Report of OpenCalphad Calculation

2021-08-17

Materials

Element	MG	SI	ZN	AL
Mole-frac	0.02	0.03	0.02	0.93

Database

COST507R.TDB

Equilibrium calculations

Equilibrium 1:

Output for equilibrium: 1, DEFAULT_EQUILIBRIUM 2021.08.17

Conditions :

```
 1:T=1000, 2:P=100000, 3:N=1, 4:X(MG)=.02, 5:X(SI)=.03, 6:X(ZN)=.02
 Degrees of freedom are 0
```

Some global data, reference state SER :

```
 T= 1000.00 K ( 726.85 C), P= 1.0000E+05 Pa, V= 0.0000E+00 m3
 N= 1.0000E+00 moles, B= 2.7730E+01 g, RT= 8.3145E+03 J/mol
 G= -4.51331E+04 J, G/N=-4.5133E+04 J/mol, H= 3.1602E+04 J, S= 7.673E+01 J/K
```

Some data for components :

```
  Component name   Moles        Mass-fr   Chem.pot/RT   Activities   Ref.state
  AL               9.3000E-01   0.90493   -5.2039E+00   5.4951E-03   SER (default)
  MG               2.0000E-02   0.01753   -1.0013E+01   4.4800E-05   SER (default)
  SI               3.0000E-02   0.03038   -6.1675E+00   2.0964E-03   SER (default)
  ZN               2.0000E-02   0.04716   -1.0166E+01   3.8475E-05   SER (default)
```

Some data for phases :

```
  Name             Status  Mass         Volume     Form.Units    Cmp/FU    dGm/RT     Comp:
  LIQUID#1         E       2.773E-02    0.00E+00   1.00E+00      1.00      0.00E+00   W:
    AL  9.04930E-01   ZN  4.71555E-02   SI  3.03846E-02   MG  1.75301E-02
```

