

PELE - New in Version 5

Starting with version 5, CO₂ and S were added as additional system components. This allows one to exsolve both a C-O-H-S fluid and to precipitate sulfide and C-bearing phases from the liquid.

CO₂ solubility essentially incorporates the model of Papale (1999, *Am Min* 84:477-492). It has been modified as follows: the CO₂-oxide liquid interaction parameters have been recalibrated to the liquid components and interaction parameters used in PELE/MELTS. Also, the thermodynamic properties of pure CO₂ and all other gas species are now calculated by the general EOS for supercritical gases of Duan et al. (1996, *GCA* 60:1209-1216). Gases are otherwise assumed to mix ideally. Possible gas species include H₂O, CO₂, CO, H₂S, and SO₂. Graphite (C) is a possible precipitating solid.

The silicate liquid component for sulfur is FeS (liquid troilite). An error will be generated if there is S but no FeO entered. Sulfur fugacity is calculated by the method of Wallace and Carmichael (1992, *GCA* 56:1863-1874).

Immiscible sulfide liquid is assumed to be an ideal solution of two components, FeS and FeO. Other possible sulfide phases that can precipitate are pyrrhotite, pyrite and troilite.

FeS-oxide liquid interaction parameters were calibrated (with some arbitrary adjustment because of uncertain sulfide liquid compositions in the experimental data) from the data of O'Neill and Mavrogenes (2002, *J Pet* 43:1049-1087), Wentlandt (1982, *Am Min* 67:877-885); Mavrogenes and O'Neill (1999, *GCA* 63:1173-1180) and Haughton et al. (1974, *Econ Geol* 69:451-467). These are mostly of basalt-intermediate composition, but the lower solubility calculated for more acid compositions appear reasonable. Above ~10 kbar, sulfide saturation values are significantly lower than expected.

Examples of Gas Calculations Using PELE:

Equilibrium degassing:

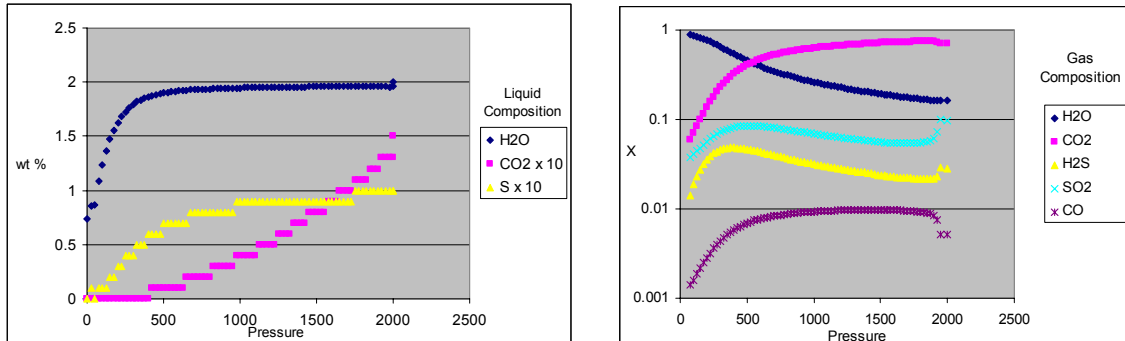


Figure 1. Volatile concentrations in silicate liquid (left) and vapor (right) for equilibrium degassing. Initial MORB liquid with 2.0 wt. % H₂O, 0.15 wt. % CO₂ and 0.1 wt % S at 1225 °C. Liquid undergoes degassing without loss of vapor while undergoing an isothermal pressure change from 2,001 to 1 bar. Steps seen in the left graph are the result of data saved to only the second decimal place.

Fractional degassing:

