Thermodynamic, Kinetic, and Properties Databases

Databases

Overview 2024a



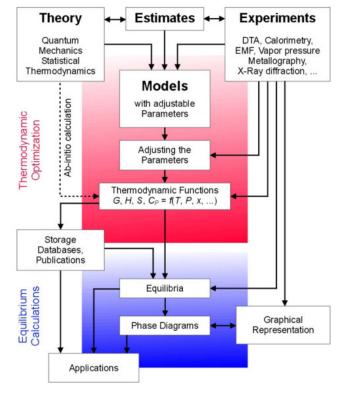


www.thermocalc.com/databases

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.

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 <u>https://thermocalc.com</u>. 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, such as the elements included, whether the database includes molar volume data which allows for the calculation of density and coefficients of thermal expansion, whether there is a corresponding mobility database for use with the Add-on Kinetic Modules, and more. 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 <u>info@thermocalc.com</u> for more information related to a specific type of problem which may interest you.

Steels and Fe-Alloys

TCFE13: 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:	435 phases 371 binary systems, 316 ternary systems, 80 quaternary systems			
Additional Properties Data:	Molar volume, surface tension of liquid, viscosity of liquid, electrical resistivity, thermal conductivity			
Mobility Database:	MOBFE8	Compatible with AM Module:	Yes	

Nickel-based Alloys

TCNI12: 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:				
	371 binary systems, 431 ternary systems			
Additional Properties Data:	Molar volume, surface tension of liquid, viscosity of liquid, electrical resistivity, thermal conductivity			
Mobility Database:	MOBNI6	Compatible with AM Module:	Yes	

Aluminum-based Alloys

TCAL9: 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, Mo, Mn, 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:	722 phases 313 binary systems, 119 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

TCMG7: 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:	541 phases 223 binary systems, 124 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		

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	

Titanium and Titanium Aluminide-based Alloys

TCTI5: 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:	433 solution and intermetallic phases 279 binary systems, 111 ternary systems			
Additional Properties Data:	Molar volume, surface tension of liquid, viscosity of liquid, electrical resistivity, thermal conductivity			
Mobility Database:	MOBTI4	Compatible with AM Module:	Yes	

Noble Metals-based Alloys

TCNOBL3: 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:	324 phases 204 binary systems, 66 ternary systems			
Additional Properties Data:	Molar volume, surface tension of liquid, viscosity of liquid, electrical resistivity, thermal conductivity			
Mobility Database:	MOBNOBL1	Compatible with AM Module:	Yes	

High Entropy Alloys

TCHEA7: 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:	540 phases 319 binary systems, 526 ternary systems			
Additional Properties Data:	Molar volume, surface tension of liquid, viscosity of liquid, electrical resistivity, thermal conductivity			
Mobility Database:	MOBHEA3	Compatible with AM Module:	Yes	

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	Compatible with AM Module:	No	

Silicon-based Alloys

TCSI1: TCS Ultrapure Silicon	Database				
Elements (34):	Ag, Al, As, A V, W, Zn, Zr		ia, Ge, In, Li,	Mg, Mn, Mo, N, Na, Ni, O, P, S, Sb, Si, Sn,	Te, Ti,
Assessed Phases and Systems:	In addition	to the diamond phase, at least ontent are included in each Si-	•	nd the corresponding stable silicide phase inary.	e with
Additional Properties Data:	None	Mobility Database:	MOBSI1	Compatible with AM Module: No	1

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	

Oxides and Slag Database

TCOX13: TCS Metal Oxide Solutions Database				
Elements (32):	Al, Ar, B, C, Ca, Co, Cr, Cu, F, Fe, Gd, H, Hf, K, La, Mg, Mn, Mo, N, Na, Nb, Ni, O, P, S, Si, Ti, V, W, Y, Yb, Zr			
Assessed Phases and Systems:	606 phases 392 binary systems, 508 ternary systems, 246 quaternary systems, 32 higher order systems			
Additional Properties Data:	Molar volume, surface tension of molten slags, viscosity of molten slags, electrical conductivity of molten slags			
Mobility Database:	None	Compatible with AM Module:	No	

Permanent Magnetic Materials

TCPMAG2: TCS Permanent Magnetic Materials Database						
Elements (9):	3, 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 li	Molar volume, surface tension of liquid, viscosity of liquid				
Mobility Database:	None	Compatible with AM Module:	No			

