Thermodynamic, Kinetic, and Properties Databases

Databases

Overview 2025b

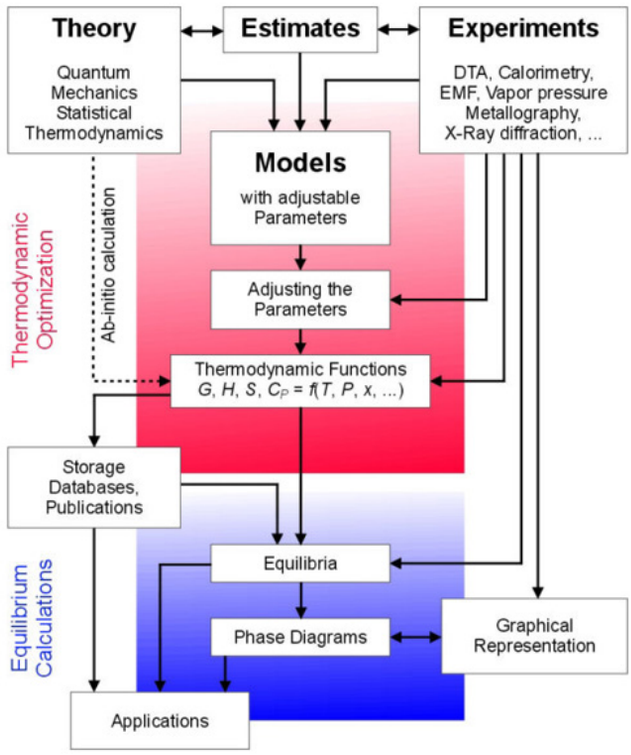
Thermo-Calc Software

www.thermocalc.com/databases

Introduction to CALPHAD Databases

To make a calculation with Thermo-Calc, it is necessary to select a database from which the thermodynamic and properties data is obtained. These databases are developed using the CALPHAD (CALculation of Phase Diagrams) approach, which describes both the thermodynamics and phase equilibria of a system as a function of chemistry and temperature in a self-consistent framework. This approach enables the prediction of properties of multicomponent systems based on data obtained from the critical assessment of binary and ternary subsystems. These assessments are combined to construct a multicomponent database.

CALPHAD is a phase-based approach, whereby the thermodynamic properties of each phase are described through the Gibbs free energy, which is evaluated through a critical assessment of all experimental and theoretical information available on phase equilibria and thermochemical properties in a system. Additionally, physical and chemical properties of the system such as crystallography, type of bonding, order-disorder transitions, and magnetic properties are also considered. The goal of the CALPHAD method is to reliably predict the set of stable phases and their thermodynamic properties in regions without experimental information and for metastable states during simulations of phase transformations.



The CALPHAD Method

The CALPHAD method can also model atomic mobilities in a similar way which, when combined with the Gibbs free energies, are used as the basis for calculating properties such as inter-diffusion coefficients in order to perform simulations of kinetic processes using the add-on Diffusion and Precipitation Calculator Modules in Thermo-Calc. Learn more about the CALPHAD method at https://thermocalc.com/methodology.

The CALPHAD method has recently been extended to model additional thermophysical properties, such as electric resistivity, thermal conductivity, surface tension, viscosity, and more, which are needed to simulate the mass and heat transfer in material manufacturing processes, such as casting and 3D printing. Additional properties are being added to our databases at each release. Learn more at https://thermocalc.com/wp-content/uploads/Brochures_and_Flyers/Current/properties-that-thermo-calc-can-calculate.pdf.

Accuracy and Validation

The accuracy of the calculations using Thermo-Calc depends on the quality and completeness of the database used. In the case of the solution databases, generally the more binary, ternary and high order systems that have been assessed, the more wide-ranging the composition space will be and the more accurate the predictions as well. This information, along with examples of validation of the databases, are available in extended information documents available at https://thermocalc.com. Every effort is made to validate the databases as broadly as possible. However, since the CALPHAD approach allows for predictions to be made for multicomponent systems of any composition, critical calculations should always be verified by experimental data.

How to use this Database Overview / Database Selection

This document is intended to provide a summary listing of the thermodynamic and properties databases available for use with Thermo-Calc. Only basic information is listed here. More detailed descriptions of each database are available at https://thermocalc.com/databases.

Note that *AM Module* used in the tables is an abbreviation for the Additive Manufacturing (AM) Module.

It is possible to combine several databases to make calculations using Thermo-Calc. Please contact one of our support specialists at info@thermocalc.com for more information related to a specific type of problem which may interest you.

