

Thermo-Calc Software

**Thermodynamic and Mobility Databases Overview
2019**

Thermodynamic and Mobility Databases

Thermo-Calc Software offers a wide spectrum of high-quality thermodynamic and mobility databases for use with Thermo-Calc, the add-on Diffusion module (DICTRA) and/or Precipitation module (TC-PRISMA), as well as SDKs for various applications. The databases supplied by Thermo-Calc Software have all been produced by critical assessments and evaluations based on experimental data.

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Steels and Fe Alloys

TCFE9: TCS Steels/Fe-alloys Database

Description:	The <i>TCS Steels/Fe-alloys Database</i> (TCFE9) is a thermodynamic database for different kinds of steels and Fe-based alloys, such as stainless steels, high-speed steels, tool steels, high-strength low alloy (HSLA) steels, cast irons, corrosion-resistant high strength steels, low-density steels, and also cemented carbides. It also includes molar volume data (with no pressure dependence except for pure iron) for several phases. It can be used to calculate density and lattice parameters (for cubic structures), coefficients of thermal expansion and/or relative length change.
Elements (28):	Ar, Al, B, C, Ca, Ce, Co, Cr, Cu, Fe, H, Mg, Mn, Mo, N, Nb, Ni, O, P, S, Si, Ta, Ti, V, W, Y, Zn, Zr Argon (Ar) and hydrogen (H) are modelled to take part in the GAS phase only and no modelling of solubility in the solid solution phases or liquid is considered.
Assessed phases and systems:	<ul style="list-style-type: none"> ✓ 390 phases ✓ 255 binary systems ✓ 255 ternary systems
Database compatibility:	<i>TCS Steels/Fe-alloys Mobility Database</i> (MOBFE4)
Additional information:	Also see the Extended Information document on our website.

MOBFE4: TCS Steels/Fe-alloys Mobility Database

Description:	The <i>TCS Steels/Fe-alloys Mobility Database</i> (MOBFE4) is a kinetic database containing mobility data limited to Fe-based alloys. Data is present in a format suitable for simulation of diffusion-controlled phenomena. Its primary application is for alloy design and the optimisation of manufacturing processes through simulation of different diffusion-controlled phenomena, such as microsegregation during solidification, homogenisation, kinetics of phase transformations, precipitate growth/dissolution kinetics, carburization, nitriding and much more.
Elements (26):	Al, B, C, Ca, Ce, Co, Cr, Cu, Fe, Mg, Mn, Mo, N, Nb, Ni, O, P, S, Si, Ta, Ti, W, V, Y, Zn, Zr
Assessed phases and systems:	<ul style="list-style-type: none"> ✓ 6 phases ✓ 38 binary systems ✓ 13 ternary systems ✓ 2 higher order systems
Database compatibility:	<i>TCS Steels/Fe-alloys Database</i> (TCFE9)

Nickel-based Alloys

TCNI9: TCS Ni-based Superalloys Database

Description:	The <i>TCS Ni-based Superalloys Database</i> (TCNI9) contains all the important Ni-based superalloy phases within a 28-element framework plus Ar and H for the GAS phase only. The ordered and disordered bcc (A2 and B2) and fcc (A1/ γ and L12/ γ') are modelled with a two sublattice model using a single Gibbs energy curve.
Elements (28 + 2):	Al, Ar, B, C, Ca, Co, Cr, Cu, Fe, H, Hf, Mg, Mn, Mo, N, Nb, Ni, O, Pd, Pt, Re, Ru, S, Si, Ta, Ti, V, W, Y, Zr Argon (Ar) and hydrogen (H) are modelled to take part in the GAS phase only.
Assessed systems and phases:	<ul style="list-style-type: none"> ✓ 680 phases ✓ 350 binary systems ✓ 308 ternary systems
Database compatibility:	<i>TCS Ni-alloys Mobility Database</i> (MOBNI5)
Additional information:	Also see the Extended Information document on our website.

MOBNI5: TCS Ni-alloys Mobility Database

Description:	The <i>TCS Ni-alloys Mobility Database</i> (MOBNI5) is a kinetic database containing mobility data for Ni-based alloys in a format suitable for simulation of diffusion-controlled phenomena. Used together with the add-on modules and a thermodynamic database for Ni-based alloys (e.g. TCNI9), the database can be used to study several phenomena of interest to Ni-based superalloys design and manufacturing, such as microsegregation during solidification, homogenisation kinetics, precipitate growth/dissolution kinetics and interdiffusion in Ni-based superalloy coating/substrate compounds.
Elements (28):	Al, B, C, Ca, Co, Cr, Cu, Fe, Hf, Mg, Mn, Mo, N, Nb, Ni, O, Pd, Pt, Re, Ru, S, Si, Ta, Ti, V, W, Y, Zr
Assessed phases and systems:	<ul style="list-style-type: none"> ✓ 6 phases ✓ 45 binary systems (38 FCC_A1, 1 FCC_L12, 6 BCC_B2) ✓ 41 ternary systems (13 FCC_A1, 16 FCC_L12, 11 BCC_B2, 1 LIQUID) ✓ 1 higher order system (FCC_A1)
Database compatibility:	<i>TCS Ni-based Superalloys Database</i> (TCNI9), <i>TCS High Entropy Alloy Database</i> (TCHEA3)

Aluminium-based Alloys

TCAL6: TCS Aluminium-based Alloys Database

Description:	The <i>TCS Aluminium-based Alloys Database</i> (TCAL6) contains nearly all the stable phases and the most important metastable phases (or precipitates) in the assessed systems within a 36-element framework. It can be employed to a wide range of compositions from pure Al to complex commercial aluminium alloys.
Elements (36):	Ag, Al, B, Be, Bi, C, Ca, Cd, Ce, Co, Cr, Cu, Er, Fe, Ga, Ge, H, Hf, In, K, La, Li, Mg, Mn, Mo, Na, Ni, Pb, Sc, Si, Sn, Sr, Ti, V, Zn, Zr
Assessed phases and systems:	<ul style="list-style-type: none"> ✓ Nearly 600 solution and intermetallic phases ✓ 260 binary systems ✓ 88 ternary systems ✓ 12 quaternary systems
Database compatibility:	<i>TCS Aluminium alloys Mobility Database</i> (MOBAL5)
Additional information:	Also see the Extended Information document on our website.

