
TCES1: TCS Sintering/Incineration/Combustion Database

Database name: TCS Sintering/Incineration/Combustion Database *Database acronym:* TCES

Database owner: Thermo-Calc Software AB *Database version:* 1.1

TCES1 is a database for various solid phases and gaseous species with a general application of metals processing. It is used for environmental controls in steel and alloy production and metallurgical engineering, and environmentally-friendly treatments of industrial waste and nuclear waste.

Included Elements

Al As Br C Ca Cd Cl Cr Cu F Fe H Hg I K Mg Mn
N Na Ni O P Pb S Sb Si Sn Te Ti Zn

Included Phases

Many types of multicomponent stoichiometric and solution phases are available in the database, such as: gas (gaseous mixture containing about 400 species) and many stoichiometric solids (e.g. metals; carbides, nitrides, silicides, phosphides, borides and other inter-metallic/non-metallic compounds; oxides, hydroxides, silicates, sulfides, sulfates, nitrates, nitrites, phosphates, phosphites, carbonates, borates, halides, etc.). Total amount of different phases is 369.

Assessed Systems

All phases have been critically assessed and treated by some appropriate thermodynamic models (e.g. the Sublattice Model for solid solutions and liquid mixture phases, the Ideal Gas Model for gas mixture phase, the Inden Model for magnetic contributions, etc.), which are applicable over a wide temperature-pressure-composition range.

Validation

The database allows calculations of, for example,

- the effect of variation of ore compositions, sintering temperature, water cooling of the sinter strand at different location, etc., on the concentrations of gaseous species produced along the strand.
- the condensed species formed from the gas phase on cooling and their formation temperatures.

The information provided by the calculations allows process parameters to be adjusted to minimize or eliminate emission of hazardous species and to select suitable filtering operations to maximize removal of both desirable and undesirable species condensing from the gas phase formed during the sintering process.

The database also allows calculations that regard the composition of gas phase forming during incineration and combustion processes, and their respective amounts and temperatures of condensation of species formed on cooling the gas.

Limits

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 Models and References

See the Thermo-Calc Software reference list and reference library at:

<https://www.thermocalc.com/support/resources/>