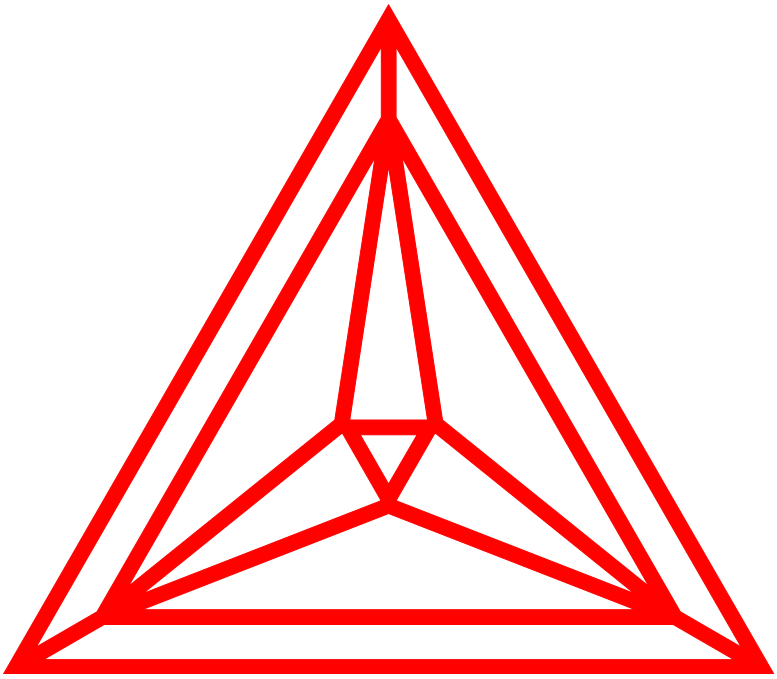
TC-API

Version 7.0

Programmer's Guide



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Chapter 1

Thermo-Calc c-api 6

The main part of this manual is a technical description of the TCAPI. To find details on the Thermodynamic applications of each library function see the section on tcapi.h.

1.1 Installed files

In the distribution of Thermo-Calc c-api 6, the following folders and files can be found.

1.1.1 TCAPI libraries.

These could be .lib, .dll, .so -files depending on your installation.

E.g. on a 64 bit Windows system you will find:

tcapi-win-x64-6.dll and tcapi-win-x64-6.lib

1.1.2 Source folder.

This is the c code for running the the different examples. Some of this code can be reused in user-written projects.

1.1.3 Project folders for building the example code

Linux:

-> Linux/Linux-Dynamic-Linking

-> Linux/Linux-Explicit-Loading

Windows:

-> Windows-Mingw32-Explicit-Loading

-> Windows-Studio-Project-Dynamic-Linking

-> Windows-Studio-Project-Explicit-Loading

1.2 Explicit loading or Dynamic linking

When using Dynamic Linking, the libraries (.so or .lib) and the header-files of the tcapi are needed when the program is being built.

When using Explicit Loading no libraries are needed for the build. They are loaded at runtime (.so or .dll).

1.3 About the source code

1.3.1 For dynamic linking

Simple thermodynmic calculations to demonstrate the use of this api.

example1.c

example2.c

example3.c

Utility functions for finding the correct environment variables

tcutils.c

tcutils.h

Declarations and documentation on all TC-API functions

tcapi.h

Thermo-Calc proprietary declarations and definitions. DO NOT EDIT. tc_data_defs.h

1.3.2 For explicit loading

Utilities to simplify working with explicitly loaded dll. libtc.c

libtc.h

Simple thermodynmic calculations to demonstrate the use of this api.

tcExamples.c

tcExamples.h

Main program to exemplify hos this api can be used

tcMain.c

Utility functions for finding the correct environment variables

tcutils.c

tcutils.h

Thermo-Calc proprietary declarations and definitions. DO NOT EDIT.

tc_data_defs.h

1.4 When starting developing proprietary projects the following code is needed

1.4.1 For dynamic linking

tcapi.h

tc_data_defs.h

1.4.2 For explicit loading

libtc.c

libtc.h

tc_data_defs.h

(tcMain.c can give an idea of how the above files can be used)

Chapter 2

Data Structure Index

2.1 Data Structures

Here are the data structures with brief descriptions:

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Chapter 3

File Index

3.1 File List

Here is a list of all documented files with brief descriptions:

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source/tcutils.h . . . 18

Chapter 4

Data Structure Documentation

4.1 _tc_function_library Struct Reference

`#include <libtc.h>`

4.1.1 Detailed Description

Data structure that holds the published and supported functions of the Thermo-Calc api.