Advanced application: Scheil-Gulliver Solidification

Figure 1: Mole fraction of solid vs. Temperature

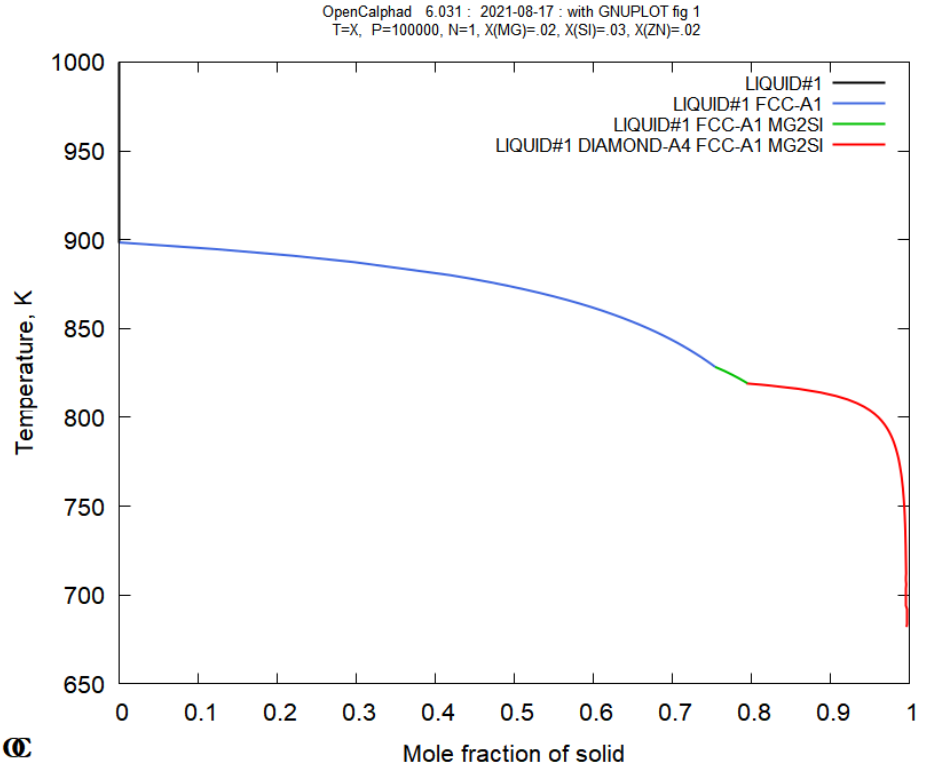

Figure 2: Equilibrium: Mole fraction of phase vs. Temperature

