

# Continuous air purification by front flow photocatalytic reactor: Modelling of the Influence of mass transfer step under simulated real conditions

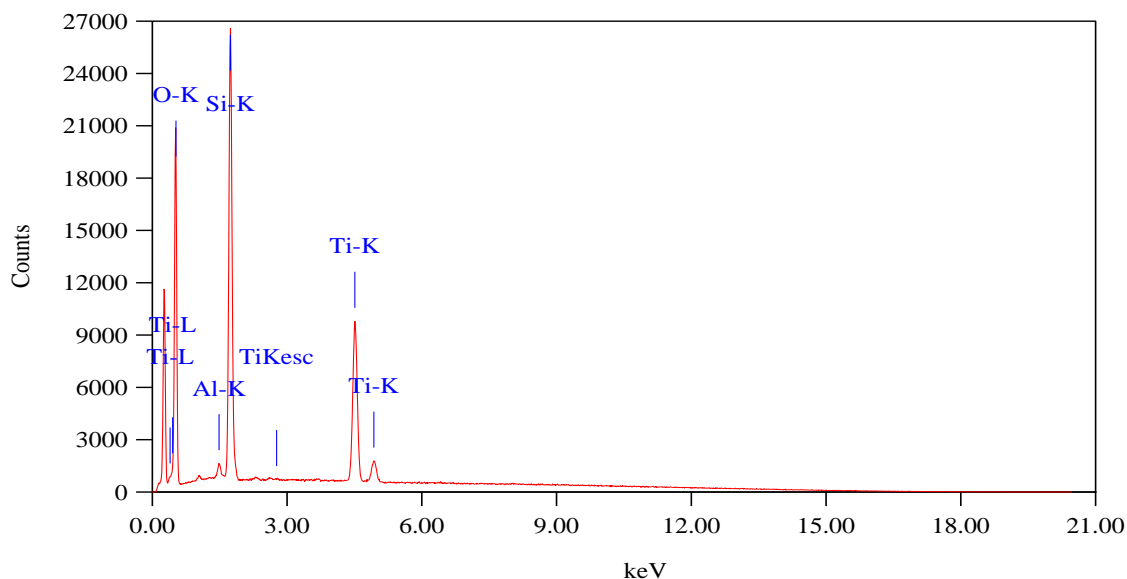
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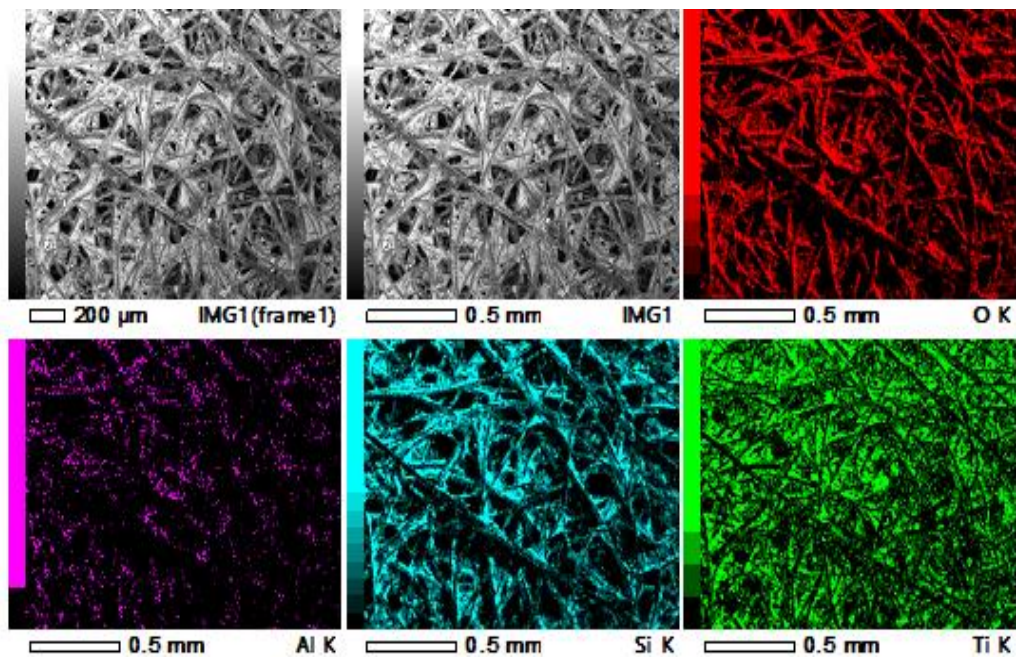


