

Early removal of weak-binding adsorbates by kinetic separation

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Supporting Information for Publication

The time constants r_1 and r_2 in Equation (5) are given by

$$r_1 = \frac{\theta - \sqrt{\theta^2 - 4\phi}}{2}; r_2 = \frac{\theta + \sqrt{\theta^2 - 4\phi}}{2} \quad (\text{S1})$$

with:

$$\begin{aligned} \theta &= \exp(\beta\mu_s) + \exp(\beta\mu_w) + \exp(\beta\varepsilon_s) + \exp(\beta\varepsilon_w), \\ \phi &= \exp(\beta\mu_s)\exp(\beta\varepsilon_w) + \exp(\beta\mu_w)\exp(\beta\varepsilon_s) + \exp(\beta\varepsilon_s)\exp(\beta\varepsilon_w) \end{aligned} \quad (\text{S2})$$

The coefficients C in Equation (5) are:

$$\begin{aligned} C_{2,s} &= \frac{1 + \exp(-\beta\mu_s)r_1n_{eq,s}}{\exp(-\beta\mu_s)(r_2 - r_1)}; C_{1,s} = -C_{2,s} - n_{eq,s} \\ C_{2,w} &= -[r_2 \exp(-\beta\mu_s) + \exp[-\beta(\varepsilon_s - \mu_s)] + 1]C_{2,s}; C_{1,w} = -C_{2,w} + n_{eq,s} \end{aligned} \quad (\text{S3})$$

Values of the cross time for several combinations of coverage for each species are given in the Table below. Notice that this time can be a considerable fraction of the total equilibration time or even coincide with it.

$n_{eq,s} \backslash n_{eq,w}$	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
0.1	1.00	0.18	0.11	0.08	0.05	0.03	0.01	0.00	0.00
0.2		1.00	0.29	0.21	0.16	0.13	0.11	0.07	
0.3			1.00	0.38	0.27	0.21	0.17		
0.4				1.00	0.45	0.31			
0.5					1.00				

Table 1. Cross time (in units of the equilibration time of the system) for several combinations of $n_{eq,s}$ and $n_{eq,w}$.