Photocatalytic Degradation of 2-propanol Over TiO₂-based Thin Films in a Simulated Pilot Microreactor

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Abstract: Background: Microreactor devices have attracted increasing attention over the last years due to their high surface-to-volume ratio, which ensures a high heat and mass transfer, short molecular diffusion distance and greater spatial illumination homogeneity compared to the traditional reactors.

Objective: The aim of this study was to model the kinetics of photo-degradation of 2-propanol over TiO₂-based thin films in a gas-phase batch-reactor and simulate their performance in a microreactor device.

Methods: The reaction was carried out in a gas-phase batch-reactor, assessing the reactivity of single-layer nitrogen (N)-doped TiO₂ and a bilayer consisting of N-doped TiO₂ as a bottom layer and copper (Cu)-doped TiO₂ as a top layer. The kinetics of the photocatalytic process was modelled by Langmuir–Hinshelwood (LH) model. The constants obtained from the LH model were used to simulate the performance of the photocatalysts in a microreactor, operating in a continuous flow mode and investigating the effect of the volumetric flow rate (Q), initial concentration of pollutant (C₀), number of microchannels (n) and microchannel length (l) on the photo-degradation of 2-propanol.

Results: N-Cu-TiO₂ exhibited a higher reactivity but a lower adsorption ability towards the target pollutant compared to N-TiO₂. To maximize and leverage the advantages of a microreactor, optimal operating conditions for a continuous flow mode, at a steady-state, should be moderately low Q and C₀, long l and n that minimizes flow maldistribution in parallel.

Conclusion: The findings in this work could serve as a basis to design and fabricate efficient microreactors for the removal of VOC in air purification applications.

Keywords: Photocatalysis, microreactor, VOCs, bilayer thin-film structure, TiO₂, nitrogen and copper doping.

1. INTRODUCTION

Volatile organic compounds (VOCs) are airborne organic chemicals classified as major contributors to air pollution due to their toxic and carcinogenic effects on humans and their tendency to act as ozone or smog precursors [1]. The growing urbanization and industrialization are the main causes behind the increasing emissions of VOCs into the atmosphere, derived from biogenic or anthropogenic sources. Examples of main VOC sources are chemical industries, petroleum refining, transportation, cleaning products, paint drying, solvents, etc. [2-4]. The emission of VOCs can be controlled by the recovery technologies, such as adsorption, membrane separation, and oxidative processes, which include (photo)catalytic oxidation, thermal oxidation, biological degradation and nonthermal plasma oxidation [5]. Photocatalytic oxidation is recognized as one of the most efficient techniques for the oxidation of VOCs to CO₂, H₂O and less harmful compounds. This is mainly due to the possibility of unselectively mineralizing various types of organic pollutants, removing even trace amount of highly hazardous refractory compounds under ambient conditions. These features are highly desirable for VOC removal because of the diversified nature of this category of pollutant and their recalcitrance to other treatments [6].

Among many candidates for photocatalytic oxidation, titanium dioxide (TiO₂) is the preferred catalyst due to its relatively low cost, availability, nontoxicity, high chemical stability and photoactivity [7, 8]. Metal and non-metal doping are widely used to boost the visible-light adsorption of this semiconductor (Due to its wide band gap (ca. 3.2 eV in anatase)), pure TiO₂ mainly absorbs UV light, accounting for only 5% of the solar spectrum [9]. Stratified thin-film
structures consisting of TiO2 with different dopants in the individual layers have been found to exhibit a superior photocatalytic activity compared to single-layer doped thin films due to the formation of an electronic heterostructure at the interface between the layers, which enhances the efficiency of charge separation. In support of this claim, we demonstrated that a bilayer configuration, made up of nitrogen(N)-doped TiO2 as the bottom layer and copper(Cu)-doped TiO2 as the top layer, ensures a significantly higher degradation of a model VOC (i.e., 2-propanol) compared to single-layer samples of TiO2, Cu-TiO2 and N-TiO2 [10]. In particular, under simulated solar radiation, the pseudo-first-order rate constant of the above-mentioned double-layer, i.e., N-Cu-TiO2, was more than twice as high as that of N-TiO2, the most reactive sample among the single-layer thin films.

