## Micropillar Photocatalytic Reactor Modeling: investigation of LEDs-to-reactor distance

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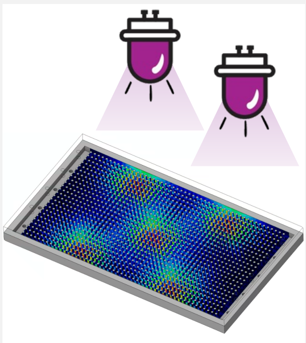


The LEDs-to-reactor distance was analyzed for an illumination system composed of 5 high power LEDs for the illumination of a micropillar photocatalytic reactor. The light behavior was simulated employing a ray tracing algorithm and the irradiation fields obtained were incorporated into computational fluid dynamics simulations. The impact of the irradiation field over the photocatalytic oxidation of n-decane was investigated. Results demonstrated that the homogeneity of the irradiation field and irradiance levels impact the pollutant degradation significantly. Simulations have shown that the homogeneity of the irradiance field increases with the distance of the LEDs to the detriment of the irradiance values. An ideal value of LEDs-to-reactor distance was encountered, and the global illumination efficiency was demonstrated to be a predictor of the reactor performance and can be useful in the illumination system optimization.

### Introduction

The design of photocatalytic reactors has two main challenges: mass and photon transfer [1]. The rate transfer can be affected by the reactor's geometry, catalyst type and thickness, and by the illumination system employed.

In the current work, the impact of the LEDs-to-reactor distance was evaluated for an illumination system composed of 5 high power LEDs. A micropillar reactor was employed for the degradation of n-decane from air. To evaluate the light behavior a ray tracing algorithm was employed and CFD simulations were used to quantify the pollutant degradation. The irradiance levels, homogeneity of the radiation field, light power absorption efficiency and the pollutant conversion were evaluated and compared.

### Material and Methods

A micropillar reactor was developed for this study. The reactor consists of a stainless-steel slab with a total of 1250 micropillars (1 mm of diameter each). A $TiO_2$ catalyst film covers the reactor, and a borosilicate glass slab closes the reaction chamber. The 5 LEDs that compose the illumination system were positioned at a distance of 6 mm, 12 mm, 24 mm, and 48 mm from the reactor. The optical properties of all materials that compose the reactor system and the LEDs properties were described in detail in Matiazzo *et al*. [2]. The software Ansys Speos was employed for the light simulations. The results obtained were then incorporated at Ansys Fluent for the simulations of n-decane degradation from an airstream. The boundary conditions employed for all cases are summarized in Table 1.

**Table 1.** Boundary conditions of the CFD simulations

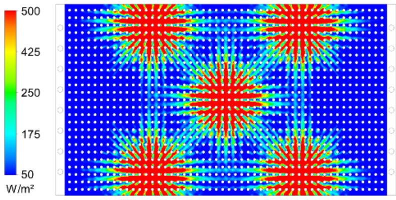
| | |
|---|---|
| **Velocity inlet:** | 0.5 m/s |
| **Molar fraction of *n*-decane:** | $7 \cdot 10^{-4}$ |
| **Molar fraction water vapor:** | $10^{-2}$ |
| **Pressure outlet:** | atmospheric |
| **Reaction rate:** | $r_{dec} = 3.09 \cdot 10^{-8}\, E C_{dec}^{0.43} C_w^{0.18}$ |

* $C_{dec}$ (kmol/m³) - Molar concentration of n-decane; $C_w$ (kmol/m³) - Molar concentration of water; E (W/m²) – Irradiance

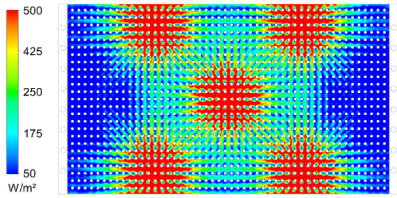
### Results and Discussion

Figure 1 shows the radiation field obtained at the $TiO_2$ catalyst surface of each of the evaluated cases. The average irradiance registered ranged from 87 W/m² to 204 W/m². The irradiance increases with the proximity of the LEDs to the reactor and regions of the catalyst that are positioned exactly below the LEDs reach higher irradiance values. The homogeneity index (γ) was evaluated along with the power absorption efficiency (φ), and the global illumination efficiency (η). The global illumination efficiency peaked for the LEDs-to-reactor distance of 12 mm, reaching the equivalent of 46.0%, demonstrating that in this distance it is possible to balance the maximization of both average irradiance and the homogeneity of the field.