Figure S1: EDX analysis of the photocatalytic medium

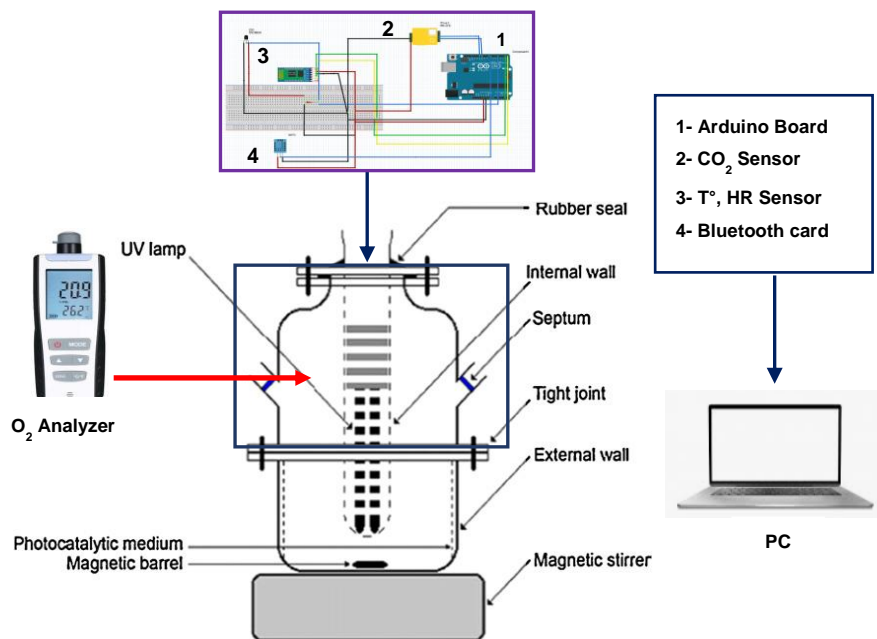


Figure S2: Schematic of the control system associated with a batch photocatalytic reactor

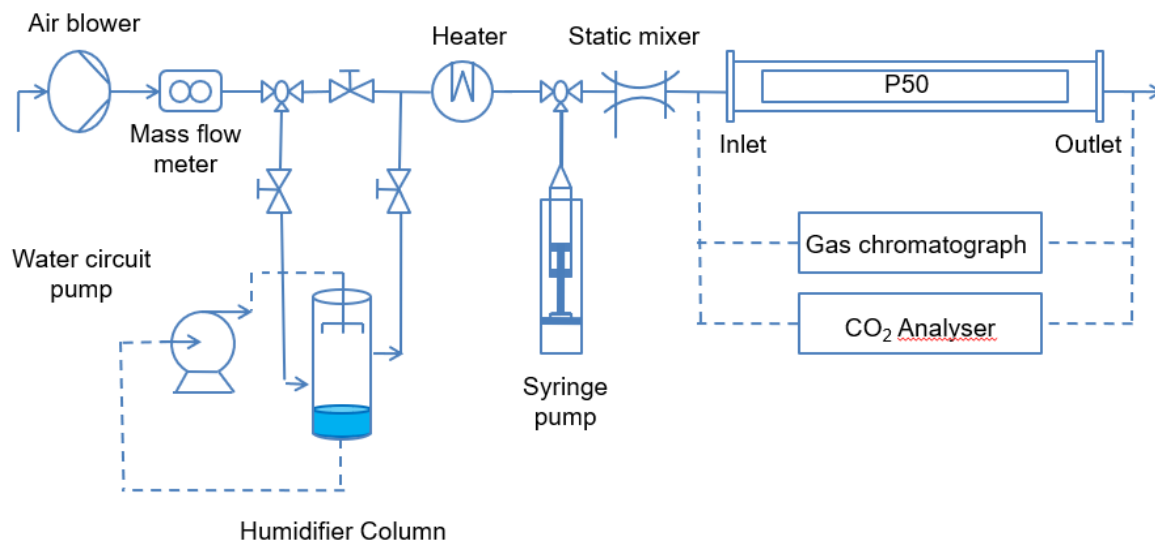


Figure S3: Diagram of the photocatalytic process using P50 for continuous treatment

