

## Properties that Can Be Calculated

with Thermo-Calc and the Add-on Modules

Thermo-Calc and the Add-on Modules can be used to calculate a broad range of materials properties for multicomponent systems as a function of temperature and composition when used in conjunction with suitable databases. This document lists a selection of the properties that can be calculated with our software for each of our primary materials databases, as of the 2025b release. Databases not included in this document can make many of the calculations in the list, particularly in the thermodynamic sections at the beginning. If you have questions about any of the products or calculations, contact us at **info@thermocalc.com**.

	Material / Database(s	): 	)BFE) Sed	<sup>BNI</sup> )	BAL)	UBMG)	<sup>OBCU)</sup> and TiAI	Noble Alloys	High Entropy Allow	<sup>AOBHEA)</sup> ovs	silicon-based Allow	' <sup>BSI</sup> ) 'VS Ma Slag		Permanent Magnes	Temp.	alts	mn	<sup>OB</sup> NO) OBNRI	(on.
	Calculations	Steel & Fe-based	Nicket-based	Aluminum (TCAL+AAC	Magnesium (TCMG+AA	Copper (TCCU+MAC)	Titanium and Tig	Noble All	High Entr	Solder Alloys	Silicon-based A	Oxides and Slag	Zirconium (TCZR+AAC)	Permane (TCPNAGC	Ultra-high Temp.	Molten Salts	Molybdenum	Niobium (TCNB+MOBNR)	/
	Amount of phases (moles, mass, mole- fraction/percent, mass- fraction/percent)	х	x	х	х	х	х	х	х	х	х	х	х	x	х	х	х	х	
	Phase constitution (moles, mass, mole- fraction/percent, mass- fraction/percent, site-fractions)	х	x	x	x	х	х	х	x	х	x	х	х	x	х	х	х	x	
Equilibria	Volume-fraction/percentage of phases	х	х	х	х	х	х	х	х	х		х	х	х	х	х	х	х	
e Equil	Solubility limits	х	х	х	х	х	х	х	х	х	х	х	х	х	х	х	х	х	
Phase	Driving forces for phase formation	x	x	x	x	х	х	x	x	x	x	х	х	x	х	х	х	х	
	Activities and Chemical potentials	х	x	х	x	х	х	х	x	х	х	х	х	x	х	x	х	x	
	Phase diagrams, Potential diagrams, and Pourbaix diagrams <sup>a</sup>	х	х	х	х	Х	Х	х	х	х	Xp	х	х	х	х	х	Х	x	

	Material / Database(s	): 	<sup>BFE</sup>	(INA)	Magnesium (TCM6+142)	<sup>OBMG)</sup>	Titanium and Tid.	<sup>BTI)</sup>	High Entropy Allow	Solder Alloys (TCSLD+hange)	silicon-based Allow	rd Slag		Permanent Magnes	Temp	alts	Molybdenum (TCMO+AA	<sup>OBMO)</sup>
	Calculations	Steel & Fe. based	Nickel-based	Aluminum (TCAL+MAC)	Magnesiu (TCMG+A	Copper (TCCU+MC)	Titanium (TCTI+Mic	Noble Alloys	High Entr	Solder Al	Silicon-based A	Oxides and Slag	Zirconium (TCZR+AAC	Permane, ""	Ultra-high Temp	Motten Salts	Molybde	Niobium (TCNB+MOBMO)
	Enthalpy, Entropy	Х	Х	Х	Х	Х	Х	Х	Х	Х	Х	Х	Х	Х	х	х	Х	х
	Specific heat	Х	х	х	х	х	х	х	х	х	х	х	х	х	х	х	х	х
	Heat capacity	х	Х	х	х	х	х	х	х	х	х	х	х	х	х	х	х	х
es	Heat of formation	Х	Х	х	Х	х	х	х	х	х	х	х	х	х	х	х	х	х
had	Interfacial energy	Х	Х	Х	Х	Х	Х	Xc	х	Х	Xc	х	Х	х	Xc	х	х	х
2	Density	х	х	х	х	х	х	х	х	х		х	х	х	х		х	х
/sical	Coefficient of thermal expansion	Х	х	х	Х	х	х	х	х	х		х	х	х	х		х	х
Inermochemical and Thermophysical Properties	Lattice parameters (for cubic structures)	х	х	х	х	х	х	х	х	х		х	х	х	х		х	х
U	Viscosity of liquid	Х	х	Х	Х	Х	Х	х	х	х		х	х	х		х	х	x
	Surface tension of liquid	х	х	х	х	х	х	х	х	х		х	х	х		х	х	х
	Thermal conductivity	Х	х	х	х	х	х	х	х	х		х					х	х
cnem	Thermal resistivity	х	х	х	х	х	х	х	х	х		х					х	х
0 E	Thermal diffusivity	х	х	х	х	х	х	х	х	х		х					х	x
Ine	Electrical resistivity	х	х	х	х	х	х	х	х	х		х					х	х
	Electrical conductivity	х	х	х	х	х	х	х	х	х		х					х	х
	Generation of Materials Properties for the Additive Manufacturing Module	х	х	х	х	х	х	х	х	х							х	х