Steels and Fe-Alloys

TCFE14: TCS Steel and Fe-alloys Database			
Elements (29 + 1):	Al, B, C, Ca, Ce, Co, Cr, Cu, Fe, H, Mg, Mn, Mo, N, Nb, Ni, O, P, Ru, S, Si, Sn, Ta, Ti, V, W, Y, Zn, Zr Plus Ar, which is for the gas phase only.		
Assessed Phases and Systems:	465 phases 371 binary systems, 335 ternary systems, 84 quaternary systems		
Additional Properties Data:	**Thermophysical properties**: Molar volume, surface tension of liquid, viscosity of liquid, electrical resistivity, thermal conductivity **Elastic properties[1]**: Elastic constants		
Mobility Database:	MOBFE8	**Compatible with AM Module:**	Yes

Nickel-based Alloys

TCNI13: TCS Nickel-based Superalloys Database			
Elements (29 + 2):	Al, B, C, Ca, Co, Cr, Cu, Fe, Hf, Mg, Mn, Mo, N, Nb, Ni, O, P, Pd, Pt, Re, Ru, S, Si, Ta, Ti, V, W, Y, Zr Plus Ar and H, which are for the gas phase only.		
Assessed Phases and Systems:	732 phases 371 binary systems, 433 ternary systems		
Additional Properties Data:	**Thermophysical properties**: Molar volume, surface tension of liquid, viscosity of liquid, electrical resistivity, thermal conductivity **Elastic properties[1]**: Elastic constants		
Mobility Database:	MOBNI6	**Compatible with AM Module:**	Yes

Aluminum-based Alloys

TCAL10: TCS Aluminum-based Alloys Database			
Elements (48):	Ag, Al, B, Ba, Be, Bi, C, Ca, Cd, Ce, Co, Cr, Cu, Er, Fe, Ga, Ge, H, Hf, In, K, La, Li, Mg, Mn, Mo, Na, Nb, Nd, Ni, P, Pb, Pr, S, Sb, Sc, Se, Si, Sn, Sr, Ta, Te, Ti, V, W, Y, Zn, Zr		
Assessed Phases and Systems:	725 phases 313 binary systems, 123 ternary systems, 14 quaternary systems		
Additional Properties Data:	Molar volume, surface tension of liquid, viscosity of liquid, electrical resistivity, thermal conductivity		
Mobility Database:	MOBAL8	**Compatible with AM Module:**	Yes

Magnesium-based Alloys

TCMG8: TCS Magnesium-based Alloys Database			
Elements (33):	Ag, Al, Bi, Ca, Ce, Cu, Dy, Er, Fe, Ga, Gd, H, 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:	575 phases 229 binary systems, 133 ternary systems, 5 quaternary systems		
Additional Properties Data:	Molar volume, surface tension of liquid, viscosity of liquid, electrical resistivity, thermal conductivity		
Mobility Database:	MOBMG2	**Compatible with AM Module:**	Yes

Titanium and Titanium Aluminide-based Alloys

TCTI6: TCS Ti/TiAl-based Alloys Database			
Elements (28):	Ag, Al, B, C, Co, Cr, Cu, 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:	423 solution and intermetallic phases 279 binary systems, 111 ternary systems		
Additional Properties Data:	**Thermophysical properties**: Molar volume, surface tension of liquid, viscosity of liquid, electrical resistivity, thermal conductivity **Elastic properties[1]**: Elastic constants		
Mobility Database:	MOBTI5	**Compatible with AM Module:**	Yes

1: Elastic properties are only available for cubic BCC (A2 and B2), cubic FCC (A1 and L12), and hexagonal HCP (A3) phases.

Ultra-high Temperature Materials

TCUHTM2: TCS Ultra-high Temperature Materials Database					
Elements (8):	B, C, Hf, N, O, Si, Ta, Zr				
Assessed Phases and Systems:	47 phases 28 binary systems, 41 ternary systems				
Additional Properties Data:	Molar volume	**Mobility Database:**	None	**Compatible with AM Module:**	No

Copper-based Alloys

TCCU6: TCS Copper-based Alloys Database			
Elements (32):	Ag, Al, Au, As, B, Be, Bi, C, Ca, Cd, Ce, Co, Cr, Cu, Fe, Ge, La, Mg, Mn, Mo, Nb, Ni, O, P, Pb, Pt, Se, Si, Sn, Ti, Zn, Zr		
Assessed Phases and Systems:	315 solution and intermetallic phases 148 binary systems, 64 ternary systems		
Additional Properties Data:	Molar volume, surface tension of liquid, viscosity of liquid, electrical resisitivity, thermal conductivity		
Mobility Database:	MOBCU5	**Compatible with AM Module:**	Yes

