TCS Cemented Carbide Database (TCCC1)

Technical Information

Available Starting with Thermo-Calc 2015a

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About the TCS Cemented Carbide Database (TCCC)

TCS Cemented Carbide Database (TCCC) is used in applications such as cemented carbide-alloy design and processing, including heat treatment. TCCC1 includes data for molar volumes enabling the calculation of density and lattice parameters (for cubic structures), coefficients of thermal expansion and/or relative length change.

The molar volume data incorporated has no pressure dependence. It can be used with satisfactory results for cemented carbides with cobalt, iron and/or nickel binder.

TCCC1 was developed to be used with nearly our entire suite of products: Thermo-Calc, the Add-on Modules, except for the Additive Manufacturing Module, and all available SDKs.

The database does not have a corresponding mobility database.

TCCC: TCS Cemented Carbide Database Revision History. The current version of the database is TCCC1. See the link for any subversion release details.

The CALPHAD Method

The Thermo-Calc databases are developed with the CALPHAD approach based on various types of experimental data and theoretical values (e.g. those from first-principles calculations). It is based on the critical evaluation of binary, ternary, and for some databases, important higher order systems. This enables predictions to be made for multicomponent systems and alloys of industrial importance. Among these, the thermodynamic database is of fundamental importance.

Learn more on our website about the CALPHAD Method and how it is applied to the Thermo-Calc databases.

Combining Databases

It is possible to combine several databases to make calculations using Thermo-Calc. For more information related to a specific type of problem, contact one of our support specialists at info@thermocalc.com. The experts are available to make recommendations on the most suitable database to use for your needs.

TCS Cemented Carbide Database (TCCC) Resources

Information about the database is available on our website and in the Thermo-Calc software online Help.

- **Website**: On our website the information is both searchable and the database specific PDFs are available to download.
- **Online Help**: Technical database information is included with the Thermo-Calc software online Help. When in Thermo-Calc, press F1 to search for the same information as is contained in the PDF documents described. Depending on the database, there are additional examples available on the website.

Database Specific Documentation

- The *TCS Cemented Carbide Database (TCCC) Technical Information* PDF document contains version specific information such as assessed systems, a list of phases, a list of the included elements, and summaries of the database revision history by version.

Go to the Cemented Carbides Database page on our website where you can access the technical information and explore the many resources such as training courses, webinars, and Getting Started Guides.

Learn more on our website about the CALPHAD Method and how it is applied to the Thermo-Calc databases.

TCCC1 Elements, Systems, and Phases

The TCS Cemented Carbide Database (TCCC) 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

Included Elements

There are 13 elements included in the most recent version of the database.

C	Co	Cr	Fe	Mo	N	Nb	Ni	Ta	Ti
V	W	Zr							

Assessed Systems and Phases

The most recent version of the database contains:

- 77 assessed binary systems, which can be calculated with the BINARY module in Thermo-Calc Console Mode.
- 76 assessed ternary systems, mostly to their full range of composition. These can be calculated with the TERNARY module in Thermo-Calc Console Mode.
- 32 quaternaries are assessed.
- 36 phases.

TCCC1 Models for the Included Phases

In Console Mode, you can list phases and constituents in the Database (TDB) module and the Gibbs (GES) module. For some phases, supplementary information is included in the definitions. To show the information, it is recommended in the Database (TDB) module to use the command LIST_SYSTEM with the option `Constituents`.

TCCC1 Systems

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TCCC1 Assessed Binary Systems

There are 77 binary systems assessed for this database.

	C	Co	Cr	Fe	Mo	N	Nb	Ni	Ta	Ti	V	W	Zr
C													
Co	x												
Cr	x	x											
Fe	x	x	x										
Mo	x	x	x	x									
N		x	x	x	x								
Nb	x	x	x	x	x	x							
Ni	x	x	x	x	x	x	x						
Ta	x	x	x	x	x	x	x	x					
Ti	x	x	x	x	x	x	x	x	x				
V	x	x	x	x	x	x	x	x	x	x			
W	x	x	x	x	x	x	x	x	x	x	x		
Zr	x	x	x	x	x	x	x	x	x	x	x	x	

TCCC1 Assessed Ternary Systems

There are 76 ternary systems assessed for this database.

