Chapter 15
Development of an Intelligent Neural Model to Predict and Analyze the VOC Removal Pattern in a Photocatalytic Reactor

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ABSTRACT

Volatile organic compounds (VOCs) belong to a new class of air pollutant that causes significant effect on human health and environment. Photocatalytic oxidation is an innovative, highly efficient, and promising option to decontaminate air polluted with VOCs, at faster elimination rates. This study pertains to the application of artificial neural networks to model the removal dynamics of an annular type photoreactor for gas – phase VOC removal. Relevant literature pertaining to the experimental work has been reported in this chapter. The different steps involved in developing a suitable neural model have been outlined by considering the influence of internal network parameters on the model architecture. Anew, the neural network modeling results were also subjected to sensitivity analysis in order to identify the most influential parameter affecting the VOC removal process in the photoreactor.

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INTRODUCTION

The rapid growth of small – medium – large scale polluting industries and the arising trend in urbanization has led to large scale emission of both point and non – point source air pollutants, particularly in developing countries. Besides, the increasing development of synthetic chemicals, particularly the petrochemicals, a new class of air pollutants, called the volatile organic compounds (VOCs) have become a matter of concern in recent years. The Clean Air Act of 1990 (CAA – 90), proposed by the United States Environmental Protection Agency (US – EPA), classifies the different organic and inorganic chemical species present in the atmosphere, that are likely to cause significant effect on human health and the environment, based on their inherent toxicity and physico – chemical properties. VOCs can be defined as "any compound of carbon, excluding CO, CO_2, carbonic acid, metallic carbides or carbonates, which participates in atmospheric photochemical reactions" (Nunez, 1998). According to the US – EPA website, VOCs are emitted as gases from certain solids or liquids that are usually chemicals, some of which might pose short – and long – term adverse health effects. The US – EPA further clarifies that the concentrations of many VOCs are consistently higher indoors (×10) than outdoors. Some typical examples are as follows: paints and lacquers, paint strippers, cleaning supplies, pesticides, building materials and furnishings, emissions from fine chemical, pharmaceutical and petroleum related industries.

Toluene is a VOC, most commonly used as a raw material for the synthesis of compounds such as tri-nitro toluene (TNT), chloroamine-T, saccharin and many dyestuffs (Rene et al., 2005). Toluene has shown to cause serious adverse human health effects. Even at low concentrations, toluene has been found to be carcinogenic, cause damage to the liver and kidney and paralyze the central nervous system (Martin et al., 1998). In human studies, the uptake of gas – phase toluene has been estimated by different authors to be 40-60% of the total amount inhaled (WHO, 1993). The results of some studies suggests that low levels of toluene exposure (3.75 mg/m^3) may have behavioural effects (Horiguchi and Inoue, 1977), electroencephalogram (EEG) changes and sleep rhythm in mice (Takeuchi and Hisanaga, 1977). The widespread use of toluene in various industrial operations, its high vapour pressure (28.6 mmHg at 25 °C) and high polarity characterized by its water solubility (0.53 g/l at 25 °C) warrants their removal before its emission into the natural environment (Spicer et al., 2002).

PHOTOREACTOR FOR VOC REMOVAL AND WORKING MECHANISM

Among the different techniques, chemical and – or biological, used for the removal of gas – phase 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''. Titanium dioxide (TiO_2) irradiating with UV or near UV light, results in the formation of 'electron – hole pairs' on the catalyst surface. These electrons and holes interact with the adsorbed species producing highly reactive hydroxyl radicals, which in turn initiate redox reactions to decompose VOCs. In some cases, it has been proved that the activity of TiO_2 could be greatly enhanced by modifying the catalyst properties. Zuo et al. (2006) gave sufficient information on the benefits of modifying a photocatalyst, as; (i) inhibiting electron–hole recombination by increasing the charge separation, (ii) increasing the wavelength response range, and (iii) changing the selectivity or yield of a particular product.

According to Wang and Ray (2000), the application of photo oxidation technique for gas – phase VOC removal is more appealing due to