The present study aims to provide further insights into the better photocatalytic performance of N-Cu-TiO2 in the degradation of 2-propanol under-simulated solar radiation. 2-propanol is a widely spread VOC due to its versatility as a reactant and solvent in many industrial processes, including semiconductor manufacturing, spraying, pharmaceutical applications, printing, coatings, etc. [11, 12].

Due to the shift towards the development and implementation of more sustainable chemical technologies, microreactor technology keeps gaining attention among several industries, such as in pharmaceuticals, chemical engineering, process technology, etc. [13]. The microreactor has remarkable properties that can be leveraged for heterogeneous photocatalytic processes, such as air cleaning. Microreactors have a high surface-to-volume ratio, superior mass and heat transfer rates, excellent light penetration and ease with which process can be optimized and controlled [14-16]. Microreactors can be implemented as slurry Taylor flow reactors or as immobilized photocatalytic reactors. A slurry Taylor flow microreactor is a multiphase reactor that possesses enhanced mass and heat transfer rates [17, 18]. However, this type of reactor is still stymied with the problem of photocatalyst recovery after use. The recovery step remains an extra operational cost when the slurry system is implemented. However, in this work, we proposed a simulated gas-immobilized solid-phase microreactor, which eliminates the extra step, thereby reducing operational cost of the photocatalyst recovery.

There are only a few studies that dealt with microreactors applied to photocatalytic processes, including both experiments and modelling aspects, especially for gas-solid phase reactions. Vesborg et al. used a wall coated TiO2 microreactor to oxidize CO and methanol [19]. Under UV irradiation, CO oxidation was achieved under 2 s, while that of methanol took few minutes due to its complex oxidation reaction, but the total mineralization was attained for both. Castedo et al. also used a microreactor device for the production of hydrogen from a gas-phase mixture of water-ethanol [20]. The channels were coated with Au/TiO2 and the system was illuminated with UVA LEDs. Odiba et al. designed a microreactor for the catalytic oxidation of propane, using CFD package COMSOL Multiphysics [13]. Their design involved a selection of the best configuration and geometry of microreactor for the oxidation of propane.

The optimal propane conversion was achieved at a low flow rate and high temperature.

Only a few studies have tested and ascertained improved performance and cost-effectiveness using microreactors for photocatalytic reactions; there is still a need for more studies that can leverage the remarkable features of this miniaturized photoreactor. Most of these studies only test the benchmark photocatalyst (P25); therefore, it is still important to explore the performance of more hierarchical photocatalysts with potentially better photocatalytic activity in the gas phase.

In light of this, here, we present a study on the performance of N-TiO2 and N-Cu-TiO2 thin films in the microreactor for the photo-degradation of 2-propanol in a continuous flow-mode (single pass). First, these thin films were tested in a gas-phase batch-reactor. The constants estimated from the Langmuir–Hinshelwood (LH) model, applied to the batch process, were then used in the CFD model of the simulated microreactor to investigate the performance of the thin films under different operating conditions.

2. EXPERIMENTAL METHODS

2.1. Sample Preparation and Characterization

TiO2-based thin films were deposited on soda-lime glass substrates (Sigma-Aldrich) and UV Fused quartz microscope slides (laser Optex), using radiofrequency (RF) magnetron sputtering (AJA ATC Orion Series). Before the deposition, the substrates were cleaned by sonication in acetone (10 min) and 2-propanol (10 min).