Assessed Ternary Systems				
C-Co-Cr	C-Co-Fe	C-Co-Nb	C-Co-Ni	C-Co-Ti
C-Co-W	C-Cr-Fe	C-Cr-Mo	C-Cr-N	C-Cr-Nb
C-Cr-Ni	C-Cr-Ta	C-Cr-V	C-Cr-Zr	C-Fe-Mo
C-Fe-N	C-Fe-Nb	C-Fe-Ni	C-Fe-Ti	C-Fe-V
C-Fe-W	C-Mo-N	C-Mo-Nb	C-Mo-Ta	C-Mo-Ti
C-Mo-V	C-Mo-W	C-Mo-Zr	C-Nb-Ti	C-Nb-V
C-Nb-W	C-Ni-W	C-Ni-Zr	C-N-Nb	C-N-Ti
C-N-Zr	Co-Cr-W	Co-Fe-N	Co-Fe-W	Co-Ni-W
Co-W-Zr	Cr-Fe-Mo	Cr-Fe-N	Cr-Fe-Ni	Cr-Fe-V
Cr-Fe-W	Cr-Mo-N	Cr-Mo-Ni	Cr-Ni-W	Cr-Ni-Zr
Cr-N-Ni	Cr-N-V	Cr-N-W	C-Ta-W	C-Ti-V
C-Ti-W	C-Ti-Zr	C-V-W	C-V-Zr	C-W-Zr
Fe-Mo-N	Fe-Mo-Ni	Fe-Mo-W	Fe-Nb-Zr	Fe-Ni-Ti
Fe-Ni-W	Fe-N-Nb	Fe-N-Ni	Fe-N-V	Fe-N-W
Mo-N-Ni	Mo-N-V	N-Nb-Ti	N-Nb-V	N-Ti-V
N-Ti-W				

TCCC1 Assessed Quaternary Systems

There are 32 quaternary systems assessed for this database.

Assessed Quaternary Systems			
C-Co-Cr-W	C-Co-Fe-Ni	C-Co-Fe-W	C-Co-Ni-W
C-Cr-Fe-Mo	C-Cr-Fe-N	C-Cr-Fe-Ni	C-Cr-Fe-V
C-Cr-Fe-W	C-Cr-Mo-V	C-Cr-V-W	C-Fe-Mo-V
C-Fe-Mo-W	C-Fe-Ni-W	C-N-Nb-Ta	C-N-Nb-Ti
C-N-Nb-V	C-N-Nb-W	C-N-Nb-Zr	C-N-Ta-Ti
C-N-Ta-V	C-N-Ta-W	C-N-Ta-Zr	C-N-Ti-V
C-N-Ti-W	C-N-Ti-Zr	C-N-V-W	C-N-V-Zr
C-N-W-Zr	Cr-Fe-Mo-N	Cr-Fe-N-Ni	Cr-Mo-N-Ni

