

Assignment #5

Computational Material Thermodynamics

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Task

Using Thermo-Calc compute how the equilibrium partial pressures of the most dominant gas specie of a gas mixture, initially consisting of equimolar amounts of SO_3 and O_2 , vary as a function of temperature from 300 to 1500 K at 2 bar. You may use PSUB database.

Solution

Plot partial pressure (refer Fig) of all gas species. MACRO file pALL.TCM can be run to obtain the same plot. From *LIST_EQUILIBRIUM*, major gas species were found to be O_2 , O_2S1 and O_3S1 (refer Fig.). MACRO file pS-O2.TCM can be run to obtain the same plot. It was found that oxygen is the most dominant gas specie in the gas mixture (refer Fig). MACRO file pO2.TCM can be run to obtain the same plot.

ALL GAS SPECIES IN S-O MIXTURE

2016.05.08.13.23.49

PSUB: O, S

P=2E5, N(O)=2.5, N(S)=0.5

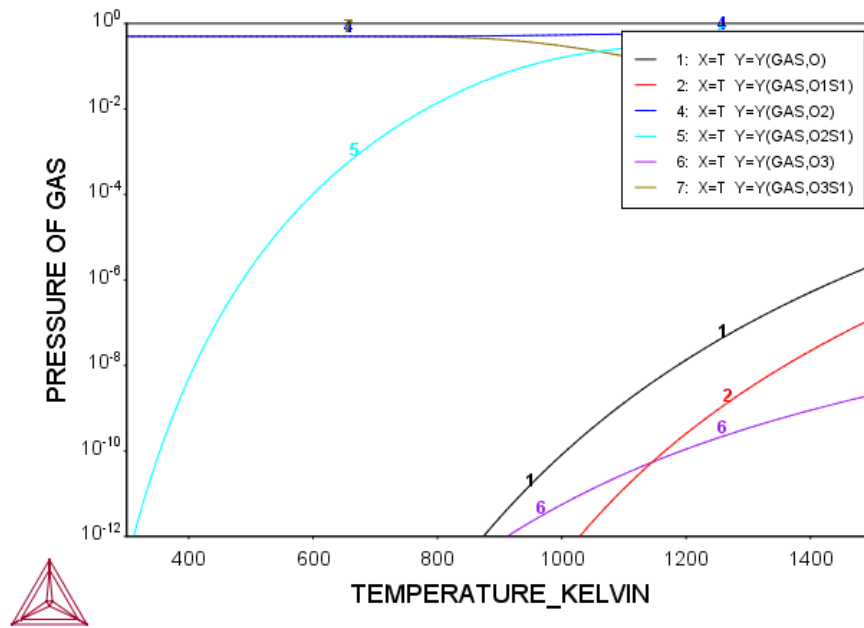


Figure 1: Partial pressure as function of temperature of all gas species

MAJOR GAS SPECIES IN S-O MIXTURE

2016.05.08.13.24.12

PSUB: O, S

P=2E5, N(O)=2.5, N(S)=0.5

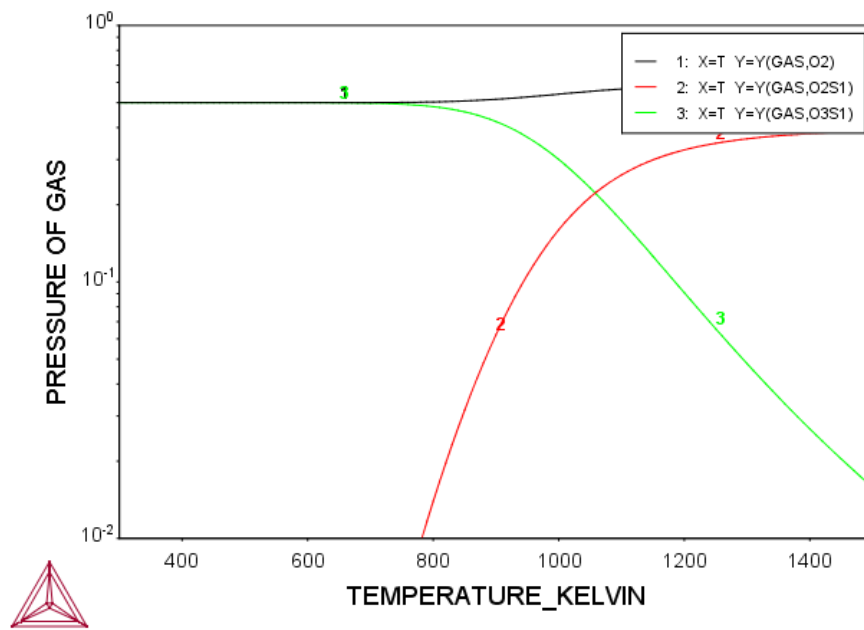


Figure 2: Partial pressure as function of temperature of three major gas species

DOMINANT GAS SPECIE IN S-O MIXTURE

2016.05.08.13.23.59

PSUB: O, S

P=2E5, N(O)=2.5, N(S)=0.5

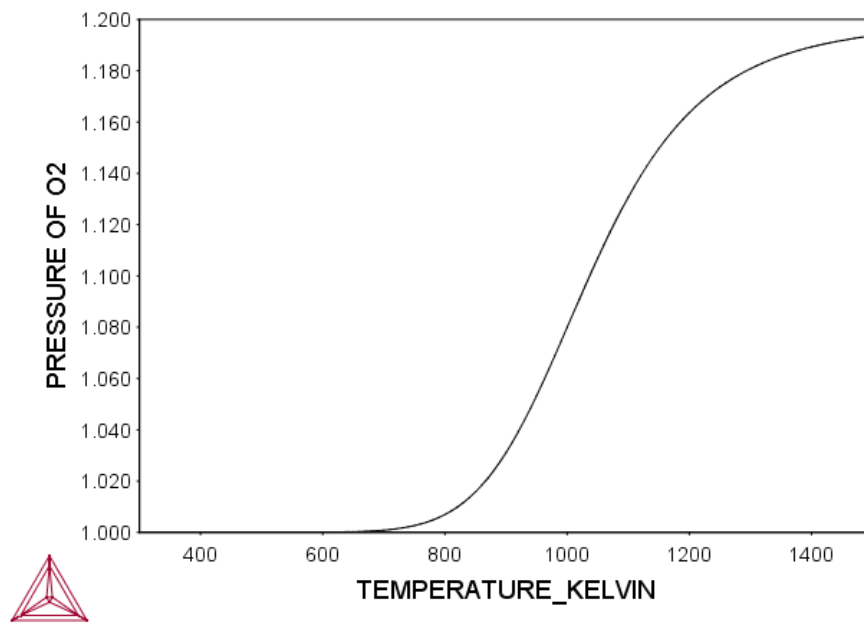


Figure 3: Partial pressure as function of temperature of O_2