Nitrogen-doped TiO2 (N-TiO2) sample was obtained from a target with atomic ratio TiO2:N = 98.5:1.5. This target was also used for the deposition of the bottom N-TiO2 layer of the bilayer, while the top copper-doped layer (Cu-TiO2) was deposited from a target with atomic ratio TiO2:Cu = 98.5:1.5. The bilayer was labelled as N-Cu-TiO2. The base pressure for all deposition was ~ 4 to 6 × 10⁻³ Torr. Before starting the depositions, targets were pre-sputtered for 10 min to remove any surface contamination. Argon was used as the sputtering gas for deposition with a constant pressure of 10 mTorr and a flow rate of 30 sccm (standard cubic centimeters per minute). The RF power applied to the cathode was 250 W and the materials were deposited at room temperature. The total film thickness was around 530 nm. Bilayer films consisted of Cu-TiO2 and N-TiO2 layers of thickness of around 250 - 280 nm, to reach an overall thickness of 530 nm. After the deposition, the thin films were annealed in the air for 4 hours at 500°C.

The crystal structure was assessed with an X-Ray diffraction machine (Empyrean from PANalytical) using a Cu-Kα source (radiation wavelength of 1.54 Å). Experiments were performed in a scan range of 10 - 90° with a step-size of 0.0167°. The crystallite size, d, was calculated by Scherrer equation Eq. 1:

$$d = \frac{0.9\lambda}{B \cos \theta}$$

(1)

Where λ is the X-ray wavelength, having a value of 1.54178 Å, B is the full width at half maximum (FWHM) and θ is the diffraction angle.
Scanning electron microscopy (SEM, FEI Nova Nano-SEM) was used to investigate the morphology of the deposited films after sputtering of a 5 nm layer of Au/Pd. Optical transmittance and reflectance of the deposited films were measured by a UV/Vis spectrophotometer (Shimadzu UV-2600) in the range of 200 - 800 nm to compute the optical band gap of the films. The optical energy gap $E_g$ was calculated from the absorption spectrum using the Tauc relation. The formula for indirect allowed transitions, which is usually applied to TiO$_2$-based materials, is given by Eq. 2:

$$\alpha = A \left( \frac{h \nu - E_g}{h \nu} \right)^2$$  \hspace{1cm} (2)

Where $\alpha$ is the absorption coefficient of the material, $h$ is the Planck’s constant, $\nu$ is the frequency of the incident photons and $B$ is a constant.

### 2.2. Photocatalytic Tests

The degradation of 2-propanol was carried out under simulated solar light using a LOT Quantum Design LS0606, equipped with a 1000 W Xenon short-arc lamp and AM1.5G Filter. The average values of radiation on the film equipped with a 1000 W Xenon short-arc lamp and simulated solar light using a LOT Quantum Design LS0606, 2.2. Photocatalytic Tests

Planck’s constant, $B$

$\text{enex}$ column Zebron ZB-WAXplus 30mL x 0.32mm ID. N$_2$ equipped with a flame ionization detector and the Phenom-monitored by a gas chromatograph (Shimadzu GC 2014), propanol and before turning the lamp on, 10 min elapsed to initial concentration. Specifically, four initial concentrations min. The degradation kinetics was studied by varying the was saturated with oxygen by continuously flowing for 30

stant at ca. 22 °C. Before injecting 2-propanol, the reactor was made of Pyrex glass with a volume of 314 mL, 9721 radiometer and matching probes. The gas-phase reac-
tor was made of Pyrex glass with a volume of 314 mL, equipped with an external jacket where water circulated continuously during the runs to keep the temperature con-
stant at ca. 22 °C. Before injecting 2-propanol, the reactor was saturated with oxygen by continuously flowing for 30 min. The degradation kinetics was studied by varying the initial concentration. Specifically, four initial concentrations were used: 3.3, 9.8, 15.3, and 23.1 μM. After injection of 2-
propanol and before turning the lamp on, 10 min elapsed to reach the adsorption/desorption thermodynamic equilibrium. During irradiation, the photooxidation of 2-propanol was monitored by a gas chromatograph (Shimadzu GC 2014), equipped with a flame ionization detector and the Phenom-
exen column Zebron ZB-WAXplus 30mL x 0.32mm ID. N$_2$ was used as the carrier gas and the column flow was set to 1.60 mL min$^{-1}$. The column temperature was 65 °C, while the detector and injection temperatures were 245°C and 250°C, respectively. Scheme and picture of the photocata-
lytic apparatus are shown in Fig. S1.

