decision must be made regarding which data source to consider. The more reliable data should be given a higher weighting factor in the optimization.

Lukas, together with co-authors Fries and Sundman, summarized guidelines for the optimization of thermodynamic descriptions in a textbook [6].

The CALPHAD community expressed its appreciation for the work of Hans Leo Lukas in 2008 by awarding him the CALPHAD Gibbs Triangle Award. This award is only given every three to five years for outstanding contributions to the development of the thermodynamic background and principles of construction for ternary and higher order phase diagrams, as well as calculation methods and assessment work. Lukas was recognized for his seminal contributions to the CALPHAD community, in particular, thermodynamic software able to incorporate various types of data to ensure consistency of Gibbs energy modeling and the development of thermodynamic descriptions for numerous binary, ternary and higher order systems.

Hans Leo Lukas is still very active. The CALPHAD community continues to use his programs and collaborators worldwide appreciate his contributions and helpful comments to ongoing projects.

Thank you, Leo, for all your good work and a happy 80th birthday!
References


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