TCCC1 Models for the Included Phases

Phase	*Prototype*	*Strukturbericht*	*Pearson Symbol*	*Space Group Symbol*	*SG#*	*Sublattices*	*Sites*	*Formula Unit*
GAS	Gas					1	[1.0]	(C, C1N1, C1N2_CNN, C1N2_NCN, C2, C2N1_CCN, C2N1_CNC, C2N2, C3, C3N1, C4, C4N1, C4N2, C5, C5N1, C60, C6N1, C6N2, C9N1, N, N2, N3, V, ZR, ZR2)1
LIQUID	Liquid					1	[1.0]	(C, CO, CR, FE, MO, N, NB, NI, TA, TI, V, W, ZR)1
BCC_A2	Body-Centered Cubic (W, A2, bcc)	A2	cI2	Im-3m	229	2	[1.0, 3.0]	(CO, CR, FE, MO, NB, NI, TA, TI, V, W, ZR)1(C, N, VA)3
CEMENTITE	Cementite (Fe3C, D011)	D011	oP16	Pnma	62	2	[3.0, 1.0]	(CO, CR, FE, MO, NB, NI, V, W)3(C, N)1
CHI_A12	alpha-Mn (A12)	A12	cI58	I-43m	217	3	[24.0, 10.0, 24.0]	(CR, FE, NI)24(CR, MO, W, ZR)10(CR, FE, MO, NI, W)24
CO3VV	Al3Pu		hP24	P6_3/mmc	194	2	[3.0, 1.0]	(CO, V)3(CO, V)1
CR3SI	Cr3Si (A15)	A15	cP8	Pm-3n	223	2	[3.0, 1.0]	(CO, CR, FE, MO, NB, V)3(CO, CR, NB, V)1
D019_CO3MO	Ni3Sn (D019)	D019	hP8	P6_3/mmc	194	2	[3.0, 1.0]	(CO)3(MO)1
DIAMOND_ FCC_A4	Diamond (A4)	A4	cF8	Fd-3m	227	1	[1.0]	(C)1
FCC_A1	Face-Centered Cubic (Cu, A1, fcc)	A1	cF4	Fm-3m	225	2	[1.0, 1.0]	(CO, CR, FE, MO, NB, NI, TA, TI, V, W, ZR)1(C, N, VA)1
FE4N_LP1	gama-Fe4N (L'10)	L'10	cP5	Pm-3m	221	2	[4.0, 1.0]	(CO, CR, FE, NI)4(C, N)1
FECN_CHI	Mn5C2 (Fe5C2 Hagg carbide)		mS28	C2/c	15	2	[2.2, 1.0]	(FE)2.2(C, N)1
GRAPHITE	Hexagonal Graphite (A9)	A9	hP4	P6_3/mmc	194	1	[1.0]	(C)1
G_PHASE	Th6Mn23 (D8a)	D8a	cF116	Fm-3m	225	3	[16.0, 6.0,	(CO, FE, NI, TI)16(NB, TI, ZR)6(CO, FE, NI)7

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Sublattices	Sites	Formula Unit
							7.0]	
HCP_A3	Hexagonal Close Packed (Mg, A3, hcp)	A3	hP2	P6_3/mmc	194	2	[1.0, 0.5]	(CO, CR, FE, MO, NB, NI, TA, TI, V, W, ZR)1(C, N, VA)0.5
KSI_CARBIDE	Mo6Fe11C5		mS44	C2/m	12	2	[3.0, 1.0]	(CR, FE, MO, W)3(C)1
LAVES_PHASE_C14	MgZn2 Hexagonal Laves (C14)	C14	hP12	P6_3/mmc	194	2	[2.0, 1.0]	(CO, CR, FE, MO, NB, NI, TA, TI, W, ZR)2(CO, CR, FE, MO, NB, NI, TA, TI, W, ZR)1
M12C	Fe6W6C		cF104	Fd-3m	227	3	[6.0, 6.0, 1.0]	(CO)6(W)6(C)1
M23C6	Cr23C6 (D84)	D84	cF116	Fm-3m	225	3	[20.0, 3.0, 6.0]	(CO, CR, FE, NI, V)20(CO, CR, FE, MO, NI, V, W)3(C)6
M3C2	Tongbaite (Cr3C2, D510)	D510	oP20	Pnma	62	2	[3.0, 2.0]	(CO, CR, MO, V, W)3(C)2
M5C2	Mn5C2 (Fe5C2 Hagg carbide)		mS28	C2/c	15	2	[5.0, 2.0]	(FE, V)5(C)2
M6C	Fe3W3C (E93)	E93	cF112	Fd-3m	227	4	[2.0, 2.0, 2.0, 1.0]	(CO, FE, NI)2(MO, NB, W)2(CO, CR, FE, MO, NB, NI, V, W)2(C)1
M7C3	C3Cr7 (D101)	D101	oP40	Pnma	62	2	[7.0, 3.0]	(CO, CR, FE, MO, NB, NI, V, W)7(C)3
MC_ETA	CMo		hP12	P6_3/mmc	194	2	[1.0, 1.0]	(MO, TI, V, W)1(C, VA)1
MC_SHP	Tungsten Carbide (Bh)	Bh	hP2	P-6m2	187	2	[1.0, 1.0]	(MO, W)1(C, N)1
MU_PHASE	Fe7W6 (D85) mu-phase	D85	hR13	R-3m	166	3	[7.0, 2.0, 4.0]	(CO, CR, FE, NB, NI, TA)7(MO, NB, TA, W)2(CO, CR, FE, MO, NB, NI, TA, W)4
NBNI3	beta-TiCu3 (D0a)	D0a	oP8	Pmmn	59	2	[1.0, 3.0]	(NB, NI)1(NB, NI)3
NI3TI	Ni3Ti (D024)	D024	hP16	P6_3/mmc	194	2	[0.75, 0.25]	(NI, TI)0.75(NI, TI)0.25
NITI2	NiTi2		cF96	Fd-3m	227	2	[0.3333,	(NI)0.3333(TI)0.6667