### 2.3. Modelling with COMSOL Multiphysics

The 2D model geometry employed for the microreactor simulations is shown in (Fig. 1). The 2D geometry of this photocatalytic microreactor has been previously reported by Yusuf et al. for the degradation of liquid-phase pollutant (4-
nitrophenol) [15]. This microreactor consists of nine micro-
channels in parallel, with each having a length of ca. 5 cm. In this previous work, only one side of the microchannels was coated with a photocatalyst. The microchannel has a square cross-section with a height and width of 0.5 mm, and all microchannels have an equal spacing of 0.3 cm. The CFD modelling of the 3D geometry of the same microreactor has been previously reported by Yusuf and Palmisano, where liquid phase pollutant degradation was modelled with the top side of each microchannel coated with photocatalyst [21]. The same microreactor configuration and geometry have been adopted here, but the total immobilization of all the microchannel walls with N-TiO$_2$ or N-Cu-TiO$_2$ was as-

umed. The 2D geometry was used to reduce computational costs and, at the same time, provide a fast and robust model, which utilized the momentum and mole transport PDEs.

The performance of the thin films was evaluated by estimating the conversion at the exit of the microreactor at a steady state (see Eq. 5).

$$\kappa = \frac{2xh}{k^2}$$  \hspace{1cm} (3)

$\kappa$ is the estimated illuminated area of the photocatalyst in contact with the pollutant solution (m$^{-1}$) and $h$ is the micro-
channel height (or reaction gap) and width (m).

$$-r''_{\text{LH}} = \frac{-r'_{\text{LH}}}{\kappa}$$  \hspace{1cm} (4)

where $-r''_{\text{LH}}$ is the LH rate, expressed in mol m$^{-2}$ s$^{-1}$ and $-r'_{\text{LH}}$ is the LH rate, expressed in mol m$^{-3}$ s$^{-1}$.

$$X = 1 - \frac{\text{c}_{\text{ex}},\text{steady state}}{C_0}$$  \hspace{1cm} (5)

where $X$ is the average conversion at the exit of the microreactor, $C_{\text{ex}}$ is the average concentration of 2-propanol at the exit and $C_0$ is the concentration of 2-propanol at the inlet.

### 2.3.1. Transport Equations

The velocity field in the microreactor was modelled using the Navier-Stokes’ equation as shown in Eq. 6:

$$\rho (u \cdot \nabla) u = -p I + \mu (\nabla u + (\nabla u)^T) + F$$  \hspace{1cm} (6)

where $\rho$ (kg m$^{-3}$) is the density, $u$ (m s$^{-1}$) is the velocity vector, $p$ (Pa) is the pressure, $I$ (dimensionless) is the identity matrix, $\mu$ (kg m$^{-1}$ s$^{-1}$) is the dynamic viscosity, $T'$ is the transpose operator and $F$ (N m$^{-2}$) is the generic body forces. Eq. 6 was simulated at a steady state and was coupled to the
mole transport PDE. The transport of 2-propanol in a gas-phase through microreactors was modeled by using steady-state PDE (Eq. 7), accounting for both diffusion and convection rates.

\[ \nabla \cdot (-D \nabla C + \mathbf{u} C) = 0 \quad (7) \]

where \( D \) is the assumed diffusivity for 2-propanol in air \( (0.11 \times 10^{-4} \text{ m}^2 \text{ s}^{-1}) \). To simulate Eq. 7, the boundary conditions reported in Eqs. 8 - 11 were used:

- \( C(0,0,0) = C_0 \) (at the inlet) \( (8) \)
- \( \nabla C = 0 \) (at the outlet) \( (9) \)
- \( \nabla C = 0 \) (at walls without catalyst) \( (10) \)
- \( \nabla C = -r_{\text{LH}}'' \) (on all catalytic surface) \( (11) \)

For the implementation of this model in COMSOL Multiphysics, the geometry of the microreactor was initially created and meshed. The single-phase laminar flow and the transport of the diluted species nodes were used to implement and simulate Eq. 6 – Eq. 11. For the velocity field, the inlet boundary condition was set as the inlet volumetric flow rate, and the exit was fixed at the atmospheric pressure. A no-slip boundary condition was assigned to all the stationary walls. The species transport equation was simulated by utilizing the boundary conditions in Eqs. 8 – Eq. 11. The inlet concentration was specified as the initial 2-propanol concentration (Eq. 8). At the outlet of the microreactor, diffusive flux was set to zero because the convective flux was dominant (Eq. 9). All the walls were assumed to be coated with a photocatalyst, so Eq. 11 was specified at those boundaries, and the non-catalytic parts, i.e., the inlet and the outlet collector zones, were fixed according to Eq. 10. The species transport PDE was simulated together with the velocity field equation using a stationary solver.

3. RESULTS AND DISCUSSION

3.1. Structural, Optical and Morphological Characterization

The structural properties of N-TiO\(_2\) and N-Cu-TiO\(_2\) were investigated by XRD. (Fig. 2a) shows the XRD patterns of N-TiO\(_2\) and N-Cu-TiO\(_2\). Both patterns exhibit diffraction peaks at \( 2\theta = 25.3^\circ, 37.8^\circ, 48.1^\circ, 53.9^\circ, 55.1^\circ, 62.7^\circ \) which can be respectively indexed to (101), (004), (200), (105), (211), (204) planes of tetragonal anatase phase (JCPDF no. 01-084-1286). The crystallite size, calculated from Eq. 1 using the main XRD peak (101), was slightly higher in N-Cu-TiO\(_2\) (\( d = 37.6 \text{ nm} \)) than in N-TiO\(_2\) (\( d = 35.9 \text{ nm} \)).

Fig. 2b shows the Tauc plots of N-TiO\(_2\) and N-Cu-TiO\(_2\). The band gap \( E_g \) was estimated from the intercept of the linear region of the curve with the energy axis (Eq. 2). The two samples show the same band gap, which is 3.35 eV.

The SEM micrographs in (Fig. 2c) reveal a homogenous surface in both samples with densely packed nanoparticles and presence of cracks between the agglomerated particles, which are more evident in the bilayer structure.

3.2. Langmuir-Hinshelwood Applied to 2-propanol Photo-degradation

The LH model is widely used to investigate the kinetics of the heterogeneous catalytic processes [23-25]. According to this model, the reaction rate \( r_{\text{LH}} \) can be obtained as:

\[ -r_{\text{LH}} = \frac{k K_{\text{obs}} C}{1 + K_{\text{obs}} C} \quad (12) \]

where \( k \) and \( K_{\text{obs}} \) are the reaction rate constant and the adsorption equilibrium constant of the target molecule on the catalyst. The above equation can be rewritten as:

\[ -r_{\text{LH}} = \frac{k K_{\text{obs}} C}{1 + K_{\text{obs}} C} = k_{\text{obs}} C \quad (13) \]

Therefore, the reaction rate is obtained once the pseudo-first-order constant, \( k_{\text{obs}} \), and the concentration of the target molecule, \( C \), are known. \( k_{\text{obs}} \) is determined by fitting the experimental data \( C(t) \) with an exponential curve at the beginning of the reaction, during which \( C \) is measured through gas chromatography. The above equations are valid under certain conditions that are reasonably met in the present case: (i) oxygen concentration does not change so that the surface coverage of the oxygen can be considered constant during the reaction; (ii) the concentration of possible intermediates is low due to the limited conversion of the target molecule at the beginning of the reaction; (iii) the adsorption constant of the target molecule and possible intermediates are similar [23].
$K_a$ and $k$ can be obtained from the initial reaction rate, $r_0$, considering that:

$$r_0 = \frac{k K_a C_0}{1 + K_a C_0}$$

and

$$\frac{1}{r_0} = \frac{1}{k K_a C_0} + \frac{1}{k}$$

(14)