Refractory Alloys

TCMO2: TCS Molybdenum-based Alloys Database					
Elements (19):	Al, B, C, Cr, Fe, Hf, Mn, Mo, Nb, Pt, Re, Rh, Ru, Si, Ta, Ti, V, W, Zr				
Assessed Phases and Systems:	249 phases 170 binary systems, 75 ternary systems, 4 quaternary systems				
Additional Properties Data:	Molar volume, surface tension of liquid, viscosity of liquid, electrical resistivity, thermal conductivity	**Mobility Database:**	MOBMO2	**Compatible with AM Module:**	Yes

TCNB1: TCS Niobium-based Alloys Database					
Elements (12):	Al, C, Cr, Hf, Mo, Nb, Si, Ta, Ti, V, W, Zr				
Assessed Phases and Systems:	101 phases 66 binary systems, 76 ternary systems				
Additional Properties Data:	Molar volume, surface tension of liquid, viscosity of liquid, electrical resistivity, thermal conductivity	**Mobility Database:**	MOBNB1	**Compatible with AM Module:**	Yes

Oxides and Slag Database

TCOX14: TCS Metal Oxide Solutions Database					
Elements (34):	Al, Ar, B, Ba, C, Ca, Co, Cr, Cu, F, Fe, Gd, H, Hf, K, La, Li, Mg, Mn, Mo, N, Na, Nb, Ni, O, P, S, Si, Ti, V, W, Y, Yb, Zr				
Assessed Phases and Systems:	744 phases 433 binary systems, 557 ternary systems, 294 quaternary systems, 33 higher order systems				
Additional Properties Data:	Molar volume, surface tension of molten slags, viscosity of molten slags, electrical conductivity/resistivity, thermal conductivity/resistivity	**Mobility Database:**	None	**Compatible with AM Module:**	No

High Entropy Alloys

TCHEA8: TCS High Entropy Alloys Database			
Elements (27):	Al, B, C, Co, Cr, Cu, Fe, Hf, Ir, Mn, Mo, N, Nb, Ni, O, Re, Rh, Ru, Si, Sn, Ta, Ti, V, W, Y, Zn, Zr		
Assessed Phases and Systems:	713 phases 342 binary systems, 643 ternary systems, 54 quaternary systems, 3 higher order systems		
Additional Properties Data:	**Thermophysical properties**: Molar volume, surface tension of liquid, viscosity of liquid, electrical resistivity, thermal conductivity **Elastic properties**[1]: Elastic constants		
Mobility Database:	MOBHEA3	**Compatible with AM Module:**	Yes

1: Elastic properties are only available for cubic BCC (A2 and B2), cubic FCC (A1 and L12), and hexagonal HCP (A3) phases.

Solder Alloys

TCSLD5: TCS Solder Alloy Solutions Database			
Elements (24):	Ag, Al, Au, Bi, Ca, Cd, Co, Cu, Ga, Ge, Hf, In, Mg, Mn, Ni, Pb, Pd, Pt, Sb, Si, Sn, Ti, Zn, Zr		
Assessed Phases and Systems:	328 phases 161 binary systems, 78 ternary systems		
Additional Properties Data:	Molar volume, surface tension of liquid, viscosity of liquid, electrical resistivity, thermal conductivity		
Mobility Database:	MOBSLD2	**Compatible with AM Module:**	Yes

Molten Salts

TCSALT2: TCS Molten Salts Database			
Elements (12):	Al, Ca, Cl, F, K, Li, Mg, Na, O, Si, Sr, Zn		
Assessed Phases and Systems:	177 phases 78 pseudo-binary systems, 65 pseudo-ternary systems, 2 higher order systems, 36 mixed systems		
Additional Properties Data:	Molar volume, surface tension of liquid, viscosity of liquid		
Mobility Database:	None	**Compatible with AM Module:**	No

SALT1: SGTE Molten Salts Database					
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:	31 phases 83 binary systems				
Additional Properties Data:	None	**Mobility Database:**	None	**Compatible with AM Module:**	No (N/A)

Noble Metals-based Alloys

TCNOBL4: TCS Noble Metal Alloy Database					
Elements (26):	Ag, Al, Au, Ca, Co, Cr, Cu, Fe, Ga, Ge, In, Ir, Li, Mn, Ni, Pd, Pt, Re, Rh, Ru, Sb, Sc, Si, Sn, Ti, Zn				
Assessed Phases and Systems:	376 phases 220 binary systems, 71 ternary systems				
Additional Properties Data:	Molar volume, surface tension of liquid, viscosity of liquid, electrical resistivity, thermal conductivity	**Mobility Database:**	MOBNOBL2	**Compatible with AM Module:**	Yes

