Editorial

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Computer coupling of phase diagram data with thermochemistry through use of the Calphad approach is a success story of the past three decades and the approach has continued to become increasingly application relevant. It is satisfying to see that thermodynamic databases are currently used worldwide to solve industrial and commercial problems. This provides a strong motivation for fundamental research in the modeling of multi-component systems. The *Journal of Phase Equilibria and Diffusion* is traditionally a platform for publication of works in this research area.

Assessing metallic or ceramic materials systems by thermodynamic optimization requires experimental key data as input for the software packages. Such experimental data are quite often lacking, especially when sophisticated models for the Gibbs free energy descriptions of solution phases need to be used. In such cases, numerous parameters and coefficients must be adjusted. Usually high quality experimental data are then required to find the best numerical values. Constraints, estimation techniques, and sophisticated assumptions may help to limit the number of coefficients to be determined, but there still remains a crucial need for experimental input data related to these coefficients. However, experimental thermodynamic techniques to provide such data are no longer frequently used. One may even feel like a rather exotic representative of an old school when publishing such data. In fact, the contrary is true and we need to find ways to push for more experimental work like this. Data from fundamental enthalpy measurements (solution calorimetry, drop calorimetry etc.), chemical potential measurements (Knudsen effusion, EMF), and phase diagram investigations are needed more than ever before. Additionally, crystal structures, crystallographic site occupancies, coordination numbers, and stability ranges of the specific system phases have to be taken into account for solution phase modeling.

The measurement of such data continuously requires innovations in experimental methodologies. For example, studying the competition between the polymorphism and surface energies in nanomaterials or the energetic characterization of order-disorder transformations involves exceedingly precise calorimetric data. However, only few research groups are left publishing data from advanced high temperature calorimetry. We must strive to convince our national funding agencies soon to once again support such type of scientific activities.

In developing multi-component phase diagrams for engineering applications, there is also tremendous need for assessment and thermodynamic optimization of more ternary systems. Numerous assessments of literature data for ternary systems were, and still are, presented by V. Raghavan and K.P. Gupta in the *Journal of Phase Equilibria and Diffusion*. Such work is highly appreciated in our community, because missing experimental key data on thermodynamics and phase diagrams can be easily defined by studying their articles. It is one of the major challenges of this field to define such key data which are doubtlessly necessary to be measured, even though some new information can certainly be derived from ab initio approaches. For those who are dealing with the development of databases by thermodynamic optimization, it is obvious that the use of just "guess values" involves numerous risks.

This is true, especially when dealing with commercial customers who may extrapolate to system regions experimentally not determined before, even though the models and data used are not sufficient. For this reason it is good practice to document as much as possible details on any database offered to customers. Encrypted databases should not be delivered; however, this is at present probably an unrealistic hope. Therefore, at least, the lists of thermodynamically optimized systems including the corresponding phases and models with an exhausting literature reference part might be given. Detailed information is also very important on the assessment and optimization procedures and the adapted methods for the development of analytical descriptions of the Gibbs free energies. Additionally, the used, and not used, input data for the optimization procedure could be documented. The challenge arises then in how to motivate commercial database suppliers to follow such customer demands. Certainly, the ever increasing competition will support the claims. Suppliers who provide clear and open database documentation will have commercial advantages over others. Additionally, an independent and international users group could be established to grade accessible databases. This certainly could support the introduction of quality standards for thermodynamic databases.

Impressive databases are available nowadays for steels, light alloys, nuclear materials, slags, ceramics, cemented carbides, Ni-base alloys etc. The ideal scenario would be the introduction of internationally accepted quality standards for such commercially offered thermodynamic databases. The quality of datasets can be given, e.g., in terms of agreement between calculated and available experimental results (phase diagram, thermodynamic properties) with regard to the binary systems or to ternary and multi-component systems.

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