

GTOX – A multipurpose oxide⁺ database

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The GTOX database has been developed over the last 9 years in very close cooperation with IEK-2 of Forschungszentrum Jülich. The database is under constant development and covers thus far twelve oxide components as well as contributions for CaF₂ and the five component sulphide subsystem CaS-MgS-MnS-FeS-CrS. The assessments of the various Gibbs-energy functions are based on experimental information on thermodynamic properties, such as enthalpies of formation or transformation or component activities, but mainly on phase diagram information from the literature.

As a source of rapid information on the contents of the database a Slag Atlas has been generated showing all calculated phase diagrams together with the available experimental data. The Slag Atlas is available on request.

For the multitude of solid solutions covered by the database in general multi-sublattice models have been applied taking into account crystallographic information where available. The liquid has been modelled with the non-ideal associate solution model which permits to treat information on the internal structure of and the strong attractive interactions in the liquid by way of formation of associate species. On the other hand, repulsive interactions which occur mainly in SiO₂-rich oxide melts can also be handled by way of composition dependent interaction parameters using Redlich-Kister-polynomials.

The presentation will highlight the very wide ranges of applicability of the database by showing examples from cement making, coal combustion and gasification, stainless steel thermochemistry, dephosphorisation of steels, sulphidic and oxidic precipitations in steels, fluidity improvements by adding CaF₂, as well as special applications based on the GTOX database for cases of vitrification of nuclear wastes or use of oxide systems in the applications of solar power for the generation of fertilisers.

Possible extensions of the database are for ashes and slags of bio-masses by the inclusion of sulphate constituents or the introduction of Cu both with respect to the oxides and the sulphides for the generation of a Cu-metallurgical database.