

Challenges in the development of large thermodynamic databases

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The power of the 'so-called' CalPhaD technique undoubtedly lies in the ability it provides to enable extremely complex calculations to be performed on chemical systems containing, in principle, any number of components. Because the data involved in making these complex calculations is based upon 'the real world' through careful experimental observation, the user performing these calculations can have a high degree of confidence in the results. In order to be able to perform these calculations, the user (and the software employed) needs access to large self-consistent databases of assessed thermodynamic data (Gibbs energy expressions). The construction of large thermodynamic databases is a non-trivial task and can be fraught with problems. The purpose of this presentation to explain how large databases are constructed, tested and to point out some of the many pitfalls that can occur during the construction process.