KINETIC MODELING OF A PHOTOCATALYTIC REACTOR DESIGNED FOR REMOVAL OF GAS–PHASE BENZENE: A STUDY ON LIMITING RESISTANCES USING DESIGN OF EXPERIMENTS

J. KRISHNAN† and T. SWAMINATHAN‡

† *Faculty of Chemical Engineering, Universti Teknologi MARA, Shah Alam - 40450, Malaysia.*
jagannathan@salam.uitm.edu.my (corresponding author)
‡ *Department of Chemical Engineering, Indian Institute of Technology Madras, Chennai - 600036, India.*
tswami@iitm.ac.in

***Abstract*— Experiments were conducted at room temperatures, in an immobilized annular tube reactor, using titanium dioxide as the photocatalyst, to identify the influence of important operational parameters, viz., catalyst load (5–20 g m^{-2}), benzene concentration (0.2–6 g m^{-3}) and flow rate (0.2–1 L min^{-1}) on the removal of benzene. Removal efficiencies for benzene ranged from 7% to 96% depending on the range of levels of these process parameters. A modified Langmuir–Hinshelwood (L−H) kinetic model has been suggested based on the experimental observations. The use of a combined plug–flow type L−H kinetic model yielded a design equation that can be used as the basis for the photoreactor scale–up as well as to find the mass transfer and reaction resistances in the photoreactor. The ratio of reaction rate resistance to the overall resistance was found to play an important role in establishing the predominant resistances between mass transfer and reaction rate occurring in the photoreactor.**

***Keywords*— Photocatalysis; gas–phase benzene; Langmuir–Hinshelwood model; immobilized photoreactor.**

I. INTRODUCTION

Both indoor and outdoor air pollution with volatile organic compounds (VOCs) has been a serious environmental problem nowadays due to their carcinogenic nature as well as their tendency to form secondary pollutant, viz., ozone by reacting with NO_x in the presence of sunlight at the ground level. Among the different treatment methods developed for the degradation of VOCs, photocatalytic oxidation process can be considered as an innovative and promising technology to completely oxidize high concentrations of VOCs to harmless end products such as H_2O and CO_2 at ambient temperatures (Wang *et al.*, 2003; Jagannathan *et al.*, 2004). TiO_2 irradiating with ultraviolet (UV) or near UV light results in the formation of electron–hole pairs on the catalyst surface. These electrons and holes interact with adsorbed species producing highly reactive hydroxyl radicals, which in turn initiate redox reactions to decompose VOCs. As the decreasing wavelength increases the radiant power output of the UV lamps, use of the germicidal lamps (254 nm) for the photodegradation of VOCs was reported to be more efficient (Shen and Ku, 2002; Pengyi *et al.*, 2003; Jeong *et al.*, 2004 and Jagannathan, Ph.D thesis, 2006). During the last decade, the gas–phase elimination of VOCs has received more attention (Pengyi *et al.*, 2003).

Photoreactors of various configurations have been developed; however, annular fixed-bed reactors with TiO_2 coated on the surface of reactor wall are the most commonly employed photoreactors for their ease of construction and operation (Ollis and Al-Ekabi, 1993; Alberici and Jardim, 1997; Hennezel *et al.*, 1998). During initial stages of reactor experiments, statistical methodology plays significant role in analyzing the data obtained by studying different process parameters, where there is a likely chance of experimental errors (Montgomery, 1991). However, determining the reaction kinetics is an important aspect of successful design of catalytic reactors. Simple kinetic models help in predicting the expected conversions and also desired size of a reactor. Heterogeneous photochemical reactions, unlike other chemical reactions, are more complex as they involve a variety of mechanisms such as adsorption, surface reaction, desorption etc. It is found from literatures that, kinetic modeling of photoreactors has not been carried out extensively; however, Langmuir–Hinshelwood (L–H) type rate expression has been widely used to describe gas–solid reactions for heterogeneous photocatalysis (Fox and Dulay, 1993; Alberici and Jardim, 1997; Kim and Hong, 2002; Lin *et al.*, 2002). Anew, a wide variety of hydrophilic and hydrophobic VOCs have been tested, that includes, trichloroethylene (Jacoby *et al.*, 1995), 1- butane (Cao *et al.*, 1999), toluene (Bouzaza and Laplanche, 2002), vinyl chloride (Mohseni and David, 2003), hexane (Zhang and Liu, 2004), benzene, toluene, ethylbenzene and xylene (BTEX) in the presence of SO_2 and NO (Ao *et al.*, 2004).

In this study, the use of 2^k factorial design to study the effect of process parameters on the removal of benzene by UV/TiO_2 process in the annular immobilized photoreactor has been described. Moreover, the effects of catalyst load, inlet benzene concentration and the gas flow rate on the resistance ratio were studied using 2^k factorial design. Later from these results, the main and interaction effects were analyzed for its statistical significance by performing an analysis of variance (ANOVA). The decomposition behavior of gas–phase