MOBAL5: TCS Al-alloys Mobility Database

Description:	The <i>TCS Aluminium-alloys Mobility Database</i> (MOBAL5) is a kinetic database containing mobility data for Al-based alloys and can be used to study several different phenomena of interest to aluminium alloys. In combination with the Diffusion module (DICTRA), it can be utilized, for example, to study microsegregation during solidification, homogenisation kinetics, growth/dissolution kinetics of precipitates, and interdiffusion in Al-compounds. Combined with the Precipitation module (TC-PRISMA) it can be used to simulate concurrent nucleation, growth and coarsening of precipitates in Al alloys.
Elements (36):	Ag, Al, B, Be, Bi, C, Ca, Cd, Ce, Co, Cr, Cu, Er, Fe, Ga, Ge, H, Hf, In, K, La, Li, Mg, Mn, Mo, Na, Ni, Pb, Sc, Si, Sn, Sr, Ti, V, Zn, Zr
Assessed phases and systems:	<ul style="list-style-type: none"> ✓ 3 phases ✓ 38 binary systems ✓ 20 ternary systems ✓ 2 quaternary systems
Database compatibility:	<i>TCS Aluminium-based Alloys Database</i> (TCAL6), <i>SGTE Solutions Database</i> (SSOL6), COST thermodynamic database

Magnesium-based Alloys

TCMG5: TCS Magnesium-based Alloys Database

Description:	The <i>TCS Magnesium-based Alloys Database</i> (TCMG5) contains all the important Mg-based alloy phases within a 31-element framework. It can be used for a wide range of compositions from pure Mg to complex commercial magnesium alloys.
Elements (31):	Ag, Al, Ca, Ce, Cu, Dy, Er, Fe, Ga, Gd, Ho, In, K, La, Li, Mg, Mn, Na, Nd, Ni, Pr, Sb, Sc, Si, Sm, Sn, Sr, Th, Y, Zn, Zr
Assessed phases and systems:	<ul style="list-style-type: none"> ✓ All the stable solution phases and intermetallic compounds that exist in each assessed system are included ✓ 195 binary systems ✓ 91 ternary systems ✓ 5 quaternary systems
Database compatibility:	<i>TCS Magnesium-alloys Mobility Database</i> (MOBMG1)
Additional information:	Also see the Extended Information document on our website.

MOBMG1: TCS Mg-alloys Mobility Database

Description:	The <i>TCS Magnesium-alloys Mobility Database</i> (MOBMG1) is a CALPHAD-type kinetic database containing atomic mobility data for Mg-based alloys. Coupled with a compatible thermodynamic database, MOBMG1 can be used to calculate various diffusivities in both solid and liquid solution phases, and most importantly to simulate diffusion-controlled phenomena such as solidification, nucleation, growth / dissolution and coarsening of precipitates in Mg-based alloys.
Elements (24):	Ag, Al, Ca, Ce, Cu, Fe, Gd, K, La, Li, Mg, Mn, Na, Nd, Ni, Pr, Sc, Si, Sn, Sr, Th, Y, Zn, Zr
Assessed phases:	<ul style="list-style-type: none"> ✓ 2 phases
Database compatibility:	<i>TCS Magnesium-based Alloys Database</i> (TCMG5)
Additional information:	All data sets are critically assessed against experimental information whenever available. Experimental diffusion data is limited for Mg-based alloys so the use of ab-initio calculations and sound empirical rules are considered extensively in the development of this kinetic database.

Copper-based Alloys

TCCU2: TCS Copper-based Alloys Database

Description:	The <i>TCS Copper-based Alloys Database</i> (TCCU2) contains most of the important Cu-based alloy phases within a 29-element framework. It can be used for a wide range of compositions from pure Cu to complex commercial copper alloys.
Elements (29):	Ag, Al, Au, As, B, Be, Bi, C, Ca, Cd, Co, Cr, Cu, Fe, Mg, Mn, Mo, Nb, Ni, O, P, Pb, Pt, Se, Si, Sn, Ti, Zn, Zr
Assessed phases and systems:	<ul style="list-style-type: none"> ✓ 234 solutions phases and intermetallic compounds ✓ 123 binary systems ✓ 48 ternary systems.
Database compatibility:	<i>TCS Copper Alloys Mobility Database</i> (MOBCU2)
Additional information:	Also see the Extended Information document on our website.

