TCAQ3: TCS Aqueous Solution Database

TCAQ3 is a database suitable for calculating thermodynamic properties of complex aqueous solutions. The database is used in applications such as materials corrosion processes, hydro-metallurgy, aqueous chemistry and geochemistry and environmental chemistry.

Database name:	**TCS Aqueous Solution Database**
Database acronym:	**TCAQ**
Database owner:	**Thermo-Calc Software AB**
Database version:	**3.1**

Included Elements (75)

Ag	Al	Ar	As	Au	B	Ba	Be	Br	C
Ca	Cd	Ce	Cl	Co	Cr	Cs	Cu	Dy	Er
Eu	F	Fe	Ga	Gd	H	He	Hg	Ho	I
In	K	Kr	La	Li	Lu	Mg	Mn	Mo	N
Na	Nd	Ne	Ni	O	Os	P	Pb	Pd	Pr
Pt	Ra	Rb	Re	Ru	S	Sb	Sc	Se	Si
Sm	Sn	Sr	Tb	Te	Th	Tl	Tm	U	W
V	Xe	Y	Yb	Zn					

Included Phases

The database contains an AQUEOUS solution phase which consists of various free cations and anions, inorganic and organic complexes. The hypothetical phase, REFERENCE_ELECTRODE, is introduced to calculate the electric potential (based on the standard hydrogen electrode) and other properties of the electron in the interaction system. Connected with this database, the non-ideality of the EOS and thermodynamic properties of H2O is calculated, using an empirical expression of the simplified HGK model. The non-ideality of the AQUEOUS solution phase in this database is described using the extended SIT model, i.e., taking into account of the Debye-Hückel Limiting Law term, as well the binary, ternary and higher-order interaction terms.

This database is compatible with PURE, SSUB, SSOL, TCFE, TCNI, TCAL, TCMG, TCCU, TCOX, TTNi/Ti/Al/Mg, and GCE databases. To make heterogeneous equilibrium calculations in complex systems involving aqueous solutions, some phases from other appropriate databases, such as gaseous mixtures and stoichiometric solids from SSUB, and solid solutions from SSOL or TCFE, should be appended.

The TCAQ3 database can be used in the POURBAIX module in Console Mode if the multiple database option is chosen with appended gas and solid phases from other available databases (e.g., SSUB and SSOL).

Assessed Systems

TCAQ3 contains evaluated thermodynamic data for a large amount of different species (approximately 350) in the AQUEOUS solution phase.

Limits

TCAQ3 can be applied to low PTX conditions (up to 100 bar, 350ºC and 3 molality). However, if investigated heterogeneous interaction processes occur at high PTX (up to 5 kbar, 1000 ºC, and 6 molality of equivalent NaCl at room PT conditions and higher concentrations at higher PT), the other aqueous solution database (i.e., AQS2) is required, which implies the complete revised HKF (Helgeson-Kirkham-Flowers) model.

As in the spirit of the CALPHAD method, predictions can be made for multicomponent systems by extrapolation into multicomponent space of data critically evaluated and assessed based on binary, ternary and in some cases higher order systems. However, critical calculations must always be verified by equilibrium experimental data; it is the user's responsibility to verify the calculations but Thermo-Calc Software AB is interested to know about any significant deviations in order to improve any future release.

Scientific Bibliography

See the Thermo-Calc Software scientific bibliography on our website.