

## TCFE8: TCS Steel and Fe-alloys Database

Thermo-Calc Software is pleased to announce the release of TCFE8, a thermodynamic database for different kinds of steels and Fe-based alloys (stainless steels, high-speed steels, tool steels, HSLA steels, cast iron, corrosion-resistant high strength steels and more) for use with the Thermo-Calc, DICTRA and TC-PRISMA software packages. In order to increase the predictive capability of the database, several significant re-assessments have been performed by Thermo-Calc Software AB which are incorporated in the new release.

The elements Zn and Y and relevant phases associated with these elements have been added in the new TCFE8.

The element Zn has been added mainly for the purpose of galvanization process with the focus on the Zn corner of Al-Cr-Fe-Zn system for, but several other binaries and ternaries are also included. The element Y has been added mainly for the purpose of oxide dispersion strengthened (ODS) steels and the Al-Cr-Cu-Fe-Mn-Ni-O-Si-Y-Zr has been included which contains many assessed oxygen containing binary and ternary systems.

The description of Cu containing systems are improved with addition of Co-Cu, Co-Cu-Fe and Cu-Fe-Si data.

The FE2SITI\_L21 phase has been added in the database which is important for the Fe-Si-Ti precipitation hardening steels.

The LIQUID, MU\_PHASE, LAVES\_PHASE\_C14, SIGMA and L12\_FCC phases have been improved due to the modifications for the LIQUID in the Mn-O-S, Mo-Si, C-Fe-Si and C-Fe-O systems, MU\_PHASE in the Co-Nb and Co-Ta systems, LAVES\_PHASE\_C14 in Co-Mo and Cu-Fe systems, SIGMA phase in the Co-Cr, Al-Nb, Mn-Ta, Mo-V, Nb-V, Ta-Ti and Ta-V systems, and L12\_FCC in Co-V system.

The description of C-Co-Cr system has also been added for cemented carbide applications.

All necessary volume data (including molar volume and thermal expansion) has been updated for all phases in this new release. However, the molar volume data incorporated has no pressure dependence.

Some of the major improvements to the TCFE8 database include improved/added thermodynamic descriptions for the following binary, ternary and quaternary systems:

Al-Nb	Al-Y	Al-Zn	B-Y
Ca-Zn	Co-Cr	Co-Cu	Co-Mo
Co-Nb	Co-Ta	Co-V	Co-Y
Co-Zn	Cr-Y	Cr-Zn	Cu-Fe
Cu-Y	Cu-Zn	C-Y	C-Zn
Fe-Y	Fe-Zn	Mg-Zn	Mn-Ta
Mn-Zn	Mo-Si	Mo-V	Mo-Y
Mo-Zn	Nb-V	Nb-Y	Nb-Zn
Ni-Y	Ni-Zn	O-Y	P-Zn
Si-Y	Si-Zn	S-Zn	Ta-Ti

Ta-V	Ta-Y	Ti-Y	Ti-Zn
V-Y	V-Zn	W-Y	Y-Zn
Y-Zr	Al-Cr-Zn	Al-Fe-Zn	Al-Mg-Zn
Al-O-Y	Al-Si-Zn	Al-Y-Zn	C-Co-Cr
C-Co-Zn	C-Fe-O	C-Fe-Si	Co-Cu-Fe
Cr-Fe-Zn	Cr-O-Y	Cu-Fe-Si	Cu-O-Y
Fe-O-Y	Fe-Si-Ti	Mn-O-S	Mn-O-Y
Ni-O-Y	O-Si-Y	O-Y-Zr	Al-Cr-Fe-Zn
Al-Cr-O-Y	Al-Fe-O-Y	Al-O-Si-Y	Cr-Fe-O-Y
Mn-O-Y-Z			

Compared with the previous version TCFE7 the new phases in the TCFE8 database are as listed below:

A_YZN2	COZN_DELTA	MO5SI3_D8M	Y2ZN17
AL12MG17_A12	COZN_GAMMA	MOSI2_C11B	Y3SI5_HT
AL13FE4	COZN_GAMMA1	MOZN22	Y3SI5_LT
AL2CR3	COZN_GAMMA2	MOZN7	Y3ZN11
AL2FE1	COZN_HT	MSI_B27	Y5SI4
AL2Y_C15	COZN_LT	MZR3_E1A	YAG:I
AL2Y3	COZN4_GAMMA	NI17Y2	YAM:I
AL3Y_HT	CRZN17	NI2Y	YAP:I
AL3Y_LT	CU2Y_H	NI2Y3	YB12
AL5FE2	CU2Y_L	NI3Y	YB4
AL5FE4	CU4Y	NI4Y	YB6
AL7CR	CU5ZN8_GAMMA_D83	NI5Y	YB66
ALMG_BETA	CU7Y1	NI7ZR2	YC_GAMMA
ALMG_EPSILON	CU7Y2	NIY	YC2_C11A
ALMGZN_PHI	CUO	NIZN_TP2	YCUO2
ALMGZN_Q	CUPRITE_C3:I	NIZN8_DELTA	YFE2O4
ALMGZN_T1	CUZN_EPSILON	PYRITE	YSI2_HT

ALMGZN_T2	CUZR_B2	TAU4_ALCRZN	YSI2_LT
ALY	D019_CO3MO	TI2ZN	YZN
ALY2	D022_AL3NB	TIZN1	YZN12
B_YZN2	DELTA_FEZN	TIZN10	YZN3
BETA1	FE2SITI_L21	TIZN15	YZN5
CA3ZN	FE3B	TIZN2	ZETA_FEZN
CA5ZN3	GAMMA	TIZN3	ZN1ZR1
CAZN11	GAMMA_D82	TIZN5	ZN1ZR2
CAZN13	GAMMA1_FEZN	V4ZN5	ZN22ZR1
CAZN3	GAMMA2_ALFEZN	VZN3	ZN2CA
CAZN5	K_PHASE	Y13ZN58	ZN2ZR1
CO17Y2	M2O3C:I	Y15C19_H	ZN2ZR3
CO3VV	M2O3H:I	Y15C19_R	ZN39ZR5
CO3Y	MG2ZN11	Y2C3_H	ZN3P2
CO3Y2	MG2ZN3	Y2C3_R	ZN3ZR1H
CO3Y4	MG51ZN20	Y2CU2O5	ZN3ZR1L
CO5Y_D2D	MGZN	Y2S2A_Y2SI2O7	ZNCA
CO5Y8	MN2YO5	Y2S2B_Y2SI2O7	ZNP2
CO7Y6	MNTA	Y2S2D_Y2SI2O7	ZNS_ALPHA_B3
COY_BF	MNYO3_HEX	Y2S2G_Y2SI2O7	ZNS_BETA_B4
COZN_BETA1	MNZN9	Y2SIO5	ZR3Y4O12

A comprehensive list of how the different phases are modelled (number of sub-lattices and atomic ratio), and which elements/constituents they contain, can be found in the extended information flyer for the TCFE8 database. In that document validation data for various types of alloys are presented as well.