

Example 2 using OCASI-TQ: Calculations in the binary Fe-Ni system including mobility data

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This is an example for the OCASI Fortran TQ interface.

The example is based on the TQ standard for interfacing thermodynamic software with application software. A more extensive interface called OpenCalphad Application Software Interface (OCASI) is under development.

If you are not familiar with compiling and linking software and do not understand the instructions here please ask some guru close to you for help. The instructions here are very brief but I do not have time to answer questions about how to compile and link software. If you find errors you are welcome to report them.

To link this example you must first install the OC main program. This installation generates two files you need: **liboceq.a** and **liboceqplus.mod**. Both of these files are needed for these applications.

You also need the **liboctq.F90** source code which is on the directory above this example.

Files on this directory:

- readme.pdf is this file.
- readme.tex is a LaTeX file to generate this pdf file.
- FENI.TDB is a small database in the TDB format.
- TQ2-feni.F90 is the test program written in Fortran95/08.
- linkmake is a text file without extension which you can use as command file a on Windows system if you add the extension .cmd and execute it a batch file in a terminal window (or if you double click on it). If you use LINUX you can edit it to create a Makefile.

In the linkmake file there are some additional comments and instructions. If you do not understand these instruction please ask a local guru for help.

Compiling and linking the test program

When you executing the linkmake file in a terminal window (or the corresponding Makefile) you should have a program called tqtest1.exe. The linking below assumes that the OC main program and the corresponding libraries will be two directories above this one.

The output during compiling and linking will be something like:

```
C:\Users\...\TQ4lib\F90\feni>linkmake

C:\Users\...\TQ4lib\F90\feni>REM Copy libraries (compiled without OpenMP)
from OC directory

C:\Users\...\TQ4lib\F90\feni>copy ..\..\..\liboceq.a .
1 fil(er) kopierad(e).

C:\Users\...\TQ4lib\F90\feni>copy ..\..\..\liboceqplus.mod
.
1 fil(er) kopierad(e).

C:\Users\...\TQ4lib\F90\feni>REM Copy tqlibrary from directory above

C:\Users\...\TQ4lib\F90\feni>copy ..\liboctq.F90 .
1 fil(er) kopierad(e).

C:\Users\...\TQ4lib\F90\feni>REM Compile and link

C:\Users\...\TQ4lib\F90\feni>gfortran -c liboctq.F90

C:\Users\...\TQ4lib\F90\feni>gfortran -o tqex2 TQ2-feni.F90
liboctq.o liboceq.a
```

When you run the program it will look like

```
C:\Users\...\TQ4lib\F90\feni>tqex2.exe

Calculation of equilibria and mobility data in Fe-Ni system
Fictitious mobility data for the liquid in the TDB file:
PARAMETER MQ&FE(LIQUID,FE;0) 298.15 -10000*IQRT-18; 6000 N BOS !
PARAMETER MQ&FE(LIQUID,NI;0) 298.15 -12000*IQRT-19; 6000 N BOS !
PARAMETER MQ&NI(LIQUID,NI;0) 298.15 -11000*IQRT-18; 6000 N BOS !
PARAMETER MQ&NI(LIQUID,FE;0) 298.15 -13000*IQRT-19; 6000 N BOS !
```

PARAMETER MQ&FE(FCC_A1,FE:VA;0) 298.15 -30000*IQRT-30; 6000 N BOS !
 PARAMETER MQ&FE(FCC_A1,NI:VA;0) 298.15 -32000*IQRT-32; 6000 N BOS !
 PARAMETER MQ&NI(FCC_A1,NI:VA;0) 298.15 -33000*IQRT-32; 6000 N BOS !
 PARAMETER MQ&NI(FCC_A1,FE:VA;0) 298.15 -25000*IQRT-31; 6000 N BOS !

tqini created: DEFAULT_EQUILIBRIUM

System with 2 elements: FE, NI,
 and 2 phases: LIQUID, FCC_A1,

Give conditions:

Temperature: /1000/:

Pressure: /100000/:

Mole fraction of FE: /0.5/: .3

3Y Composition set(s) created: 1

3Y Gridmin: 16 points 0.00E+00 s and 0 clockcycles, T= 1000.00

Phase change: its/add/remove: 16 0 2

Equilibrium calculation 21 its, 1.5600E-02 s and 15 clockcycles

Successful calculation

Amount of 2 phases: 0.0000 1.0000

Stable phase: FCC_A1, amount: 1.0000E+00, mole fractions:

FE: 0.300000, NI: 0.700000,

System volume: 5.7000E-06

Component, mole fraction, chemical potentials, lnac = mu/RT

FE 0.300000 -5.569910E+04 -6.699023E+00

NI 0.700000 -4.984943E+04 -5.995474E+00

LN(mobility of component in phase) and exp(ln(.)):

MQ&FE(LIQUID) = -2.002412E+01 2.012036E-09

MQ&NI(LIQUID) = -1.974213E+01 2.667485E-09

MQ&FE(FCC_A1) = -3.517653E+01 5.284780E-16

MQ&NI(FCC_A1) = -3.538031E+01 4.310476E-16

Calculating Darken stability matrix, dG_A/dN_B for phase 2:

Calculation required 6 its

Chemical potential derivative matrix, dG_I/dN_J for 2 endmembers

	1	2
1	3.9069E+04	-1.6744E+04

```

2 -1.6744E+04  7.1759E+03

LN(mobility) values for 2 components
1 -3.5177E+01 -3.5380E+01

Any more calculations? /N/: y

Give conditions:
Temperature: /1000/: 2000
Pressure: /100000/:
Mole fraction of FE: /0.7/: .3
3Y Composition set(s) created: 1
3Y Gridmin: 16 points 0.00E+00 s and 0 clockcycles, T= 2000.00
Phase change: its/add/remove: 5 0 3
Equilibrium calculation 10 its, 1.5600E-02 s and 15 clockcycles

Successful calculation

Amount of 2 phases: 1.0000 0.0000

Stable phase: LIQUID, amount: 1.0000E+00, mole fractions:
FE: 0.300000, NI: 0.700000,

System volume: 7.7000E-06

Component, mole fraction, chemical potentials, lnac = mu/RT
FE 0.300000 -1.504170E+05 -9.045449E+00
NI 0.700000 -1.343949E+05 -8.081949E+00

LN(mobility of component in phase) and exp(ln(..)):
MQ&FE(LIQUID) = -1.938555E+01 3.810336E-09
MQ&NI(LIQUID) = -1.899758E+01 5.616396E-09
MQ&FE(FCC_A1) = -3.327521E+01 3.538017E-15
MQ&NI(FCC_A1) = -3.353104E+01 2.739401E-15

Calculating Darken stability matrix, dG_A/dN_B for phase 1:
Calculation required 6 its

Chemical potential derivative matrix, dG_I/dN_J for 2 endmembers
1 2
1 4.7487E+04 -2.0351E+04
2 -2.0351E+04 8.7221E+03

LN(mobility) values for 2 components

```

1 -1.9386E+01 -1.8998E+01

Any more calculations? /N/:

Auf wiedersehen

C:\Users\...\TQ4lib\F90\feni>