This datastructure and it's descriptions is mostly of technical interest. For documentation of each function see tcapi.h

The documentation for this struct was generated from the following file:

- source/libtc.h

Chapter 5

File Documentation

5.1 source/example1.c File Reference

```
#include <stdio.h>
#include <string.h>
#include "tcapi.h"
#include "tcutils.h"
```

5.1.1 Detailed Description

Basic api example that calculates an equilibrium in the Fe-Cr-C system and retrieves certain quantities.

5.2 source/example2.c File Reference

```
#include <stdio.h>
#include <string.h>
#include "tcapi.h"
#include "tcutils.h"
```

5.2.1 Detailed Description

Basic api example that calculates an equilibrium in the Fe-Cr-C system and retrieves certain quantities.

5.3 source/example3.c File Reference

```
#include <stdio.h>
#include <string.h>
#include "tcapi.h"
#include "tcutils.h"
```

5.3.1 Detailed Description

Shows how to display certain values in arrays.

5.4 source/libtc.h File Reference

```
#include "tc_data_defs.h"
#include <dlfcn.h>
#include <errno.h>
#include <string.h>
```

Data Structures

- struct _tc_function_library

Typedefs

- typedef struct _tc_function_library tc_function_library

Functions

- int importFunctions (TCHANDLE tcHandle, tc_function_library *tc, char *message)

5.4.1 Detailed Description

This file contains pointers and Definitions of the published and supported Thermo-Calc functions so that it is easier to use them when explicitly loading the dll. It is all contained in one data structure _tc_function_library

For documentation of each function see tcapi.h

5.4.2 Typedef Documentation

5.4.2.1 typedef struct _tc_function_library tc_function_library

Data structure that holds the published and supported functions of the Thermo-Calc api.

This datastructure and it's descriptions is mostly of technical interest. For documentation of each function see tcapi.h

5.4.3 Function Documentation

5.4.3.1 int importFunctions (TCHANDLE *tcHandle,* tc_function_library * *tc,* char * *message*)

TCHANDLE tcHandle Handle to shared library

tc_function_library* tc pointer to data structure that holds functions. Must be allocated by caller.

char* message Error message. Must be allocated by caller.

Call this function to import functions from library.

The shared library must be loaded prior to calling this function.

The tc_function_library* tc must be allocated by caller.

