Exploring Photocatalytic Degradation of Diclofenac and Assessing Performance in the Innovative Annular Spiral Photoreactor

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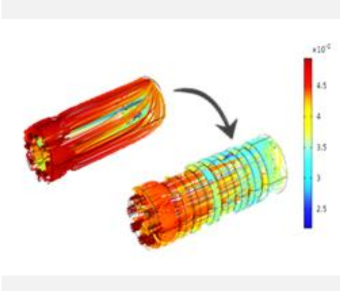

The synergy between computational fluid dynamics (CFD) and advanced oxidative processes is gaining prominence in water treatment evaluation. Addressing low-concentration pollutants, the degradation of emerging contaminants via effluent decontamination using UVC radiation, ozonation, and other Advanced Oxidative Processes (AOPs) presents a promising solution. This study advocates for the fusion of CFD with photocatalytic degradation of Diclofenac (DFC) to scrutinize both kinetic and fluid dynamic advancements in a novel photoreactor design, particularly the spiral photoreactor.

Introduction

Advanced oxidation processes (AOPs) that employ UVC radiation have been increasingly used in studies for the disinfection of organic contaminants, mainly pesticides and pharmaceuticals, in wastewater. By utilizing UV radiation, these processes show considerable promise due to their high effectiveness and wide applicability for disinfecting trace contaminants in aqueous solutions [1].

Several studies found in the literature investigate the degradation kinetics of organic contaminants during UV treatment. Investigations explored the kinetics and mechanisms of degradation in various water matrices and photocatalysts, with the aim of achieving increasingly efficient degradation rates [1, 2,3].

Diclofenac sodium, a nonsteroidal anti-inflammatory analgesic, is commonly prescribed for several conditions, including the treatment of postoperative pain. According to published data, daily doses typically range from 75 to 150 mg, with approximately 65% excreted through urine and 35% through bile after absorption by the body. In terms of topical application, only 50% of the administered dose is absorbed, while the remainder is eliminated during bathing or lost through contact with clothing [3].

In the field of research, computational fluid dynamics (CFD) simulations are gaining traction to study flow patterns and chemical reactions in such contexts. Furthermore, this computational tool allows the exploration of models that incorporate the radiative aspects of these photoreactors, further improving our understanding of the processes involved [4, 5].

The study observed the performance of jet and spiral photoreactors with respect to flow dynamics, identification of dead zones, and elimination of organic contaminants under various operating conditions and design parameters. Changes in inlet configurations, reactor diameter and number of lamps were introduced to optimize the photocatalytic degradation of diclofenac.

Within this framework, the research aims to comprehensively explore how reactor configuration influences the photocatalytic efficiency of diclofenac degradation, employing Computational Fluid Dynamics (CFD) simulations for detailed analysis.

Material and Methods

Numerical simulations were conducted using Comsol Multiphysics®, software to model the photocatalytic process and investigate the degradation activity of diclofenac (DFC). A comparison between jet and spiral reactors, the latter being an innovative design aimed at improving fluid flow, was also performed. Additionally, the dynamic behavior of the photoreactor was evaluated.

Computational Model

Figure 1 shows the geometries used in this study.

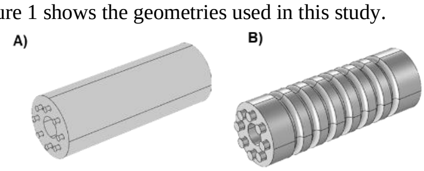

Figure 1. Geometric configuration of jet and spiral photoreactors (A) and (b), respectively**.**

Figure 2 illustrates the mesh used in the numerical simulations, with a layer of prisms added at the inlets and outlets of the reactors. The mesh used in the simulations has a tetrahedral shape and comprises approximately 1.000.000 elements.

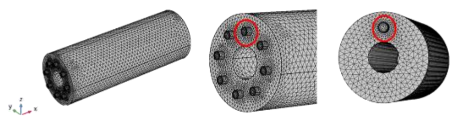

Figure 2. Representation of the mesh and layer of prisms used in the study

Results and Discussion

To validate the numerical simulation, we conducted a comparative analysis with experimental data from the jet photoreactor. Figure 3 illustrates this comparison, revealing a noteworthy concordance between the experimental and numerical results. Notably, the observed error was less than 5%, suggesting a high level of accuracy in our evaluated model. Thus, it is reasonable to conclude that the model effectively captures the photocatalytic degradation kinetics under examination.

