TCAL5 is a thermodynamic database for Al-based alloys for use with Thermo-Calc and the add-on Diffusion Module (DICTRA) and/or Precipitation Module (TC-PRISMA). TCAL5 is based on the critical evaluation of binary, ternary and important higher-order systems which enables predictions to be made for multi-component systems and alloys of industrial importance.

A hybrid approach of experiments, first-principles calculations and CALPHAD modeling has been used to obtain thermodynamic descriptions of the constituent binary and ternary systems over the whole composition and temperature ranges. The database has been validated where possible against higher-order systems and is the result of a long-term collaboration with academia that has involved extensive experimental work, theoretical calculations and critical assessments of the published literature. The database has been developed in a 35-element framework:

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In total, 258 of the binary systems in this 35-element framework have been assessed, mostly to their full range of composition, and can be calculated with the BINARY Module in Thermo-Calc. TCAL also contains assessments of 87 ternaries, and these can be calculated with the TERNARY Module in Thermo-Calc. Many quaternaries with Al as one element have also been assessed.

TCAL contains nearly 600 solution and intermetallic phases in total. The GAS phase is rejected by default when retrieving the data from the database. When this phase is required for a calculation, it has to be manually restored. Phase diagrams of assessed binary and ternary systems can be conducted using the BINARY and TERNARY modules, respectively. The complete list of phases is given at the end of this document. First there is a list of all phases and then a detailed description of their models, e.g. number of sublattices and constituents on each sublattice.

TCAL includes nearly all stable phases in the assessed systems and most important metastable phases (or precipitates) that may form in as-cast and aged Al-based alloys. The database can be used to calculate various phase diagrams and property diagrams in the assessed systems or even extrapolated higher-order systems. The extrapolation to higher-order systems helps to understand the phase equilibria in multi-component industrial aluminum alloys to be able to predict the phase formation, phase fractions and phase compositions or to calculate the driving force of forming a phase. Note that the extrapolation to higher-order systems might not be valid beyond the Al-rich region. The database can also be used for predicting solidification behaviour of Al-alloys with the SCHEIL_GULLIVER module in Thermo-Calc and simulating multi-particle precipitation during aging treatment with the add-on Precipitation Module (TC-PRISMA).

Some ordered compounds with the structure of L12 or B2 were modeled as stoichiometric phases, and named as L12_FCC and B2_BCC, respectively. The L12-type precipitate that forms in Er, Li and Sc containing aluminum alloys was modeled as Al3X, and its solubility of Ti, Zr and Mg was described. In general, however, the ordered B2 and L12 phases, together with bcc_A2 and fcc_A1, respectively, have been modeled with the so-called partition model, which describes an ordered phase and its disordered counterpart using a single Gibbs energy curve. This type of description is of particular importance to be able to predict second order transformations between a disordered phase and its ordered structures. Also note that there may be several possible composition sets for the phases.
named FCC_L12 and BCC_B2, due to the co-existence of disordered and ordered structures or the presence of miscibility gap.

**Database Revision History**

If you are interested in the revision history for this database, the information is available in the online help (from Thermo-Calc go to Help>Online Help) or in the release notes on our [website](http://www.thermocalc.com).
Assessed binary systems in full range of composition and temperature

|   | Al | Ag | B  | Be | Bi | C  | Ca | Co | Cd | Cr | Cu | Er | Fe | Ga | Ge | H  | Hf | In | K  | La | Li | Mg | Mn | Na | Ni | P  | Pb | Sc | Si | Sn | Sr | Ti | V  | Zn | Zr |
|---|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
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Assessed ternary systems, mostly in full compositional ranges

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Assessed Quaternary Systems

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Examples of Calculations

**Note**: Phase diagrams shown in this document have been calculated with various versions of the TCAL database, so small differences might be observed if they are recalculated with TCAL5. For the systems, which have been considerably or significantly improved, however, their phase diagrams should have already been updated.

