1 Sorption Rates

It has been found that the rate of sorption to the magnetic beads may be expressed by a rate law of arbitrary order n, as shown below,

$$\frac{\mathrm{d}\omega^{is}}{\mathrm{d}t} = \hat{k}\left(\omega_{eq}^{is} - \omega^{is}\right)^{n} \ , \tag{1}$$

where ω_{eq}^{is} is the mass fraction at equilibrium, and $\hat{\mathbf{k}}$ and n are empirically fit constants. The equilibrium mass fraction may be calculated from the Langmuir isotherm, given by

$$\omega_{eq}^{is} = \frac{Q_0 b C_{eq}^{iw}}{1 + b C_{eq}^{iw}} \ , \tag{2}$$

where C_{eq}^{iw} is the equilibrium concentration in the fluid phase and Q_0 and b are empirically fit constants. The issue that has been found, is that we need to calculate the rate of change of species i in the fluid phase. We know that, for constant fluid density,

$$V^{w}\frac{\mathrm{d}C^{iw}}{\mathrm{d}t} = -\frac{\mathrm{d}m^{is}}{\mathrm{d}t} \ , \tag{3}$$

where m^{is} is the mass of species i in the solid phase and V^{w} is the volume of fluid. We may calculate mass fraction from

$$\omega^{is} = \frac{m^{is}}{m_0^{s} + m^{is}} \ , \tag{4}$$

where m_0^{s} is the original mass of the solid phase at time zero, before the experiment begins. Thus, we find that

$$\frac{\mathrm{d}\omega^{is}}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{m^{is}}{m_0^{s} + m^{is}}\right) \ . \tag{5}$$

Applying the quotient rule, we get

$$\frac{\mathrm{d}\omega^{is}}{\mathrm{d}t} = \frac{\left(m_0^{s} + m^{is}\right)\frac{\mathrm{d}m^{is}}{\mathrm{d}t} - m^{is}\frac{\mathrm{d}m^{is}}{\mathrm{d}t}}{\left(m_0^{s} + m^{is}\right)^2} \ , \tag{6}$$

which rearranges to

$$\frac{\mathrm{d}\omega^{is}}{\mathrm{d}t} = \frac{m_0^{s}}{\left(m_0^{s} + m^{is}\right)^2}\frac{\mathrm{d}m^{is}}{\mathrm{d}t} \ . \tag{7}$$

Noting that

$$m^{is} = \frac{\omega^{is}}{1 - \omega^{is}} m_0^{s} \ , \tag{8}$$

we can write Eqn. (7) as

$$\left(1 + \frac{\omega^{is}}{1 - \omega^{is}}\right)^2 m_0^{s}\frac{\mathrm{d}\omega^{is}}{\mathrm{d}t} = \frac{\mathrm{d}m^{is}}{\mathrm{d}t} \ . \tag{9}$$

Plugging the above into Eqn. (3), and plugging in our rate law, gives us

$$V^{w}\frac{\mathrm{d}C^{iw}}{\mathrm{d}t} = -\left(1 + \frac{\omega^{is}}{1 - \omega^{is}}\right)^2 m_0^{s}\frac{\mathrm{d}\omega^{is}}{\mathrm{d}t} \ . \tag{10}$$

This form is convenient, because it does not require that we calculate the total mass of the solid phase, it does not require that ρ^{s} is constant, and because m_0^{s}/V^{w} is available from the experiments, and may be input into the model with ease.