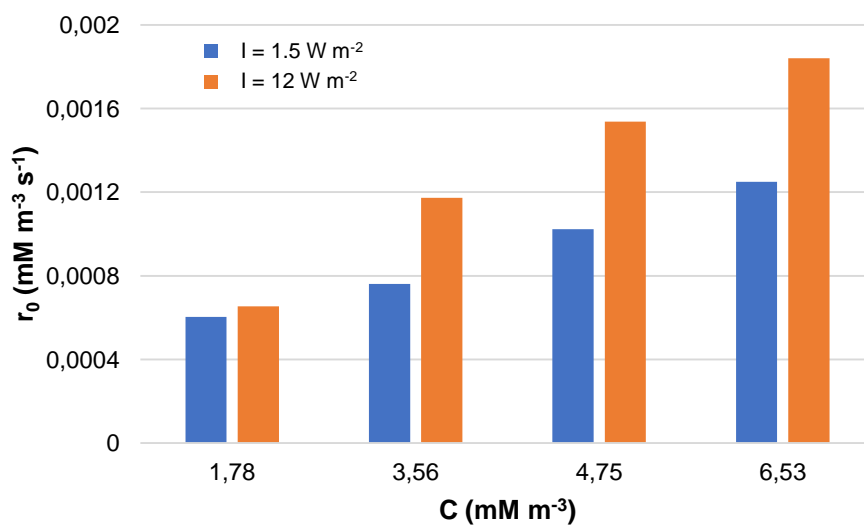


Figure S4: Initial degradation rate of Cyclohexane with TiO<sub>2</sub> (Cellulosic) at different concentrations

under different Intensities ( $HR = 40 \pm 2\%$ ,  $T = 20 \pm 2 \text{ C}^\circ$ ,  $m_{TiO_2} = 0.13 \text{ g cm}^{-2}$ )

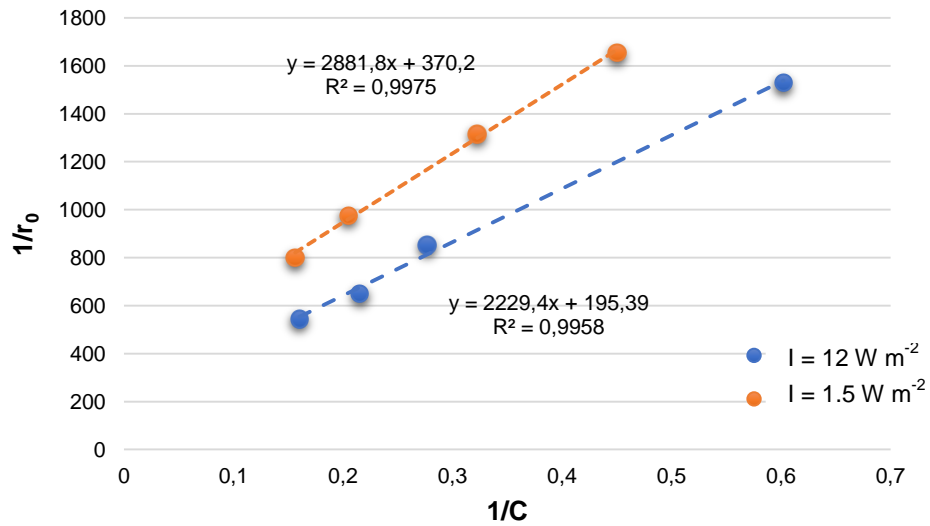


Figure S5: Linear regression of the results with Eq. (5) for UV intensity =  $1.5 \text{ W m}^{-2}$  and  $12 \text{ W m}^{-2}$

