

Multiscale analysis of reactive transport within a photocatalytic textile

DEGRAVE Robin^{1, 2, 3}, SCHMITZ Philippe^{1, 2, 3}, COCKX Arnaud^{1, 2, 3*}

1 Université de Toulouse; INSA, UPS, INP; LISBP, 135 Avenue de Rangueil, F-31077 Toulouse, France

2 INRA UMR792, Ingénierie des Systèmes Biologiques et des Procédés, F-31400 Toulouse, France

3 CNRS UMR 5504, Ingénierie des Systèmes Biologiques et des Procédés, F-31400 Toulouse, France

**Corresponding author: arnaud.cockx@insa-toulouse.fr*

Highlights

- The present work deals with the multi-scale modelling of the reactive transport within a UV-light photocatalytic textile.
- Experiments were performed on a specific designed plane reactor composed of a single textile unit.
- A local model is numerically solved using Comsol Multiphysics software on a representative volume element (RVE) of the textile.
- An accurate analysis of the coupling phenomena (hydrodynamic, transport and reaction) is then carried out to characterize the photocatalytic reactor.

1. Introduction

Advanced Oxidation Processes (AOP) have been described as a solution for degrading organic pollutants found in liquids (pesticides, industrial compounds, pharmaceutical products) [1]. One of them is photocatalysis, which uses a catalyst activated by UV radiation. The present paper focuses on a new and original technology named UV photocatalytic textile. This textile consists of an assembly of fabric and optical fibres linked by bonding points. The catalyst is directly deposited on the whole “fabric + optical fibres” surface. Because of the contact between the catalyst and the UV-light source, i.e. the optical fibres, this system ensures a maximum surface area of activated catalyst.

The goal of the study is to develop a numerical approach in order to further design a new photocatalytic reactor composed of an assembly of photocatalytic textile units. A numerical model at the optical fibre scale is proposed to perform numerical simulations in a geometrical domain consisting of a Representative Volume Element (RVE) of the photocatalytic textile with periodic boundary conditions. The complete investigation of the flow in such a complex structure has already been described in detail by Degrave et al. [2]. In the present paper, we deal with the photocatalytic degradation of formic acid by UV textile. A simplified unidimensional stationary model is implemented in order to quickly characterize the global reactor behaviour. Kinetic constants are used as fitting parameters to match the macroscopic model with experimental measurements. The regressed constants are then used in the RVE to reproduce the depollution along the total length of the textile microscopically. An accurate analysis of the coupling phenomena (hydrodynamic, transport and reaction) shows the microscopic characteristics of the photocatalytic reactor.

2. Methods

The spatial periodicity of the photocatalytic textile geometry permitted the domain to be reduced to the form of a representative volume element (RVE, Figure 1). The RVE was composed of three cylinders representing the optical fibres. They were supported by a porous rectangular prism representing the fabric. The first step in modelling fluid depollution by a UV photocatalytic reactor is to consider the hydrodynamics within such a system. Then we deal with the modelling of the reactive transport within the flat reactor composed of a single textile unit: the Langmuir-Hinshelwood model is used for the transport to the surface reaction. Figure 1 shows also the stationary velocity field at the RVE outlet. Degrave et al. [2] studied the hydrodynamics within the photocatalytic textile and have already shown the heterogeneous properties of the flow. As expected, the velocity is higher between optical fibres.

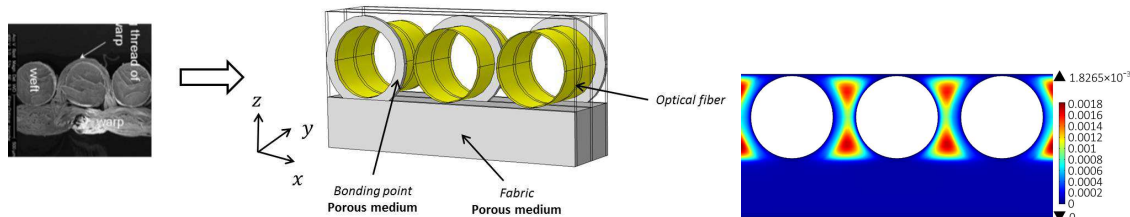


Figure 1. Representative Volume Element of the assembly of fabric / optical fibres and simulated velocity field

3. Results and discussion

In the following, the RVE model associated with pseudo-periodic boundaries is computed with the kinetic parameters calculated by the regression of a macroscopic model with experimental measurements. The degradation after flowing through 30 cm of the textile is then compared with the experimental value. Moreover, a spatial microscopic description is provided by the microscopic simulations. Figure 2 shows the pollutant concentration field at the RVE outlet after 30 cm along the UV-light textile. For all simulations, low concentrations are observed within the fabric and high concentrations are observed in the upper part of the RVE. The errors between simulation results and experimental measurements are lower than 6%. The performance of the flat plate reactor is then well represented by the RVE model.

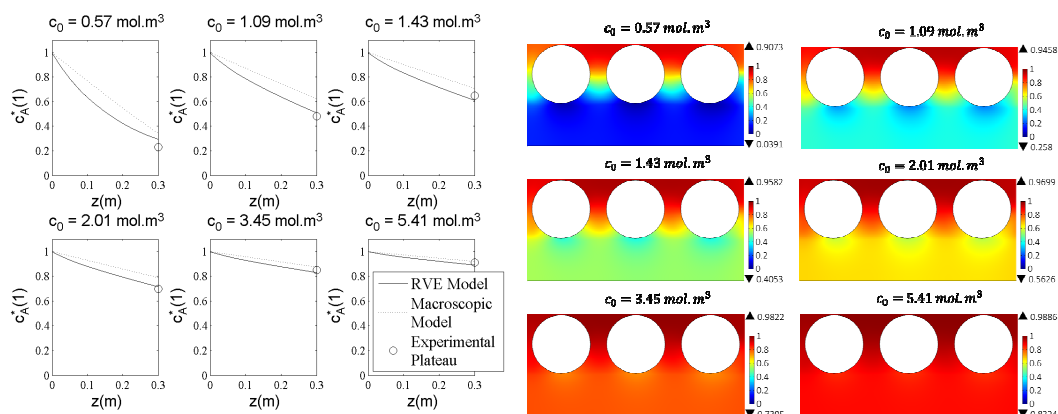


Figure 2. Spatial evolution of pollutant concentration along the textile.

4. Conclusions

In this paper, both numerical and experimental approaches to the reactive transport within a UV-light photocatalytic textile were developed. Measurements of the degradation of formic acid by photocatalytic reaction were detailed. These experiments were reproduced numerically by a microscopic model applied to a representative volume element (RVE) of the photocatalytic textile. This microscopic approach describes the coupling between hydrodynamic, transport and heterogeneous reactions in a complex geometry. The reaction model based on Langmuir-Hinshelwood's model, was integrated to simulate the formic acid degradation within the flat plate reactor. The numerical results led to suggestions for improving the reactor.

References

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Keywords

photocatalysis, cfd, reactive adsorption, multiscale