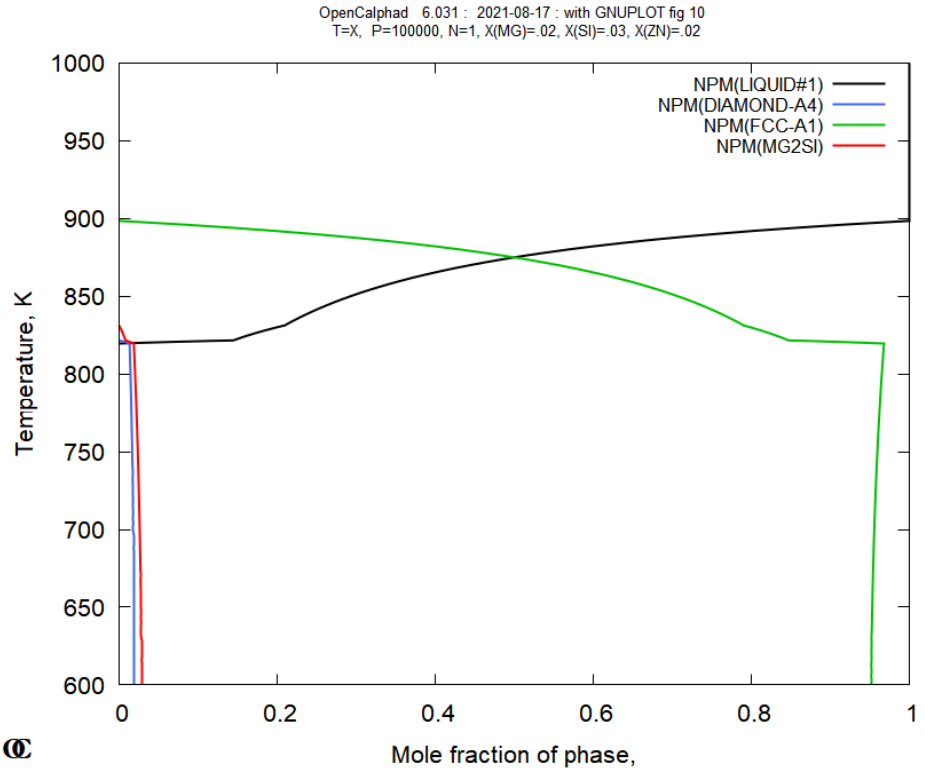

Figure 3: Mole fraction of solid vs. Composition of phase

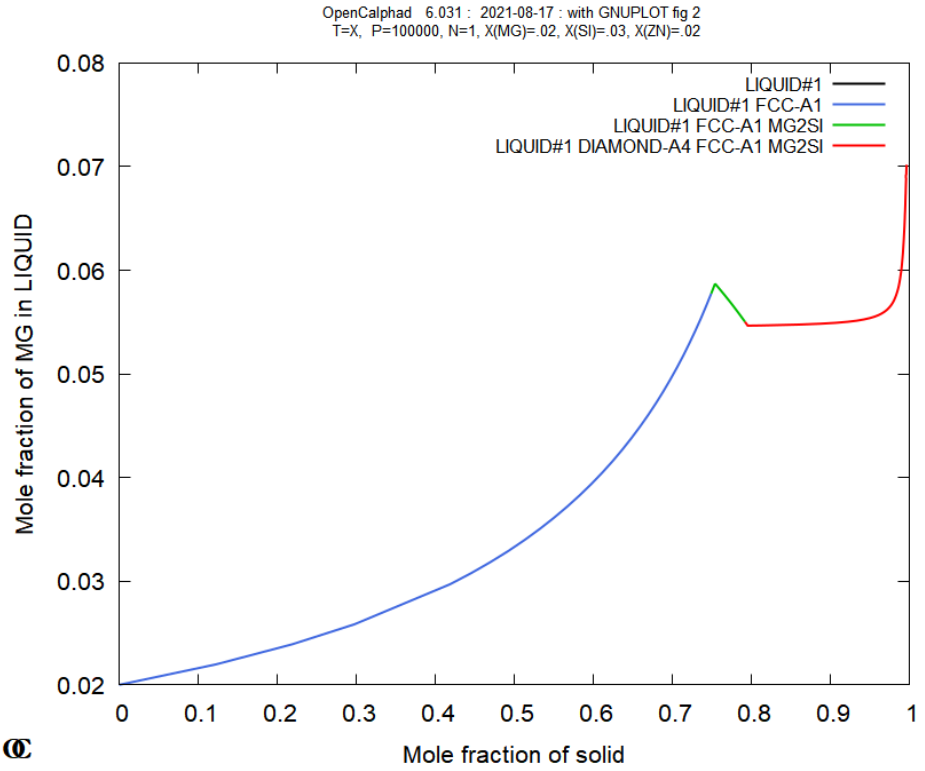

Figure 4: Mole fraction of solid vs. Composition of phase