MOBCU2: TCS Copper Alloys Mobility Database

Description:	The <i>TCS Copper Alloys Mobility Database</i> (MOBCU2) is a kinetic database containing mobility data for Cu-based alloys. When combined with the Diffusion module (DICTRA), it is used to study diffusion-controlled phenomena in copper alloys, e.g. microsegregation during solidification, homogenisation kinetics, growth/dissolution kinetics of precipitates, interdiffusion, and so forth. You can also use it with the Precipitation module (TC-PRISMA) to simulate concurrent nucleation, growth, and coarsening of precipitates in Cu-based alloys.
Elements (29):	Ag, Al, As, Au, B, Be, Bi, C, Ca, Cd, Co, Cr, Cu, Fe, Mg, Mn, Mo, Nb, Ni, O, P, Pb, Pt, Se, Si, Sn, Ti, Zn, Zr
Assessed phases and systems:	<ul style="list-style-type: none"> ✓ 2 phases ✓ 49 binary systems (37 in FCC_A1 and 12 in LIQUID) ✓ 26 ternary systems (FCC_A1) ✓ 1 quaternary system (FCC_A1)
Database compatibility:	<i>TCS Copper-based Alloys Database</i> (TCCU2)

Titanium-based Alloys

TCTI2: TCS Ti/TiAl-based Alloys Database

Description:	The <i>TCS Ti/TiAl-based Alloys Thermodynamic Database</i> (TCTI2) contains.
Elements (27):	Ag, Al, B, C, Co, Cr, Fe, H, Hf, Mn, Mo, N, Nb Ni, O, Pd, Pt, Re, Ru, Si, Sn, Ta, Ti, V, W, Y, Zr
Assessed phases and systems:	<ul style="list-style-type: none"> ✓ 470 solution and intermetallic phases ✓ 269 binary systems ✓ 95 ternary systems
Database compatibility:	<i>TCS Ti-alloys Mobility Database</i> (MOBTI3)
Additional information:	Also see the Extended Information document on our website.

MOBTI3: TCS Ti-alloys Mobility Database

Description:	The <i>TCS Ti-alloys Mobility Database</i> (MOBTI3) is a kinetic database containing mobility data for Ti-based alloys. The database can be used to study several diffusion-controlled phenomena in Ti/TiAl based alloys, such as microsegregation during solidification, homogenisation kinetics, growth/dissolution kinetics of precipitates, and much more by using the add-on Diffusion module (DICTRA). In a similar way, MOBTI3 is suitable for simulating concurrent nucleation, growth, and coarsening of precipitates in Ti/TiAl-alloys by using the Precipitation module (TC-PRISMA).
Elements (27):	Ag, Al, B, C, Co, Cr, Fe, H, Hf, Mn, Mo, N, Nb Ni, O, Pd, Pt, Re, Ru, Si, Sn, Ta, Ti, V, W, Y, Zr
Assessed phases and systems:	<ul style="list-style-type: none"> ✓ 4 phases ✓ 29 binary systems ✓ 11 ternary systems
Database compatibility:	<i>Thermo-Calc Ti/TiAl-based Alloys Thermodynamic Database</i> (TCTI2)

High Entropy Alloys

TCHEA3: TCS High Entropy Alloys Database

Description:	The <i>TCS High Entropy Alloys Database</i> (version TCHEA3) is a thermodynamic database for high entropy alloys (HEA) and is developed within a 26-element framework. A hybrid approach of combining experiments, first-principles calculations and CALPHAD modelling is used to obtain reliable thermodynamic descriptions of the BCC, FCC and HCP solutions. That enables predictions to be made for multi-component alloy systems, especially for HEAs.
Elements (26):	Al, B, C, Co, Cr, Cu, Fe, Hf, Ir, Mn, Mo, N, Nb, Ni, Re, Rh, Ru, Si, Sn, Ta, Ti, V, W, Y, Zn, Zr
Assessed phases and systems:	<ul style="list-style-type: none"> ✓ 449 solution phases and intermetallic compounds ✓ 294 binary systems ✓ 137 ternary systems ✓ 308 tentatively assessed ternary systems
Database compatibility:	<i>TCS High-entropy Alloy Mobility Database</i> (MOBHEA1)
Additional information:	Also see the Extended Information document on our website.

MOBHEA1: TCS High Entropy Alloy Mobility Database

Description:	The <i>TCS High Entropy Alloy Mobility Database</i> (MOBHEA1) is a kinetic database containing atomic mobility data for high-entropy alloys (HEA). A systematic validation has been conducted for this mobility database and it was found that a majority of experimental diffusion couple composition profiles could be satisfactorily simulated with the Diffusion module (DICTRA) in Thermo-Calc by using MOBHEA1 and TCHEA3.
Elements (22):	Al, B, C, Co, Cr, Cu, Fe, Hf, Mn, Mo, N, Nb, Ni, Re, Ru, Si, Ta, Ti, V, W, Y, Zr
Assessed phases and systems:	<ul style="list-style-type: none"> ✓ 5 phases ✓ The MOBHEA1 database is based on MOBNI4, and all relevant binary and ternary descriptions from MOBNI4 have been adopted. More importantly, the MOBHEA1 database includes newly assessed atomic mobility data for the FCC_A1 phase in the HEA systems containing Al, Co, Cr, Cu, Fe, Mn, and Ni.
Database compatibility:	<i>Thermo-Calc High Entropy Alloys Database</i> (TCHEA3)

Noble Metal-based Alloys

TCNOBL1: TCS Noble Metal Alloys Database

Description:	The <i>TCS Noble Metal-based Alloy Database</i> (TCNOBL1) is a thermodynamic database that is primarily for gold, silver, platinum, palladium, and their alloys. It is used for jewellery, decoration industries and dental alloys, as well as delicate components for scientific equipment, such as thermal couples and calorimetry elements.
Elements (21):	Ag, Al, Au, Co, Cr, Cu, Fe, Ga, Ge, In, Ir, Mn, Ni, Pd, Pt, Re, Rh, Ru, Sn, Ti, and Zn.
Assessed phases and systems:	<ul style="list-style-type: none"> ✓ 321 solution phases and intermetallic compounds ✓ 204 binary systems ✓ 61 ternary systems
Additional information:	Also see the Extended Information document on our website.