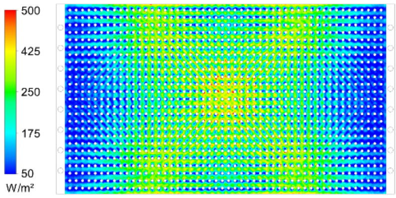
Figure 2 depicts the n-decane degradation rate obtained at the catalyst surface. It is noticeable that the reaction rate is higher where the irradiance reaches elevated values. The pollutant conversion ranged from 42.7% to 70.0%. The highest pollutant conversion was reached at a LEDs-to-reactor distance equivalent to 12 mm, demonstrating that the global illumination efficiency is a good parameter to predict and optimize photocatalytic reactors.



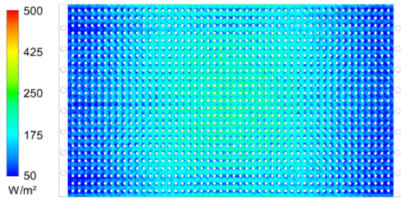

a) LEDs-to-reactor distance: 6 mm
E = 204 W/m², $\gamma$ = 47.1%, $\varphi$ = 84.4%, $\eta$ = 39.8%




b) LEDs-to-reactor distance: 12 mm
E = 177 W/m², $\gamma$ = 62.8%, $\varphi$ = 73.2%, $\eta$ = 46.0%

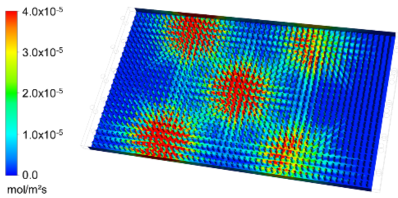



c) LEDs-to-reactor distance: 24 mm
E = 139 W/m², $\gamma$ = 72.0%, $\varphi$ = 57.3%, $\eta$ = 41.2%

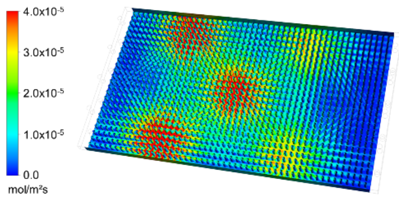



d) LEDs-to-reactor distance: 48 mm
E = 87 W/m², $\gamma$ = 72.2%, $\varphi$ = 35.9%, $\eta$ = 25.9%

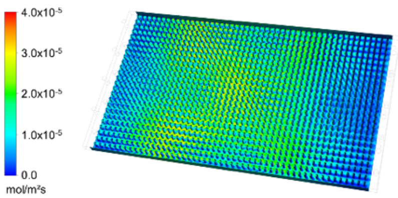
**Figure 1.** Irradiance maps incident at the micropillar reactor catalyst surface.



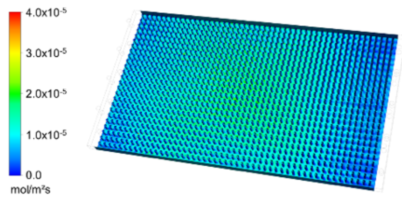

a) LEDs-to-reactor distance: 6 mm; X = 69.6%




b) LEDs-to-reactor distance: 12 mm; X = 70.0%




c) LEDs-to-reactor distance: 24 mm; X = 61.2%




d) LEDs-to-reactor distance: 48 mm; X = 42.7%

**Figure 2.** Reaction rate over the $TiO_2$ catalyst surface of the micropillar reactor.

## Conclusions

The LEDs-to-reactor distance has been evaluated for an illumination system composed of 5 high power LEDs. The photocatalytic conversion of n-decane was simulated considering the distinct LEDs-to-reactor distance in a micropillar reactor. The geometrical position of the LEDs had great impact over the pollutant conversion. Variations in the LEDs-to-reactor distance led to an increase in the average irradiance of up to 135% and improvement of up to 64% in the pollutant conversion.

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