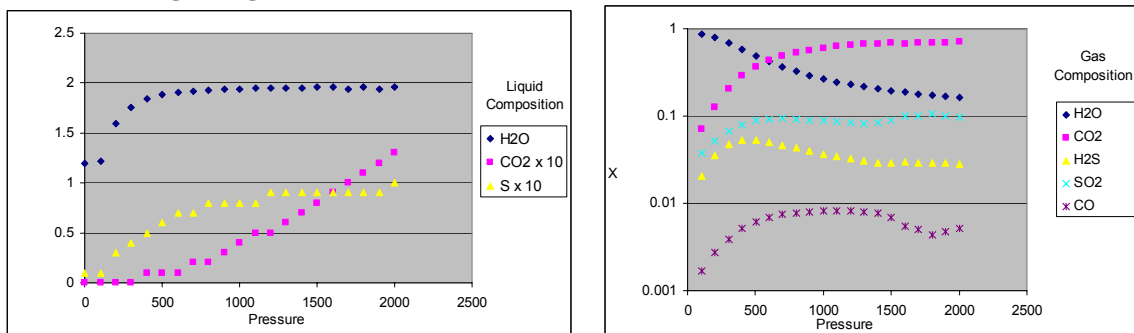


Figure 2. Volatile concentrations in silicate liquid (left) and vapor (right) for fractional degassing. Initial MORB liquid with 2.0 wt. % H₂O, 0.15 wt. % CO₂ and 0.1 wt % S at 1225 °C. Liquid undergoes degassing with loss of vapor while undergoing an isothermal pressure change from 2,001 to 1 bar.

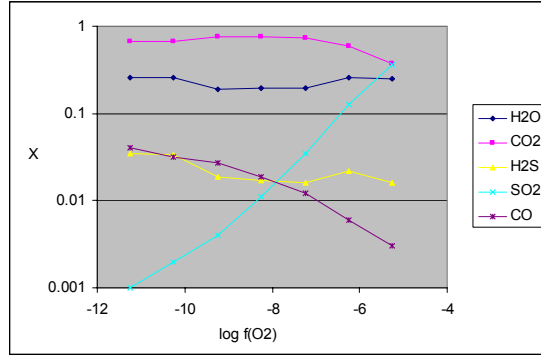


Figure 3. Composition of gas phase (in mole fractions) as a function of $\log f(\text{O}_2)$. Initial bulk composition = MORB liquid with 2.0 wt. % H_2O , 0.15 wt. % CO_2 and 0.1 wt % S, equilibrated at 1225 °C, 1000 bars. $\log f(\text{O}_2)$ varies between QFM +3 to QFM -3.

Examples of Sulfide Calculations using PELE:

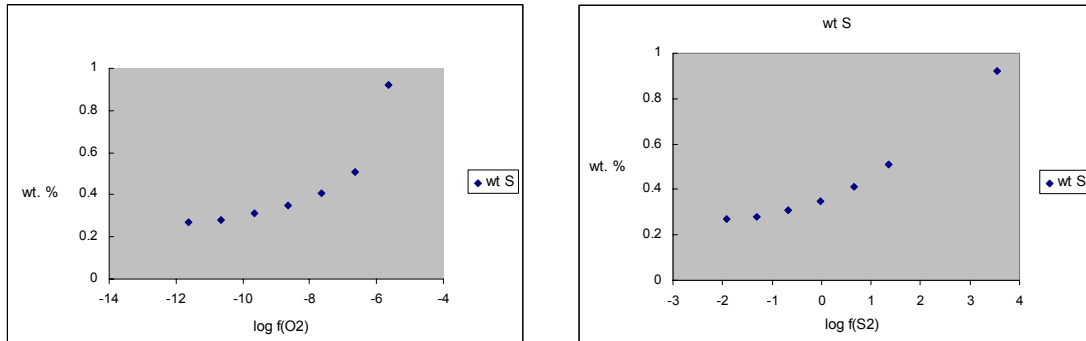


Figure 4. Sulfur concentration in silicate liquid at sulfide saturation as a function of $\log f(\text{O}_2)$ (left) and $\log f(\text{S}_2)$ (right) at 1200 °C and 1 bar. Sample 8F1 for Haughton et al (1974); $\text{FeO}_t = 26.2$ wt. %.

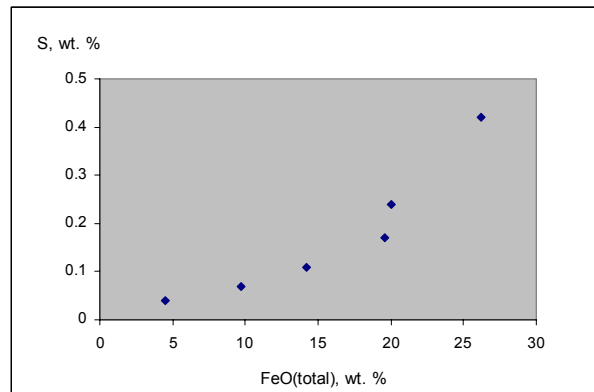


Figure 5. Sulfur concentration at sulfide saturation in liquids of basaltic composition as a function of $\text{FeO}_{\text{total}}$ concentration at 1200 °C, 1 bar and $f(\text{O}_2) = \text{Ni-NiO}$.