Report of OpenCalphad Calculation

2021-08-17

Materials

Element	C	CR	MO	SI	V	FE
Wt%	0.9	4.5	10.0	0.1	0.9	83.6

Database

STEEL1.TDB

Equilibrium calculations

Equilibrium 1:

Output for equilibrium: 1, DEFAULT_EQUILIBRIUM 2021.08.01

Conditions :

```
 1:T=1200, 2:P=100000, 3:N=1, 4:W(C)=.009, 5:W(CR)=.045, 6:W(MO)=0.1,
 7:W(SI)=.001, 8:W(V)=.009
 Degrees of freedom are 0
```

Some global data, reference state SER :

```
 T= 1200.00 K ( 926.85 C), P= 1.0000E+05 Pa, V= 6.2488E-06 m3
 N= 1.0000E+00 moles, B= 5.6057E+01 g, RT= 9.9774E+03 J/mol
 G= -5.95658E+04 J, G/N=-5.9566E+04 J/mol, H= 3.3261E+04 J, S= 7.736E+01 J/K
```

Some data for components :

```
  Component name   Moles        Mass-fr   Chem.pot/RT   Activities   Ref.state
  C                4.2005E-02   0.00900   -3.8815E+00   2.0621E-02   SER (default)
  CR               4.8515E-02   0.04500   -7.2654E+00   6.9934E-04   SER (default)
  FE               8.3915E-01   0.83600   -5.7515E+00   3.1780E-03   SER (default)
  MO               5.8430E-02   0.10000   -7.7491E+00   4.3114E-04   SER (default)
  SI               1.9960E-03   0.00100   -2.0233E+01   1.6327E-09   SER (default)
  V                9.9040E-03   0.00900   -1.3631E+01   1.2028E-06   SER (default)
```

Some data for phases :

```
  Name             Status  Mass        Volume     Form.Units    Cmp/FU    dGm/RT     Comp:
  FCC_A1#1         E       4.756E-02   6.24E-06   8.45E-01      1.02      0.00E+00   W:
    FE  9.30246E-01   MO  1.86557E-02   V   1.33998E-03   SI  1.17863E-03
    CR  4.45427E-02   C   4.03696E-03
  FCC_A1_AUTO#2    E       7.958E-04   6.09E-09   1.07E-02      1.84      0.00E+00   W:
    V   4.38981E-01   C   1.36662E-01   FE  3.89593E-03   SI  4.50528E-10
    MO  3.73157E-01   CR  4.73040E-02
  M6C              E       7.700E-03   0.00E+00   1.70E-02      7.00      0.00E+00   W:
    MO  5.74221E-01   CR  4.75864E-02   V   1.18768E-02   SI  0.00000E+00
    FE  3.39854E-01   C   2.64622E-02
```