	Material / Database(s)	Steel & Fe. based	Nickerbased	Aluminum (TCAL+MC)	Magnesium (TCMG+10)	Copper (TCCU+AAC	Titanium and Tidi	Noble Alloys	High Entropy Allow	Solder Alloys (TCSLD+110ys	Silicon-based Allow	Oxides and Slag	Zirconium (TCZR+hac	Permanent Magnes	Ultra-high Temp	Salts	Molybdenum (TCMO4402	Niobium (TCNB+MC)
	Calculations	Steel & (TCFE+)	Nickel-4	Aluminu (TCAL+A	Magnes	Copper (TCCU+1	Titaniur, (TCTI+N	<b>Noble A</b> (TCNOBL	High En (TCHEA,	Solder ,	Silicon-1 (TCSI+N	Oxides (TCOX)	Zirconiu (TCZR+A	Perman (TCPMA	Ultra-hi (TCUHT	Molten Salts	Molyba (TCMO+	Niobiun (TCNB+)
S	Atomic mobility	Х	Х	Х	Х	Х	Х	Х	Х	Х	Х		Х				Х	Х
Kinetic Coefficients	Tracer diffusion	х	х	х	х	х	х	х	х	х	х		х				х	х
Kin oeffi	Intrinsic diffusion	Х	х	х	х	х	х	х	х	х	х		х				х	х
U	Interdiffusion	Х	х	х	х	х	х	х	х	х	х		х				Х	х
Mechanical Properties	Yield strength <sup>d</sup>	х	х	х	х	х	х	х	х	х	х		х					
Mech Prop	Hardness <sup>d</sup>	х	х	х	х	х	х	х	х	х	х		х					
Se	Bulk modulus	х	х				х		х									
Elastic Properties <sup>e</sup>	Shear modulus	х	х				х		х									
astic Pr	Young's modulus	х	х				х		х									
Ξ	Elastic constants	х	х				х		х									
ies	Liquidus, solidus, incipient melt temperatures, freezing range	х	х	х	х	х	х	х	х	х	х		х	х	х		х	х
m Solidification Properties	Fraction solid curves, solidification path, fraction eutectic	х	х	х	х	х	х	х	х	х	х		х	х	х		х	х
ation I	Microsegregation, partition coefficients	х	х	х	х	х	х	х	х	х	х		х	х	х		х	x
solidific	Latent heat, total or apparent heat release	х	х	х	х	х	х	х	х	х	х		х	х	х		х	x
um S	Shrinkage	Х	х	х	х	х	х		х	х	х		х	х	х		Х	х
Non-equilibriu	Accounting for back diffusion in Scheil module	х	х	х	х	х	х	х	х	х	х		х				х	х
Non-ec	Columnar to Equiaxed Transition	х	х	х	х	х	х	х	х	х			х				х	х
	Hot tearing tendency <sup>f</sup>	Х	Х	Х	Х	Х	Х	Х	Х	Х	Х		Х	Х	Х		Х	х

