

**Thermo-Calc
Software**

**Overview of Thermodynamic and
Properties Databases - 2021b**

A Strong Foundation



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 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.

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/methodology>

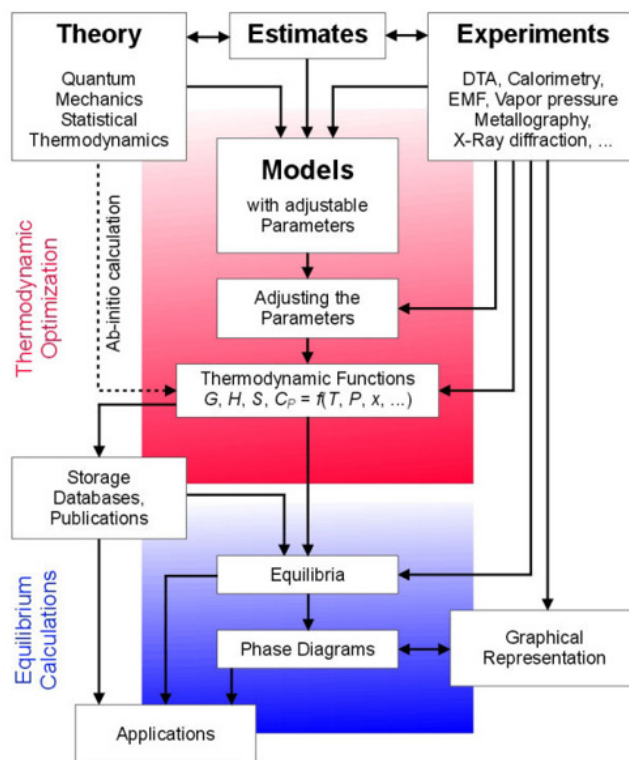
Accuracy and Validation

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 www.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 only to provide a summary listing of the more than 30 thermodynamic and properties databases available for use with Thermo-Calc. Only basic information is listed here, such as the elements included, the number of phases, the number of assessed binary and ternary systems, whether the database includes molar volume data which allows for the calculation of density and coefficients of thermal expansion and whether there is a corresponding mobility database for use with the Add-on Kinetic Modules. More detailed descriptions of each database are available at www.thermocalc.com.

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 and we will be more than happy to make recommendations on the most suitable database to use.



The CALPHAD Method

Steels and Fe-Alloys

TCFE11: TCS Steel and Fe-alloys Database	
Elements (28 + 1):	Al, B, C, Ca, Ce, Co, Cr, Cu, Fe, H, Mg, Mn, Mo, N, Nb, Ni, O, P, Ru, S, Si, Ta, Ti, V, W, Y, Zn, Zr Plus Ar, which is for the gas phase only.
Assessed Phases and Systems:	437 phases 345 binary systems, 290 ternary systems, 79 quaternary systems
Additional Properties Data:	Molar volume, surface tension of liquid, viscosity of liquid
Mobility Database:	MOBFE6

Nickel-based Alloys

TCNI11: TCS Nickel-based Superalloys Database	
Elements (28 + 2):	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 Plus Ar and H, which are for the gas phases only.
Assessed Phases and Systems:	680 phases 350 binary systems, 309 ternary systems
Additional Properties Data:	Molar volume, electrical resistivity, surface tension of liquid, thermal conductivity, viscosity of liquid
Mobility Database:	MOBNI5

Aluminum-based Alloys

TCAL8: TCS Aluminum-based Alloys Database	
Elements (44):	Ag, Al, B, Be, Bi, C, Ca, Cd, Ce, Co, Cr, Cu, Er, Fe, Ga, Ge, H, Hf, In, K, La, Li, Mg, Mo, Mn, Na, Nb, Nd, Ni, P, Pb, Pr, S, Sc, Se, Si, Sn, Sr, Te, Ti, V, Y, Zn, Zr
Assessed Phases and Systems:	662 phases 275 binary systems, 108 ternary systems, 14 quaternary systems
Additional Properties Data:	Molar volume, surface tension of liquid, viscosity of liquid, thermal conductivity, electrical resistivity
Mobility Database:	MOBAL6

Titanium and Titanium Aluminide-based Alloys

TCTI3: 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:	495 phases 278 binary systems, 108 ternary systems
Additional Properties Data:	Molar volume, surface tension of liquid, viscosity of liquid
Mobility Database:	MOBTI4

Magnesium-based Alloys

TCMG6: 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:	540 phases 208 binary systems, 102 ternary systems, 5 quaternary systems
Additional Properties Data:	Molar volume, surface tension of liquid, viscosity of liquid, electrical resistivity, thermal conductivity
Mobility Database:	MOBMG2