![Fig.1: Calculated Al-Ni phase diagram. [Ansara et al., 1997]](image1)

![Fig.2: Calculated Al-Zn phase diagram. [an Mey, 1993]](image2)

![Fig.3: Calculated Al-Mn phase diagram. [Du et al, 2007]](image3)

![Fig.4: Calculated Al-Er phase diagram, where the Er solubility in (Al) was evaluated [Chen, 2017a]](image4)
Fig. 5: Calculated Al-Li phase diagram [Saunders, 1989 and Chen, 2012/2017b]

Fig. 6: Calculated (Al) solvi in the Al-Li system [Saunders, 1989 and Chen, 2012/2017b], in comparison with the data from [Fujikawa, 1986]

Fig. 7: Calculated Al-Fe-Si liquidus projection ($\tau_5$: $\alpha$-AlFeSi; $\tau_6$: $\beta$-AlFeSi), (a) in the Al-rich corner. The invariant points are from Pontevichi et al. (2004) and Bosselet et al (2004). The remaining data from Takeda and Mutuzaki (1940), Munson (1967) and Zakharov et al. (1988); (b) over the entire compositional range, with the data from Takeda and Mutuzaki (1940).
Fig. 8: Al-Mn-Si vertical section at 4 wt. % Si ($\beta$-AlMnSi: $\tau_8$; $\alpha$-AlMnSi: $\tau_9$) [Chen et al., 2014]

Fig. 9: Al-Fe-Mn-Si liquidus surface at 0.3 wt. % Mn. ($\alpha$-AlFeSi: $\tau_5$; $\beta$-AlFeSi: $\tau_6$; $\gamma$-AlFeSi: $\tau_7$; $\delta$-AlFeSi: $\tau_4$; $\alpha$-AlMnSi: $\tau_9$) [Chen et al., 2014a]

Fig. 10: Isothermal section of Al-Mg-Zn at 335°C. [Liang et al., 1998]

Fig. 11: Liquidus projection with isothermal lines in the Cu–Mn–Ni system. [Sun et al., 2009]
Fig. 12: Al-Sn-Zn isothermal section at 300°C [Chen, 2017c]

Fig. 13: Al-Sn-Zn Liquidus surface projection with isotherms [Chen, 2017c]

Fig. 14: Calculated Al-Si-Sn isothermal sections at 536 °C, 544 °C and 550 °C [Chen, 2017c], with data read from Schmid-Fetzer (1993)

Fig. 15: Al-Ce-Mg isothermal section at 400 °C [Chen, 2017d]
Fig. 16: Equilibrium solidification and Scheil solidification simulations of alloy AA7075, compared with experimental result [Backerud, et al., 1990]. (Al), Al13Fe4, Mg2Si, T-Phase and V-Phase (MgZn2) are found in the microstructure as predicted from the calculation. Al45Cr7 forms primarily as a Cr-bearing phase, which may have been overlooked in experimental investigation due to its small amount. S-Phase was shown at the late stage of the Scheil solidification and its amount is small. Al2Cu was experimentally observed but not shown in the calculation.

Fig. 17: Equilibrium solidification and Scheil solidification simulations of alloy 204.2, compared with experimental result [Backerud, et al., 1990]. (Al), Al13Fe4, Al7Cu2Fe and Al2Cu are found in the microstructure as predicted from the calculations. Al3Ti appeared as the primary phase since this alloy contains 0.22 wt. % Ti.
Fig. 18: Calculated isothermal sections of the Al-Cu-Mg-Zn system at 460°C: at 8 wt.% Zn [Chen, 2012b] (experimental data are from Strawbridge et al., 1947).

Fig. 19: Calculated isothermal sections of the Al-Cu-Mg-Zn system at 90 wt.% Al (experimental data are from Wright, n.d.).
Fig. 20: Calculated molar volumes of the Al-X (X=Li, Mg, Si, Zn) fcc_A1 phase.

Fig. 21: Calculated densities of pure Al and Al-Si alloys versus the temperature, in comparison with experimental data from Magnusson and Arnberg (2001).
Fig. 22: Calculated volume thermal expansivity for Al₃Sc, Al₃Ti and Al₃Zr [Chen, 2017e]

Fig. 23: Lattice mismatch between Al₃Sc and (Al), at different Zr contents and temperatures [Chen, 2017e]

Fig. 24: Calculated Al-rich Al-Cr binary phase diagram. Experimental data are from Fink and Freche (1933), Raynor and Little (1945) and Eremenko et al., (1980).
Fig. 25: Calculated Al-rich Al-V binary phase diagram. Experimental data were read from Gong et al. (2004).