5.5 source/tcapi.h File Reference

```
#include "tc_data_defs.h"
```

Functions

- void tc_append_database (TC_STRING name)
- TC_BOOL tc_check_license (TC_STRING name, TC_STRING message, TC_STRING_LENGTH strlen_message)
- TC_STRING tc_component_status (TC_STRING component_name)
- void tc_compute_equilibrium ()
- void tc_create_new_equilibrium (TC_INT equilibrium)
- TC_INT tc_database (TC_STRING datan, TC_INT linelen)
- void tc_define_components (TC_STRING component_name, TC_INT strlen, TC_INT number_of_components)
- TC_INT tc_degrees_of_freedom ()
- void tc_delete_condition (TC_STRING condition)
- void tc_delete_symbol (TC_STRING symbol)
- TC_INT tc_element (TC_STRING elements, TC_INT linelen)
- void tc_element_reject (TC_STRING element_name)
- void tc_element_select (TC_STRING element_name)
- void tc_enter_ges5_parameter (TC_STRING parameter, TC_STRING expression)
- void tc_enter_symbol (TC_STRING symbol, TC_STRING type, TC_INT argument_type, TC_INT integer_argument, TC_FLOAT double_argument, TC_STRING string_argument)
- TC_BOOL tc_error (TC_INT *error_number, TC_STRING message, TC_INT strlen)
- void tc_ges5 (TC_STRING command)
- void tc_get_data ()
- void tc_get_derivatives (TC_STRING phase_name, TC_FLOAT *arr1, TC_FLOAT *arr2)
- void tc_get_ges5_parameter (TC_STRING parameter, TC_STRING expression, TC_INT strlenExpression)
- TC_FLOAT tc_get_value (TC_STRING symbol)
- TC_INT tc_init_root ()
- TC_INT tc_init_root3 (TC_STRING tmppath, TC_STRING tcpath)
- TC_INT tc_list_component (TC_STRING component_name, TC_INT strlen)
- TC_INT tc_list_conditions (TC_STRING conditions, TC_INT strlen)
- TC_INT tc_list_phase (TC_STRING phase_name, TC_INT strlen)
- TC_INT tc_list_species (TC_STRING species_name, TC_INT strlen)
- TC_INT tc_list_symbols (TC_STRING symbols, TC_INT strlen, TC_INT *type)
- void tc_open_database (TC_STRING name)
- TC_INT tc_phase (TC_STRING phases, TC_INT linelen)
- TC_INT tc_phase_all_constituents (TC_STRING phase_name, TC_INT *constituent_array, TC_STRING element_array, TC_INT strLenElem, TC_FLOAT *number_of_sites)
- TC_INT tc_phase_constituents (TC_STRING phase_name, TC_INT *constituent_array, TC_STRING element_array, TC_INT strLenElem, TC_FLOAT *number_of_sites)
- void tc_phase_reject (TC_STRING phase_name)
- void tc_phase_select (TC_STRING phase_name)
- TC_STRING tc_phase_status (TC_STRING phase_name)
- TC_INT tc_phase_structure (TC_STRING phase_name, TC_INT *constituent_array, TC_STRING species_array, TC_STRING_LENGTH strLenSpecies, TC_FLOAT *number_of_sites)
- void tc_poly3 (TC_STRING command)
- void tc_read_poly3_file (TC_STRING filename)
- void tc_reject_constituent (TC_STRING phase_name, TC_INT sublattice, TC_STRING constituent)
- void tc_reset_error ()
- void tc_restore_constituent (TC_STRING phase_name, TC_INT sublattice, TC_STRING constituent)

- void tc_save_poly3_file (TC_STRING filename)
- void tc_select_equilibrium (TC_INT equilibrium)
- void tc_set_component_status (TC_STRING component_name, TC_STRING status)
- void tc_set_condition (TC_STRING condition, TC_FLOAT value)
- void tc_set_minimization_option (TC_INT *global_flag, TC_INT *max_gridpoints, TC_INT *frequency, TC_INT *mesh_flag)
- void tc_set_phase_addition (TC_STRING phase_name, TC_FLOAT addition)
- void tc_set_phase_status (TC_STRING phase_name, TC_STRING status, TC_FLOAT value)
- void tc_set_start_value (TC_STRING state_variable, TC_FLOAT starting_value)
- TC_STRING tc_species_status (TC_STRING species_name)
- void tc_version (TC_STRING str, TC_INT str_len)

5.5.1 Detailed Description

Complete description of the available functions in the TCAPI.

5.5.2 Function Documentation

5.5.2.1 void tc_append_database (TC_STRING *name*)

Appends the named database

5.5.2.2 TC_BOOL tc_check_license (TC_STRING *name*, TC_STRING *message*, TC_STRING_LENGTH *strlen_message*)

Returns true if the checked license is available and valid, currently accepts: TC_DLL, TC_GUI and TC_TC4U

5.5.2.3 TC_STRING tc_component_status (TC_STRING *component_name*)

Returns the status of "component_name" where status may be one of "ENTERED" or "SUSPENDED"

5.5.2.4 void tc_compute_equilibrium ( )

Computes the equilibrium in POLY-3 using the currently set conditions

5.5.2.5 void tc_create_new_equilibrium (TC_INT *equilibrium*)

Creates a new equilibrium in POLY-3 with number "equilibrium number".

