

Contamination Assessment and Remediation of the Environment

CFD Simulation of a Honeycomb Monolith Photoreactor

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Aim and Objectives:

1. To obtain an appropriate model for the design of a monolith photoreactor.
2. To validate the model with experimental results for conversions of formaldehyde and toluene.
3. To investigate major parametric effects.

Characteristics:

1. Instead of modeling only a single channel, the entire monolith photoreactor was simulated.
2. The monoliths were treated as *Porous Zones*, and Porous Media Formulations were applied.
3. User-defined function (UDF) was used to define the reaction rates involving local radiation intensity.

Computation Domain:

(a) Simulation Tool: FLUENT®

(b) Physical System:

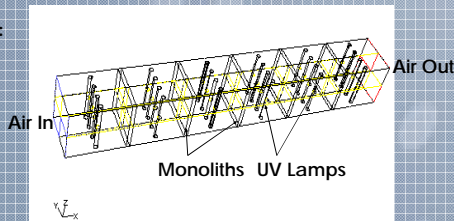


Fig.1 Physical system

(c) Assumptions:

1. Constant density and diffusivity.
2. Diffusely reflecting reactor wall.
3. Negligible absorption, scattering or emission by the gaseous medium.
4. Negligible homogeneous reactions.

Model:

(a) Radiation Model: Discrete Ordinates (DO) Model

(b) Reaction Model: Langmuir-Hinshelwood Kinetics

$$-r = K_0 \frac{K_1 X_C}{1 + K_1 X_C + K_2 X_W} \frac{K_4 X_W}{1 + K_3 X_C + K_4 X_W}, \text{ where } K_0' = K_0 \left(\frac{I}{I_G} \right)^{0.5}$$

Table 1. Rate constants (Obee, 1996)

Gas	K_0	K_1	K_2	K_3	K_4
Toluene	0.34	1.93	0.00036	1.93	0.00036
Formaldehyde	1.05	1.02	0.00020	1.11	0.015

X_C, X_W : mass fraction of VOC, water (ppm)
 K_0, K_1, K_2, K_3, K_4 : Langmuir constants (ppm⁻¹)
 I : Light intensity (W/m²)
 I_G : Light intensity on flat plate reactor (W/m²)

Results and Discussions:

(a) VOC Removal:

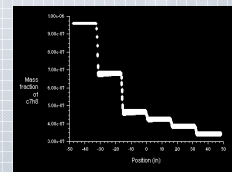


Fig.3 Mass fraction profile

1. The VOC amount decreased (red to blue) whenever the flow encountered a monolith.
2. The VOC amount decreased by 50% when the flow reached 15% of the photoreactor length (second monolith).

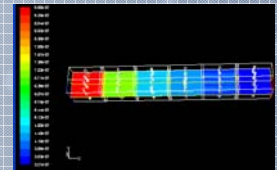


Fig.2 Mass fraction contour

(b) Model Validation:

1. 5 and 6 cases of different geometries (Fig.4) were carried out respectively for formaldehyde and toluene conversions at different operating conditions in a pilot-scale reactor (Hossain et al., 1999).

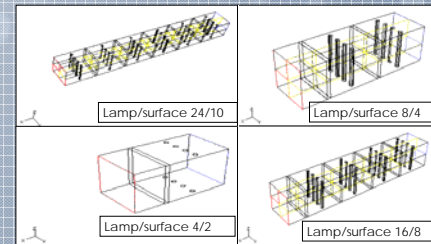


Fig.4 Different geometries for experimental tests

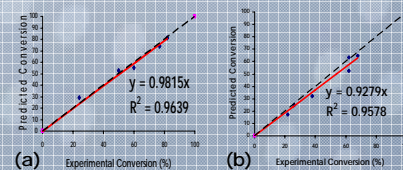


Fig.5(a) formaldehyde, (b) toluene cases

2. Slopes of best fit lines of the data points for formaldehyde and toluene cases were 0.98 and 0.93 respectively, $R^2 = 0.96$, high enough to warrant model reliability.

(c) Parametric Studies:

Light Intensity:

The degradation was first-order followed by power law of exponential 0.5 from low to high intensity.

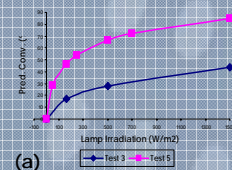
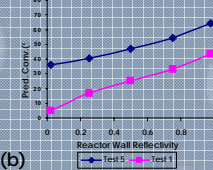


Fig.6 Effects of (a) Irradiation, (b) Adsorption, (c) Reactor wall reflectivity on conversion

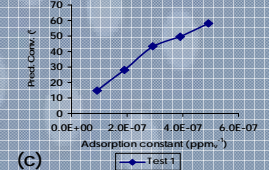
Adsorption:

The conversion was enhanced by increased adsorption constants.



Reactor Wall Reflectivity:

The reactor wall reflectivity is important for this optically-thin system.



Conclusion:

1. A full simulation of photocatalytic oxidations of formaldehyde and toluene using Fluent® in a monolith photoreactor was shown.
2. Porous media modeling using DO model efficiently described the process.
3. Parametric studies were carried out to assist in future design.

References:

1. Obbe T.N., (1996), *Environ.Sci.Technol.*, 30, 3578-3584.
2. Hossain M.M., Raupp G.B., Hay S.O., Obbe T.N., (1999), *AIChE J.*, 45, 1309-1321.