Solder Alloys

TCSLD3: TCS Solder Alloy Solutions Database

Description:	The <i>TCS Solder Alloy Solutions Database</i> (TCSLD3) is for thermodynamic calculations of Sn-/Au-/Bi-/Zn-based solder systems (Pb-containing/Pb-free).
Elements (21):	Ag, Al, Au, Bi, Ca, Cd, Co, Cu, Ga, Ge, In, Mg, Mn, Ni, Pb, Pd, Pt, Sb, Si, Sn, Zn
Assessed phases and systems:	<ul style="list-style-type: none"> ✓ 271 solution phases and intermetallic compounds ✓ 139 binary systems ✓ 72 ternary systems
Database compatibility:	<i>TCS Solder Alloy Solutions Mobility Database</i> (MOBSLD1)
Additional information:	Also see the Extended Information document on our website.

MOBSLD1: TCS Solder Alloy Solutions Mobility Database

Description:	The <i>TCS Solder Alloy Solutions Mobility Database</i> (MOBSLD1) is a kinetic database containing mobility data for solder alloys.
Elements (21):	Ag, Al, Au, Bi, Ca, Cd, Co, Cu, Ga, Ge, In, Mg, Mn, Ni, Pb, Pd, Pt, Sb, Si, Sn, Zn
Assessed phases and systems:	<ul style="list-style-type: none"> ✓ 9 phases ✓ 49 binary systems (17 for LIQUID, 31 for FCC_A1, 1 for DIAMOND_A4) ✓ 22 ternary systems (6 for LIQUID, 16 for FCC_A1) ✓ 2 quaternary systems (FCC_A1)
Database compatibility:	<i>TCS Solder Alloy Solutions Thermodynamic Database</i> (TCSLD3)

Silicon-based Alloys

TCSI1: TCS Silicon-based Alloys Database

Description:	The <i>TCS Silicon-based Alloys Database</i> (TCSI1) focuses on the impurity solubility in silicon with diamond structure within a 34-element framework. This database is used in applications involving solar grade silicon materials.
Elements (34):	Ag, Al, As, Au, B, Bi, C, Ca, Co, Cr, Cu, Fe, Ga, Ge, In, Li, Mg, Mn, Mo, N, Na, Ni, O, P, S, Sb, Si, Sn, Te, Ti, V, W, Zn, Zr
Assessed phases and systems:	<ul style="list-style-type: none"> ✓ 84 phases ✓ In addition to the diamond phase, at least the liquid and the corresponding stable silicide phase with highest Si content are included in each Si-containing binary.
Database compatibility:	<i>TCS Silicon-alloys Mobility Database</i> (MOBSI1)
Additional information:	Also see the Extended Information document on our website.

MOBSI1: TCS Si-alloys Mobility Database

Description:	The <i>TCS Silicon-alloys Mobility Database</i> (MOBSI1) is a kinetic database developed for calculating self and impurity diffusivities in both solid and liquid Si. Data for all elements, except Cr in liquid silicon, are provided. Due to the difficulty in measuring diffusivity in melt, most of mobility data in liquid silicon are estimated by using empirical rules, which are found reliable for practical applications.
Elements (28):	Ag, Al, As, Au, B, Bi, C, Co, Cr, Cu, Fe, Ga, Ge, In, Li, Mn, N, Ni, O, P, S, Sb, Si, Sn, Te, Ti, V, Zn
Assessed phases:	✓ 2 phases
Database compatibility:	<i>TCS Silicon-based Alloys Thermodynamic Database</i> (TCSI1)
Additional information:	Also see the Extended Information document on our website.

Oxides and Slag Databases

TCOX8: TCS Metal Oxide Solutions Database

Description:	The <i>TCS Metal Oxide Solutions Database</i> (TCOX8) contains critically assessed data for many multicomponent oxides, fluorides and sulfides. The intended application is for solid and liquid ionized materials, such as the development of ceramics, metallurgical processing and materials corrosion, thermal barrier coatings (TBC) and Yttria-Stabilised-Zirconia (YSZ).
Elements (24):	Al, Ar, C, Ca, Co, Cr, Cu, F, Fe, Gd, La, Mg, Mn, Mo, Nb, Ni, O, P, S, Si, V, W, Y, Zr
Assessed phases and systems:	<ul style="list-style-type: none"> ✓ 352 phases ✓ 241 binary systems ✓ 218 ternary systems ✓ 88 pseudo-ternary oxide systems ✓ 28 oxy-fluoride and oxy-sulfide systems
Additional information:	Also see the Extended Information document on our website.

SLAG4: TCS Fe-containing Slag Database

Description:	The <i>TCS Fe-containing Slag Database</i> (SLAG4) is for liquid slag phase, Fe-rich liquid phase (dilute solution), pure FeO liquid phase, a large gaseous mixture phase, and many stoichiometric solids and solid solution phases (e.g., oxides, silicates, sulfides, phosphates, halites and so forth).
Elements (30):	Ag, Al, Ar, B, C, Ca, Co, Cr, Cu, F, Fe, H, Mg, Mn, Mo, N, Na, Nb, Ni, O, P, Pb, S, Si, Sn, Ti, U, W, V, Zr
Assessed phases:	✓ 115 phases
Additional information:	Also see the Extended Information document on our website.