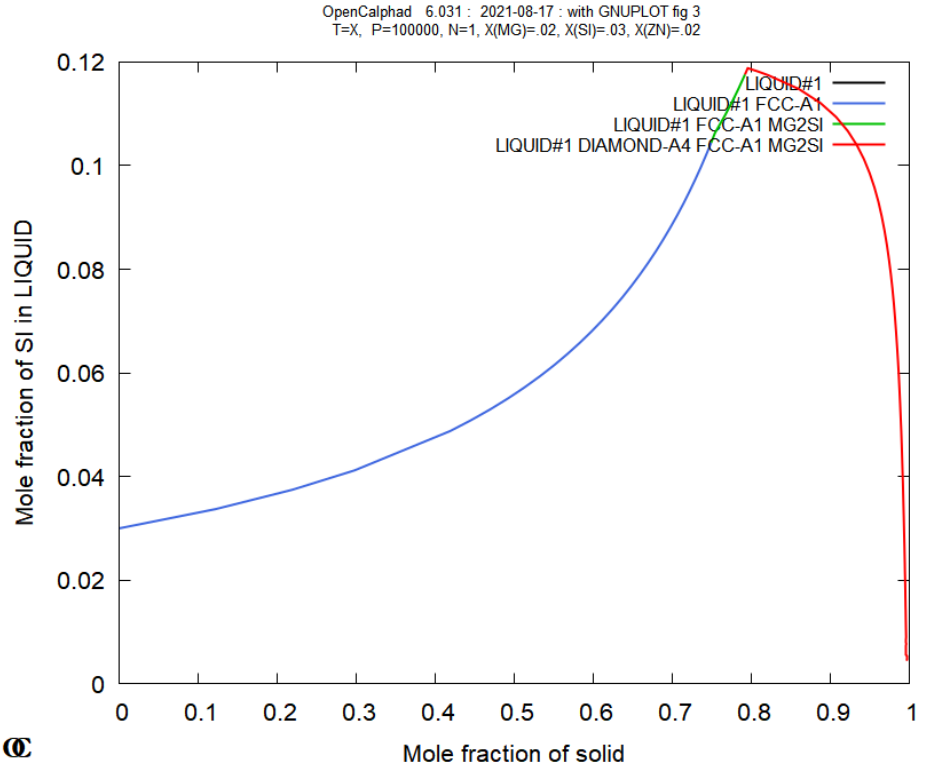

Figure 5: Mole fraction of solid vs. Composition of phase

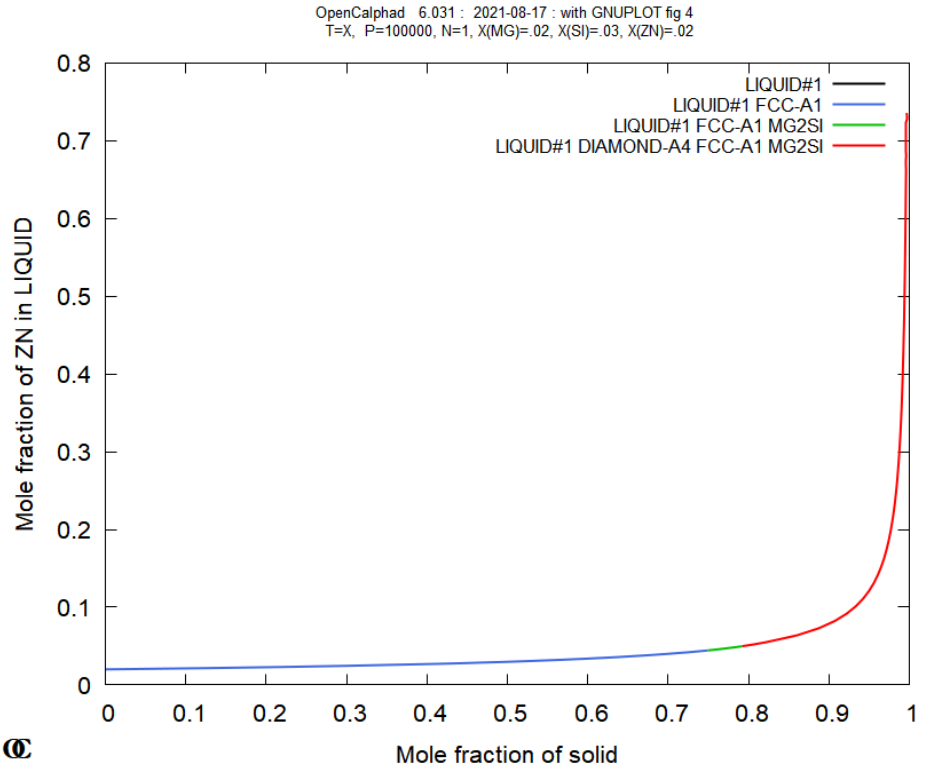

Figure 6: Mole fraction of solid vs. Composition of phase

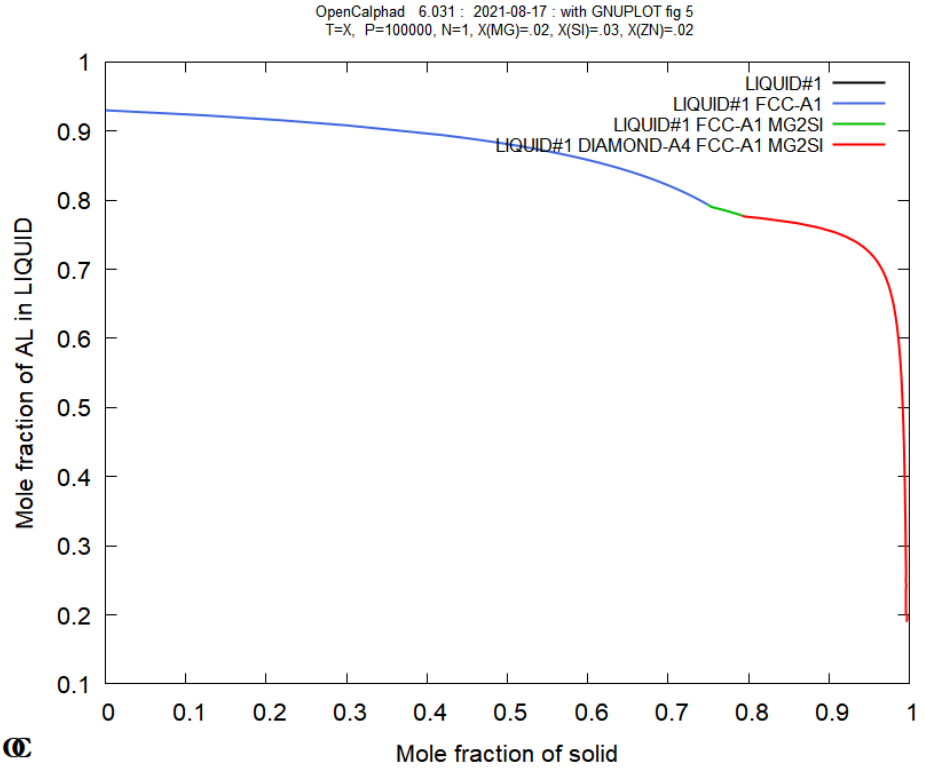

