Electronic Supplementary Information

Liquid-phase catalytic hydrodechlorination of chlorinated organic compounds in continuous flow micro-packed bed reactor over Pd/AC catalyst

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1. Calculation of internal diffusion

In order to determine the effect of internal mass transfer, the Thiele modulus and efficiency factor were calculated using equations (S1, S2, S3) and the equation (S4), respectively:

$$D_m = 7.4 \times 10^{-8}[\frac{(\varphi M)^{0.5} T}{\mu V^{0.6}}] \quad \#\ (S1)$$

$$D_{eff} = D_m \frac{\varepsilon}{tortuoxity} \quad \#\ (S2)$$

$$\emptyset = L\sqrt{\frac{k}{D_{eff}}} \quad \#\ (S3)$$

$$\eta = \frac{\varepsilon}{\emptyset}\left(\frac{1}{tanh\emptyset} - \frac{1}{\emptyset}\right) \quad \#\ (S4)$$

The values supporting this calculation are summarized in Table S1.

Table S1 Values of symbols in internal diffusion of chlorobenzene.

Symbols	Significance	Value
φ	"Association parameter" for the solvent	1.0[1]
M	Molecular weight of solvent (methanol)	32.04 g/mol
T	Temperature	353.15 K
μ	Viscosity of solvent (methanol)	1.16 mPa·s[2]
V	Molar volume of solute at its normal boiling point	101.3 for CB[3]
ε	porosity	0.38[1]
	tortuoxity	2.7[1]
L	Characteristic length of catalyst particles (L=R/3 for sphere)	0.12 mm
k	Apparent reaction rate constant	0.0042 s^{-1}
D_m (CB)	Molecular diffusion coefficient of CB	7.98×10^{-10} m^2/s
D_{eff} (CB)	Effective diffusion coefficient of CB	1.09×10^{-10} m^2/s

$\emptyset$ (CB)	Thiele modulus of CB	0.905
η (CB)	Efficiency factor of CB	0.948

[1] C. Yang, A.R. Teixeira, Y. Shi, S.C. Born, H. Lin, Y. Song, B. Martin, B. Schenkel, M.P. Lachegurabi and K.F. Jensen, Catalytic Hydrogenation of N-4-nitrophenyl Nicotinamide in a Micro-Packed Bed Reactor, Green Chem., 2018, **20,** 886-893.
[2] R. A. Lewis, Hawley's condensed chemical dictionary, John Wiley & Sons, 2016.
[3] N.T. Program, National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina: NTP via httn. canieochemicals. noaa. gov/chemical/20568.

2. Determination of adsorption equilibrium

Based on the adsorption characteristics accompanied by high specific surface area of the carrier, we experimentally determined the conditions for adsorption saturation of the system and then tested these samples. The experimental result is shown in the Fig. S1.

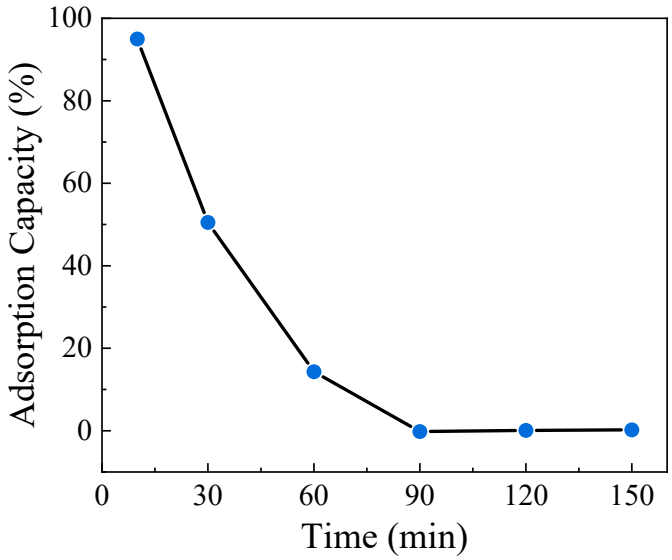

Fig. S1. The curve of adsorption capacity as a function of reaction time.