Ultra-high Temperature Materials

TCUHTM1: TCS Ultra-high Temperature Materials Database						
Elements (7):	B, C, Hf, N, S	s, C, Hf, N, Si, Ta, Zr				
Assessed Phases and Systems:		5 phases 1 binary systems, 26 ternary systems				
Additional Properties Data:	None	Mobility Database:	None	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:	Covers the complete and critical as	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			

Aqueous Solutions

Elements (75):	n Database 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:	organic con hypothetica standard hy	Si, Sm, Sn, Sr, Ib, Ie, Ih, II, Im, U, V, W, Xe, Y, Yb, Zn 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:	organic con hypothetica standard hy HKF model	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		

Semiconductors

SEMC2: TCS Semiconductors Database						
Elements (10):	Al, As, C, Ga	Al, As, C, Ga, H, In, P, Pb, Sb, Sn				
Assessed Phases and Systems:	18 phases	L8 phases				
	15 binary sy	15 binary systems, 18 ternary systems, 135 gas species				
Additional Properties Data:	None	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:							
Additional Properties Data:	Molar volume	Mobility Database:	None	Compatible with AM Module:	No		

General Alloys and Substances

SSOL8: SGTE Solutions Database

Owner:	Scientific G	Scientific Group Thermodata Europe (SGTE)				
Elements (79):	Ag, Al, Am, In, Ir, K, La, Sb, Sc, Se, S	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, n, 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:		2023 phases 783 binary systems, 144 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 G	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:	Contains as	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)		

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:	mixture pha	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:	mixture pha	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)	

NUMIZ: ICS 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:	Contains cr calculations					
Additional Properties Data:	None	Mobility Database:	None	Compatible with AM Module: No		

Molten Salts

TCSALT1: TCS Molten Salts Database									
Elements (11):	Al, Ca, Cl, F,	l, Ca, Cl, F, K, Mg, Na, O, Si, Sr, Zn							
Assessed Phases and Systems:	154 phases 57 pseudo-	54 phases 7 pseudo-binary systems, 41 pseudo-ternary systems, 2 higher order systems, 28 mixed systems							
Additional Properties Data:	None	one							
Mobility Database:	None	None Compatible with AM Module: No							
SALT1: SGTE Molten Salts Da	atabase								
Owner:	Scientific G	Scientific Group Thermodata Europe (SGTE)							
Elements (17):	Br, C, Ca, Cl	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								
	83 binary S	ystems							

Thermotech Ltd. Thermodynamic Databases

TTAL8: Thermotech Al-based Alloys Database							
Owner:	Thermotec	hermotech Ltd.					
Elements (25):	Al, B, Bi, C,	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	Compatible with AM Module:	No (N/A)		

TTNI8: Thermotech Ni-based Superalloys Database

Owner:	Thermotec	nermotech Ltd.					
Elements (23):	Al, B, C, Co,	l, 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	Compatible with AM Module:	No (N/A)		

TTMG5: Thermotech Mg-based Alloys Database

Owner:	Thermotech	hermotech Ltd.					
Elements (17):	Al, Ca, Ce, C	Al, Ca, Ce, Cu, Fe, Gd, La, Mg, Mn, Nd, Sc, Si, Sn, Sr, Y, Zn, Zr					
Additional Properties Data:	None	one Mobility Database: None Compatible with AM Module: No (N/A)					

TTTI3: Thermotech Ti-based Alloys Database								
Owner:	Thermotecl	Thermotech Ltd.						
Elements (21):	Al, B, C, Cr,	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	Compatible with AM Module:	No (N/A)			

TTTIAL1: Thermotech TiAl-based Alloys Database

Owner	: Thermotec	hermotech Ltd.					
Elements (13)	Al, B, Cr, M	Al, B, Cr, Mn, Mo, Nb, O, Si, Ta, Ti, V, W, Zr					
Additional Properties Data	None	Mobility Database:	None	Compatible with AM Module:	No (N/A)		

TTZR1: Thermotech Zr-based Alloys Database							
Owner:	Thermotec	Thermotech Ltd.					
Elements (12):	C, Cr, Fe, H,	C, Cr, Fe, H, Hf, N, Nb, Ni, O, Si, Sn, Zr					
Additional Properties Data:	None	Mobility Database:	None	Compatible with AM Module:	No (N/A)		



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/databases