(15)

In a plot of $1/r_0$ vs. $1/C_0$, the values of $K_a$ and $k$ can be extrapolated from the slope and the intercept. The value of $k_{obs}$ can thus be used to find the exponential decrease of the target molecule during the reaction:

$$C = C_0 e^{-k_{obs} t}$$

(16)

The parameters $K_a$ and $k$ can be finally adjusted to compute the modeled $k_{obs}$ by minimizing the sum of the quadratic errors, obtained by the difference with the correspondent values recorded from the experimental runs. (Fig. 3) shows that LH kinetics satisfactorily fit the experimental runs at different initial concentrations in both samples. It should be noted that the initial slope, and thus the reaction rate, increased with increasing $C_0$ to reach a constant value beyond a certain concentration. The standard error of the fitting, calculated for the different initial concentrations, is reported in Table 1, while the values of $k$ and $K_a$ obtained from the model are summarized in Table 2. The kinetic constant for N-Cu-TiO$_2$ was almost twice the value obtained for N-TiO$_2$, giving evidence of the faster degradation over the bilayer thin film. On the other hand, the adsorption constant was larger in N-TiO$_2$. However, the use of a higher adsorption constant does not always result in a better performance. Despite the lower $K_a$ in N-Cu-TiO$_2$, which indicates a slightly reduced adsorption capacity of the top layer of Cu-TiO$_2$ towards the target molecule compared to N-TiO$_2$, the bilayer showed the best reactivity. This is due to the enhanced charge separation in this sample, impacting on $k$ and on the efficiency of the photocatalytic process to a greater extent [10]. Overall, the final performance based on LH model depends simultaneously on $k$ and $K_a$ and their product, which is reported in Table 2.

3.3. Simulation Results and Discussion

The CFD simulation results depict the effect of changing inlet volumetric flow rate ($Q$), initial concentration of
Fig. (3). 2-propanol concentration vs. time curves from the LH model and experimental points obtained during the photocatalytic runs under simulated solar light; Initial 2-propanol concentrations: 3.3 μM (blue), 9.8 μM (orange), 15.3 μM (grey), 23.1 μM (yellow). (A higher resolution / colour version of this figure is available in the electronic copy of the article).

Table 1. The standard error of the fitting calculated for the different $C_0$

<table>
<thead>
<tr>
<th>Sample</th>
<th>$C_0 = 3.3 \text{ μM}$</th>
<th>$C_0 = 9.8 \text{ μM}$</th>
<th>$C_0 = 15.3 \text{ μM}$</th>
<th>$C_0 = 23.1 \text{ μM}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>N-TiO$_2$</td>
<td>0.30</td>
<td>0.14</td>
<td>0.59</td>
<td>0.25</td>
</tr>
<tr>
<td>N-Cu-TiO$_2$</td>
<td>0.34</td>
<td>0.36</td>
<td>0.37</td>
<td>0.57</td>
</tr>
</tbody>
</table>

Table 2. $k$, $K_a$, $kK_a$ for N-TiO$_2$ and N-Cu-TiO$_2$.