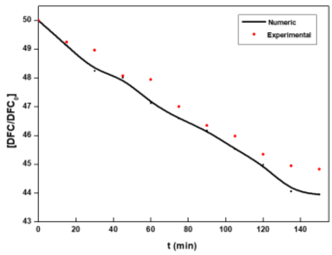

Figure 3 Comparison between experimental and numerical results: validation of the CFD simulation

Figure 4 depicts the fluid flow through streamlines, offering insights into the preferential paths and dead zones within the photoreactor. Additionally, it illustrates the development of turbulent motion within the system. A comparative examination of the two figures highlights enhancements in flow dynamics, notably characterized by the emergence of helical movements. These helical movements play a crucial role in facilitating solution mixing, thereby promoting increased contact between the solution and UVC radiation. Consequently, this results in elevated degradation rates of the contaminant.

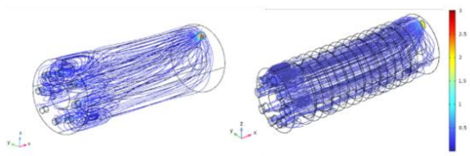

Figure 4 Representation of the mesh and layer of prisms used in the study

The Grafiph abstract, we can discern the concentration evolution within the jet and spiral photoreactors. A significant disparity in concentration development is evident between the two reactors. In the spiral photoreactor, distinct peaks are observable, indicating variations in concentration decay along its length. Conversely, in the jet photoreactor, the photodegradation kinetics progress more uniformly. Furthermore, it's notable that the degradation rate in the spiral reactor surpasses that of the jet reactor, underscoring how geometric modifications can optimize the reaction process and enhance performance.

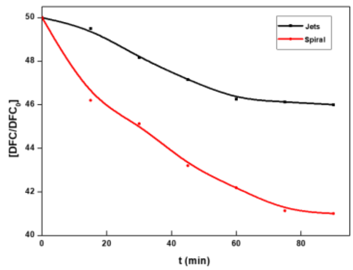

Figure 5 Comparative analysis of the performance of jet and spiral photoreactors

Upon evaluating the results derived from the numerical simulation of both photoreactors, it becomes apparent that the spiral photoreactor holds a significant advantage in terms of photocatalytic degradation compared to the jet photoreactor. Despite maintaining identical inlet and outlet configurations, the performance of the spiral reactor surpasses that of the jet reactor owing to modifications in the reactor walls. These alterations facilitate enhanced solution mixing, prolonged residence time, and consequently, heightened contact with UVC radiation. This, in turn, yields a greater degradation rate.

Conclusions

Based on the findings, it is evident that degradation of Diclofenac (DFC) was not only achieved but also attained satisfactory levels. The jet reactor achieved approximately 65% degradation, while the spiral reactor exhibited even higher performance, with around 75% degradation of the contaminant. Notably, the development of the spiral photoreactor showcased substantial enhancements in both fluid dynamics and degradation rates, attributed to the innovative geometry introduced in its design

Acknowledgments

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References

[1] J. Rodríguez-Chueca, J. Carbajo, P. García-Muñoz, Catalysts, 401 (2023)

[2] R. N. Brodgen, R. C. Heel, G. E. Pakes, T. M. Speight, G. S. Avery, Diclofenac Sodium: A Review of its Pharmacological Properties and Therapeutic Use in Rheumatic Diseases and Pain of Varying Origin, Drugs,.24, 20 (2012)

[3] R. Altman, B. Bosch, K. Brune, P. Patrignani, C. Young, Advances in NSAID Development: Evolution of Diclofenac Products Using Pharmaceutical Technology. 859, 75. (2015).

[4] R. L. P. Carvalho, E.C. P. Leal-Júnior, M. C. Petrellis, R. L. Marcos, M. H. C. de Carvalho, G. de Nucci, R. A. B. Lopes-Martins. Effects of Low-Level Laser Therapy (LLLT) and Diclofenac (Topical and Intramuscular) as Single and Combined Therapy in Experimental Model of Controlled Muscle Strain in Rats. Photochemistry and Photobiology, 508. 89. (2023)

[5] V. M. Avargani, S. Zendehboudi, S. Osfouri, A. Rastami, Performance evaluation of a solar nano-photocatalytic reactor for wastewater treatment applications: Reaction kinetics, CFD, and scale-up perspectives 421 (2023)