Fig. 26: Calculated Al-Cu (Al) solvus curves equilibrated with $\theta$, $\Omega$, $\theta'$, $\theta''$ (or GPII zones) and GPI zones, respectively. A metastable miscibility gap of fcc_A1 is shown. The GPI zones were modeled as the second composition set of fcc_A1, i.e. fcc_A1#2. It is assumed that experimentally observed GPI zones are usually tiny (say $< 3$ nm), so the interfacial and elastic energy are considered. The line for GPI zones was calculated with adding +800 J/mole-atoms to the energy of fcc_A1#2 [Chen, 2014b]
Fig. 27: Calculated fcc_A1 solvi in alloys at 0.73 at.% Si and varying Mg content, relative to different Al-Mg-Si precipitates, including the stable $\beta$-Mg$_2$Si phase, pre-$\beta$ precipitates ($\beta'$, U1, U2 and B') and the pre-$\beta'$ precipitate, i.e. $\beta''$. The symbols indicate certain precipitates have been experimentally observed in alloys of given compositions and aged at given temperatures [Chen, 2014b].

Fig. 28: Scheil solidification of an A206 alloy (Al-4.58Cu-0.28Mg-0.51Fe-0.07Si-0.003Mn, wt.%) with the Al$_3$Fe$_4$ phase suspended [Chen, 2014b]. According Liu et al. (2012), the metastable Al$_m$Fe phase formed after (Al) during the solidification. The phase formation sequence and phase transformation temperatures can be well accounted for with this calculation.
References


[2017a, Chen] H.-L. Chen, "Thermodynamic modeling of the Er-X (X = Ag, Al, Fe, Si, Zr) binary and Al-Er-X (X=Cu, Fe, Mg) ternary systems", unpublished work, 2017a.


[2017d, Chen] H.-L. Chen, "Thermodynamic modeling of the Al-Ce-X (X = Cr, Fe, Mg, Mn, Ni, Si) ternary systems", unpublished work, 2017d.

Phases included in TCAL5

The elements in phase names are rearranged in the alphabetical order except for carbides and borides, where B and C appear at the end. In order to designate the high-temperature and the low-temperature modifications of a phase, respectively, suffixes of “_HT” and “_LT” are used instead of using prefixes of “alpha-”, “beta-” or “gamma”.

One can list phases and constituents in the Database module and the GES module. For some phases, supplementary information has been included in their definitions. In order to show the information, it is recommended to use “List-System” or “List-Database” with the option of “Constituents” in the Database module.

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> Si2Zr, Ge2Zr

SI2TI_C54: 2 2 1
> Ge2Ti, Si2Ti, Sn2Zr

ZRM5_C15B: 2 5 1
> Cu5Zr, Ni5Zr

FEM_B35: 2 1 1
> FeSn, FeGe

SN5TI6_OI44: 2 5 6
> Sn5Ti6, Si5V6, Ge5Ti6

M7C3_D101: 2 7 3
> Cr7C3, Mn7C3

M23C6_D84: 2 23 6
> Cr23C6, Mn23C6, Mn23SC6

V_PHASE: 3 5 6 2
> solution of Mg2Zn11, Al5Cu6Mg2; aka Z

AGER: 2 1 1

AG2ER: 2 2 1

AG51ER14: 2 0.77 0.23

AGLA: 2 1 1

AG2LA: 2 1 2

AG51LA14: 2 14 51
ALCU_ZETA  2   9  11  > a Al-Mg-Zn ternary phase known as PHI
:AL:CU FE :

GAMMA_D83  3   4  1  8  AL12MN  2   12  1
:AL FE NI SI ZN:AL CU NI SI ZN:AG CU MN
:AL:MN :
FE NI ZN :
> solution between Al8Cu5 (rt) and Cu5Zn8

GAMMA_H   3   4  1  8  AL6MN  2   6  1
:AL ZN:AL CU ZN:CU MN FE NI :
> Cu5Zn8-type Al8Cu5 (ht) phase
:AL ZN:MN FE :

ALER       2   0.5 0.5  AL4MN_R  2 0.81162 0.18838
:AL MG:ER :

