Report of OpenCalphad Calculation

2021-08-17

Materials

Element	CR	NI	FE
Wt%	18.0	8.0	74.0

Database

SAF2507.TDB

Equilibrium calculations

Equilibrium 1:

Output for equilibrium: 1, DEFAULT_EQUILIBRIUM 2021.08.17

Conditions :

```
 1:T=1800, 2:P=100000, 3:N=1, 4:W(CR)=0.18, 5:W(NI)=.08
 Degrees of freedom are 0
```

Some global data, reference state SER :

```
 T= 1800.00 K ( 1526.85 C), P= 1.0000E+05 Pa, V= 7.3721E-06 m3
 N= 1.0000E+00 moles, B= 5.5324E+01 g, RT= 1.4966E+04 J/mol
 G= -1.15072E+05 J, G/N=-1.1507E+05 J/mol, H= 6.9549E+04 J, S= 1.026E+02 J/K
```

Some data for components :

```
  Component name   Moles        Mass-fr   Chem.pot/RT   Activities   Ref.state
  CR               1.9152E-01   0.18000   -7.5640E+00   5.1881E-04   SER (default)
  FE               7.3307E-01   0.74000   -7.4753E+00   5.6690E-04   SER (default)
  NI               7.5412E-02   0.08000   -1.0082E+01   4.1834E-05   SER (default)
```

Some data for phases :

```
  Name             Status  Mass        Volume     Form.Units    Cmp/FU    dGm/RT     Comp:
  LIQUID#1         E       5.532E-02   7.37E-06   1.00E+00      1.00      0.00E+00   W:
    FE  7.40000E-01   CR  1.80000E-01   NI  8.00000E-02
```