Molten Salts

SALT1: SGTE Molten Salts Database

Description:	The <i>SGTE Molten Salts Database</i> (SALT1) is a database for molten salts and is used in applications such as hot salt corrosion of alloys, high energy lamp design and more.
Owner:	Scientific Group Thermodata Europe (SGTE)
Elements (17):	Br, C, Ca, Cl, Cr, Cs, F, H, I, K, Li, Mg, Na, O, Rb, S, Zn
Assessed phases and systems:	<ul style="list-style-type: none"> ✓ 31 phases ✓ 83 binary systems

General Alloys and Substances

SSOL6: SGTE Solutions Database

Description:	The <i>SGTE Solutions Database</i> (SSOL6) is an important thermochemical database for many non-ideal multicomponent solution phases.
Owner:	Scientific Group Thermodata Europe (SGTE)
Elements (79):	Ag, Al, Am, As, Au, B, Ba, Be, Bi, C, Ca, Cd, Ce, Co, Cr, Cs, Cu, Dy, Er, Eu, Fe, Ga, Gd, Ge, H, Hf, Hg, Ho, In, Ir, K, La, Li, Lu, Mg, Mn, Mo, N, Na, Nb, Nd, Ni, Np, O, Os, P, Pa, Pb, Pd, Pr, Pt, Pu, Rb, Re, Rh, Ru, S, Sb, Sc, Se, Si, Sm, Sn, Sr, Ta, Tb, Tc, Te, Th, Ti, Tl, Tm, U, V, W, Y, Yb, Zn, Zr
Assessed phases and systems:	<ul style="list-style-type: none"> ✓ 1331 solution phases and intermetallic compounds ✓ 575 binary systems ✓ 133 ternary systems ✓ 20 quaternary systems
Additional information:	Also see the Extended Information document on our website.

SSUB6: SGTE Substances Database

Description:	The <i>SGTE Substances Database</i> (SSUB6.0) is a large thermochemical database used for alloy and process design and engineering in various applications such as with inorganic materials, gas phase chemistry and solid-melts-aqueous interactions.
Owner:	Scientific Group Thermodata Europe (SGTE)
Elements (99 + 2):	Ac, Ag, Al, Am, Ar, As, At, Au, B, Ba, Be, Bi, Br, C, Ca, Cd, Ce, Cf, Cl, Cm, Co, Cr, Cs, Cu, Dy, Er, Es, Eu, F, Fe, Fm, Fr, Ga, Gd, Ge, He, Hf, Hg, Ho, I, In, Ir, K, Kr, La, Li, Lu, Mg, Mn, Mo, N, Na, Nb, Nd, Ne, Ni, Np, O, Os, P, Pa, Pb, Pd, Pm, Po, Pr, Pt, Pu, Ra, Rb, Re, Rh, Rn, Ru, S, Sb, Sc, Se, Si, Sm, Sn, Sr, Ta, Tb, Tc, Te, Th, Ti, Tl, Tm, U, V, W, Xe, Y, Yb, Zn, Zr, plus 2 hydrogen isotopes (D, T)
Assessed phases and systems:	✓ 5746 substances (3188 condensed stoichiometric compound phases and 2558 gaseous species)

MOB2: TCS Alloys Mobility Database

Description:	The <i>TCS Alloys Mobility Database</i> (MOB2) is a kinetic database containing mobility data primarily but not limited to Fe-based alloys. Data is present in a format suitable for simulation of diffusion-controlled phenomena. Its primary application is for alloy design and the optimization of manufacturing processes, through simulation of different diffusion-controlled phenomena, such as e.g. microsegregation during solidification, homogenisation, kinetics of phase transformations, precipitate growth/dissolution kinetics, carburization, nitriding and much more.
Elements (75):	Ag, Al, Am, As, Au, B, Ba, Be, Bi, C, Ca, Cd, Co, Cr, Cs, Cu, Dy, Er, Fe, Ga, Gd, Ge, Hf, Hg, Ho, In, Ir, K, La, Li, Lu, Mg, Mn, Mo, N, Na, Nb, Nd, Ni, Np, Os, P, Pa, Pb, Pd, Pr, Pt, Pu, Rb, Re, Rh, Ru, S, Sb, Sc, Se, Si, Sm, Sn, Sr, Ta, Tb, Tc, Te, Th, Ti, Tl, Tm, U, V, W, Y, Yb, Zn, Zr
Assessed phases and systems:	<ul style="list-style-type: none"> ✓ 6 phases ✓ 20 binary systems ✓ 4 ternary systems ✓ 2 higher order systems
Database compatibility:	<i>SGTE Solutions Thermodynamic Database</i> version 6 (SSOL6), <i>TCS Steel and Fe-Alloys Thermodynamic Database</i> version 5 (TCFE5) and earlier

Specific Materials

TCCC1: TCS Cemented Carbides Database

Description:	The <i>TCS Cemented Carbides Database</i> (TCCC1) is used for design and processing of cemented carbides.
Elements (13):	C, Co, Cr, Fe, Mo, N, Nb, Ni, Ta, Ti, V, W, Zr
Assessed phases and systems:	<ul style="list-style-type: none"> ✓ 35 phases ✓ Covers the complete and critical assessments of many important binary and ternary systems, as well as some critical higher order systems within the 13-element framework.

SEMC2: TCS Semiconductor Database

Description:	The <i>TCS Semiconductor Database</i> (SEMC2) is for semiconductor engineering and electronic components processing and utility.
Elements (10):	Al, As, C, Ga, H, In, P, Pb, Sb, Sn
Assessed phases and systems:	<ul style="list-style-type: none"> ✓ 18 phases ✓ 15 binary systems ✓ 18 ternary systems ✓ 135 gas species

TCSC1: TCS Superconductor Database

Description:	The <i>TCS Superconductor Database</i> (TCSC1) is for superconducting materials as well as for other oxide calculations.
Elements (6):	Ag, Bi, Ca, Cu, O, Sr
Assessed phases and systems:	<ul style="list-style-type: none"> ✓ 43 phases ✓ 10 binary systems ✓ 8 ternary systems ✓ 6 quaternary systems ✓ 2 higher order oxide-containing systems (Bi-Sr-Ca-Cu-O and Ag-Bi-Sr-Ca-Cu-O) are also assessed