Property calculations

Figure 1: Temperature vs. Amount of phase

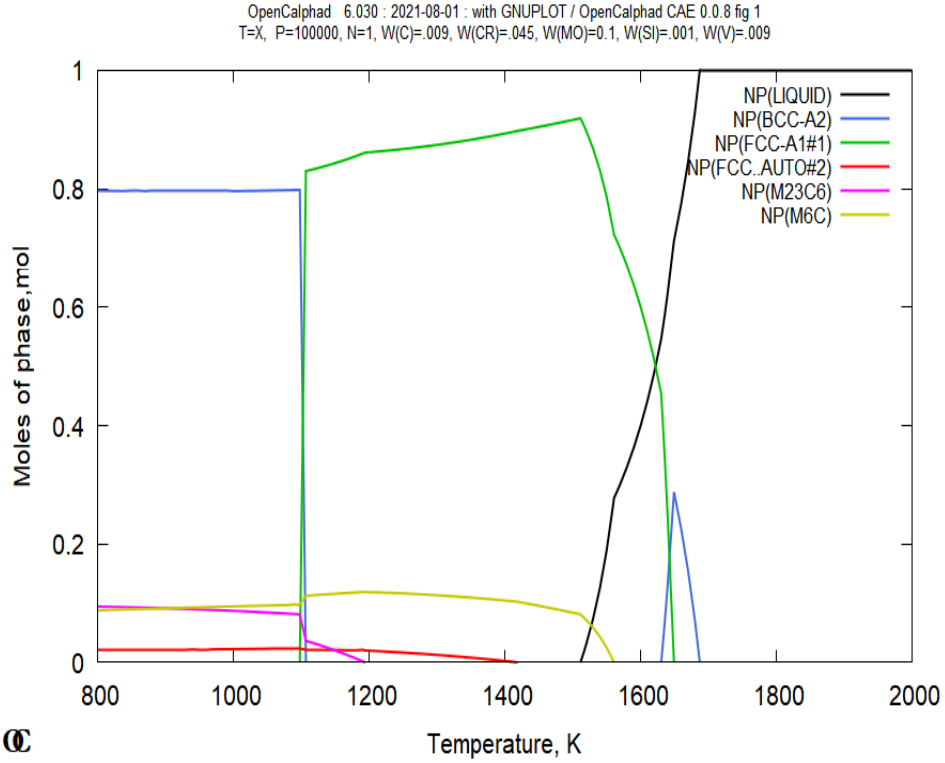

Figure 2: Temperature vs. Composition of phase

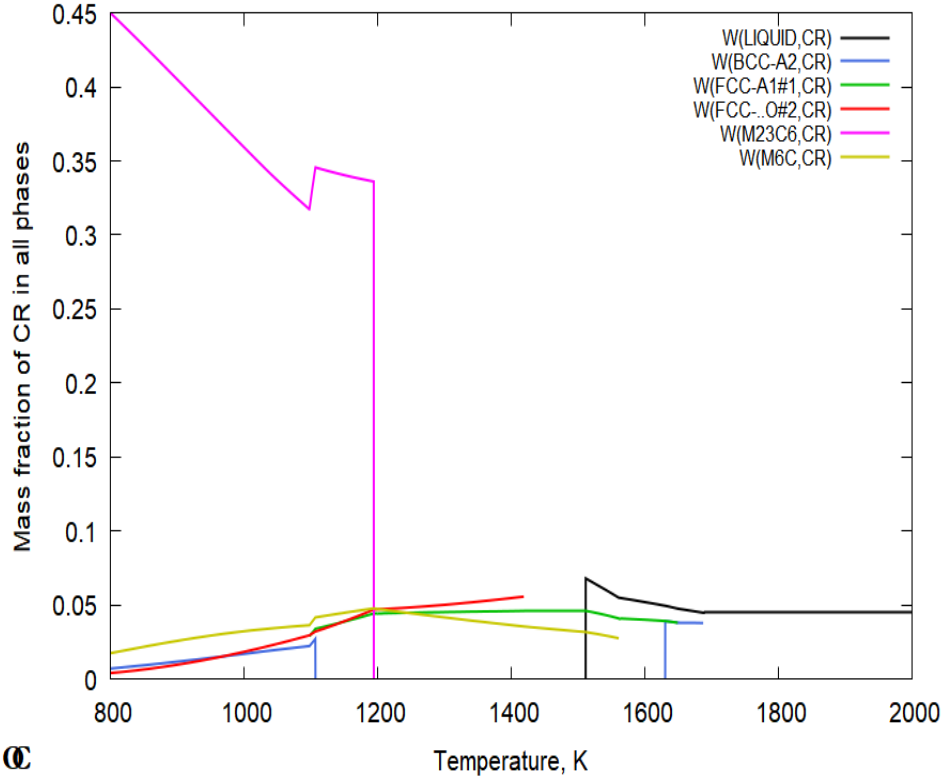

Figure 3: Temperature vs. Composition of phase