5.5.2.6 TC_INT tc_database (TC_STRING *datan*, TC_INT *linelen*)

Returns the number of databases in the system and their names in "names_of_databases"

5.5.2.7 void tc_define_components (TC_STRING *component_name*, TC_INT *strlen*, TC_INT *number_of_components*)

Redefines the components in the system to the components in "component_name".

5.5.2.8 TC_INT tc_degrees_of_freedom ( )

Returns the degrees of freedom in the system. This must be zero in order to perform an equilibrium calculation.

5.5.2.9 void tc_delete_condition (TC_STRING *condition*)

Deletes the condition for the expression in "condition".

5.5.2.10 void tc_delete_symbol (TC_STRING *symbol*)

Deletes a symbol in the system.

5.5.2.11 TC_INT tc_element (TC_STRING *elements,* TC_INT *linelen*)

Returns the number of elements in the database and their names in "elements"

5.5.2.12 void tc_element_reject (TC_STRING *element_name*)

Rejects "element name" in the currently selected database.

5.5.2.13 void tc_element_select (TC_STRING *element_name*)

Selects "element name" in the currently selected database.

5.5.2.14 void tc_enter_ges5_parameter (TC_STRING *parameter,* TC_STRING *expression*)

Enters a parameter expression

5.5.2.15 void tc_enter_symbol (TC_STRING *symbol,* TC_STRING *type,* TC_INT *argument_type,* TC_INT *integer_argument,* TC_FLOAT *double_argument,* TC_STRING *string_argument*)

Enters a symbol in the system, the symbol type may be one of "CONSTANT", "VARIABLE", "FUNCTION" or "TABLE", "argument type" defines which of the following arguments will be used, 1 indicates the integer argument, 2 the double argument and 3 the string argument.

5.5.2.16 TC_BOOL tc_error (TC_INT * *error_number,* TC_STRING *message,* TC_INT *strlen*)

Returns true if an error has been set, returning the error number in "error number" and its corresponding message in "error message"

5.5.2.17 void tc_ges5 (TC_STRING *command*)

Sends a command to the GES5 module as defined in the argument "command"

5.5.2.18 void tc_get_data ( )

Executes the database command "GET_DATA"

5.5.2.19 void tc_get_derivatives (TC_STRING *phase_name,* TC_FLOAT * *arr1,* TC_FLOAT * *arr2*)

Returns Gm and the first derivatives with respect to site-fractions in "arr1" and the second derivatives in "arr2" as GM.Y1.Y1, GM.Y1.Y2, GM.Y2.Y2, GM.Y1.Y3, GM.Y2.Y3 ... GM.YN.YN

5.5.2.20 void tc_get_ges5_parameter (TC_STRING *parameter,* TC_STRING *expression,* TC_INT *strlenExpression*)

Retrieves the expression of a parameter name

5.5.2.21 TC_FLOAT tc_get_value (TC_STRING *symbol*)

Retrieves the symbol or state variable value from the POLY-3 module.

5.5.2.22 TC_INT tc_init_root ( )

Initializes the Thermo-Calc system, must be called prior to anything else.

5.5.2.23 TC_INT tc_init_root3 (TC_STRING *tmppath,* TC_STRING *tcpath*)

Initializes the Thermo-Calc system, must be called prior to anything else. tmppath Path to directory for log file tcpath Path to Thermo-Calc installation (Used to find databases)

5.5.2.24 TC_INT tc_list_component (TC_STRING *component_name,* TC_INT *strlen*)

Returns the number of components in the system and their names in "component_name".

5.5.2.25 TC_INT tc_list_conditions (TC_STRING *conditions,* TC_INT *strlen*)

Returns the number of conditions set and their values in "conditions"

5.5.2.26 TC_INT tc_list_phase (TC_STRING *phase_name,* TC_INT *strlen*)

Returns the number of phases in the system and their names in "phase_name".