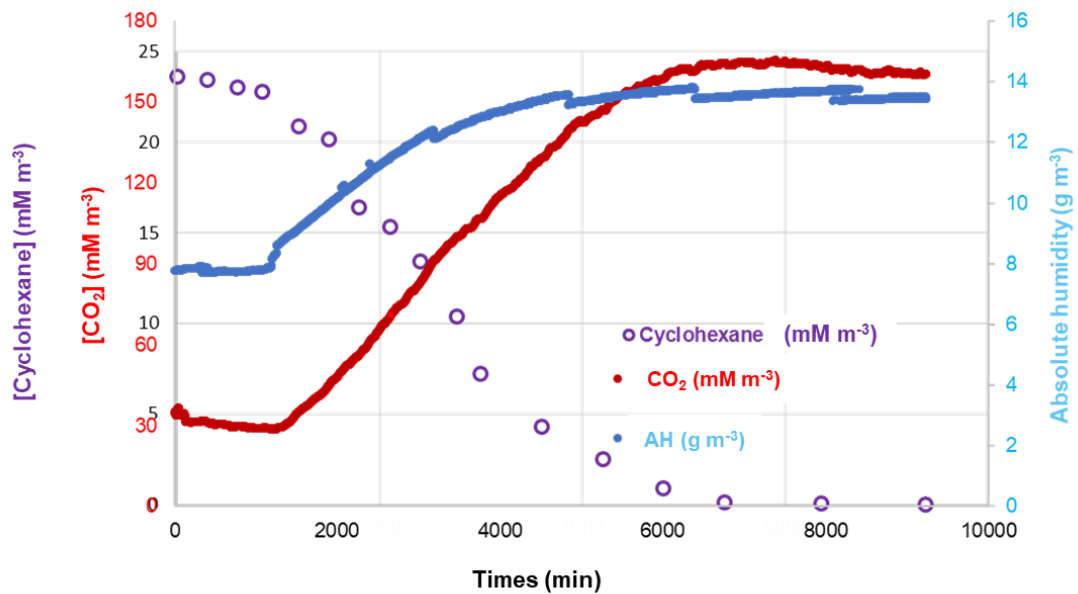


Figure S6: Monitoring of cyclohexane degradation and accumulation of  $\text{CO}_2$  and  $\text{H}_2\text{O}$  formed

$(T=20 \pm 2 \text{ }^\circ\text{C}, \text{UV intensity} = 12 \text{ W m}^{-2})$

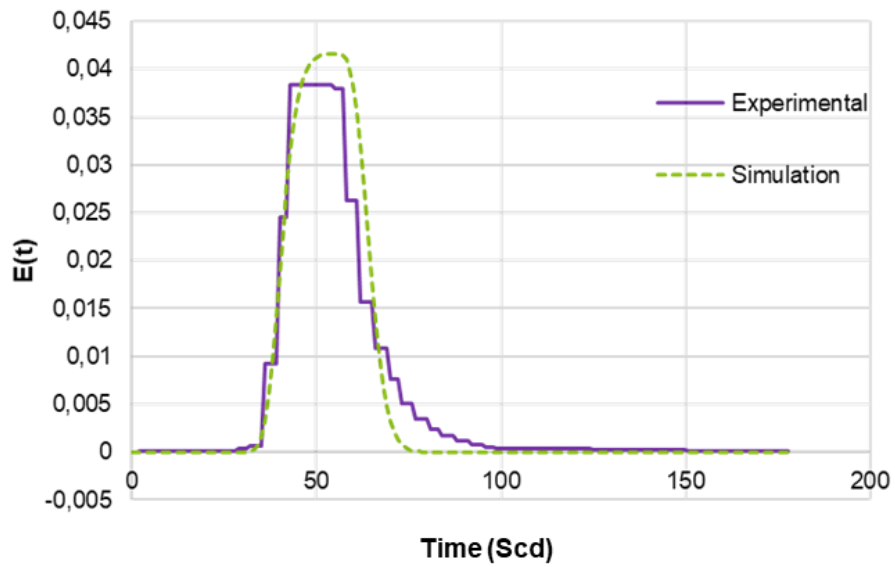


Figure S7: Residence time distribution  $E(t)$  of the immobilized photoreactor ( $J=18$ ). For a flow rate of  $18 \text{ L min}^{-1}$  corresponding to 10 seconds ( $HR = 5\%$ ,  $T=20 \pm 2 \text{ }^\circ\text{C}$ )