Phase	Prototype	Strukturbericht	Pearson Symbol	Space Group Symbol	SG#	Sublattices	Sites	Formula Unit
							0.6667]	
PI	beta-Mn (A13)	A13	cP20	P4_132	213	3	[12.8, 7.2, 4.0]	(CR)12.8(FE, NI)7.2(N)4
P_PHASE	Cr9Mo21Ni20		oP56	Pnma	62	3	[24.0, 20.0, 12.0]	(CR, FE, NI)24(CR, FE, MO, NI)20(MO)12
R_PHASE	R-(Co, Cr, Mo)		hR53	R-3	166	3	[27.0, 14.0, 12.0]	(CO, CR, FE, NI)27(MO, W)14(CO, CR, FE, MO, NI, W)12
SIGMA	sigma-CrFe (D8b)	D8b	tP30	P4_2/mnm	136	3	[10.0, 4.0, 16.0]	(CO, CR, FE, NI, TA, V)10(CR, MO, NB, TA, TI, V, W)4(CO, CR, FE, MO, NB, NI, TA, TI, V, W)16
TAN_EPS	TaN-eps		hP6	P-62m	189	2	[1.0, 1.0]	(TA)1(N)1
TI2N	Rutile (TiO2, C4)	C4	tP6	P4_2/mnm	136	2	[2.0, 1.0]	(TI)2(C, N)1
Z_PHASE	CrNbN		tP6	P4/nmm	129	3	[1.0, 1.0, 1.0]	(CR, FE)1(MO, NB, V)1(N, VA)1

TCCC1 Calculation Examples

The TCS Cemented Carbide Database (TCCC) 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. Below are two calculation examples for this database.

TCCC1 Assessed Systems

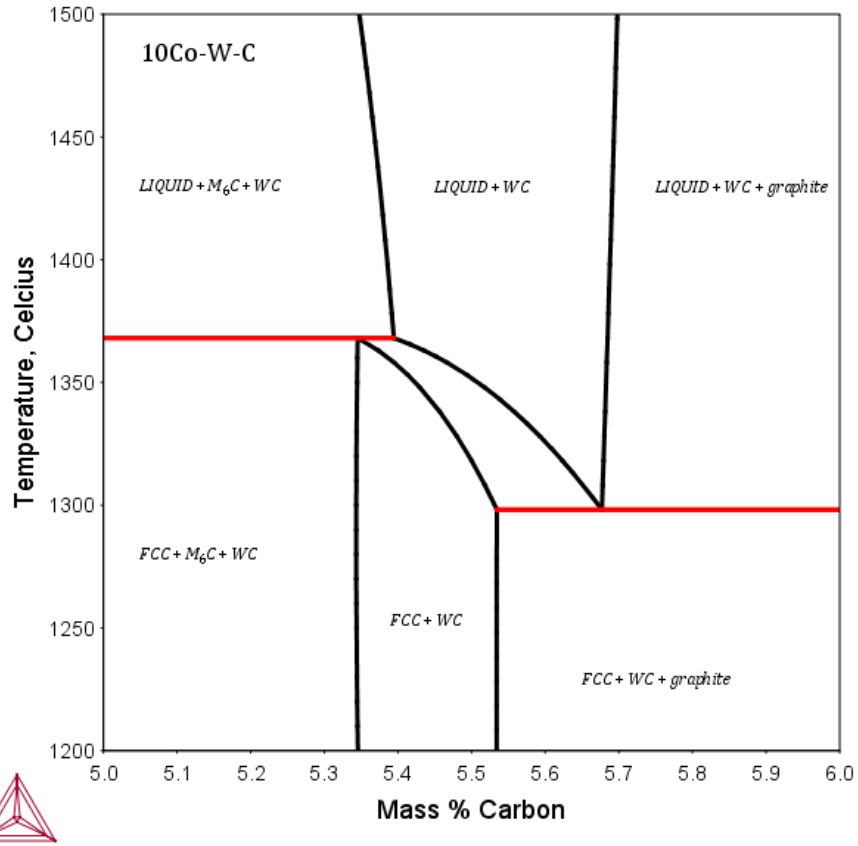

Figure 1: Phase diagram for 10w%Co-W-C.