TCFC1: TCS Solid Oxide Fuel Cell Database

Description:	The <i>TCS Solid Oxide Fuel Cell Database</i> (TCFC1) is for solid oxide fuel cell (SOFC) materials and for other oxide calculations.
Elements (6):	La, Mn, O, Sr, Y, Zr
Assessed phases and systems:	<ul style="list-style-type: none"> ✓ 42 phases ✓ 9 binary systems ✓ 9 ternary systems ✓ 5 higher order systems

Metallurgical & Materials Processing & Environmental Applications

TCMP2: TCS Materials Processing Database

Description:	The <i>TCS Materials Processing Database</i> (TCMP2) is for liquid slag, metallic liquid, various solid phases and gaseous species. It has applications in materials processing and environmental controls in steel/alloy production and metallurgical engineering, recycling / re-melting / re-processing treatments of industrial, chemical and nuclear wastes, as well as sintering, incineration and combustion processes.
Elements (35):	Ag, Al, Ar, B, Bi, C, Ca, Cd, Cl, Co, Cr, Cu, F, Fe, H, K, Mg, Mn, Mo, N, Na, Nb, Ni, O, P, Pb, S, Sb, Si, Sn, Ti, U, W, V, Zn
Assessed phases and systems:	All 734 phases are critically assessed and treated by some appropriate thermodynamic models (e.g. the Sublattice Model for solid solutions and liquid mixture phases, the Kapoor-Frohberg-Gaye Cell Model for slag phase, 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.

TCES1: TCS Sintering/Incineration/Combustion Database

Description:	The <i>TCS Sintering/Incineration/Combustion Database</i> (TCES1) is a database for solid phases and gaseous species. It has applications in environmental controls in steel and alloy production and metallurgical engineering, and treatment of industrial waste and nuclear waste.
Elements (30):	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
Assessed phases and systems:	All 369 phases are 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.

Aqueous Solutions

TCAQ3: TCS Aqueous Solution Database

Description:	The <i>TCS Aqueous Solution Database</i> (TCAQ3) is a database suitable for calculating thermodynamic properties of complex aqueous solution phases. It has applications in materials corrosion processes, hydro-metallurgy, aqueous chemistry, geochemistry and environmental chemistry.
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
Assessed phases and systems:	Contains an AQUEOUS solution phase consisting of various free cations and anions, and inorganic and organic complexes and the thermodynamic data is evaluated for approximately 350 species. The hypothetical phase, REFERENCE_ELECTRODE, is used to calculate the electric potential (based on the standard hydrogen electrode) and other properties of the electron in the interaction system.

AQS2: TCS Aqueous Solution Database

Description:	The <i>TCS Aqueous Solution Database</i> (AQS2) is suitable for calculating thermodynamic properties of complex aqueous solution phases. It has applications in materials corrosion processes; hydro-metallurgy, aqueous chemistry, geochemistry and environmental chemistry.
Elements (82):	Ag, Al, Ar, As, Au, B, Ba, Be, Bi, Br, C, Ca, Cd, Ce, Cl, Co, Cr, Cs, Cu, Dy, Er, Eu, F, Fe, Fr, Ga, Gd, H, He, Hf, Hg, Ho, I, In, K, Kr, La, Li, Lu, Mg, Mn, Mo, N, Na, Nb, Nd, Ne, Ni, O, P, Pb, Pd, Pm, Pr, Pt, Ra, Rb, Re, Rh, Rn, Ru, S, Sb, Sc, Se, Si, Sm, Sn, Sr, Tb, Tc, Th, Tl, Tm, U, W, V, Xe, Y, Yb, Zn, Zr
Assessed phases and systems:	Contains an AQUEOUS solution phase consisting of various free cations and anions, and inorganic and organic complexes and the thermodynamic data is evaluated for approximately 1600 species. The hypothetical phase, REFERENCE_ELECTRODE, is used to calculate the electric potential (based on the standard hydrogen electrode) and other properties of the electron in the interaction system.

Nuclear Materials

MEPH15: IRSN Mephista Nuclear Fuels Database

Description:	The <i>IRSN Mephista-15_1 Nuclear Fuels Database</i> (MEPH15) contains critically-assessed and internally-consistent thermodynamic data for the entire field from metal to oxide domains within a 14-element framework plus Ar and H for the GAS phase and for hydrides and hydrous oxides/silicates.
Owner:	ISRN
Elements (14 + 2):	Ba, C, Ce, Cs, Fe, La, Mo, O, Pu, Ru, Si, Sr, U, Zr (+Ar and H for the gaseous phase and for hydrides and hydrous oxides/silicates)
Assessed phases and systems:	<ul style="list-style-type: none"> ✓ 439 phases (46 condensed solution phases, 236 condensed stoichiometric phases, and 157 gaseous mixture phases) ✓ 91 binary systems ✓ 16 ternary systems ✓ 43 pseudo-binary systems ✓ 2 pseudo-ternary systems
Additional information:	Also see the Extended Information document on our website.

NUCL15: IRSN NUCLEA Nuclear Alloys-Oxides Database

Description:	The <i>IRSN NUCLEA-15_4 Nuclear Alloys-Oxides Database</i> (NUCL15) contains critically-assessed and internally-consistent thermodynamic data for the entire field from metal to oxide domains within an 18-element framework plus Ar and H for the GAS phase and for hydrides and hydrous oxides/silicates. It is useful for metal to oxide domains and is used to calculate the thermochemical equilibrium state at any step of a severe accident and to use the results of the thermodynamic approach for improving the predictions of thermo-hydraulic or other accidents codes.
Owner:	ISRN
Elements (18 + 2):	Ag, Al, B, Ba, C, Ca, Cr, Fe, In, La, Mg, Ni, O, Ru, Si, Sr, U, Zr (+Ar and H for the gaseous phase and for hydrides and hydrous oxides/silicates)
Assessed phases and systems:	<ul style="list-style-type: none"> ✓ 773 phases (59 condensed solution phases, 507 condensed stoichiometric phases, and 207 gaseous mixture phases) ✓ 153 binary systems ✓ 22 ternary systems ✓ 105 pseudo-binary systems ✓ 27 pseudo-ternary systems
Additional information:	Also see the Extended Information document on our website.

