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 2024a 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**.

Calculations \ Material / Database(s):		**Steel & Fe-based** *(TCFE+MOBFE)*	**Nickel-based** *(TCNI+MOBNI)*	**Aluminum** *(TCAL+MOBAL)*	**Magnesium** *(TCMG+MOBMG)*	**Copper** *(TCCU+MOBCU)*	**Titanium and TiAl** *(TCTI+MOBTI)*	**Noble Alloys** *(TCNOBL+MOBNOBL)*	**High Entropy Alloys** *(TCHEA+MOBHEA)*	**Solder Alloys** *(TCSLD+MOBSLD)*	**Silicon-based Alloys** *(TCSI+MOBSI)*	**Oxides and Slag** *(TCOX)*	**Zirconium** *(TCZR+MOBZR)*	**Permanent Magnets** *(TCPMAG)*	**Ultra-high Temp.** *(TCUHTM)*	**Molten Salts** *(TCSALT)*
Phase Equilibria	Amount of phases (moles, mass, mole-fraction/percent, mass-fraction/percent)	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
	Phase constitution (moles, mass, mole-fraction/percent, mass-fraction/percent, site-fractions)	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
	Volume-fraction/percentage of phases	X	X	X	X	X	X	X	X	X		X	X	X		
	Solubility limits	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
	Driving forces for phase formation	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
	Activities and Chemical potentials	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X

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Physical Properties	Phase diagrams, Potential diagrams, and Pourbaix diagrams*	X	X	X	X	X	X	X	X	X	(X)**	X	X	X	X	X
	Enthalpy, Entropy	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
	Specific heat	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
	Heat capacity	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
	Heat of formation	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
	Interfacial energy	X	X	X	X	X	X	(X)***	X	X	(X)***	X	X	X	(X)***	X
	Density	X	X	X	X	X	X	X	X	X		X	X	X		
	Coefficient of thermal expansion	X	X	X	X	X	X	X	X	X		X	X	X		
	Lattice parameters (for cubic structures)	X	X	X	X	X	X	X	X	X		X	X	X		
	Viscosity of liquid	X	X	X	X	X	X	X	X	X		X	X	X		
	Surface tension of liquid	X	X	X	X	X	X	X	X	X		X	X	X		
	Thermal conductivity	X	X	X	X	X	X	X	X							
	Thermal resistivity	X	X	X	X	X	X	X	X							
	Thermal diffusivity	X	X	X	X	X	X	X	X							
	Electrical resistivity	X	X	X	X	X	X	X	X			X******				
	Electrical conductivity	X	X	X	X	X	X	X	X			X******				
	Generation of Materials Properties for the Additive Manufacturing Module	X	X	X	X	X	X	X	X							

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Kinetic Coefficients	Atomic mobility	X	X	X	X	X	X	X	X	X	X		X			
	Tracer diffusion	X	X	X	X	X	X	X	X	X	X		X			
	Intrinsic diffusion	X	X	X	X	X	X	X	X	X	X		X			
	Interdiffusion	X	X	X	X	X	X	X	X	X	X		X			
Mechanical Properties	Yield strength****	X	X	X	X	X	X	X	X	X	X		X			
	Hardness****	X	X	X	X	X	X	X	X	X	X		X			
Non-equilibrium Solidification Properties	Liquidus, solidus, incipient melt temperatures, freezing range	X	X	X	X	X	X	X	X	X	X		X	X	X	
	Fraction solid curves, solidification path, fraction eutectic	X	X	X	X	X	X	X	X	X	X		X	X	X	
	Microsegregation, partition coefficients	X	X	X	X	X	X	X	X	X	X		X	X	X	
	Latent heat, total or apparent heat release	X	X	X	X	X	X	X	X	X	X		X	X	X	
	Shrinkage	X	X	X	X	X	X		X	X	X		X	X		
	Accounting for back diffusion in Scheil module	X	X	X	X	X	X	X	X	X	X		X			
	Hot tearing tendency*****	X	X	X	X	X	X	X	X	X	X		X	X	X	

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Steel Model Library	Martensite start temperature	X														
	Martensite fractions	X														
	Martensitic Steel Strength	X														
	Pearlite kinetics	X														
	Bainite kinetics	X														
	Ferrite kinetics	X														
	Critical transformation temperatures	X														
Nickel Model Library	Antiphase boundary energy - Ni		X													
	Coarsening - Ni		X													
	Equilibrium with freeze-in temperature		X													
	Solvus for ordered phase		X													
	Strain-Age Cracking (SAC)		X													
Process Metallurgy Module	Optimizing slag chemistries											X				
	Simulating steel refining											X				

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Diffusion Module (DICTRA)	Microsegregation during solidification	X	X	X	X	X	X	X	X	X	X		X			
	Homogenization of alloys	X	X	X	X	X	X	X	X	X	X		X			
	Growth/dissolution of secondary phases such as carbides, nitrides, intermetallic phases	X	X	X	X	X	X	X	X	X	X		X			
	Coarsening of precipitate phases	X	X	X	X	X	X	X	X	X	X		X			
	Allotropic phase transformations such as, for example, austenite to ferrite transformations in steel	X	X	X	X	X	X		X	X	X		X			
	Carburization, nitriding, and carbonitriding of steel and other alloys	X	X	X	X	X	X		X	X	X					

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Precipitation Module (TC-PRISMA)	Concurrent nucleation, growth/dissolution, and coarsening of precipitates	X	X	X	X	X	X	X	X	X	X		X			
	Temporal evolution of particle size distribution	X	X	X	X	X	X	X	X	X	X		X			
	Temporal evolution of grain size distribution	X	X	X	X	X	X	X	X	X	X		X			
	Average particle radius, number density, and volume fraction	X	X	X	X	X	X	X	X	X	X		X			
	Matrix and precipitate composition	X	X	X	X	X	X	X	X	X	X		X			
	Estimated yield strength of your material	X	X	X	X	X	X	X	X	X	X		X			
	Time-Temperature-Precipitation (TTP) diagrams	X	X	X	X	X	X	X	X	X	X		X			
	Continuous-Cooling-Transformation (CCT) diagrams	X	X	X	X	X	X	X	X	X	X		X			

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

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

***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.

****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.

***** 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 Al- 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.

****** For ionic liquid ONLY