OPTIMIZATION OF THE FLOW IN PHOTOELECTROCATALYTIC CELLS FOR WATER TREATMENT

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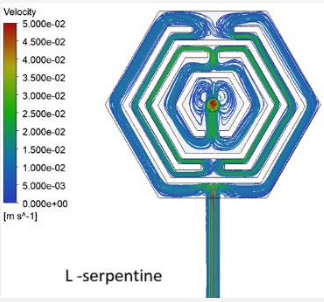

This work address freshwater scarcity through water reuse, particularly focusing on improving photoelectrocatalytic (PEC) cells' design using computational fluid dynamics (CFD) tools. Various geometries were explored to enhance mass transfer in individual PEC cells, with the "L-serpentine" geometry proving most effective. Experimental validation was conducted through 3D printing. Scaling up designs allowed for increased treated volume without compromising mass transfer. A LED board replicating the solar spectrum was designed, enabling a combined study of fluid dynamics and radiation transport towards the PEC cells. This integration ensures both flow homogeneity and adequate radiation exposure on photoactive surfaces.

Introduction

The scarcity of freshwater has become one of the most concerning issues worldwide and is expected to increase as a consequence of climate change. Water reuse is a key element in mitigating the problem of scarcity; however, conventional treatment techniques cannot achieve complete removal of most complex contaminants. Photoelectrocatalyc (PEC) cells have shown great promise to remove them, with even an opportunity for energy recovery by capturing CO_2. Improving the design of PEC cells is a necessary challenge before scaling up and commercial use. This work focuses on developing a methodology to model the behavior of PEC reactors with the aid of computational fluid dynamics tools. A LED-illuminated PEC cell is designed and modeled, including fluid dynamics, mass and radiation transport. CFD allows an economic and time saving alternative over physical experimentation.

Different studies have aimed to optimize flow and improve mass transfer in electrochemical cells [1]. In the case of PEC, the design is more complex, since the radiative transfer equation must also be considered to ensure adequate illumination of the photocatalyst. On the other hand, to the best of the author's knowledge, there are not many studies that focus on scaling PEC to treat larger volumes while still obtaining homogeneous illumination [2]. More efforts in the study of stacked cells to obtain designs that can be used at industrial level are still needed.

Material and Methods

First, different geometries were considered in order to improve the mass transfer coefficients for an individual sandwich-like PEC cell. Different turbulence promoters and flow distributors were considered to achieve a better distribution of the fluid and try to avoid dead zones (Figure 1). The same electrode area is kept for comparison.

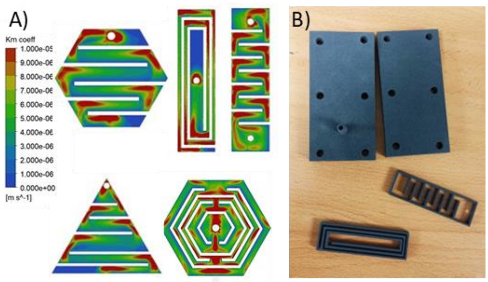

Figure 1. A) Mass transfer coefficients in the channeled geometries. B) 3D printed geometry for model validation.

The influence of inlet and outlet ports location, considering the obtaining of an unobstructed illuminated surface, is also studied.

A LED board simulating the solar spectrum is designed (Figure 3). Then PEC cells are stacked. Geometry is considered for improve LED illumination and their advantages for the scaling-up process are studied. Hydrodynamics calculations have been carried out considering a three-dimensional and steady-state flow through the resolution of the continuity equation and the classical Navier-Stokes equation. The transport of a tracer was considered to calculate the mass transfer coefficient. The radiation field was calculated using the Discrete Ordinate Method (DOM). The incident radiation in each spatial cell is calculated by integrating the radiation intensity in the spherical space directions.

Results and Discussion

Channeling the flow considerably improves mass transport, resulting in an increase in the average transport coefficient and, above all, in greater homogeneity. Specifically, the L-serpentine geometry is the one that offers the best results (See Figure 1). Several pieces have been 3D printed with the aim of experimentally validating these results. With the scaled designs (Figure 2), it is possible to increase the treated volume without affecting mass transfer. The average mass transfer coefficient in the scaled geometries is slightly improved with respect to the individual equivalent case.

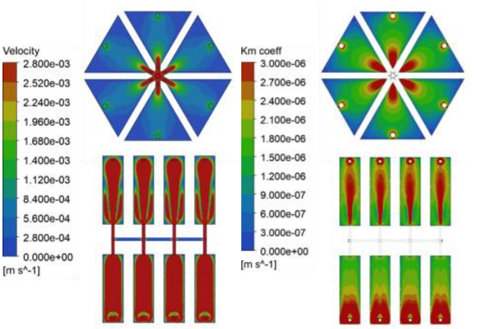

Figure 2. A) Velocity and B) mass transfer distribution in different stacked cell designs. Mass transfer coefficients in the channeled geometries. B) 3D printed geometry for model validation.

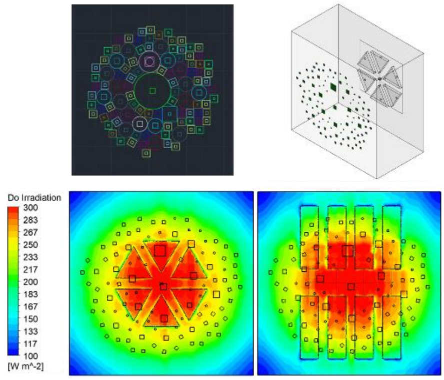

Figure 3. A) Velocity and B) mass transfer distribution in different stacked cell designs. Mass transfer coefficients in the channeled geometries. B) 3D printed geometry for model validation.

Based on the commercial LEDs available, a LED-board with 103 LEDs has been designed to replicate the solar spectrum. The combined study of fluid-dynamics and radiation transport from the LED-board towards the cathodic surfaces, allows taking into account both the homogeneity in the flow and the radiation received in the PEC cells.

Conclusions

The methodology that is being developed allows researchers to be guided towards the scaling-up of this technology. Future work will include electrochemical kinetics in the design of more effective PECs. We consider that this work can help boost the technology, aiding in the scaling-up process.

Acknowledgments

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