Figure 7: Equilibrium: Mole fraction of solid vs. Temperature

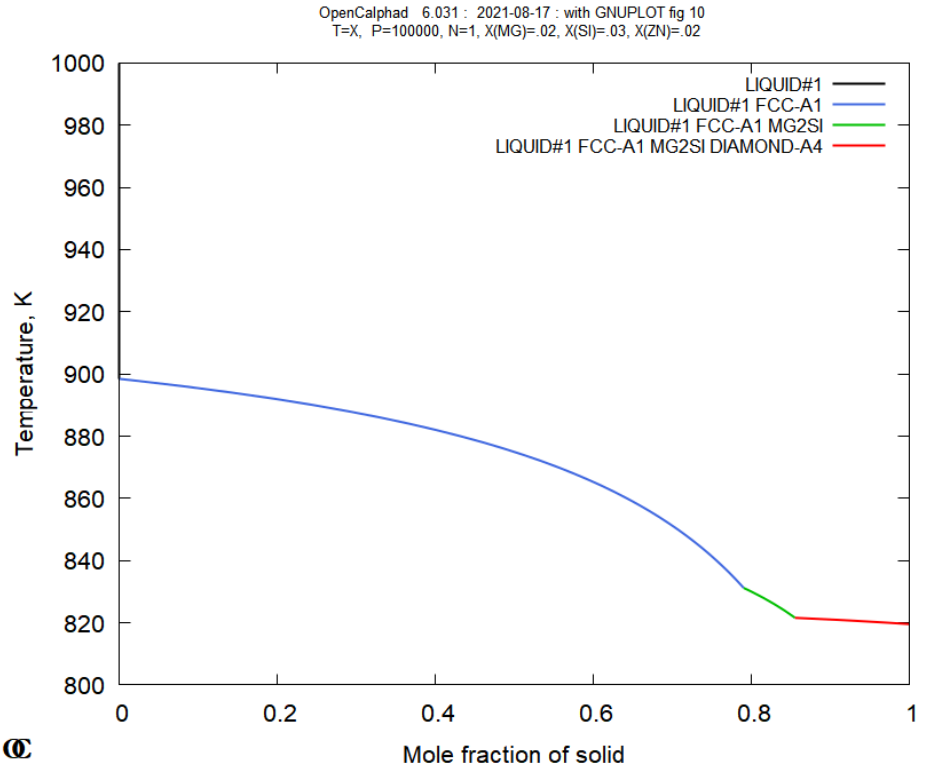

Figure 8: Comparison between Equilibrium and Scheil: Mole fraction of solid vs. Temperature