Advanced application: Scheil-Gulliver Solidification

Figure 1: Mole fraction of solid vs. Temperature

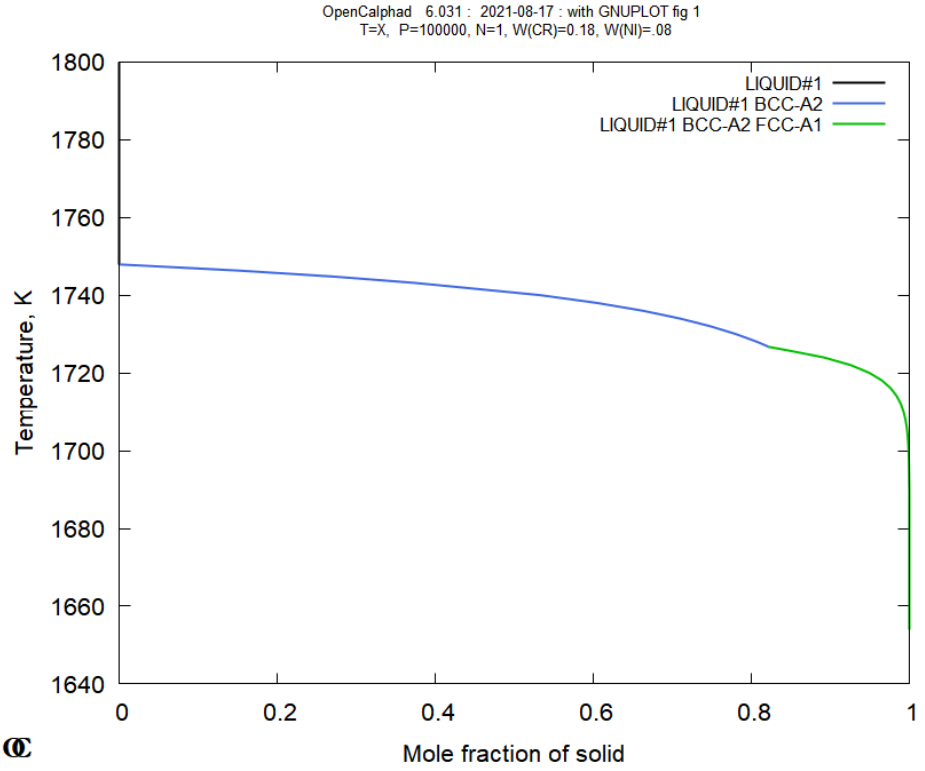

Figure 2: Equilibrium: Mole fraction of phase vs. Temperature

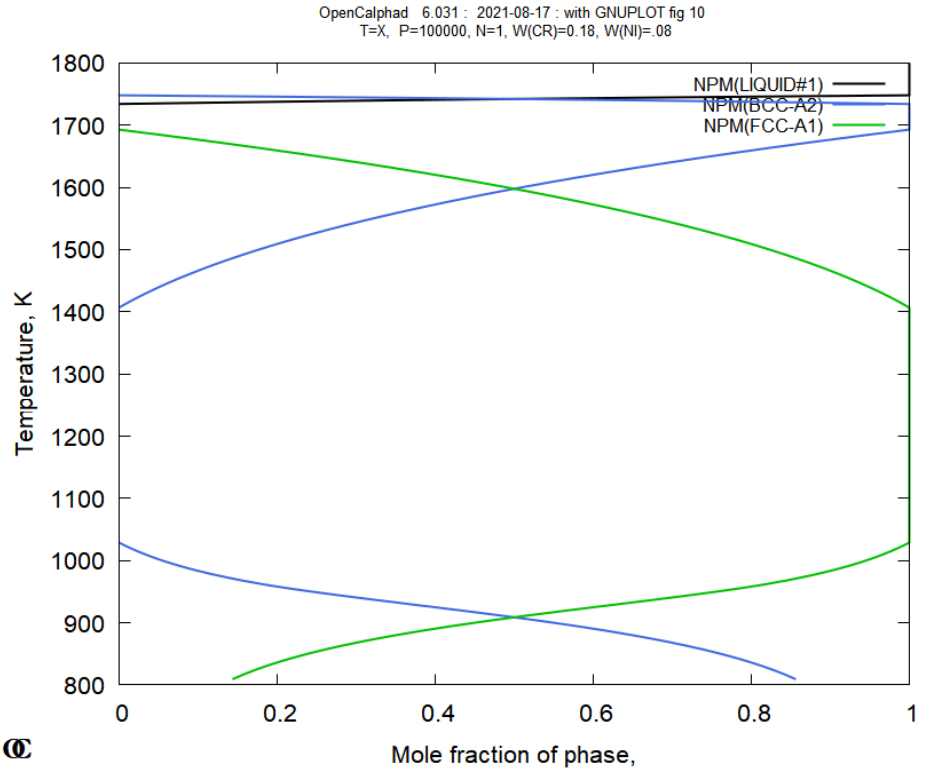

