

Appendix

Computation methods for expanded empirical Cl solubility model

This model follows on the 2000 bar method of Webster and De Vivo (2002) modified for subtle issues of composition and accounting for changes in pressure and temperature. At ca. 1 to 7000 bars, 700 to 1250 °C, the quantity of Cl that dissolves in aluminosilicate melts of rhyolitic to basaltic composition is described by [i.e., all (X) quantities are in moles per 100 g of melt and are calculated as the (wt% component/molecular or atomic weight of the component)]:

$$\begin{aligned}
 & (1) \text{ The 2000-bar molar solubility of Cl (moles Cl in 100 g of melt) not accounting for } \\
 & \text{pressure or temperature =} \\
 & \quad [[\text{Cl}]\text{@2000bar}] = \\
 & \quad (((0.00566)\text{x}[\text{Al}]) + ((0.0105)\text{x}[\text{K}]) + ((0.04)\text{x}[\text{Na}]) + ((0.143)\text{x}[\text{Fe}]) + ((0.24)\text{x}[\text{Ca}]) + \\
 & ((0.25)\text{x}[\text{Mg}]) + ((0.0636)\text{x}[\text{F}])) \\
 & \quad - ([\text{Ti}]\text{x}(1)) \text{ IF } [\text{Si}] < 0.975 \\
 & \quad \{ \text{FOR Ti-BEARING, MAFIC MELTS} \} \\
 & \quad - ([\text{P}]\text{x}(1.3)) \text{ IF } [\text{P}] < 0.08 \text{ AND } [\text{Si}] < 1 \\
 & \quad \{ \text{FOR P-BEARING, MAFIC MELTS} \} \\
 & \quad - (((0.02)\text{x}([\text{Ca}]+(2\text{x}[\text{Na}])+(2\text{x}[\text{K}])))/(2\text{x}[\text{Al}]) \text{ IF } \\
 & (2\text{x}[\text{Al}])/([\text{Ca}]+(2\text{x}[\text{Na}])+(2\text{x}[\text{K}])) < 0.7 \text{ AND } \\
 & ([\text{Na}])/([\text{Na}]+([\text{K}])) < 0.32 \\
 & \quad \{ \text{FOR RELATIVELY POTASSIC, ALKALINE MELTS} \} \\
 & \quad + ([\text{P}]\text{x}(0.07)) \text{ IF } [\text{Si}] > 1 \\
 & \quad \{ \text{FOR P-BEARING, INTERMEDIATE AND FELSIC MELTS} \} \\
 & \quad + ((([\text{Al}]-([\text{Na}]+[\text{K}]+[\text{Ca}]+[\text{Li}]))\text{x}(0.15)) \text{ IF } [\text{Si}] > 1.1 \text{ AND } ([\text{Al}])/([\text{Ca}]+[\text{Na}]+[\text{K}]+[\text{Li}])) > \\
 & 1.19 \\
 & \quad \{ \text{FOR ALUMINOUS FELSIC MELTS} \} \\
 & \quad + ((([\text{Na}]+[\text{K}]+[\text{Ca}]+[\text{Li}])-\text{[Al]})\text{x}(0.0055)) \text{ IF } [\text{Si}] > 1.0 \text{ AND } (([\text{Ca}]+[\text{Na}]+[\text{K}]+[\text{Li}])/[\text{Al}]) > \\
 & 1.1 \\
 & \quad \{ \text{FOR ALKALINE, INTERMEDIATE AND FELSIC MELTS} \} \\
 & \quad + ((([\text{Al}]+[\text{Ca}]+[\text{Mg}])/([\text{Na}]+[\text{K}]+[\text{Li}])\text{x}(0.0015)) \text{ IF } (([\text{Al}]+[\text{Ca}]+[\text{Mg}])/([\text{Na}]+[\text{K}]+[\text{Li}])) > \\
 & 10 \\
 & \quad \{ \text{FOR Al-, Ca-, AND Mg-ENRICHED MAFIC MELTS} \}
 \end{aligned}$$

$$\begin{aligned}
 & (2) \text{ The molar solubility of Cl in 100 g of melt at all pressures (in bars) and temperatures (in } \\
 & \text{degrees Celsius) =} \\
 & \quad [[\text{Cl}]\text{@P\&T}] = \\
 & \quad [[\text{Cl}]\text{@2000bar}] \\
 & \quad + ((([\text{Cl}]\text{@2000bar}) \text{ x } ((\text{pressure}) - (1999)) \text{ x } (0.00011)) \text{ IF } \text{pressure} > 2100 \\
 & \quad + ((([\text{Cl}]\text{@2000bar}) \text{ x } ((\text{pressure}) - (1999)) \text{ x } (0.0001)) \text{ IF } \text{pressure} < 2000 \\
 & \quad + ((([\text{Cl}]\text{@2000bar}) \text{ x } ((\text{temperature}) - (1050)) \text{ x } (0.0008)) \text{ IF } \text{temperature} > 1050 \text{ AND } [\text{Si}] > \\
 & 0.93
 \end{aligned}$$

$$\begin{aligned}
 & (3) \text{ The wt\% of Cl in 100 g of melt (at all pressures and temperatures) =} \\
 & \quad ([[\text{Cl}]\text{@P\&T}] \times (35.453))
 \end{aligned}$$