NUMT2: TCS Pure Radionuclides Database

Description:	The <i>TCS Pure Radionuclides Database</i> (NUMT2) is for about 600 condensed and gas phase substances, including pure radio nuclides. This database can be applied to a wide range of nuclear-related applications, which can be modelled adequately, or to a first approximation, using pure substances.
Elements (44):	Ag, Al, Am, B, Ba, Bi, C, Ca, Cd, Ce, Cl, Co, Cr, Cs, Eu, F, Fe, H, I, In, Kr, La, Mg, Mn, Mo, Na, Nb, Nd, Ni, O, Pd, Pr, Pu, Rh, Ru, Sb, Si, Sn, Sr, Tc, Te, U, Xe, Zr
Assessed phases and systems:	<ul style="list-style-type: none"> ✓ 248 phases ✓ Contains critically-assessed thermodynamic data for pure substances, which are of relevance to calculations for various nuclear applications. ✓ It contains pure radionuclides in the following 15-element framework: Ba, Ce, Cs, I, La, Mo, Pd, Pr, Pu, Rh, Ru, Sr, Te, U and Zr.

NUOX4: TCS Nuclear Oxides Database

Description:	The <i>TCS Nuclear Oxides Database</i> (NUOX4) is for nuclear oxide solution systems, gas excluded. It is primarily for studying molten core-concrete interactions although it can also be applied to any relevant system or application which comprises the constituent oxides.
Elements (11):	Al, Ba, Ca, Ce, La, Mg, O, Si, Sr, U, Zr
Assessed phases and systems:	<ul style="list-style-type: none"> ✓ 88 phases ✓ Contains data for a collection of assessed binary and ternary systems relevant to nuclear applications, although it excludes the gas phase data. ✓ Full description of the system $UO_{2+x}-ZrO_2-SiO_2-CaO-Al_2O_3-MgO-BaO-SrO-La_2O_3-CeO_2-Ce_2O_3$ where all the component binary interactions are assessed.

Minerals

GCE2: TCS Geochemical/Environmental Database

Description:	The <i>TCS Geochemical/Environmental Database</i> (GCE2) is for about 600 minerals with applications in the fields of geochemistry, geophysics, hydro-metallurgy, aqueous chemistry and environmental chemistry.
Elements (46):	Ag, Al, Ar, As, Au, B, Ba, Be, Br, C, Ca, Cd, Cl, Co, Cr, Cs, Cu, F, Fe, Ga, Gd, H, Hg, I, K, Li, Mg, Mn, Mo, N, Na, Ni, O, P, Pb, Rb, S, Se, Si, Sn, Sr, Ti, U, W, V, Zn
Assessed phases and systems:	It contains critically assessed temperature-, pressure- and composition-dependent data for minerals (silicates, oxides, hydroxides, halides, carbonates, sulfides, sulfates, nitrates, phosphates, etc.).

Thermotech Ltd. Thermodynamic Databases

TTAL8: Thermotech Al-based Alloys Database

Description:	The <i>Thermotech Al-based Alloys Database</i> (TTAL8) is a comprehensive database for Al-alloys that can be used for all major types of commercial Al-alloys ranging from commercial pure Al to complex alloys.
Owner:	Thermotech Ltd.
Elements (25):	Al, B, Bi, C, Ca, Co, Cr, Cu, Fe, H, La, Li, Mg, Mn, Mo, Ni, Pb, Sc, Si, Sn, Sr, Ti, V, Zn, Zr
Database compatibility:	<i>TCS Al-alloys Mobility Database</i> (MOBAL1)

TTNI8: Thermotech Ni-based Superalloys Database

Description:	The <i>Thermotech Ni-based Superalloys Database</i> (TTNI8) is for commercial Ni-based superalloys, high Fe-containing and single crystal Ni-based superalloys.
Owner:	Thermotech Ltd.
Elements (23):	Al, B, C, Co, Cr, Cu, Fe, Hf, Mn, Mo, N, Nb, Ni, O, Pt, Re, Ru, Si, Ta, Ti, W, V, Zr
Database compatibility:	<i>TCS Ni-alloys Mobility Database</i> (MOBNI1)

TTMG5: Thermotech Mg-based Alloys Database

Description:	The <i>Thermotech Mg-based Alloys Database</i> (TTMG5) is a comprehensive database for Mg-alloys that can be used for all major types of commercial Mg-alloys ranging from pure Mg to complex commercial alloys.
Owner:	Thermotech Ltd.
Elements (17):	Al, Ca, Ce, Cu, Fe, Gd, La, Mg, Mn, Nd, Sc, Si, Sn, Sr, Y, Zn, Zr

TTTI3: Thermotech Ti-based Alloys Database

Description:	The <i>Thermotech Ti-based Alloys Database</i> (TTTI3) is for Ti-alloys that can be used for all major types of commercial Ti-alloys ranging from commercial pure Ti to complex alloys.
Owner:	Thermotech Ltd.
Elements (21):	Al, B, C, Cr, Cu, Fe, H, Mn, Mo, N, Nb, Ni, O, Re, Ru, Si, Sn, Ta, Ti, V, Zr
Database compatibility:	<i>TCS Ti-alloys Mobility Database</i> (MOBT1)

TTTIAL1: Thermotech TiAl-based Alloys Database

Description:	The <i>Thermotech TiAl-based Alloys Database</i> (TTTIAL1) is for the prediction of stable and metastable phase equilibria in multicomponent γ -TiAl based alloys.
Owner:	Thermotech Ltd.
Elements (13):	Al, B, Cr, Mn, Mo, Nb, O, Si, Ta, Ti, W, V, Zr

