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Multiscale analysis and modelling of fluid flow within a photocatalytic textile

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HIGHLIGHTS

- Modelling of photocatalytic textile by a Representative Volume Element.
- Implementation of free and porous media model.
- Determination of hydrodynamic parameters at microscale.
- Scale-up to reactor scale.

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ABSTRACT

This paper deals with a multiscale strategy for the design of an original reactor that will be an assembly of light photocatalytic textiles. This process is intended to decontaminate industrial effluents such as water containing pesticides. The reactor comprises a fabric and optical fibres and the performance of such a complex textile has to be carefully analysed in terms of fluid flow and the resulting ability to degrade target pollutants.

We present an experimental set-up based on classical 1D flow experiments to obtain data on fluid flow through the photocatalytic textile. We also propose a numerical model at the optical fibre scale using COMSOL Multiphysics to perform numerical simulations in a geometrical domain consisting of a Representative Volume Element (RVE) of the photocatalytic textile with periodic boundary conditions.

A good fit is found between the permeability of the fabric given by the numerical model and that obtained from experimental measurements, which is also in agreement with the value calculated from an experimental determination of the fabric porosity using a permeability model for fibrous media. Then, the effect of geometrical parameters on fluid flow distribution in the textile is characterized numerically. A short optical fibre pitch maximizes the amount of fluid circulating per unit time in the neighbourhood of the region where the degradation reaction takes place. Finally, a simplified analytical model based on a combination of hydraulic resistances in series and in parallel is implemented and validated with the numerical model mentioned above. This simplified model can be advantageously used for further simulations at industrial reactor scale. Additional simulations on the whole textile are performed to better understand the edge effect currently encountered in 1D flow experiments, which could degrade experimental data. It is found that the edge effect can be neglected in the present experiments.

1. Introduction

To meet the growing demand for water while respecting the environment, wastewater must be reused. In this context, the removal of refractory compounds, such as pesticides or herbicides in agricultural water, has become a major issue. Today, the efficiency of traditional water treatment processes in eliminating target pollutants appears to be poor. Advanced technologies such as advanced Oxidation Processes, including photocatalysis, have thus emerged to meet current legislation. Photocatalysis allows the degradation of pollutants through their reaction with a catalyst activated by UV irradiation. Like other advanced oxidation processes, it can be considered as a pre-treatment for industrial wastewater (for instance in oil recovery or in agriculture). The

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treated water can also be reused directly, depending on the local context.

In 2010, Chong et al. (Chong et al., 2010) reviewed technological progress in water treatment by photocatalysis, especially the photoreactor configurations. In the most common set-ups, the catalyst is in suspension within the effluent to be treated (Chong et al., 2009), so these devices have to be coupled with a filtration system to separate the catalyst and the solution after the treatment. Such processes cannot work continuously. An alternative solution is to immobilize the catalyst on an inert support (Pozzo et al., 2000) or within a membrane (Molinari et al., 2002). Nevertheless, the major challenge for all these photocatalytic processes remains the way to optimize the UV light source and to maximize the irradiated catalyst surface per unit volume (Pareek et al., 2008).

The present study focuses on an original new technology called UV photocatalytic textile. This textile consists of an assembly of a fabric and optical fibres. The catalyst is deposited on the whole "fabric+optical fibre" surface. When it is irradiated by UV light coming from the side wall of the optical fibres, a surface reaction occurs during the contact between the pollutant and the catalyst. Both the main challenges mentioned above are expected to be solved with an immobilized catalyst and an optimal UV light source but the process performance needs to be better analysed in terms of fluid flow and subsequent ability to degrade target pollutants. Here, we intend to analyse and model the flow within the photocatalytic textile as a first necessary step towards modelling the complete process, including heterogeneous reaction.

It is obvious that the flow depends on the geometrical and physical properties of the "fabric+optical fibre" assembly. At fibre scale, the crucial physical parameter is the fabric permeability. Here, the study focuses on the flow distribution within the complex geometry of the textile. This requires the prior determination of the fabric permeability.

For clarity in the rest of the paper:

- 'textile' or 'photocatalytic textile' will refer to the assembly of fabric and optical fibres,
- 'fibre' will refer to the woven fibres composing the fabric,
- 'optical fibre' will refer to the UV light source for the photocatalytic textile.