	Material / Database(s	): .pased	<sup>BF</sup> EJ	BNIJ	BAL)	<sup>OBING</sup>	)BCU) md TiAl	Noble Alloys	High Entropy Allow	OBHEA)	Silicon-based Allon	asi) -rs d'slag		Permanent Magnes	Temp.	Its	un la	UBNIO) BNIC:	(Bhra
	Calculations	Steel & Fe.based	Nicket-based	Aluminum (TCAL+MCC	Magnesium (TCNIG+IA2	Copper (TCCU+MAC)	Titanium and Tial	Voble Allo	High Entro	Solder Alloys (TCSLD+hac	Silicon-bas	Oxides and Slag	Zirconium (TCZR+MAC	Permanen (TCPNAG)	Ultra-high Temp.	Molten Salts (TCSALT)	Molybadenum	Niobium (TCNB+MOBNG)	/
	Martensite start temperature	Х																	
	Martensite fractions	Х																	
ar V	Martensitic steel strength	х																	
Steel Model Library	Flow stress (Martensitic steel strength)	х																	
δοχ	Pearlite kinetics	х																	
Steel	Bainite kinetics	Х																	
•,	Ferrite kinetics	Х																	
	Critical transformation temperatures	х																	
	Antiphase boundary energy		Х																
orary	Coarsening (Ni)		х																
odel Lik	Equilibrium with freeze-in temperature		х																
Nickel Model Library	Solvus for ordered phase		х																
z	Strain-Age Cracking (SAC)		Х																
tel m	Alloy strength						х												
Titanium Model Librarv	Martensite start temperature						х												
Noble Metal Alloys Model Librarv								x											
Process Metallurgy Module	Optimizing slag chemistries											х							
Proc Metal Moo	Simulating steel refining											х							

	Material / Database(s)		d d	(IN)	4()	<sup>BMG)</sup>	<sup>BCU)</sup> Na Tial		DBNOBL)	BHEA) S	<sup>BSLD</sup> ) ed Allous	Slag		(A) Magner	emp.	: .	E	BNB) SNB)
	Calculations	Steel & Fe-based	Nickel-based	Aluminum (TCAL+NAC	Magnesium (TCMG+AAC)	Copper (TCCU+MAC)	Titanium and Tid	Noble Alloys	High Entropy Allow	Solder Alloys	Silicon-based Allow	Oxides and Slag	Zirconium (TCZR+MAC)	Permanent Magnos	Ultra-high Temp	Molten Salts	Molybdenum	Niobium (TCNB+MOBNB)
	Microsegregation during solidification	х	х	х	х	х	х	х	х	х	х		х				х	х
2	Homogenization of alloys	х	х	х	х	х	х	х	х	х	х		х				х	х
ile (DICTRA)	Growth/dissolution of secondary phases such as carbides, nitrides, intermetallic phases	х	х	х	х	х	х	х	х	х	х		х				х	х
Jodu	Coarsening of precipitate phases	х	х	х	х	Х	х	х	Х	х	х		Х				х	х
Diffusion Module	Allotropic phase transformations such as, for example, austenite to ferrite transformations in steel	х	х	х	х	х	х		х	х	х		х				х	х
	Carburization, nitriding, and carbonitriding of steel and other alloys	х	х	х	х	х	х		х	х	х						х	x