AL2ER3  2   0.4 0.6  AL11MN4_LT  2  11.4
:AL MG:ER :

ALER2  2   0.33333 0.66667  AL11MN4_HT  2  29 10
:AL MG:ER :

AL2FE1  2   2  1  AL8MN5  3   12.5 9
:AL CU SI ZN:FE MN NI :
:AL ZN:MN:AL MN SI CU :

AL5FE2  2   5  2  AL3NI_D011  2  0.75 0.25
:AL CU SI ZN:FE MN NI :
:AL MN NI:FE NI B C :

AL5FE4  2   0.5 0.5  AL3NI2  3   3  2  1
:AL CU FE MN :
:AL SI ZN:AL CU FE MG NI:NI VA :

AL13FE4  3  0.6275 0.235 0.1375  AL3NI5  2  0.375 0.625
:AL CU:FE MN NI ZN:AL SI VA ZN :
:AL NI :
> solution phases based on Al13Fe4, aka Al3Fe

AL4FE  2   4.2 1  CA2CU  2  2 1
:AL:FE :
:CA:CU :

ALMG_BETA  2   89 140  CACU  2  1 1
:MG LI:AL ZN :
:CA:CU :

ALMG_EPS  2   23 30  HCP_CA  2  1 0.5
:MG:AL ZN :
:CA:H VA :

ALMG_GAMMA  3  5 12 12  CAH2_LT  2 12
:LI MG:AL MG ZN:AL MG ZN :
:CA:H :

ALMGZN_PHI  2   6  5  CAH2_HT  2 12
:MG:AL ZN :
:CA:H :

ALMGZN_PHI  2   6  5  CAH2_HT  2 12
:MG:AL ZN :
:CA:H :

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FESI_B20 2 1 1

> FeSi, MnSi, CrSi, CrGe

> Mn5Si3, Cr3Si5, Fe5Si3, Ge3Mn5, Ge3Zr5, Si3Zr5, Sn3Ti5

MN5Si3_D88 2 5 3

> Mn5Si3, Cr3Si5, Fe5Si3, Ge3Mn5, Ge3Zr5, Si3Zr5, Sn3Ti5

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LA2NI7_LT 2 2 7

LA2NI7_HT 2 2 7

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LA5SI4 2 0.5556 0.4444

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LA2NI2_A2 2 0.3333 0.6667

LAZN2 2 0.333 0.667

LAZN4 2 0.2 0.8

LAZN5 2 0.1667 0.8333
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:Ni:HF :

Ni10HF7 2 0.588 0.412
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Ni11HF9 2 0.55 0.45
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NiHF_HT 2 0.5 0.5
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HF2Si 2 0.6666667 0.3333333
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HF3Si2 2 0.6 0.4
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HF5Si3 2 0.625 0.375
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HFi 2 0.5 0.5
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HFSi2 2 0.333333 0.666667
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> L12 phase, Ni3Si.rt, AlZr3, GeNi3, TiZn3, VZn3

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NiSi_B31 2 1 1
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AL4C3 2 4 3
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AL5Cr 2 5 1
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AL4Cr 2 1 4
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GAMMA_D810 3 12 5 9
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| AL11CU5MN3 | 3 | 11 3 5 |
| :AL:MN:CU : | | |
| ALCU3MN2 | 3 | 1 2 3 |
| :AL:MN:CU : | | |
| AL7CU4NI | 2 | 1 1 |
| :AL:FE CU NI VA : | | |
| ALCUSC_TAU | 3 | 0.6154 0.3077 |
| 7.69E-2 | | |
| :AL CU:AL CU:SC : | | |

| AL6ER2FE11 | 3 | 6 2 11 |
| :AL:ER:FE : | | |
| AL7ERMG2 | 3 | 0.66667 0.1 0.23333 |
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| AL9FENI | 2 | 9 2 |
| :AL:FE NI : | | |
| AL10FE3NI | 2 | 5 2 |
| :AL:FE NI : | | |
| AL71FE5NI24 | 3 | 0.71 5E-2 0.24 |
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| ALFESI_T1 | 2 | 5 3 |
| :AL SI:FE : | | |
| > Al-Fe-Si ternary phase, tao 1 / tao 9 |

