Report of OpenCalphad Calculation

2021-08-16

Materials

Element	O	H
Mole-frac	0.333	0.667

Database

HOGAS.TDB

Equilibrium calculations

Equilibrium 1:

Output for equilibrium: 1, DEFAULT_EQUILIBRIUM 2021.08.16

Conditions :

```
 1:T=3000, 2:P=100000, 3:N=3, 4:X(O)=0.333
 Degrees of freedom are 0
```

Some global data, reference state SER :

```
 T= 3000.00 K ( 2726.85 C), P= 1.0000E+05 Pa, V= 2.8353E-01 m3
 N= 3.0000E+00 moles, B= 1.8000E+01 g, RT= 2.4944E+04 J/mol
 G= -9.83265E+05 J, G/N=-3.2776E+05 J/mol, H=-4.6434E+04 J, S= 3.123E+02 J/K
```

Some data for components :

```
  Component name   Moles        Mass-fr   Chem.pot/RT   Activities   Ref.state
  H                2.0010E+00   0.11205   -1.1450E+01   1.0644E-05   SER (default)
  O                9.9900E-01   0.88795   -1.6524E+01   6.6656E-08   SER (default)
```

Some data for phases :

```
  Name             Status  Mass        Volume     Form.Units    Cmp/FU    dGm/RT     Comp:
  GAS              E       1.800E-02   2.84E-01   1.14E+00      2.64      0.00E+00   W:
    O   8.87954E-01   H   1.12046E-01
    Constituents:     There are 6 constituents:
    H2O17.24199E-01   O2  6.31116E-02   O   2.84341E-02   O3  2.07533E-08
    H2  1.27699E-01   H   5.65564E-02
```

Property calculations

Figure 1: Temperature vs. Site fraction