

# Evaluation of TiO<sub>2</sub>-SiO<sub>2</sub> Microhoneycomb Photocatalysts Using Model Simulation

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## Introduction

Photocatalytic systems can generally be categorized into suspended systems and immobilized systems. Suspended systems usually provide more surface area per unit volume. However, the necessity of separation step prevents scaling up of this type of systems. Immobilization of photocatalysts can be used to avoid separation step, although the surface area is generally lower than suspended systems [1]. Therefore, the improvement of the configuration of photocatalytic systems is desired.

Previously, we have suggested the use of photocatalyst having microhoneycomb (MH) morphology [2]. This morphology not only provides high specific surface area, but also causes minimal pressure drop to a fluid flow.

In this work, to evaluate the performance of systems with MH photocatalysts, as well as to predict the behavior of such systems, a simplified model based on mass transfer and reaction kinetics is proposed.

## Experimental

TiO<sub>2</sub>-SiO<sub>2</sub> MHs (10 mol% TiO<sub>2</sub>) were prepared by the method modified from Ref. 2. In short, two sources of TiO<sub>2</sub> sol were added to SiO<sub>2</sub> sol so that pH of the mixture can be controlled independently from TiO<sub>2</sub> content. The MHs were calcined in air at 873 K.

Decolorization of methylene blue (MB) was used as a model reaction in continuous flow system (Fig.1). Synthesized photocatalyst having bulk density of  $\rho$  was held vertically while aqueous solution of MB of concentration  $C_0$  was fed to the system from the bottom ( $z = 0$ ). Outlet solution at  $z = L$  was analyzed by a UV-vis spectrophotometer.

A model proposed assumes plug flow at a superficial velocity of  $v$  and 1<sup>st</sup> order rate law

with respect to amount of adsorbed MB ( $q$ ). At steady state, reaction rate is equal to rate of mass transfer of MB to the solid surface (Eq. 1). Rate constant  $k(z)$  includes the effect of light attenuation from blank monolith ( $\varepsilon_1$ ) and adsorbed MB ( $\varepsilon_2$ ) (Eq. 2). The equations were solved at  $C(0) = C_0$  and varied  $k(L)$  so that the deviation of  $C(L)$  from experimental data of uncalcined samples is the lowest. Mass transfer coefficient  $K_f a$  and constants in Freundlich isotherm,  $K$  and  $n$ , were determined from separate batch adsorption experiments.

$$-v \frac{dC}{dz} = k(z) \rho q = K_f a \left( C - \left( \frac{q}{K} \right)^n \right) \quad (1)$$

$$\frac{d \ln k}{dz} = \varepsilon_1 + \varepsilon_2 q \quad (2)$$

## Results and Discussion

From Fig.2, the same rate constant from experimental data of uncalcined samples can be used to predict the conversion of systems with calcined samples as well. The model also indicates that the irradiation depth is shallower in calcined samples than in uncalcined ones. However, higher adsorption capacity of calcined samples leads to higher overall activity. These results suggest the potential of the model to be used for improvement of the configuration of photocatalytic systems.

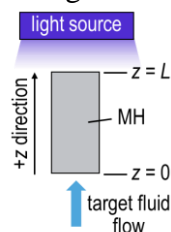


Fig.1 Schematic drawing of photocatalytic system.

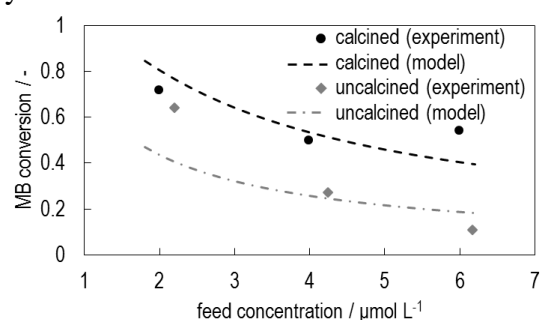


Fig.2 MB decolorization catalyzed by TiO<sub>2</sub>-SiO<sub>2</sub> MHs

## REFERENCES

- [1] C. McCullagh et al., J. Chem. Technol. Biotechnol., 86 (2011) 1002.
- [2] S.R. Mukai et al., ISCRE 22, Maastricht, The Netherlands, 2-5 Sept. 2012.