Report of OpenCalphad Calculation

2021-08-22

Materials

Element	C	CR	FE
Wt%	1.0	13.0	86.0

Database

STEEL7.TDB

Equilibrium calculations

Equilibrium 1:

Output for equilibrium: 1, DEFAULT_EQUILIBRIUM 2021.08.22

Conditions :

```
1:T=1198.15, 2:P=100000, 3:N=1, 4:W(C)=.01, 5:W(CR)=0.13
Degrees of freedom are 0
```

Some global data, reference state SER :

```
T= 1198.15 K ( 925.00 C), P= 1.0000E+05 Pa, V= 6.4632E-06 m3
N= 1.0000E+00 moles, B= 5.3385E+01 g, RT= 9.9620E+03 J/mol
G= -5.80270E+04 J, G/N=-5.8027E+04 J/mol, H= 3.3731E+04 J, S= 7.658E+01 J/K
```

Some data for components :

Component name	Moles	Mass-fr	Chem.pot/RT	Activities	Ref.state
C	4.4446E-02	0.01000	-4.5659E+00	1.0400E-02	SER (default)
CR	1.3347E-01	0.13000	-6.6220E+00	1.3308E-03	SER (default)
FE	8.2208E-01	0.86000	-5.7635E+00	3.1402E-03	SER (default)

Some data for phases :

Name	Status	Mass	Volume	Form.Units	Cmp/FU	dGm/RT	Comp:
FCC_A1#1	E	4.888E-02	6.46E-06	8.78E-01	1.01	0.00E+00	W:
FE 9.18045E-01	CR 7.92069E-02	C 2.74774E-03					
M7C3	E	4.507E-03	0.00E+00	1.11E-02	10.00	0.00E+00	W:
CR 6.80843E-01	FE 2.30508E-01	C 8.86495E-02					

Phase diagram calculations

Figure 1: Isopleth phase diagram