

Thermo-Calc Software

Overview of Thermodynamic and Properties Databases - 2021a



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>

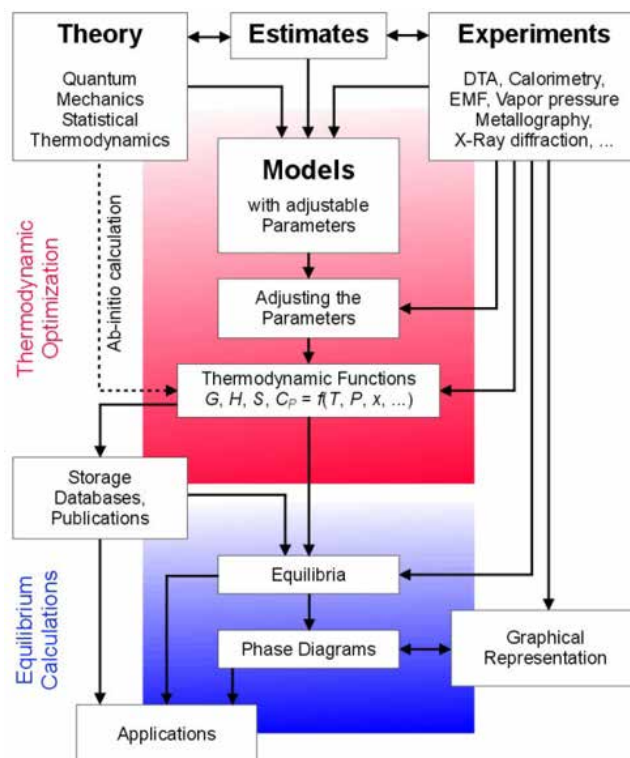
Accuracy and Validation

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

| TCNI10: 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, surface tension of liquid, viscosity of liquid | |
| Mobility Database: | MOBNI5 | |

Aluminum-based Alloys

| TCAL7: TCS Aluminum-based Alloys Database | | |
|---|---|--|
| Elements (39): | 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, Ni, P, Pb, Sc, Si, Sn, Sr, Ti, V, Y, Zn, Zr | |
| Assessed Phases and Systems: | 637 phases 267 binary systems, 99 ternary systems, 12 quaternary systems | |
| Additional Properties Data: | Molar volume, surface tension of liquid, viscosity of liquid, thermal conductivity, electric 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 207 binary systems, 102 ternary systems, 5 quaternary systems | |
| Additional Properties Data: | Molar volume, surface tension of liquid, viscosity of liquid, electric resistivity, thermal conductivity | |
| Mobility Database: | MOBMG2 | |

Copper-based Alloys

| TCCU3: 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 133 binary systems, 50 ternary systems | | |
| Additional Properties Data: | Molar volume | Mobility Database: | MOBCU3 |

High Entropy Alloys

| TCHEA4: 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, viscosity of liquid | | |
| Mobility Database: | MOBHEA2 | | |

Solder Alloys

| TCSLD3: 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 | 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

| TCOX10: TCS Metal Oxide Solutions Database | | | |
|--|--|--|--|
| Elements (28): | Al, Ar, C, Ca, Co, Cr, Cu, F, Fe, Gd, H, La, Mg, Mn, Mo, N, Na, Nb, Ni, O, P, S, Si, Ti, V, W, Y, Zr | | |
| Assessed Phases and Systems: | 459 phases 288 binary systems, 288 ternary systems, 152 quaternary systems | | |
| Additional Properties Data: | Molar volume, viscosity of liquid | | |
| 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