Figure 3: Mole fraction of solid vs. Composition of phase

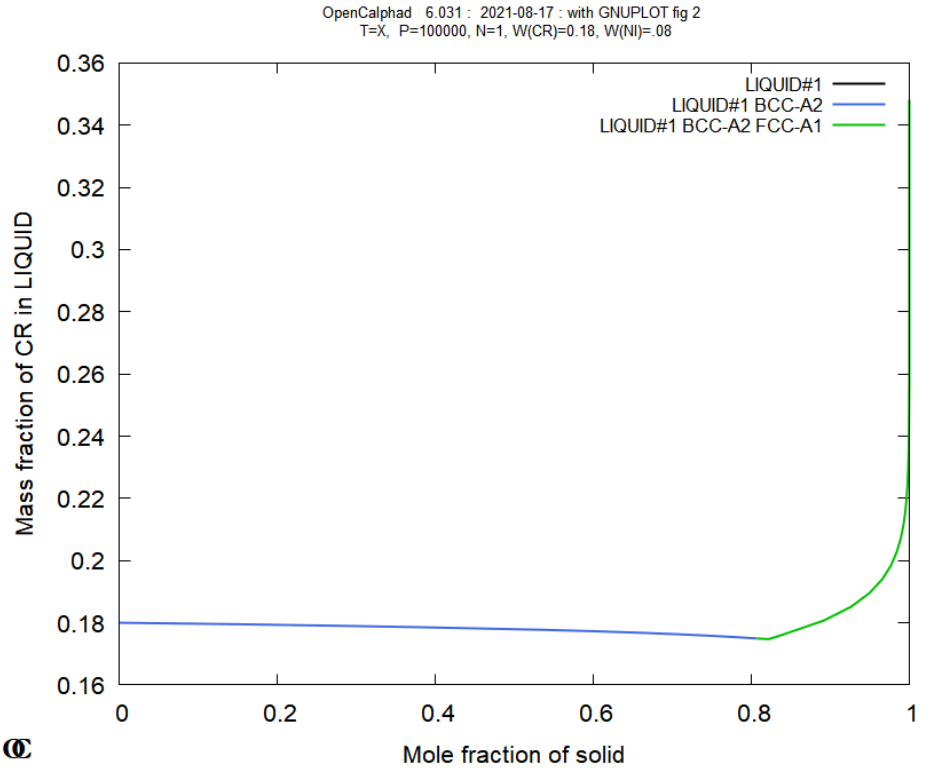

Figure 4: Equilibrium: Mole fraction of solid vs. Temperature

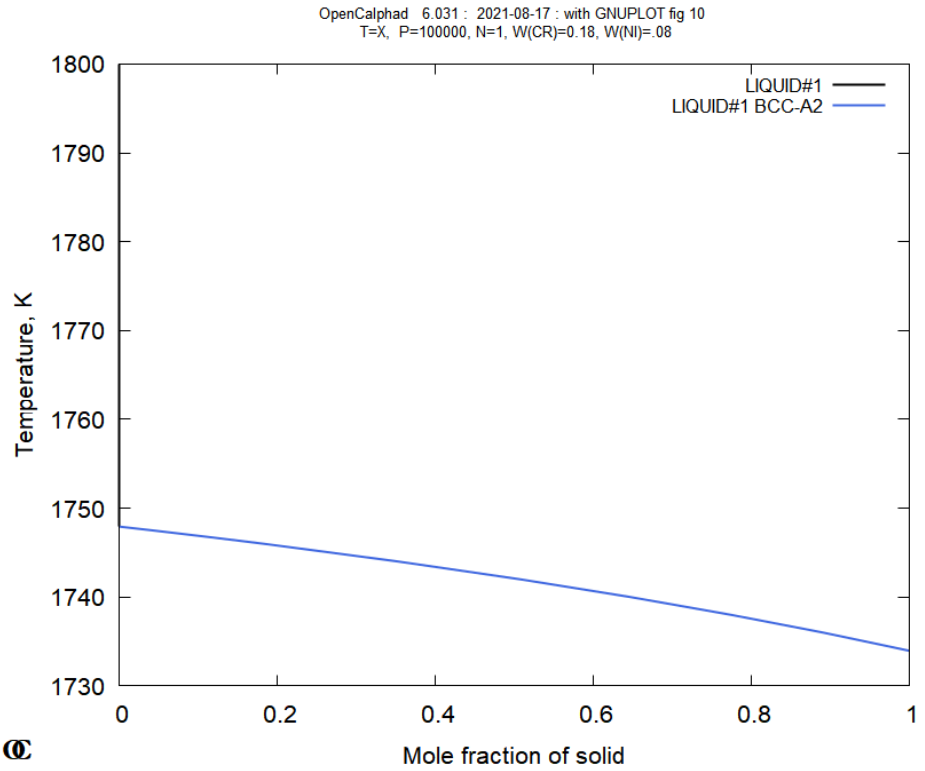

Figure 5: Comparison between Equilibrium and Scheil: Mole fraction of solid vs. Temperature

