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Simple Chemical Model for Facilitated Transport with an Application to Wyman-Murray Facilitated Diffusion

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Supporting Information

In the Supporting Information, we have gathered some of the details that are left out of the main text in the paper.

Section 1:

The D_i from King-Altman-Hill method in (5) are given by:

$$D_0 = k_{-5}k_{+4}k_{-3} + k_{-2}k_{-5}k_{-3} + k_{-2}k_{-5}k_{-4} + k_{-2}k_{-4}k_{+3}c_P, \tag{26a}$$

$$D_1 = k_{-2}k_{+5}k_{-4} + k_{-2}k_{+5}k_{-3} + k_{+5}k_{+4}k_{-3} + k_{+2}k_{+4}k_{-3}c_S, \tag{26b}$$

$$D_2 = k_{+2}k_{-5}k_{-3}c_S + k_{+2}k_{-5}k_{-4}c_S + k_{+2}k_{-4}k_{+3}c_Sc_P + k_{+5}k_{-4}k_{+3}c_P, \tag{26c}$$

$$D_3 = k_{+2}k_{-5}k_{+4}c_S + k_{+2}k_{+4}k_{+3}c_Sc_P + k_{+5}k_{+4}k_{+3}c_P + k_{-2}k_{+5}k_{+3}c_P. \tag{26d}$$

Section 1.1:

The general form of (7) for any values of the parameters is given by

$$\begin{aligned}
\frac{c_{ES}}{c_E} &= K_2 c_S \frac{1 + \frac{k_{+3}k_{-4}k_{+5}c_P}{k_{+2}c_S(k_{-3}k_{-5}+k_{-4}k_{-5}+k_{+3}k_{-4}c_P)}}{1 + \frac{k_{-3}k_{+4}k_{-5}}{k_{-2}(k_{-3}k_{-5}+k_{-4}k_{-5}+k_{+3}k_{-4}c_P)}}, \\
\frac{c_{\widetilde{E}P}}{c_{\widetilde{E}}} &= K_3 c_P \frac{1 + \frac{k_{+2}k_{+4}k_{-5}c_S}{k_{+3}c_P(k_{-2}k_{+5}+k_{+4}k_{+5}+k_{+2}k_{+4}c_S)}}{1 + \frac{k_{-2}k_{-4}k_{+5}}{k_{-3}(k_{-2}k_{+5}+k_{+4}k_{+5}+k_{+2}k_{+4}c_S)}}.
\end{aligned}$$

Section 1.2:

The general form of v_N and v_F are given by

$$v_N = k_{+1}s_0 - k_{-1}p_0, \tag{27a}$$

$$v_F = \frac{k_{+4}k_{-5}K_2 e_0^{tot}\left(k_{+1}s_0 - k_{-1}p_0\right)}{k_{+1}\Omega} \tag{27b}$$

where

$$\begin{aligned}\Omega &= (k_{-5}+k_{+5}) + (k_{-4}+k_{+4})\,K_2K_3s_0p_0 + (k_{+4}+k_{-5})\,K_2s_0 \\ &\quad + (k_{-4}+k_{+5})\,K_3p_0 + (k_{-5}+k_{+5})\left(\frac{k_{-4}}{k_{-3}}+\frac{k_{+4}}{k_{-2}}\right) \\ &\quad + (k_{-4}+k_{+4})\left(\frac{k_{-5}}{k_{-3}}K_2s_0+\frac{k_{+5}}{k_{-2}}K_3p_0\right). \qquad (28)\end{aligned}$$

Section 2:

The scaling factor is determined as follows. From Wittenberg's experiments, we know the cross-sectional area of the milipore filter, $A = 11.5\,cm^2$, as well as the (dimensionless) porosity of the filter, $\rho = 0.79$, so the effective cross-sectional area across which the ligands can diffuse is ρA. A one-dimensional diffusion process and a two-compartment kinetics transport model can be related by the distance across which the ligands and enzymes diffuse, ℓ. Therefore, we choose our "volume factor" to be the effective volume: $V_{eff} = \rho A \ell$. In order to convert the total ligand flux, J, to Wittenberg's units of $\mu L \cdot min^{-1}$, we also need to use a conversion factor determined using the ideal gas law for Wittenberg's experimental conditions, $\alpha = 1.344 \times 10^9 \mu L \cdot s \cdot min^{-1} \cdot mol^{-1}$. Thus our scaling factor is given by $\gamma = \alpha \rho A \ell$.