5.5.2.27 TC_INT tc_list_species (TC_STRING *species_name,* TC_INT *strlen*)

Returns the number of species in the system and their names in "species_name".

5.5.2.28 TC_INT tc_list_symbols (TC_STRING *symbols,* TC_INT *strlen,* TC_INT * *type*)

Returns the number of defined symbols in the system with their expression and value in "symbols" and their corresponding type in "type of symbol", where the type may be one of 1="CONSTANT", 2="VARIABLE" 3="FUNCTION" 4="TABLE"

5.5.2.29 void tc_open_database (TC_STRING *name*)

Opens the named database "name_of_database"

5.5.2.30 TC_INT tc_phase (TC_STRING *phases,* TC_INT *linelen*)

Returns the number of phases in the system with the selected elements. NOTE: the routine returns the number of all available phases.

5.5.2.31 TC_INT tc_phase_all_constituents (TC_STRING *phase_name,* TC_INT * *constituent_array,* TC_STRING *element_array,* TC_INT *strLenElem,* TC_FLOAT * *number_of_sites*)

Returns the number of sublattices in the phase (including phases with the status SUSPENDED), the number of constituents on each sublattice in "constituents", the name of the selected species on each sublattice one after each other in "species names" and the "number of sites" on each sublattice.

5.5.2.32 TC_INT tc_phase_constituents (TC_STRING *phase_name,* TC_INT * *constituent_array,* TC_STRING *element_array,* TC_INT *strLenElem,* TC_FLOAT * *number_of_sites*)

Returns the number of sublattices in the phase, the number of constituents on each sublattice in "constituents", the name of the selected species on each sublattice one after each other in "species names" and the "number of sites" on each sublattice.

5.5.2.33 void tc_phase_reject (TC_STRING *phase_name*)

Rejects the phase in "phase_name"

5.5.2.34 void tc_phase_select (TC_STRING *phase_name*)

Selects the phase in "phase_name"

5.5.2.35 TC_STRING tc_phase_status (TC_STRING *phase_name*)

Returns the status of "phase_name" where status may be one of "FIXED", "SUSPENDED" or "ENTERED"

5.5.2.36 TC_INT tc_phase_structure (TC_STRING *phase_name,* TC_INT * *constituent_array,* TC_STRING *species_array,* TC_STRING_LENGTH *strLenSpecies,* TC_FLOAT * *number_of_sites*)

Returns the number of sublattices in the phase, the number of constituents on each sublattice in "constituents", the name of the species on each sublattice one after each other in "species names" and the number of sites in "number of sites".

5.5.2.37 void tc_poly3 (TC_STRING *command*)

Sends a command to POLY-3 module as defined in the argument "command"

5.5.2.38 void tc_read_poly3_file (TC_STRING *filename*)

Loads the workspace from file "filename" in POLY-3.

5.5.2.39 void tc_reject_constituent (TC_STRING *phase_name,* TC_INT *sublattice,* TC_STRING *constituent*)

Rejects the constituent "constituent" on sublattice "sublattiice" from phase "phase_name".

5.5.2.40 void tc_reset_error ( )

Resets the error if an error has been set

5.5.2.41 void tc_restore_constituent (TC_STRING *phase_name,* TC_INT *sublattice,* TC_STRING *constituent*)

Restores the constituent "constituent" on sublattice "sublattiice" from phase "phase_name".

5.5.2.42 void tc_save_poly3_file (TC_STRING *filename*)

Stores/overwrites the current workspace in POLY-3 on the file "filename".

5.5.2.43 void tc_select_equilibrium (TC_INT *equilibrium*)

Selects an equilibrium in POLY-3 with number "equilibrium number".

5.5.2.44 void tc_set_component_status (TC_STRING *component_name,* TC_STRING *status*)

Sets the status of "component_name" to "status" to one of "ENTERED" or "SUSPENDED"

5.5.2.45 void tc_set_condition (TC_STRING *condition,* TC_FLOAT *value*)

Sets a condition for the expression in "condition" to value in "value".