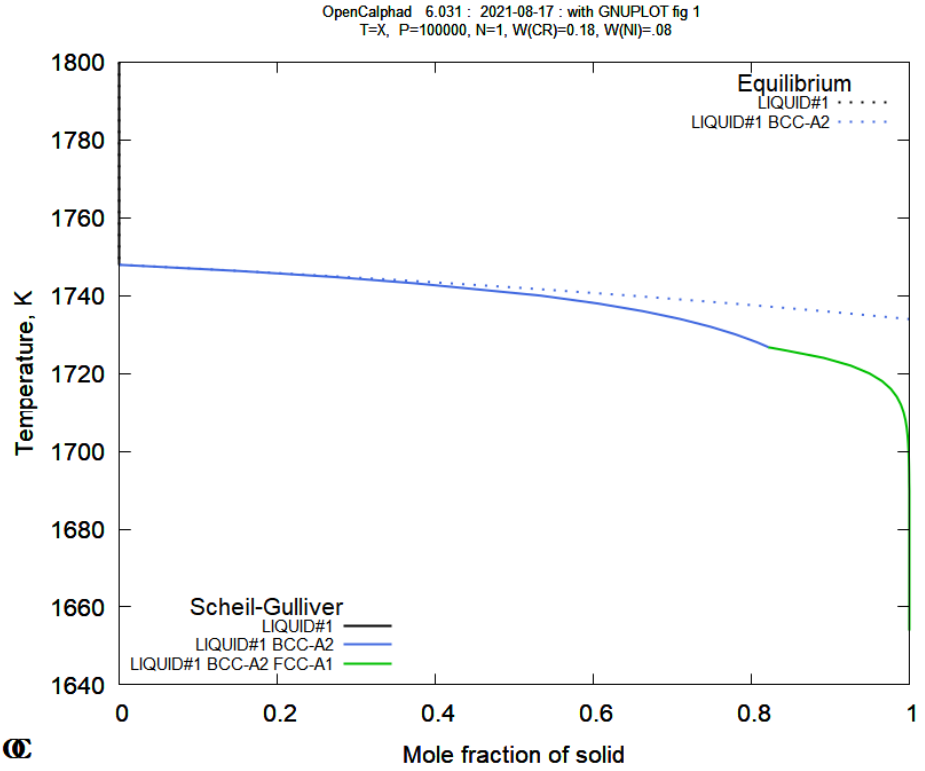

Figure 6: Equilibrium: Mole fraction of phase vs. Temperature

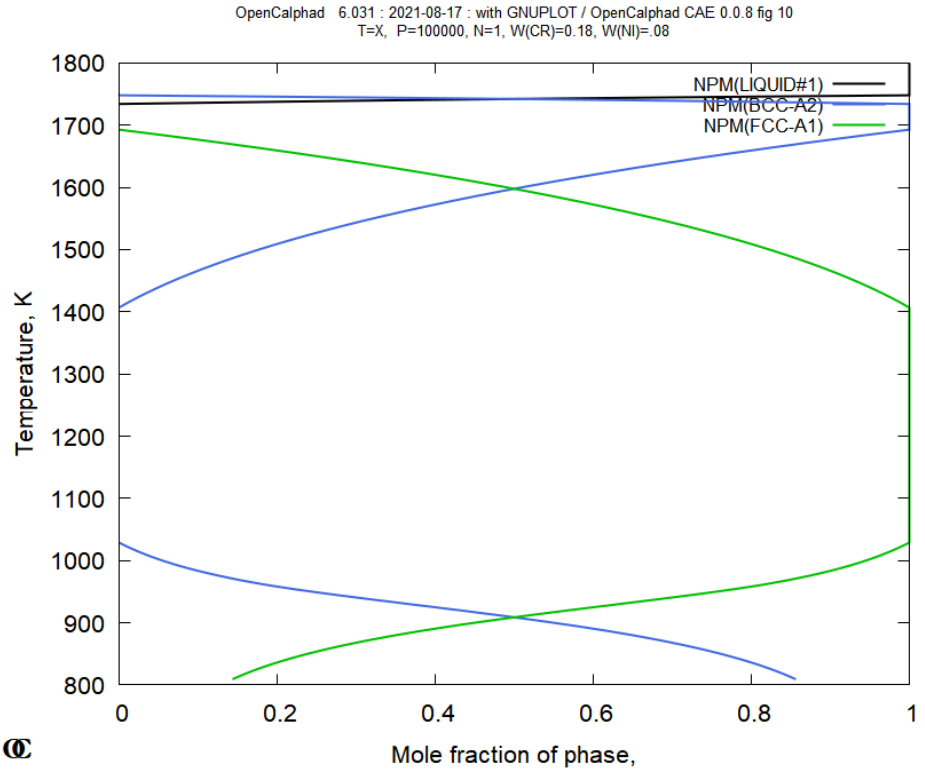

Figure 7: Equilibrium: Mole fraction of phase vs. Temperature