Supplementary Information

Microreactor with Mesoporous Silica Support Layer for Lipase Catalyzed Enantioselective Transesterification

Sho Kataoka, Yasutaka Takeuchi, Atsuhiro Harada, Mitsuhiko Yamada, Akira Endo*

National Institute of Advanced Industrial Science and Technology (AIST), 1-1-1 Higashi, Tsukuba, Ibaraki 305-8565, Japan

* Corresponding author: Tel.: +81-29-861-4653; Fax: +81-29-861-4660; e-mail: endo-akira@aist.go.jp (Akira Endo)

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Estimation of Effective Diffusivity inside Mesoporous Silica Films

The mesoporous silica film (less than 50 nm) was designed to minimize the diffusion limitation. In order to ensure the validity, we calculated the modified Thiele modulus (φ) using values obtained in the current study. We assumed that the 3D cubic film as a catalytic layer was flat and that the reaction expressed with Ping-Pong Bi Bi model in the main text was simplified in a first-order form.

First, the diffusive flux is expressed as follows:

$$N_{As} = -\frac{\varepsilon D}{\tau} \cdot \frac{dC}{dx}$$

In this model, x is defined as a position in the direction of thickness. If a material balance is expressed over the differential elements of porous materials, one could find at steady state,

$$\left(N_{As}\right)_x - \left(N_{As}\right)_{x+dx} + mR \cdot dx = 0$$

When the initial concentration is low, the reaction rate per unit lipase weight R can be simplified in a first order form as follows:

$$R=kC$$

When we take the limit as dx goes to zero, the rearrangement gives

$$\frac{\varepsilon D}{\tau}\frac{d^2C}{dx^2} = mkC$$

Based on the second-order differential equation, the modified Thiele modulus, φ is expressed as follows:

$$\varphi = d\sqrt{\frac{mk}{(\varepsilon D/\tau)}} \cong 5.6\times10^{-3}$$

In general, when φ is smaller than 0.1, its diffusion limitation is absent. Since φ is sufficiently small, the diffusion limitation is minimal.

Values of parameters used in the model:

Diffusion coefficient (estimated), D= 1 x10^{-9} $m^2 \cdot s^{-1}$:

Porosity, ε= 0.3 (from Fig 1):

Tortuosity (estimated), τ= 3:

Thickness of the film, d= 45 nm (from Fig. 1):

Amount of enzyme per unit volume, *m* is calculated from ΔM = 1.55 x 10^{-2} $g \cdot m^{-2}$ in Table 1:

$$m = \frac{\Delta M}{d} = \frac{1.55\times10^{-2}}{4.5\times10^{-8}} = 3.4\times10^{5}\ g\cdot m^{-3}:$$

Reaction rate, $R = C \cdot V_{max}/K_{VA} = k\ C$, where k = 4.5 x 10^{-6} m^3 s^{-1} $g_{-lipase}^{-1}$ (from Table 2)