

# Multiscale Simulation of a Photocatalytic Reactor for Water Treatment

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## Abstract

This study deals with the 3D modeling of a light photocatalytic textile. This process aims to decontaminate industrial effluents such as water with pesticides. The present study describes the implementation of a reactive transport model in a computational fluid dynamics model developed on a Representative Volume Element (RVE) of the textile, i.e. at the microscopic scale.

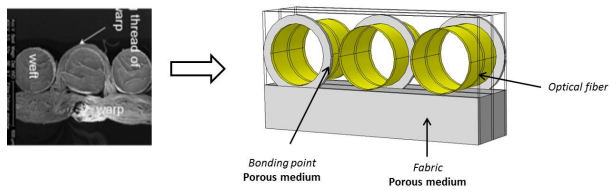
The final challenging task will be to design a new photocatalytic reactor from the microscopic model to the macroscopic scale by change scale. On one hand, the fluid dynamics model coupling the free flow and the porous media flow that takes place in the present RVE using the Free and Porous Media Flow interface of COMSOL Multiphysics®.

On the other hand, the species transport by the fluid flow is simulated using the Species Transport in Porous Media interface. This module, coupled with a Weak Form Equation, allows to model physical mechanisms of photocatalysis within the RVE.

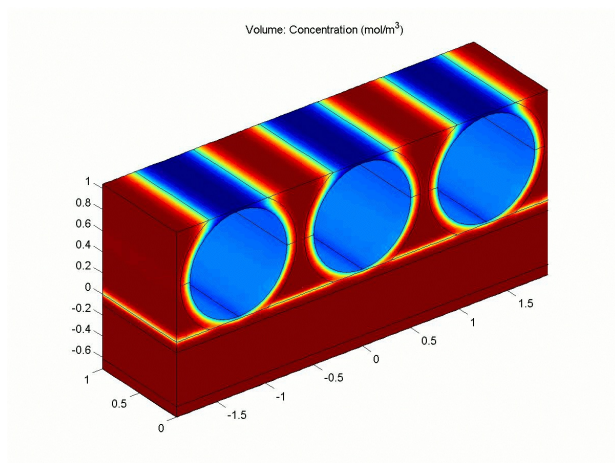
Moreover, the temporal degradation along the photocatalytic textile can be follow-up using the LiveLink™ for MATLAB®. By applying periodic conditions, the reaction phenomena can be simulated in a complete slice of the textile. An algorithm allows managing the inlet and outlet boundary conditions. The degradation is reproduced along the photocatalytic textile in the flow direction. The depollution efficiency is analyzed in terms of mass balance at the scale of the whole textile.

Finally, a study on structural parameters will be lead to maximize the fluid quantity passing in the neighborhood of the photoactive region. The results obtained on the RVE will be scaling-up to design a reactor which will be an assembly of photocatalytic textiles.

## Figures used in the abstract



**Figure 1:** Modeling of the assembly of fabric and optical fibers



**Figure 2:** Pollutant concentration field within the Representative Volume Element