TTZR1: Thermotech Zr-based Alloys Database

Description:	The <i>Thermotech Zr-based Alloys Database</i> (TTZR1) is for Zr-alloys that can be used for major types of commercial Zr-alloys.
Owner:	Thermotech Ltd.
Elements (12):	C, Cr, Fe, H, Hf, N, Nb, Ni, O, Si, Sn, Zr

Mobility Databases for Thermotech Ltd. Databases

MOBAL1: TCS Al-alloys Mobility Database

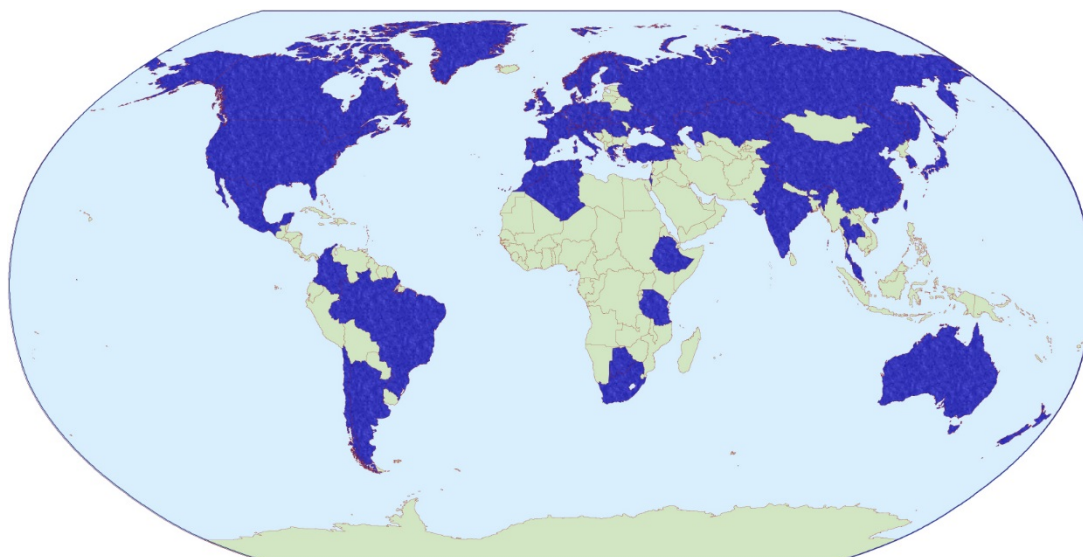
Description:	The <i>TCS Al-alloys Mobility Database</i> (MOBAL1) is a kinetic database containing mobility data for Al-based alloys present in a format suitable for simulation of diffusion-controlled phenomena. Used together with the add-on modules and a thermodynamic database for Al-alloys (TTAL) the MOBAL1 database can be used in order to study several phenomena of interest to aluminium alloys, such as microsegregation during solidification, homogenisation kinetics, growth/dissolution kinetics of precipitates, interdiffusion in Al-compounds, and much more.
Elements (41):	Ag, Al, Au, B, Be, C, Ca, Cd, Ce, Co, Cr, Cs, Cu, Fe, Ga, Ge, H, In, La, Li, Mg, Mn, Mo, Na, Nb, Nd, Ni, Pb, Pd, Pr, Sb, Sc, Si, Sm, Sn, Sr, Ti, Tl, V, Zn, Zr
Assessed phases:	✓ 2 phases
Database compatibility:	<i>Thermotech Al-based Alloys Thermodynamic Database</i> (TTAL8), <i>SGTE Solutions Thermodynamic Database</i> (SSOL6), <i>COST thermodynamic database</i>

MOBNI1: TCS Ni-alloys Mobility Database

Description:	The <i>TCS Ni-alloys Mobility Database</i> (MOBNI1) is a kinetic database containing mobility data for Ni-based alloys presented in a format suitable for simulation of diffusion-controlled phenomena. Used together with the add-on modules it can be used to study several phenomena of interest to Ni-based superalloys design and manufacturing, such as microsegregation during solidification, homogenisation kinetics, precipitate growth/dissolution kinetics and interdiffusion in Ni-base superalloy coating/substrate compounds.
Elements (22):	Al, B, C, Co, Cr, Cu, Fe, Hf, Mn, Mo, N, Nb, Ni, O, Re, Ru, Si, Ta, Ti, W, V, Zr
Assessed phases and systems:	<ul style="list-style-type: none"> ✓ 2 phases ✓ 21 binary systems ✓ 6 ternary systems ✓ 1 higher order system
Database compatibility:	<i>Thermotech Ni-based Superalloys Thermodynamic Database</i> (TTNI8)

MOBT11: TCS Ti-alloys Mobility Database

Description:	The <i>TCS Ti-alloys Mobility Database</i> (MOBT11) is a kinetic database containing mobility data for Ti-based alloys. It can be used for simulation of diffusion-controlled phenomena of interest to titanium alloys such as solidification, growth/dissolution kinetics of alpha and minor precipitates.
Elements (9):	Al, Cr, Mo, Nb, Sn, Ta, Ti, V, Zr
Assessed phases and systems:	<ul style="list-style-type: none">✓ 3 phases✓ 13 binary systems✓ 1 ternary system
Database compatibility:	<i>Thermotech Ti-based Alloys Thermodynamic Database</i> (TTT13)



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Thermo-Calc Software AB

Råsundavägen 18

SE-169 67 Solna, SWEDEN

info@thermocalc.com

Phone: +46 8 545 959 30

www.thermocalc.com

Org.No: 556540-6138

VAT No: SE556540613801

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