Report of OpenCalphad Calculation

2021-08-22

Materials

Element	CR	FE
Mole-frac	0.2	0.8

Database

STEEL1.TDB

Equilibrium calculations

Equilibrium 1:

Output for equilibrium: 1, DEFAULT_EQUILIBRIUM 2021.08.22

*** The results listed below may be inconsistent with the current conditions

Conditions :

```
 1:T=700, 2:P=100000, 3:N=1, 4:X(CR)=0.2
 Degrees of freedom are 0
```

Some global data, reference state SER :

```
 T= 700.00 K ( 426.85 C), P= 1.0000E+05 Pa, V= 7.2179E-06 m3
 N= 1.0000E+00 moles, B= 5.5410E+01 g, RT= 5.8202E+03 J/mol
 G= -2.46290E+04 J, G/N=-2.4629E+04 J/mol, H= 1.3954E+04 J, S= 5.512E+01 J/K
```

Some data for components :

```
  Component name   Moles        Mass-fr   Chem.pot/RT   Activities   Ref.state
  CR               1.1345E-01   0.10646   -3.7420E+00   2.3706E-02   SER (default)
  FE               8.8655E-01   0.89354   -4.2943E+00   1.3646E-02   SER (default)
```

Some data for phases :

```
  Name             Status  Mass        Volume     Form.Units    Cmp/FU    dGm/RT     Comp:
  BCC_A2#1         E       5.541E-02   7.22E-06   1.00E+00      1.00      0.00E+00   W:
    FE  8.93536E-01   CR  1.06464E-01
  BCC_A2_AUTO#2    E       0.000E+00   0.00E+00   0.00E+00      1.00      0.00E+00   W:
    CR  9.17511E-01   FE  8.24891E-02
```

*** The results listed above may be inconsistent with the current conditions

Equilibrium 2:

Output for equilibrium: 1, DEFAULT_EQUILIBRIUM 2021.08.22

Conditions :

```
 1:T=1400, 2:P=100000, 3:N=1, 4:X(CR)=0.1
 Degrees of freedom are 0
```

Some global data, reference state SER :

```
 T= 1400.00 K ( 1126.85 C), P= 1.0000E+05 Pa, V= 7.4180E-06 m3
 N= 1.0000E+00 moles, B= 5.5462E+01 g, RT= 1.1640E+04 J/mol
 G= -7.44752E+04 J, G/N=-7.4475E+04 J/mol, H= 4.2826E+04 J, S= 8.379E+01 J/K
```

Some data for components :

```
  Component name   Moles        Mass-fr   Chem.pot/RT   Activities   Ref.state
  CR               1.0000E-01   0.09375   -6.9761E+00   9.3393E-04   SER (default)
  FE               9.0000E-01   0.90625   -6.3338E+00   1.7753E-03   SER (default)
```

Some data for phases :

```
  Name             Status  Mass        Volume     Form.Units    Cmp/FU    dGm/RT     Comp:
  FCC_A1#1         E       5.546E-02   7.42E-06   1.00E+00      1.00      0.00E+00   W:
    FE  9.06249E-01   CR  9.37508E-02
```

Equilibrium 3:

Output for equilibrium: 1, DEFAULT_EQUILIBRIUM 2021.08.22

Conditions :

```
1:T=1900, 2:P=100000, 3:N=1, 4:X(CR)=0.2
Degrees of freedom are 0
```

Some global data, reference state SER :

```
T= 1900.00 K ( 1626.85 C), P= 1.0000E+05 Pa, V= 8.0527E-06 m3
N= 1.0000E+00 moles, B= 5.5077E+01 g, RT= 1.5798E+04 J/mol
G= -1.21169E+05 J, G/N=-1.2117E+05 J/mol, H= 7.4702E+04 J, S= 1.031E+02 J/K
```

Some data for components :

Component name	Moles	Mass-fr	Chem.pot/RT	Activities	Ref.state
CR	2.0000E-01	0.18881	-7.7630E+00	4.2518E-04	SER (default)
FE	8.0000E-01	0.81119	-7.6469E+00	4.7752E-04	SER (default)

Some data for phases :

Name	Status	Mass	Volume	Form.Units	Cmp/FU	dGm/RT	Comp:
LIQUID#1	E	5.508E-02	8.05E-06	1.00E+00	1.00	0.00E+00	W:
FE 8.11187E-01	CR 1.88813E-01						

Phase diagram calculations

Figure 1: Binary phase diagram