Copper-based Alloys

TCCU4: TCS Copper-based Alloys Database		
Elements (30):	Ag, Al, Au, As, B, Be, Bi, C, Ca, Cd, Co, Cr, Cu, Fe, Ge, Mg, Mn, Mo, Nb, Ni, O, P, Pb, Pt, Se, Si, Sn, Ti, Zn, Zr	
Assessed Phases and Systems:	Over 250 phases 135 binary systems, 53 ternary systems	
Additional Properties Data:	Molar volume, surface tension of liquid, viscosity of liquid	
Mobility Database:	MOBCU4	

High Entropy Alloys

TCHEA5: TCS High Entropy Alloys Database		
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:	500 phases 310 binary systems, 493 ternary systems	
Additional Properties Data:	Molar volume, electrical resistivity, surface tension of liquid, thermal conductivity, viscosity of liquid	
Mobility Database:	MOBHEA2	

Solder Alloys

TCSLD4: TCS Solder Alloy Solutions Database		
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:	272 phases 142 binary systems, 72 ternary systems	
Additional Properties Data:	Molar volume, surface tension of liquid, viscosity of liquid	
Mobility Database:	MOBSLD1	

Noble Metals-based Alloys

TCNOBL1: TCS Noble Metal Alloy Database		
Elements (21):	Ag, Al, Au, Co, Cr, Cu, Fe, Ga, Ge, In, Ir, Mn, Ni, Pd, Pt, Re, Rh, Ru, Sn, Ti, Zn	
Assessed Phases and Systems:	251 phases 204 binary systems, 61 ternary systems	
Additional Properties Data:	None	Mobility Database: None

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

Oxides and Slag Database

TCOX11: TCS Metal Oxide Solutions Database		
Elements (29):	Al, Ar, C, Ca, Co, Cr, Cu, F, Fe, Gd, H, K, La, Mg, Mn, Mo, N, Na, Nb, Ni, O, P, S, Si, Ti, V, W, Y, Zr	
Assessed Phases and Systems:	550 phases 324 binary systems, 327 ternary systems, 238 quaternary systems	
Additional Properties Data:	Molar volume, surface tension of molten slags, viscosity of molten slags	
Mobility Database:	None	

General Alloys and Substances

SSOL7: 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:	1711 phases 682 binary systems, 143 ternary systems, 19 quaternary systems, 1 quinary system		
Additional Properties Data:	None	Mobility Database:	MOB2

SSUB6: 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:	3188 condensed stoichiometric compound phases and one huge gaseous mixture phase Contains assessed thermochemical data for 5746 substances (3188 condensed compounds and 2558 gaseous species)		
Additional Properties Data:	None	Mobility Database:	None

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

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

Molten Salts

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

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

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

Nuclear Materials

MEPH19: IRSN Mephista Nuclear Fuels Database			
Owner:	IRSN		
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:	446 phases (47 condensed solution phases, 242 condensed stoichiometric phases, and 159 gaseous mixture phases) 91 binary subsystems, 50 ternary subsystems, 2 quaternary subsystems		
Additional Properties Data:	None	Mobility Database:	None

NUCL19: 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, 16 quaternary subsystems		
Additional Properties Data:	None	Mobility Database:	None

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

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

Thermotech Ltd. Thermodynamic Databases

TTAL8: Thermotech Al-based Alloys Database			
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		
Additional Properties Data:	None	Mobility Database:	MOBAL1

TTNI8: Thermotech Ni-based Superalloys Database			
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, V, W, Zr		
Additional Properties Data:	None	Mobility Database:	MOBNI1

TTMG5: Thermotech Mg-based Alloys Database			
Owner:	Thermotech Ltd.		
Elements (17):	Al, Ca, Ce, Cu, Fe, Gd, La, Mg, Mn, Nd, Sc, Si, Sn, Sr, Y, Zn, Zr		
Additional Properties Data:	None	Mobility Database:	None

TTTI3: Thermotech Ti-based Alloys Database			
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		
Additional Properties Data:	None	Mobility Database:	MOBTI1

TTTIAL1: Thermotech TiAl-based Alloys Database			
Owner:	Thermotech Ltd.		
Elements (13):	Al, B, Cr, Mn, Mo, Nb, O, Si, Ta, Ti, V, W, Zr		
Additional Properties Data:	None	Mobility Database:	None

TTZR1: Thermotech Zr-based Alloys Database			
Owner:	Thermotech Ltd.		
Elements (12):	C, Cr, Fe, H, Hf, N, Nb, Ni, O, Si, Sn, Zr		
Additional Properties Data:	None	Mobility Database:	None



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.

www.thermocalc.com