Permanent Magnetic Materials

TCPMAG2: TCS Permanent Magnetic Materials Database					
Elements (9):	B, Ce, Co, Dy, Fe, La, Nd, Pr, Tb				
Assessed Phases and Systems:	54 phases 36 binary systems, 29 ternary systems				
Additional Properties Data:	Molar volume, surface tension of liquid, viscosity of liquid	**Mobility Database:**	None	**Compatible with AM Module:**	No

Silicon-based Alloys

TCSI1: TCS Ultrapure Silicon Database					
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:	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.				
Additional Properties Data:	None	**Mobility Database:**	MOBSI1	**Compatible with AM Module:**	No

Cemented Carbides

TCCC1: TCS Cemented Carbides Database					
Elements (13):	C, Co, Cr, Fe, Mo, N, Nb, Ni, Ta, Ti, V, W, Zr				
Assessed Phases and Systems:	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.				
Additional Properties Data:	Molar volume	**Mobility Database:**	None	**Compatible with AM Module:**	No

Minerals

GCE2: TCS Geochemical/Environmental Database					
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, V, W, 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.).				
Additional Properties Data:	Molar volume	**Mobility Database:**	None	**Compatible with AM Module:**	No

Semiconductors

SEMC2: TCS Semiconductors Database					
Elements (10):	Al, As, C, Ga, H, In, P, Pb, Sb, Sn				
Assessed Phases and Systems:	18 phases 15 binary systems, 18 ternary systems, 135 gas species				
Additional Properties Data:	None	**Mobility Database:**	None	**Compatible with AM Module:**	No

Aqueous Solutions

TCAQ3: TCS Aqueous Solution Database					
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, V, W, 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. Uses the SIT model (Specific Interaction Theory model) which is valid up to 350°C, 100 bar and 3 molality.				
Additional Properties Data:	None	**Mobility Database:**	None	**Compatible with AM Module:**	No

AQS2: TCS Aqueous Solution Database					
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, V, W, 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. Uses the HKF model (complete revised HKF Model (Helgeson-Kirkham-Flowers)) which is valid up to 1000°C, 5 kbar and 6 molality.				
Additional Properties Data:	None	**Mobility Database:**	None	**Compatible with AM Module:**	No

Zirconium-based Alloys

TCZR1: TCS Zirconium-based Alloys Database					
Elements (8):	Cr, Fe, H, Nb, Ni, O, Sn, Zr				
Assessed Phases and Systems:	69 phases 28 binary systems, 19 ternary systems				
Additional Properties Data:	Molar volume, surface tension of liquid, viscosity of liquid	**Mobility Database:**	MOBZR1	**Compatible with AM Module:**	No

Nuclear Materials

MEPH20: IRSN Mephista Nuclear Fuels Database					
Owner:	IRSN				
Elements (15 + 2):	Ba, C, Ce, Cr, 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:	479 phases (51 condensed solution phases, 263 condensed stoichiometric phases, and 165 gaseous mixture phases) 105 binary subsystems, 61 ternary subsystems, 2 quaternary subsystems				
Additional Properties Data:	None	**Mobility Database:**	None	**Compatible with AM Module:**	No (N/A)

NUCL20: IRSN NUCLEA Nuclear Alloys-Oxides Database					
Owner:	IRSN				
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:	784 phases (65 condensed solution phases, 510 condensed stoichiometric phases, and 209 gaseous mixture phases) 153 binary subsystems, 105 ternary subsystems, 18 quaternary subsystems				
Additional Properties Data:	None	**Mobility Database:**	None	**Compatible with AM Module:**	No (N/A)

NUMT2: TCS Pure Radionuclides Database					
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:	248 phases. Contains critically-assessed thermodynamic data for pure substances, which are of relevance to calculations for various nuclear applications. 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.				
Additional Properties Data:	None	**Mobility Database:**	None	**Compatible with AM Module:**	No

General Alloys and Substances

SSOL9: SGTE Solutions Database					
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:	2352 phases 879 binary systems, 154 ternary systems, 19 quaternary systems, 1 quinary system				
Additional Properties Data:	None	**Mobility Database:**	MOB2	**Compatible with AM Module:**	No (N/A)

SSUB7: SGTE Substances Database					
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, H, 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:	3388 condensed stoichiometric compound phases and one huge gaseous mixture phase. Contains assessed thermochemical data for 5985 substances (3388 condensed compounds and 2597 gaseous species)				
Additional Properties Data:	None	**Mobility Database:**	None	**Compatible with AM Module:**	No (N/A)

Thermo-Calc Software

For more information...

Visit our website for additional information about each database, such as which specific binaries and ternaries are assessed, which phases are included, and validation and calculation examples.

If you are unsure about which databases are most suited for your specific needs, we are happy to discuss your application with you. Just send an email to info@thermocalc.com.