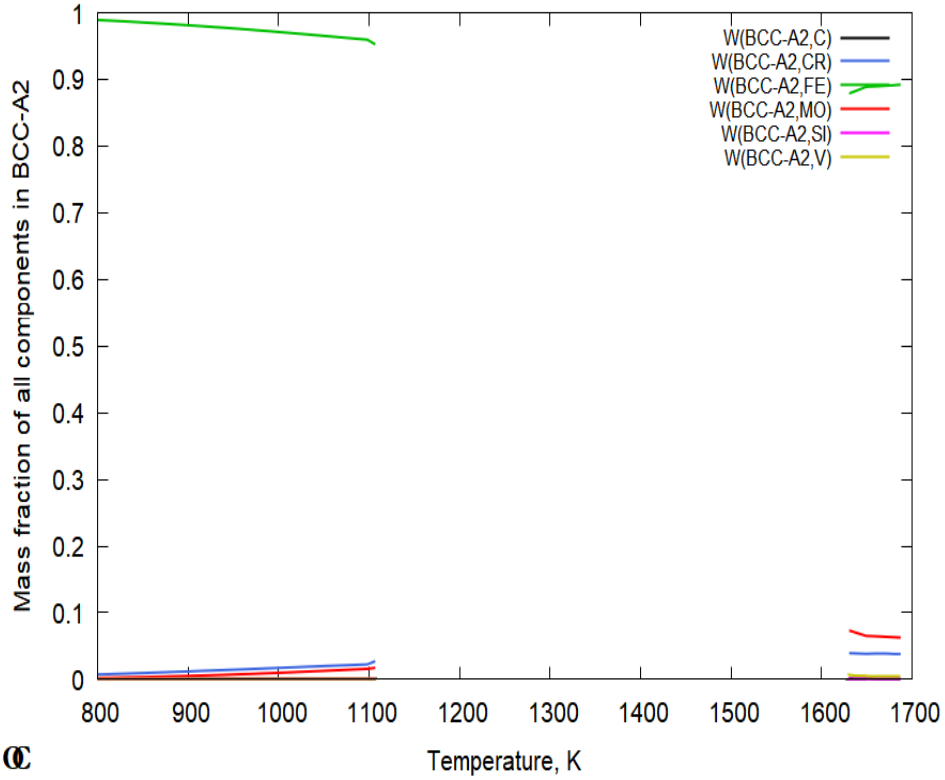

Figure 4: Temperature vs. Enthalpy

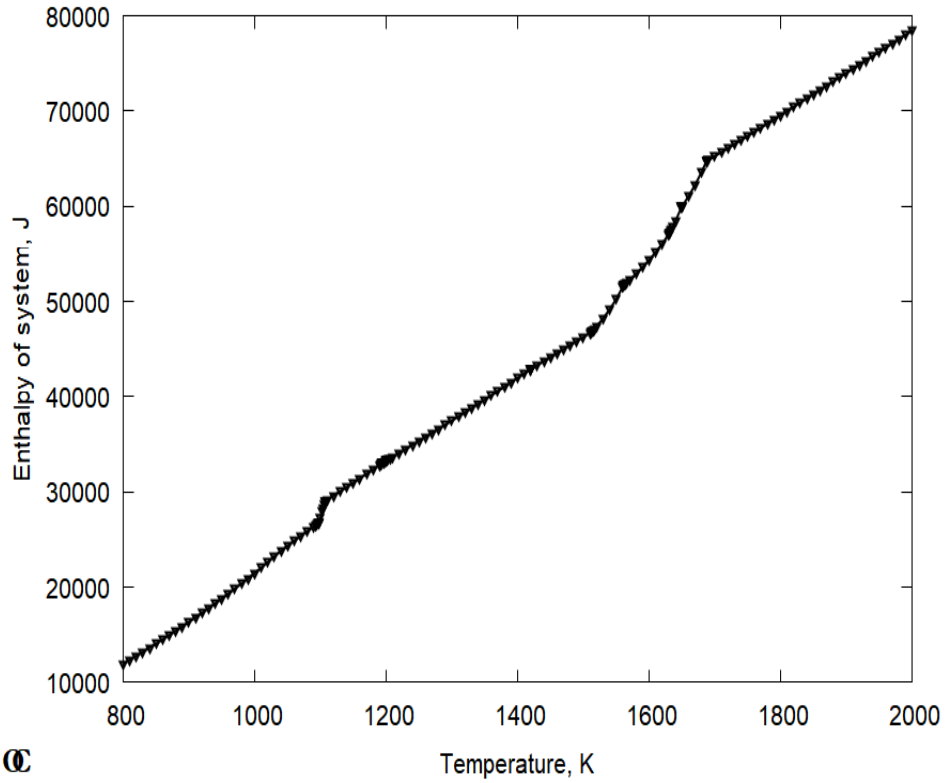

Figure 5: Temperature vs. Heat capacity

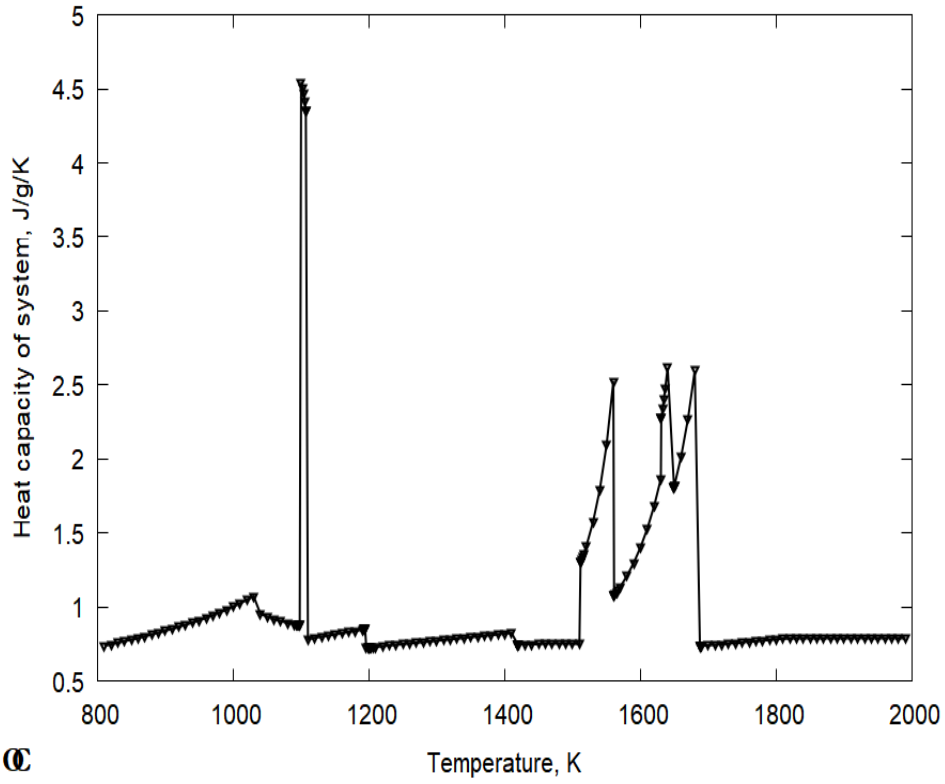

Figure 6: Temperature vs. Amount of phase