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A model to predict the sulfur concentration at sulfide saturation (SCSS) in anhydrous mafic melts

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Sulfur is a low concentration volatile element present in all magmatic systems. It plays an important role in many igneous processes ranging from volcanic degassing to magmatic sulfide ore deposition. Because of the importance of sulfur in magmatic systems an accurate model for the prediction of sulfide solubility in silicate melts provides insight into magmatic processes and also can be applied to investigate ore-deposit formation conditions.

Using experimental data from the literature we constructed a model to predict the SCSS in silicate melts of mafic composition, at pressures from 1 bar to 9 GPa, temperature from 1115 to 1800˚C and oxygen fugacities between 4.5 log units below the fayalite–magnetite–quartz buffer to 1 log units above it. All experiments were saturated with FeS melt or pyrrhotite crystals. The coefficients were obtained by multiple linear regression of experimental data and the model for the prediction of the SCSS is:

$\ln X_S$ = - 36.16 P/T + 123.27 - 0.05 $\lg fO_2$ - 130.41X_{SiO2}−118.15X_{TiO2}−128.94$X_{AlO1.5}$- 170.31$X_{FeO1.5}$- 123.37X_{FeO} - 128.33X_{MgO} - 127.11X_{CaO} - 126.72$X_{NaO0.5}$- 147.73$X_{KO0.5}$

where P is total pressure in kbar, T is temperature in degrees Kelvin, fO_2 is oxygen fugacity, $X$is mole fraction. Total iron in silicate melts is converted to FeO and Fe_2O_3 using the equation of Killinc (Killinc et al., 1983). The accuracy of an empirical model may be evaluated by comparison of the average squared deviation between the data sets calculated and measured values and with the χ^2 value, which is defined as:

χ^2 = Σ[calculated ln $X_{S(ppm)}$ – measured ln $X_{S(ppm)}$]^2/measured ln X_S.

Our empirical equation yields an average squared deviation of 0.07 and a χ^2 value of 0.45 for the 253 experimental samples used for calibration.

Using the SCSS model we can calculate the saturation of natural magmas with a sulfide phase and evolution of the SCSS during magmatic differentiation. The proposed model predicts the appearance of the sulfide phase in the vertical perspective of intrusions with an accuracy of $\pm$ 25 meters.