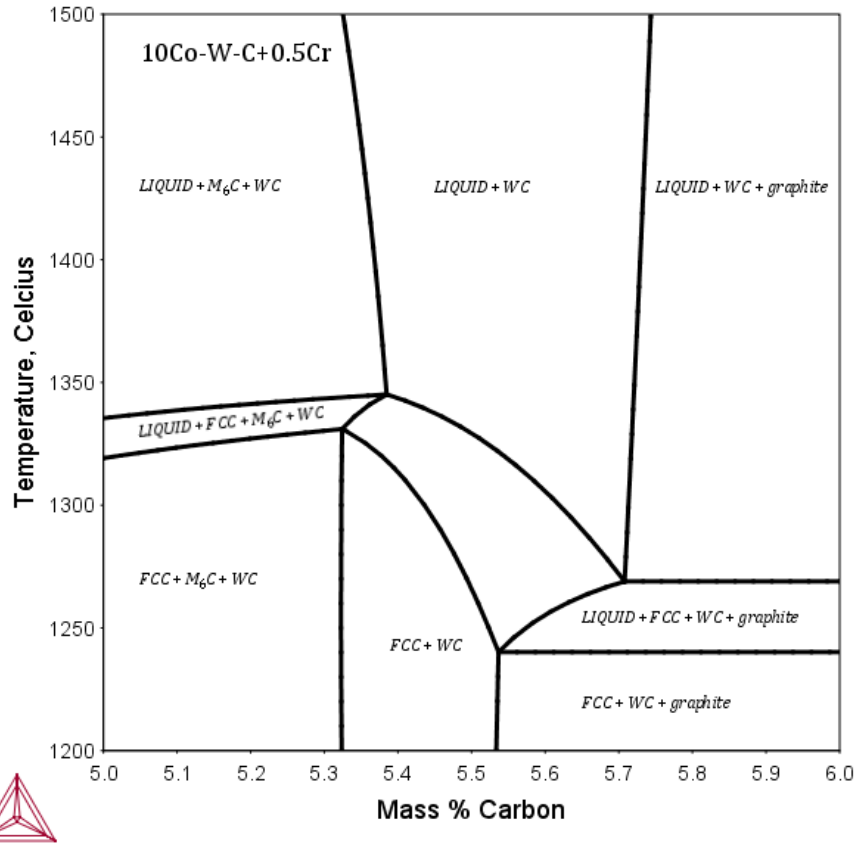

Figure 2: Phase diagram of 10w%Co-W-C with the addition of 0.5w%Cr.

Table 1. Predicted invariant temperatures of solid/liquid equilibria including WC, (cubic carbide), and graphite or M6C compared with experimental data [2001Kru; 2006Bra].

System	Invariant temperature graphite, °C	Invariant temperature M_6C, °C

	Experimental	Calculated	Experimental	Calculated
Co-W-C	1298	1298	1368	1368
+Nb	1282	1287	1345	1349
+Ta	1289	1288	1352	1348
+Ti	1289	1292	1361	1363
+Zr	1283	1291	1358	1362

References

[2001Kru] O. Kruse, B. Jansson, K. Frisk, Experimental Study of Invariant Equilibria in the Co-W-C and Co-W-C-Me (Me = Ti, Ta, Nb) Systems. J. Phase Equilibria. 22, 552–555 (2001).

[2006Bra] J. Bratberg, B. Jansson, Thermodynamic evaluation of the C−Co−W−Hf−Zr system for cemented carbides applications. J. Phase Equilibria Diffus. 27, 213–219 (2006).

TCCC: TCS Cemented Carbide Database Revision History

Current Database Version

Database name (acronym):	**TCS Cemented Carbide Database (TCCC)**
Database owner:	**Thermo-Calc Software AB**
Database version:	**1.1**
First release:	**TCCC1 was released with 2015a**

Changes in the Most Recent Database Release

TCCC1.0 to TCCC1.1

Software release 2023b Update 1 (September 2023)

- Volume description for all phases added
- Volume description for M3C2 phase updated