Strong metal-support interaction in Pt/TiO₂ induced by mild HCHO and NaBH₄ solution reduction and its effect on catalytic toluene combustion

Zebao Rui, Lingye Chen, Huayao Chen, Hongbing Ji*

Department of Chemical Engineering, School of Chemistry & Chemical Engineering, and The Key Lab of Low-carbon Chem & Energy Conservation of Guangdong Province, Sun Yat-Sen University, Guangzhou 510275, P.R. China

^{*} Corresponding author. Tel.: +86 20 84113658. E-mail address: jihb@mail.sysu.edu.cn (H. Ji).

In this work, the Weisz-Prater Criterion (Eq.S1) was used to estimate the influence of pore diffusion on reaction rates. It is particularly useful because it provides a dimensionless number containing only observable parameters that can be readily measured or calculated.^{1, 2}

$$N_{W-P} = \frac{\Re R_p^2}{C_s D_{eff}}$$
(S1)

Here, \Re is the reaction rate per volume of catalyst, which can be calculated from the molar flow rate and conversion of toluene at a given temperature, and the mass $(2 \times 10^{-4} \text{ kg})$ and density (188.7 kg/m³) of the packed catalyst. R_p is the catalyst particle radius, which has a largest value of $R_p = 2.25 \times 10^{-4}$ m due to the mesh screen. C_s is the reactant concentration at the particle surface. As the catalyst used in this study is in the form of a fine powder ($Rp \leq 225 \mu m$), it may be assumed that external diffusion is not effective in the reaction, and

$$C_s \cong C_0 = \frac{P_{0,C_7H_8}}{RT} \tag{S2}$$

The effective diffusivity D_{eff} is related to the mean free path (λ , m) and the mean velocity (\bar{v} , m²/s) of the gas phase toluene. Here,

$$\overline{v} = \left(\frac{8RT}{\pi M}\right)^{1/2} \tag{S3}$$

$$\lambda = \frac{k_B T}{\sqrt{2}\pi d^2 P_{C_7 H_8}} \tag{S4}$$

where $k_{\rm B}$ is the Boltzmann constant in J/K, $P_{C_7H_8}$ is partial pressure of toluene in Pa, *d* is the diameter of toluene in meters, and *M* is the molar mass of toluene in kg/mol. Use of the initial toluene P_{0,C_7H_8} and T = 473.15 K, the calculated $\lambda = 1.08 \times 10^5$ nm is much larger than the pore sizes of the catalysts (d_P , 11.0~22.8 nm). Consequently, pore diffusion will be dominated by Knudsen diffusion and

$$D_{eff} \cong D_{Kn} = \overline{\nu} \frac{d_p}{3} \tag{S5}$$

where D_{Kn} is the Knudsen diffusivity.²

References

- (1) Weisz, P.B.; Prater, C.D. Interpretation of measurements in experimental catalysis. *Adv. Catal.* **1954**, *6*, 143-196.
- (2) Vannice, M.A.; Joyce, W.H. *Kinetics of Catalytic Reactions*. New York: Springer, 2005, 134, 63-65.