In the literature, many studies have established the relationship between the arrangement of the fibres in a fibrous medium and its permeability. Davies (1970) proposed an empirical law based on many experimental results for different fibrous materials. More recently, the experimental work of Rahli et al. (1995) led to a new formula that takes the ratio between fibre length and diameter into account. The empirical models presented above have been used as references for many numerical models expressing the permeability as a function of the porosity. All models have a common geometrical approach: a unit cell containing fibres is designed and the influence of the arrangement of fibres on the permeability is studied. A numerical law is then determined for a homogeneous fibrous medium by scaling up. The advantage of a numerical model is that parameters can be changed quickly and thus many numerical experiments can be performed in a short time. Happel (1959) and Kuwabara (1959) determined a permeability law in which the unit cell consisted of a single fibre centred in a free flow domain. Drummond and Tahir (1984) and Sangani and Acrivos (1982) used a more realistic representation of the fibrous medium. They modelled one fibre in a rectangular domain, taking the existence of the neighbouring fibres into consideration. Spielman and Goren (1968) approached the problem with a new vision using an effective medium approximation. They included the permeability of the closest assembly of fibres in their model. More recently, Tamayol and Bahrami found new permeability expressions in 2009 (Tamayol and Bahrami, 2009) and 2010 (Tamayol and Bahrami, 2010), resulting from work on various arrays of parallel cylinders. All previous numerical models have studied plane geometries. The superposition principle resulting from the linearity of the Stokes and Brinkman equations make it possible to extrapolate from the plane to a spatial volume. Jackson and James (1986) generalized the Drummond and Tahir (1984) models to obtain the permeability in terms of a three-dimensional model. Higdon and Ford (1996) solved the flow with numerical simulations in a cube where several basic configurations of fibres were studied (simple cubic, centred cubic, face-centred cubic). Moreover, some authors, like Nabovati et al. (2009), used the Lattice-Boltzmann method to determine an analytical expression linking the volume fraction and the permeability. Nowadays, with the impressive increase of calculating power, numerous researchers, such as Hosseini and Vahedi Tafreshi (2012), use Computational Fluid Dynamics (CFD) tools to simulate the hydrodynamic phenomena in fibrous media.

All these models have the common goal of defining a relationship between porosity and permeability. To adapt this approach to our photocatalytic textile, the microscopic structure of the fabric supporting the optical fibres has to be known. It appears that the models described above are too basic to fully account for the complex geometry of the fabric as seen in Fig. 1. Many approximations would be necessary to model the fabric as an array of aligned fibres. The fabric is clearly a complex assembly of woven fibres. The numerical calculation could be improved by applying more accurate imaging techniques to the fabric, such as tomography (as done by Petrasch et al., 2008) or DVI (Jaganathan et al., 2008), to refine the description of the geometry. A specific representative unit cell would be built and the flow solved through the representative element. However, these techniques are costly, time consuming and difficult to apply in such a complex case study.

A more traditional way to determine a component of the permeability tensor is to acquire experimental data. The 1-D flow device (Parnas et al., 1995, 1997; Gauvin et al., 1996, Roy et al., 2007; Lundström et al., 1999) is well known and has been in common use for years. In this experiment, a test fluid of known physical properties is injected at constant flow rate or constant pressure drop through a porous medium and the behaviour of the flow is analysed with respect to Darcy's law. This method is accurate for a pure porous medium but, unfortunately, the fabric and the optical fibres cannot be separated from one another in the photocatalytic textile. So Darcy's law cannot be applied directly after the measurements. The alternative approach chosen here to determine the permeability of the fabric is to match numerical

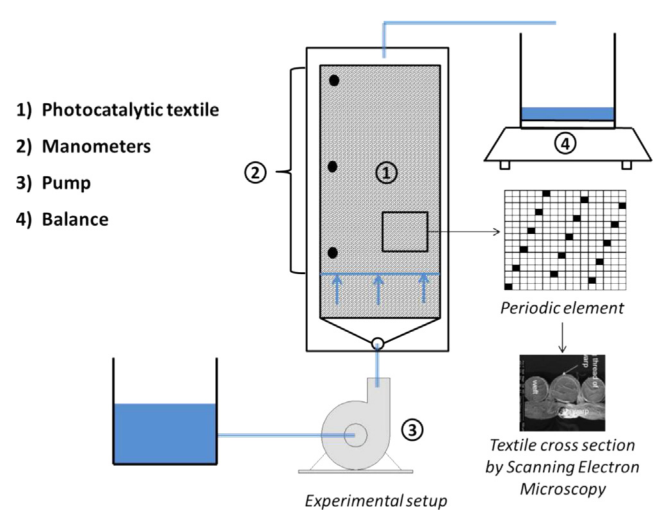

Fig. 1. Diagram of experimental device, woven textile and periodic element.