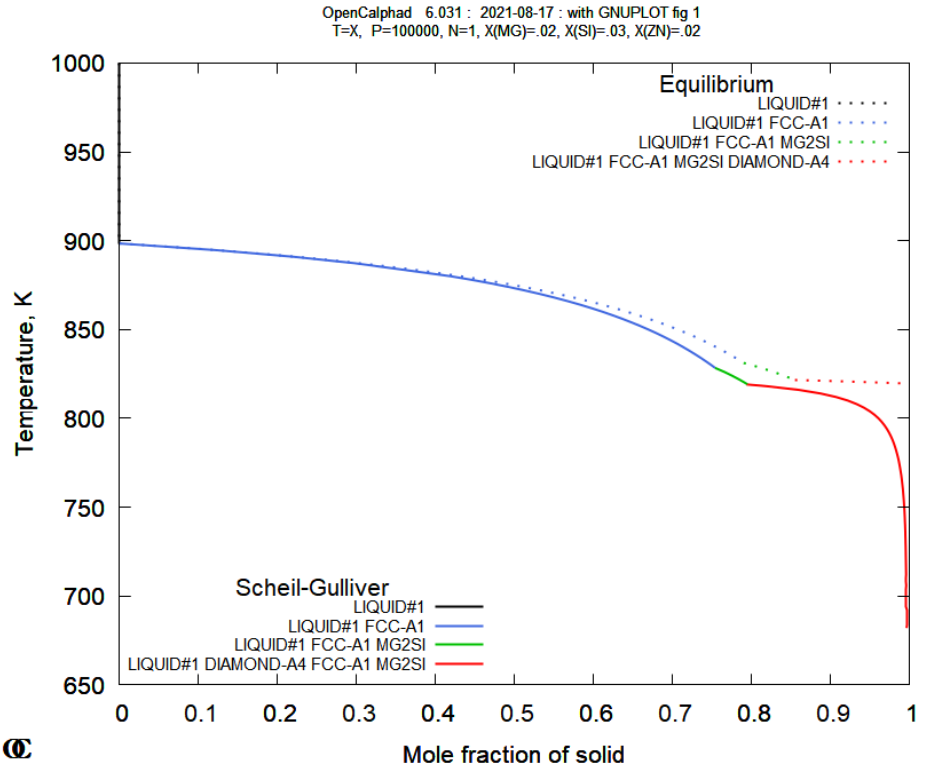

Figure 9: Equilibrium: Mole fraction of phase vs. Temperature

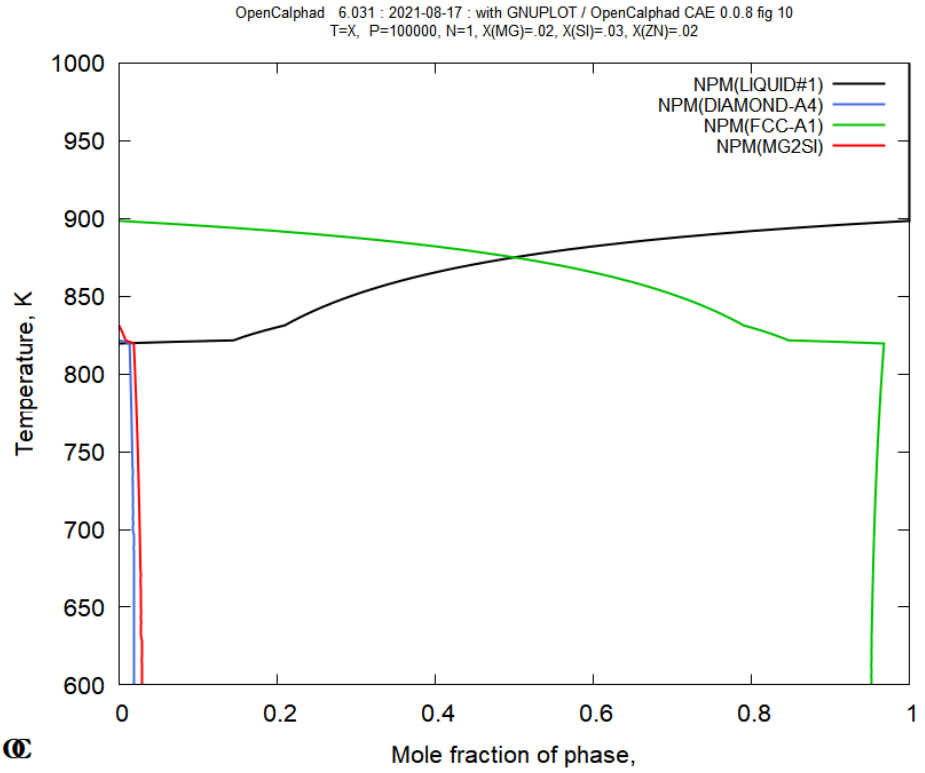

Figure 10: Equilibrium: Mole fraction of phase vs. Temperature