| ALFESI_T2 | 4 | 0.5 0.2 0.1 0.2 |
| :AL:FE:SI:AL SI : | | |
| > Al-Fe-Si ternary phase, tao 2, |
| gamma_AlFeSi |

| ALFESI_T3 | 3 | 0.56 0.24 0.2 |
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| > Al-Fe-Si ternary phase, AL56FE24SI10, tao 3 |

| ALFESI_T4 | 4 | 0.4166 0.1667 0.25 |
| :AL:FE:SI:AL SI : | | |
| > Al-Fe-Si ternary phase, tao 4, delta_AlFeSi |
| AL8FE2SI | 4 | 0.6612 0.19 4.96E-2 |
| 9.92E-2 | | |
| :AL:FE:SI:AL SI : | | |
| > solution of the Al-Fe-Si ternary phase, tao 5, alpha_AlFeSi |

| AL9FE2SI2 | 4 | 0.598 0.152 0.1 0.15 |
| :AL:FE:SI:AL SI : | | |
| > Al-Fe-Si ternary phase, tao 6, aka Al5FeSi, beta_AlFeSi |

| ALFESI_T7 | 2 | 3 1 |
| :AL SI:FE : | | |
| > Al-Fe-Si ternary phase, AL9FE5SI6, tao 7 |

| ALFESI_T8 | 2 | 2 1 |
| :AL SI:FE : | | |
| > Al-Fe-Si ternary phase, AL2FE3SI4, tao 8 |

| ALFESI_T9 | 3 | 0.6 0.25 0.15 |
| :AL:FE:SI : | | |
| > Al-Fe-Si ternary phase, AL60FE25SI15, tao 10 |

| ALFESI_T10 | 3 | 0.65 0.25 0.1 |
| :AL:FE:SI : | | |
| > Al-Fe-Si ternary phase, AL85FE30SI15, tao 11 |

| ALFEZN_GAMMA | 2 | 0.255 0.745 |
| :AL FE ZN:ZN : | | |
| > Al-Fe-Zn ternary phase, aka gamma 2, no detailed structure |

| ALFESI_T11 | 3 | 0.65 0.25 0.1 |
| :AL:FE:SI : | | |
| > Al-Fe-Si ternary phase, AL85FE30SI15, tao 11 |

| ALLIMG_T | 3 | 0.53 0.33 0.14 |
| :AL:LI:MG : | | |

| ALLISI | 3 | 0.333333 0.333333 |
| :LI:AL:SI : | | |
| 0.333334 |

<p>| AL3LI8SI5 | 3 | 0.5 0.1875 0.3125 |
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**MNNISI_T5**
:MN:NI:SI:
> Mn-Ni-Si ternary phase, T5 or "tao 1"

**MNNISI_T6**
:MN:NI:SI:
> Mn-Ni-Si ternary phase, T6 or "tao 2"

**MN3NI2SI**
:MN:NI:SI:
> Mn-Ni-Si ternary phase, T7 or Omega

**MN2NI5SI**
:MN:NI:SI:
> Mn-Ni-Si ternary phase, T8 or S

**MN6NI5SI3**
:MN:NI:SI:
> Mn-Ni-Si ternary phase, T9 or R

**MN66NI4SI30**
:MN:NI:SI:
> Mn-Ni-Si ternary phase, T10 or U

**MN52NI29SI19**
:MN:NI:SI:
> Mn-Ni-Si ternary phase, T11 or W

**MN7NI7ZN86**
:MN:NI:ZN:

**NI2SIZN_T1**
:NI:SI:ZN:

**NI9SI2ZN_T2**
:NI:SI:ZN:

**NI2SIZN3_T3**
:NI:SI:ZN:

**NISIZN_T4**
:NI:SI:ZN:

**Q_ALCUMGS1**
:AL:CU:MG:SI:
> Quaternary phase, aka Q, Al5Cu2Mg8Si6, Al3Cu2Mg9Si7 & Al4Cu2Mg8Si7

**AL18FE2MG7SI10**
:AL:FE:MG:SI:
> Quaternary phase, aka Al8FeMg3Si6 and Q_/PHI/H_PHASE