Supporting information

The partitioning of a trace element between a carbonate mineral and aqueous solution is generally expressed by the distribution coefficient, K_d, which is defined as

$$K_d = \left(\frac{X_{TrCO_3}}{X_{MCO_3}} \right) \Big/ \left(\frac{m_{Tr}}{m_M} \right) \tag{A1}$$

McIntire (1963) calculated that, K_d is related to the quotient of the thermodynamic solubility products of major element carbonate (MCO_3) and trace element carbonate ($TrCO_3$) and K_d can be expressed:

$$K_d = \left(\frac{K_{MCO_3}}{K_{TrCO_3}} \right)^{\frac{1}{V\tau}} \left(\frac{\gamma_{Tr}}{\gamma_M} \right) \left(\exp\left(\frac{-\Delta\mu}{\upsilon_a RT} \right) \right) \tag{A2}$$

The amount of Ca and Tr precipitated per kilogram of water passing through the reactor is:

$$n_{Ca} = \left(m(in)_{Ca} \right) - \left(m(out)_{Ca} \right)(1\,kg) \tag{A3}$$

$$n_{Tr} = \left(m(in)_{Tr} \right) - \left(m(out)_{Tr} \right)(1\,kg) \tag{A4}$$

From the definition of mole fraction;

$$X_{TrCO_3} = \frac{n_{TrCO_3}}{n_{TrCO_3} + n_{CaCO_3}} \tag{A5}$$

$$X_{CaCO_3} = \frac{n_{CaCO_3}}{n_{TrCO_3} + n_{CaCO_3}} \tag{A6}$$

So, the Eq.A3, A4, A5 and A6 can be written as:

$$\frac{X_{TrCO_3}}{X_{CaCO_3}} = \frac{n_{TrCO_3}}{n_{CaCO_3}} = \frac{\left(m(in)_{Tr} - m(out)_{Tr} \right)}{\left(m(in)_{Ca} - m(out)_{Ca} \right)} \tag{A7}$$

Also because, the effluent stream (out) is simply the contents of the reactor, and the concentration ratio of Tr to Ca in the reactor is;

$$\frac{m(out)_{Tr}}{m(out)_{Ca}}$$

This ratio and Eq. A7 can be substituted into the definition of K_d, to give;

$$K_d = \left(\frac{X_{TrCO_3}}{X_{CaCO_3}} \right) \Big/ \left(\frac{m_{Tr}}{m_{Ca}} \right) = \left(\frac{m(in)_{Tr} - m(out)_{Tr}}{m(in)_{Ca} - m(out)_{Ca}} \right) \Big/ \left(\frac{m(out)_{Tr}}{m(out)_{Ca}} \right) \tag{A8}$$

After measuring the $m(in)_{Tr}$, $m(in)_{Ca}$, $m(out)_{Tr}$, $m(out)_{Ca}$ and each sampling time, the K_d can be given. Eq. A8 can be rearranged to;

$$\left(\frac{m(out)_{Tr}}{m(in)_{Tr}} \right) = \frac{1}{K_d \left(\frac{m(in)_{Ca}}{m(out)_{Ca}} \right) - K_d + 1} \tag{A9}$$

f_i, indicates the fraction of species i remaining in solution, as:

$$f_i = \frac{m(out)_i}{m(in)_i} \tag{A10}$$

So, the Eq. A10 becomes:

$$f_{Tr} = \frac{1}{(K_d/f_{Ca}) - K_d + 1} \tag{A11}$$

And F_i defines the fraction of species i precipitated from solution, as

$$F_i = 1 - f_i \tag{A12}$$

So that, the Eq. A12 becomes:

$$f_{Tr} = \frac{1}{\left(\dfrac{K_d}{1-F_{Ca}}\right) - K_d + 1} \tag{A13}$$

This can be rearranged to:

$$f_{Tr} = \frac{1}{\left(\dfrac{K_d}{1-F_{Ca}}\right) - K_d + 1} \tag{A14}$$

Notation

M	major element
Tr	trace element
m_{Ca}	concentration of Ca element in aqueous solution, mol/kg
m_{Tr}	concentration of a trace element in aqueous solution, mol/kg
n_{Ca}	number of moles of Ca element
n_{Tr}	number of moles of the trace element
R	the gas constant, 8.314 J/mol K
T	temperature, K
v_a	ratio of the number of anions in Tr_nCO_3 to the number of anions in M_mCO_3
X_{CaCO3}	mole fraction of calcite component in the solid solution
X_{TrCO3}	mole fraction of the trace element carbonate component in the solid solution
$\Delta\mu$	difference between the chemical potential of $TrCO_3$ in a pure crystal of $TrCO_3$ and its chemical potential as a solid solution component in MCO_3
γ	activity coefficient of element in aqueous solution
Fe_w-OH	weak-sites of $Fe(OH)_3$
Fe_s-OH	strong-sites of $Fe(OH)_3$
Al_w-OH	weak-sites of $Al(OH)_3$
Al_s-OH	strong-sites of $Al(OH)_3$