<table>
<thead>
<tr>
<th>Sample</th>
<th>$k$ (μM h$^{-1}$)</th>
<th>$K_a$ (μM$^{-1}$)</th>
<th>$kK_a$ (h$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>N-TiO$_2$</td>
<td>0.789</td>
<td>0.1024</td>
<td>0.081</td>
</tr>
<tr>
<td>N-Cu-TiO$_2$</td>
<td>1.517</td>
<td>0.087</td>
<td>0.132</td>
</tr>
</tbody>
</table>

2-propanol ($C_o$), the number of microchannels ($n$) and microchannel length ($l$), on the photo-degradation of 2-propanol in a microreactor with multiple microchannels in parallel and operating in a single pass continuous flow mode. In particular, (Fig. 4) shows the effect of changing $Q$ on the photo-degradation of 2-propanol on N-TiO$_2$ and N-Cu-TiO$_2$, respectively. These results indicate that steady-state conversion, $X$, decreases as $Q$ increases. This is because the contact or residence time of the 2-propanol species decreases as the $Q$ increases and fewer 2-propanol molecules are converted. The same trend can be observed for both thin films, but N-Cu-TiO$_2$ showed higher conversion than N-TiO$_2$ at a fixed $Q$. (Fig. 5) shows the effect of changing $C_o$ on the steady-state conversion of 2-propanol at the exit of the microreactor. As $C_o$ was increased, the steady-state conversion $X$ decreased. A similar trend can be observed for both thin films and N-Cu-TiO$_2$ showed better performance as expected.

The result of changing the length of the nine microreactors while keeping other conditions constant is shown in (Fig. 6). Varying the length of the microchannels at a fixed $Q$ will change the residence or contact time of 2-propanol molecules as well. Higher contact time with catalyst surface has been previously established, leading to a higher steady-state conversion. It can be seen that the longer the microchannel length, the higher the conversion for both thin films, but N-Cu-TiO$_2$ showed a higher conversion than N-TiO$_2$. The results reported herein, are in agreement with the previous study by Odiba et al. [13]. (Fig. 7) shows the result for changing the number of microchannels ($n$) in parallel for only N-Cu-TiO$_2$ because of its better performance than N-TiO$_2$. Increasing $n$ will increase the total volume of air treated, and it is evident that as $n$ increases, steady-state conversion increases. The effect of $n$ (in parallel) on flow maldistribution has been previously studied by Odiba et al. [13] and they found that, for a known fluid viscosity, the flow maldistribution increases with $n$. Flow maldistribution may lead to the unequal conversion of the model pollutant in all the channels. However, this phenomenon can be minimized using symmetrical inlet and outlet manifold, small width and moderately long microchannel and depth [26].
CONCLUSION

In the present study, photocatalytic degradation of 2-propanol over single-layer and double-layer thin films has been simulated in microreactors connected in a parallel configuration. The rate constant and the adsorption equilibrium constant, used as input for the simulation, were extrapolated from the LH model applied to the photo-degradation of the target pollutant in a gas-phase reactor. As confirmed by the higher rate constant achieved by N-Cu-TiO₂, bilayer configuration yielded a better separation of the photocarriers and, in turn, a better photocatalytic performance than that obtained by a single-layer thin film. The performance of the simulated microreactor was studied at different volumetric flow rates (Q), initial concentration of 2-propanol (C₀), number of the microchannel (n) and microchannel length (l). The results showed that sufficiently low Q (< 100 mL h⁻¹) allowed laminar regime, which favored fast photo-degradation of 2-propanol, while the steady-state conversion also increased as C₀ decreased. Similarly, longer and more microchannels resulted in an enhanced contact time, enabling higher air volume to be treated, thereby leading to higher steady-state conversion. This work can serve as a basis for optimizing the design strategies of gas-phase microreactors. The target gas-phase reaction can be investigated in a simple configuration, such as in a small batch reactor, in order to obtain the input for the CFD model, which is used to design the microreactor device and optimize its operation.

CONSENT FOR PUBLICATION

Not applicable.

AVAILABILITY OF DATA AND MATERIALS

Not applicable.

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CONFLICT OF INTEREST

The authors declare no conflict of interest, financial or otherwise.
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SUPPLEMENTARY MATERIAL

Supplementary material is available on the publisher’s web site along with the published article.

REFERENCES