	Material / Database(s	e.based	<sup>BFE</sup>	(INB)	1981() 1	<sup>OBMG)</sup>	Titanium and Tid.	Noble Alloys	High Entropy Allow	Solder Alloys	Silicon-based Allow	as (iso		Permanent Magnes	h Temp.	alts	Molybdenum (TCNDA)	<sup>OBMO)</sup>
	Calculations	Steel & Fe-based	Nickel-based	Aluminum (TCAL+NACC	Magnesium (TCMG+MAG	Copper (TCCU+MAC)	Titanium (TCTI+Muc	Noble All	High Entr	Solder Al	Silicon-b <sub>e</sub>	Oxides and Slag	Zirconium (TCZR+MAC)	Permane, (TCP/MAG	Ultra-high Temp.	Molten Salts	Molybde,	Niobium (TCNB+MOBNB)
	Concurrent nucleation, growth/dissolution, and coarsening of precipitates	х	х	х	х	х	х	х	х	х	х		х				х	х
	Temporal evolution of particle size distribution	х	х	х	х	х	х	х	х	х	х		х				х	х
odule A)	Temporal evolution of grain size distribution	х	х	х	х	х	х	х	х	х	х		х				х	х
Precipitation Module (TC-PRISMA)	Average particle radius, number density, and volume fraction	х	х	х	х	х	х	х	х	х	х		х				х	x
ecipita (TC-I	Matrix and precipitate composition	х	х	х	х	х	х	х	х	х	х		х				х	х
2	Estimated yield strength of your material	х	х	х	х	х	х	х	х	х	х		х				х	х
	Time-Temperature-Precipitation (TTP) diagrams	х	х	х	х	х	х	х	х	х	х		х				х	х
	Continuous-Cooling-Transformation (CCT) diagrams	х	х	х	х	х	х	х	х	х	х		х				х	x

	Material / Database(s)	:.	<sup>BFE</sup>	(INB)	<sup>1</sup> BAL)	OBMG)	<sup>JBCU)</sup> and Tidl	Noble Alloys (TCN08L+112	High Entropy Allow	<sup>OBHEA)</sup> ovs	silicon-based Allow	d Slag		Permanent Magnos	Temp	its	mn	<sup>OBMO</sup> ) <sup>OBMD</sup> ,
	Calculations	Steel & Fe.based	Nickel-based	Aluminum (TCAL+MAC	Magnesium (TCMG+AAC)	Copper (TCCU+MC)	Titanium and Tid	Noble All	High Entr	Solder Alloys	Silicon-based ,	Oxides and Slag	Zirconium (TCZR+MAC	Permaner (TCP/MAG	Ultra-high Temp	Molten Salts	Molybdenum	Niobium (TCUB+MOBNE)
	Melt pool dimensions	Х	х	х	х	х	х	х	х	х							х	х
0	Peak temperatures	х	х	х	х	х	х	х	х	х							х	x
Module	Velocity of fluid flow	х	х	х	х	х	х	х	х	х							х	х
Additive Manufacturing Module	Location specific Thermophysical properties (viscosity, thermal conductivity, density)	х	х	х	х	х	х	х	х	х							х	х
Manu	Location specific thermal history	х	х	х	х	х	х	х	х	х							х	х
dditive	Heat source calibration using experimental data	х	х	х	х	х	х	х	х	х							х	x
٩	Keyhole modeling	х	х	х	х	х	х	х	х	х							х	х
	Printability Maps	х	х	х	х	х	х	х	х	х							х	х
	Thermal gradient and solidification rate	х	х	х	х	х	х	х	х	х							х	х
	Absorptivity of liquid	Х	х	х	х	х	х	х	х	х							х	х

a: Calculation of so-called Pourbaix diagrams requires an additional aqueous solutions database.

**b**: Phase-diagram calculations are not recommended, since only the Si-rich corner has been assessed.

c: Estimation of interfacial energy requires molar volume, which is lacking in this database. Because of that, a default molar volume value equal to 7E-6 is used in the estimate.

d: The model takes each contribution (intrinsic, solid solution, grain boundary, and precipitation strength) to the yield strength into account in a general way. The user can select between

different models and model parameters, and may need to give input data, e.g. mean particle size, unless it has been simulated using the Precipitation Module (TC-PRISMA). The model

does not account for contributions to the strength from structures like Bainite, Pearlite, or Martensite, and there is no account for deformation hardening. Hardness is estimated based on

a correlation between microhardness and Yield strength.

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

f: The model for hot tearing is general since it is based on the Scheil solidification model and the concept of estimating the time spent where the casting is vulnerable to cracking. However, the model has only been validated for AI- and Mg-alloys. Other crack mechanisms, such as precipitation of brittle grain boundary phases, segregation of brittle phosphor to grain boundaries in steels, and many others, may be predominant in other alloy systems.