Analysis of Trichloroethylene Degradation in a Millireactor with Varying Irradiance and Flow Rate

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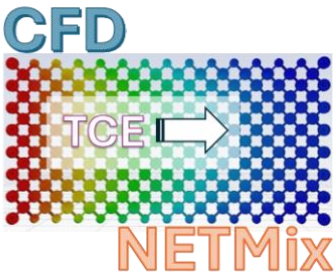


Volatile organic compounds (VOCs), such as trichloroethylene (TCE), are significant air pollutants, posing serious concerns due to their toxicity and carcinogenic potential. This study explores the degradation of TCE through photocatalysis in a millireactor utilizing Degussa P25 titanium dioxide as the catalyst. Simulations were conducted by varying the irradiance and flow rate within the reactor. The results revealed a positive correlation between TCE degradation and irradiance, and a negative correlation with flow speed. The highest degradation rate (77.25%) was achieved under conditions of high irradiance and low flow rate. These findings offer valuable insights for the development of effective air pollutant treatment methods.

Introduction

Although technological innovations have helped reduce pollution, human practices appear to be the primary drivers of environmental degradation and ecosystem disruption. These actions diminish the quality of our environment and create significant challenges for human life.

Air pollution is one of the most alarming and harmful forms of contamination, posing a severe threat to human life. The air quality is closely tied to the overall quality of life, especially due to its significant impact on public health.

Volatile organic compounds (VOCs) represent a major class of air pollutants, characterized by their high volatility. The most common VOCs include aromatic hydrocarbons and halogenated hydrocarbons, such as chloroethylene and trichloroethylene (David & Niculescu, 2021).

Trichloroethylene is a colorless compound with a sweet odor, primarily used in industry as a chemical solvent (Stettiner, Gomes, & Colacciopo, 1977). Increasing concern surrounds TCE exposure due to its toxicity and carcinogenic potential (Guha et al., 2012).

More powerful and promising methodologies for the degradation of TCE are being employed, including advanced oxidation processes (AOPs). AOPs are characterized by their ability to generate hydroxyl radicals ($^{\cdot}OH$) with a high oxidation potential (Liu & Adewuyi, 2016). Techniques such as Fenton (Bamiduro & Zahran, 2023; Farooq et al., 2023), photocatalysis (Joo et al., 2013), and others have been extensively studied over the years for the degradation of TCE.

In contrast to conventional macro-scale reactors, new strategies for applying AOP methods in micro- and milli-scale reactors are being explored. This approach is driven by the numerous advantages micro- and milli-scale reactors offer, such as higher surface area-to-volume ratios, reduced reactant diffusion distances, faster and more efficient heat and mass transfer, and improved control over process conditions (Dong et al., 2022; Tanimu et al., 2017). These benefits represent a significant innovation, not only in pollutant treatment but also in various chemical processes.

This study evaluates the degradation of trichloroethylene through photocatalysis in a millireactor, utilizing Degussa P25 titanium dioxide as the catalyst.

Material and Methods

The NETMIX millireactor model was employed to analyze the degradation of trichloroethylene in the photocatalytic device. This model features a static mixer composed of multiple circular chambers interconnected by a series of prismatic channels. The channels are 2 mm in length and 1 mm in width, while the chambers have a diameter of 6.5 mm and walls that are 3 mm high.

The reactor simulations were conducted under three-dimensional, steady-state, and laminar flow assumptions. The reactor geometry was modeled using the 3D software SpaceClaim, and the mesh was generated using Ansys Meshing.

The software Ansys Fluent was used to model the fluid dynamics within the reactor. The mathematical representation of the system is captured by the mass balance, momentum conservation, and species conservation equations, denoted as Equations (1), (2), and (3), respectively. The mesh employed consists of 5,527,670 elements. This mesh refinement level, identified by Matiazzo (2022), was found to yield satisfactory results relative to more refined meshes while maintaining lower computational costs.

$$\nabla \cdot (\rho\mu) = 0 \quad (1)$$

$$\nabla \cdot (\rho\mu\mu) = -\nabla P + \nabla \cdot (\tau) \quad (2)$$

$$\nabla \cdot (\rho\mu\, C_i) = -\nabla \cdot J_i \quad (3)$$

The reactor walls were modeled as stationary with no-slip boundary conditions. For the catalytic walls, the diffusive molar flux of the pollutant was set to match the heterogeneous reaction rate. In contrast, the non-catalytic walls were assigned a zero-molar flux for all species. The intrinsic reaction rate, defined in Equation (4), was implemented in the software as a boundary condition using a user-defined function.

$$r_{TCE} = [I(x,y)]^n \frac{k \cdot K \cdot C_{TCE}}{1 + K \cdot C_{TCE}} \quad (4)$$

A total of nine simulations were conducted as detailed in Table 1. In these simulations, the model, materials, and concentrations were kept constant, with only the irradiance and velocity values in the reactor being varied. The molar fraction of trichloroethylene was maintained at 4.487×10^{-5}, while the molar fraction of water was set at 0.00498.

Table 1. Simulated cases

Case	Catalytic disposition	E (W/m²)	Velocity (m/s)
1	FSI	495	0.2
2	FSI	495	0.45
3	FSI	495	0.7
4	FSI	795	0.2
5	FSI	795	0.45
6	FSI	795	0.7
7	FSI	1095	0.2
8	FSI	1095	0.45
9	FSI	1095	0.7

[a] Source: Elaborated by the author 2024.

This study assumed a homogeneous irradiance distribution throughout the reactor. However, in practical experimental scenarios, the distribution of light may vary, as discussed by Matiazzo (2022).

Results and Discussion

Table 2 illustrates the variation in degradation values. The results indicate that degradation increases with higher irradiance and decreases with higher flow rate. The optimal degradation value of 77.25% was achieved in Case 7, which had the highest irradiance and the lowest velocity.

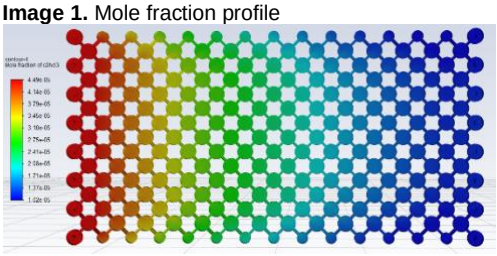
Table 2. Results

Case	E (W/m²)	Velocity (m/s)	Degradation (%)
1	495	0.2	49.11
2	495	0.45	27.96
3	495	0.7	20.00
4	795	0.2	70.56
5	795	0.45	40.99
6	795	0.7	30.20
7	1095	0.2	77.25
8	1095	0.45	51.53
9	1095	0.7	39.01

[a] Source: Elaborated by the author 2024.

This demonstrates that operating at lower flow rates, thereby increasing the residence time in the reactor, enhances the degradation of TCE. The simulated irradiance values are within the feasible range for the NETmix reactor and could potentially be increased further, likely resulting in even greater degradation values.

Image 1. Mole fraction profile



[a] Source: Elaborated by the author 2024.

Conclusions

By simulating the degradation of trichloroethylene in the NETmix reactor, it was possible to demonstrate the dependence of the process on irradiance values and on flow rate. The best set was found to be high values of irradiance and low values of flow rates, i.e., simulation 9. Other parameters were maintained so as not to interfere with the results. The maximum degradation value for trichloroethylene under these conditions was 77.25%.

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