Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Simulation of Intermediate Transport in Nanoscale Scaffolds for Multistep Catalytic Reactions

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Supporting Information

Domain Size Study

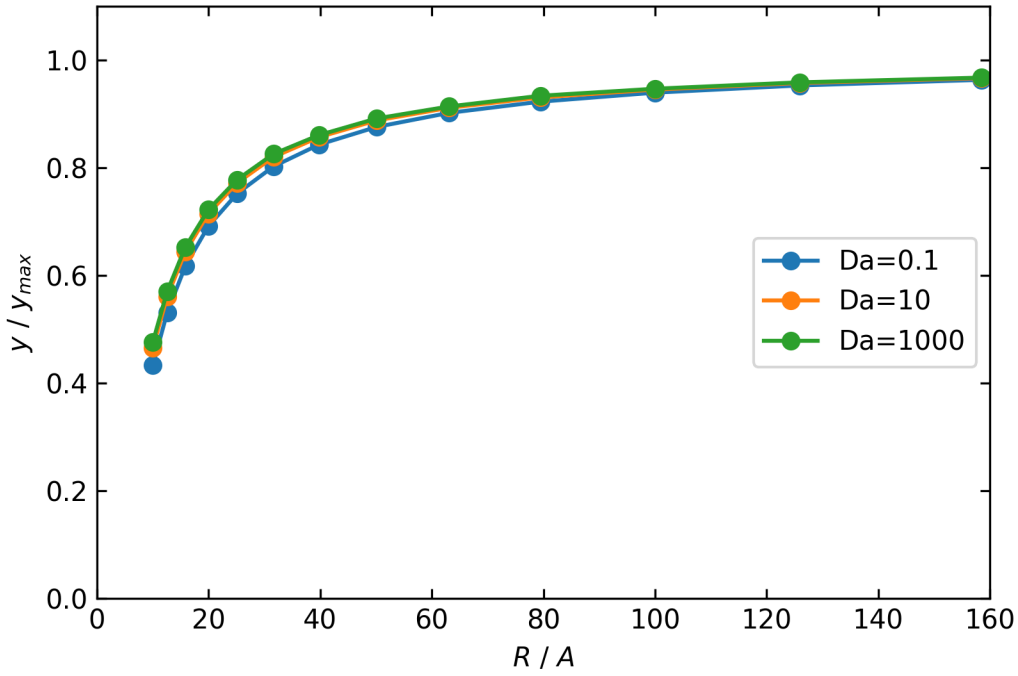

Figure S1. Effect of domain size, *R*, on simulation results in absence of electrostatic interactions. R was set to 20 nm for this study, which represents a minimal domain size that does not significantly affect yield. Other parameter values given in Table 1.

Analysis of Experimental Data for Fig. 11

Horizontal Axis

To calculate $\mathbf{Da} = k_2 A/D$, the heterogeneous rate constant k_2 (nm s^{-1}) was estimated from experimental rate data, and values of A was assumed to be in the range 0.1–1.0 nm. Unless otherwise noted, the Diffusivity, D, was assumed to be 10^{-5} cm^2 s^{-1} or 10^9 nm^2 s^{-1}.

The heterogeneous rate constant, k_2, was calculated from a homogeneous first order rate constant, k_2' (s^{-1}), determined by experiment, using the following conversion:

$$k_2 = \frac{k_2'}{C_{cat}} \frac{10^{24}}{N_A\, 2\pi A^2}$$

where C_{cat} (mol L^{-1}) is the catalyst concentration and N_A= 6.02×10^{23} (molec/mole) is Avogadro's number. The factor 10^{24} accomplishes the volumetric conversion from L to nm^3.

Input Data

Reference	k_2' / s^{-1}	C_{cat} / nm	D / cm^2 s^{-1}	τ_0 / s	τ / s
6. Trujillo	0.031	1.4	10^{-5}	30	10[a]
10. Lindbladh	0.095	79	10^{-5}	9.5	4.8
19. Zhang	0.012	1	1.7×10^{-5}	137	143
23. Liu	9.5×10^{-3}	7.8	10^{-5}	105	69

[a]*Minimum detectable value. Actual value was below detection limit.*