5.5.2.46 void tc_set_minimization_option (TC_INT * *global_flag,* TC_INT * *max_gridpoints,* TC_INT * *frequency,* TC_INT * *mesh_flag*)

Sets parameters for global minimization

5.5.2.47 void tc_set_phase_addition (TC_STRING *phase_name,* TC_FLOAT *addition*)

Sets the addition "addition" to the Gibbs

5.5.2.48 void tc_set_phase_status (TC_STRING *phase_name,* TC_STRING *status,* TC_FLOAT *value*)

Sets the status of "phase_name" to "status" to one of "FIXED", "SUSPENDED", DORMANT" or "ENTERED".

5.5.2.49 void tc_set_start_value (TC_STRING *state_variable,* TC_FLOAT *starting_value*)

Sets a starting value for the "state variable" to "start value".

5.5.2.50 TC_STRING tc_species_status (TC_STRING *species_name*)

Returns the status of "species_name" where status may be one of "ENTERED" or "SUSPENDED"

5.5.2.51 void tc_version (TC_STRING *str,* TC_INT *str_len*)

Returns the version of Thermo-Calc in "version_name"

5.6 source/tcExamples.h File Reference

```
#include "libtc.h"
```

Functions

- void example1 (tc_function_library *tc)
- void example2 (tc_function_library *tc)
- void example3 (tc_function_library *tc)

5.6.1 Detailed Description

Runs the equivalent examples of example1.c, example2.c, example3.c

5.6.2 Function Documentation

5.6.2.1 void example1 (tc_function_library * *tc*)

Basic api example that calculates an equilibrium in the Fe-Cr-C system and retrieves certain quantities.

5.6.2.2 void example2 (tc_function_library * *tc*)

Basic api example that calculates an equilibrium in the Fe-Cr-C system and retrieves certain quantities.

5.6.2.3 void example3 (tc_function_library * *tc*)

Shows how to display certain values in arrays.

5.7 source/tcMain.c File Reference

```
#include <stdio.h>
#include <string.h>
#include "tcExamples.h"
#include "tcutils.h"
```

Functions

- TCHANDLE loadTCLibraryInCurrentDir ()
- int importLibThermoCalc (tc_function_library *tc, char *message)
- int main (int argc, char *argv[])

5.7.1 Detailed Description

This is the main file to run the Thermo-Calc examples. It contains a short example how the dll can be loaded and How to fetch the Thermo-Calc functions.

To get started, build this project and run it. The executable will be placed next to a copy of the tcapi dll/library.

5.7.2 Function Documentation

5.7.2.1 int importLibThermoCalc (tc_function_library * *tc*, char * *message*)

Parameters

tc	pointer to data structure that contains Thermo-Calc functions.
message	error message. Should be allocated by caller

This function does two things.

1) Loads the library

2) Calls importFunctions that fetches the functions to the data structure.

5.7.2.2 TCHANDLE loadTCLibraryInCurrentDir ( )

Loads the library (os specific) and returns a handle to the library.

This function expects that the executable is placed next to the library. However, the library can be placed anywhere as long as the correct path is given.

5.7.2.3 int main (int *argc*, char * *argv[]*)

Main function

Start here to run the different examples Each example needs the path to a temporary directory to store log files, and the path to the thermo-calc installation where it looks for the databases.

This can be changed if for example another set of databases should be used.

5.8 source/tcutils.h File Reference

```
#include <unistd.h>
```

Functions

- void getThermoCalcEnvironmentPath (char *pathBuffer)
- void getTempEnvironmentPath (char *pathBuffer)

5.8.1 Detailed Description

Simple utility functions to work with environment variables.

5.8.2 Function Documentation

5.8.2.1 void getTempEnvironmentPath (char * *pathBuffer*)

Get path to temp directory If it can't find it - default to current working directory

5.8.2.2 void getThermoCalcEnvironmentPath (char * *pathBuffer*)

Get path from the values of Thermo-Calc environment variables TC3_HOME (Thermo-Calc 3.0) TCPATH Older versions and fallback

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