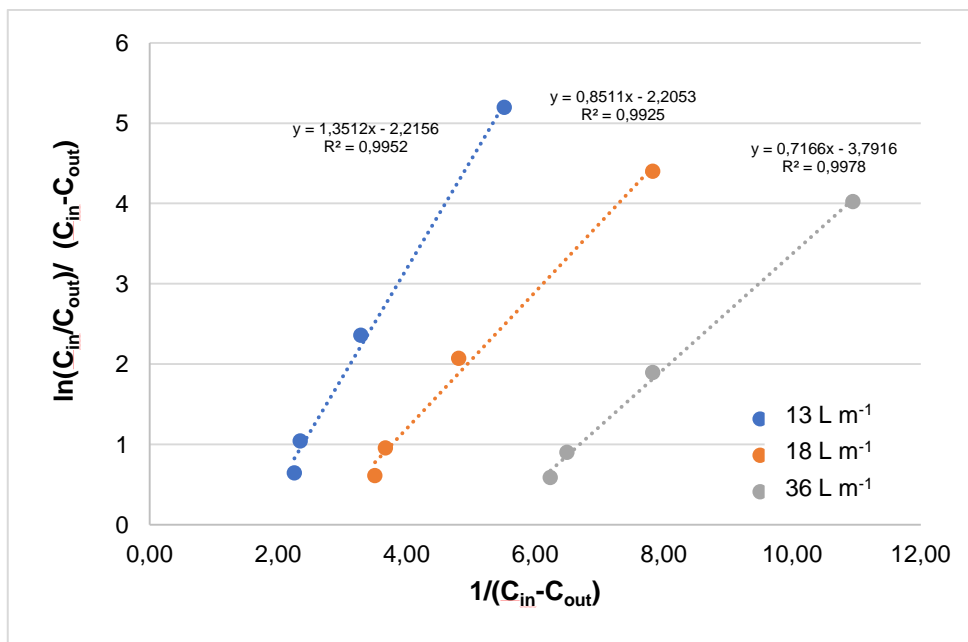


Figure S8: Linear regression of the results with Eq. (16) for Cyclohexane for different flow rates

(HR = 5 %, T = 20 ± 2 C°, UV intensity = 20 W m<sup>-2</sup>)

**List of tables:**

|                              |                                  |                                 |                                      |
|------------------------------|----------------------------------|---------------------------------|--------------------------------------|
| <b>Brute formula</b>         | C <sub>6</sub> H <sub>12</sub>   | <b>N° CAS</b>                   | 110-82-7                             |
| <b>Molar mass</b>            | 84.16 g M <sup>-1</sup>          | <b>Density</b>                  | 0.779-0.784                          |
| <b>Boiling point (1 atm)</b> | 80.75 °C                         | <b>Vapor pressure</b>           | 10.3 kPa à 20 °C<br>24.6 kPa à 40 °C |
| <b>Odor threshold</b>        | Low : 0.52 ppm<br>High : 784 ppm | <b>Exposure limits (France)</b> | 200 ppm / 700 mg m <sup>-3</sup>     |

Table S1: Physicochemical properties of cyclohexane

|   |        |        |
|---|--------|--------|
| <b>Intensity (W m<sup>-2</sup>)</b>                       | 1.5    | 12     |
| <b>k<sub>app</sub> (mM m<sup>-3</sup> s<sup>-1</sup>)</b> | 0.0027 | 0.0051 |
| <b>K (m<sup>3</sup> mM<sup>-1</sup>)</b>                  | 0.128  | 0.0876 |
| <b>R<sup>2</sup> (%)</b>                                  | 99.8   | 99.6   |

Table S2: Value of Langmuir-Hinshelwood reaction rate constants (k) and Langmuir adsorption constants (K)

|                                       |   |  |                          |
|---------------------------------------|---|--|--------------------------|
| <b>Flow rate (L min<sup>-1</sup>)</b> | <b>k<sub>app</sub> (mM m<sup>-3</sup> s<sup>-1</sup>)</b> | <b>K (m<sup>3</sup> mM<sup>-1</sup>)</b> | <b>R<sup>2</sup> (%)</b> |
| 13                                    | 0.031   | 2.216                                    | 99.5                     |
| 18                                    | 0.029   | 2.205                                    | 99.3                     |
| 36                                    | 0.028   | 3.792                                    | 99.8                     |

Table S3: Values of Langmuir-Hinshelwood constants for model I. (HR = 5 %,  $T=20 \pm 2$  C°,  
UV intensity =  $20 \text{ W m}^{-2}$ )

| Flow rate ( $\text{L min}^{-1}$ ) | Reynolds | Mass transfer coefficient<br>( $\text{k}_m \cdot 10^{-3}, \text{ m s}^{-1}$ ) |
|-----------------------------------|----------|---|
| 13                                | 1598     | 2.02  |
| 18                                | 2397     | 2.67  |
| 36                                | 4662     | 4.22  |

Table S4: Reynolds number and mass transfer coefficients in the P50.