Computational Fluid Dynamics to Estimate Residence Time Distribution: Application to an Aqueous Enzymatic Flow

Gusthavo Silva[1], Frederico Costa[2], Natalia Klanovicz[2], Bruno Ramos[1,2*], João Guilherme Poço[1], Luís Fernando Novazzi[1], Helen Treichel[3], Antônio Carlos Teixeira[2], Gustavo Olivieri[1]

1 Department of Chemical Engineering, Centro Universitário FEI, Avenida Humberto de Alencar Castelo Branco 3972, 09850-901, São Bernardo do Campo, Brazil; 2 Department of Chemical Engineering, Escola Politécnica, Universidade de São Paulo, Avenida Prof. Luciano Gualberto (Travessa 3) 380, 05508-010, São Paulo, Brazil; 3 Department of Environmental Sciences, Universidade Federal da Fronteira Sul, Rodovia ERS 135 km 72, 99700-000, Erechim, Brazil

**Corresponding author: brunoramos@fei.edu.br*

Highlights

- Coupling between Computational Fluid Dynamics and Residence Time Distribution;
- Enzyme flow in microreactors;
- Effect of different micromixers.

1. Introduction

The removal of pollutants from aqueous systems can be efficiently performed in bioprocesses, by employing enzymes to catalyze degradation reactions. Particularly, peroxidases consist of an enzyme group which degrade pollutants by the generation of free radicals from peroxides. The peroxidases have been studied for applications in effluent treatment plants (degradation of dyes, pharmaceuticals, pesticides, etc.) and in the development of biosensors (detection of toxins, pathogens, tumors, etc.) [1-3].

The peroxidases are typically studied in batch systems, while studies in continuous reactors are scarce in the literature. Microreactors consist of tubular reactors with reduced dimensions (diameters in the order of μm-mm), which tend to enhance heat and mass transfer effects. Studies involving the employment of peroxidases in microreactors are useful for developing new processes. Although preliminary studies with other enzymes indicate challenges in efficiency associated with enzyme catalysis in microreactors [4], these devices remain particularly useful when considering continuous biosensor applications.

The Residence Time Distribution (RTD) of substances in continuous reactors is important to analyze diffusion effects that may impact the performance of those substances during the reaction. Particularly, the flow of particulate systems may also be impacted by accumulation in dead zones, which can also lead to different RTD behaviors.

Within this context, the present study aimed to analyze the RTD of a commercial peroxidase in three different continuous microreactors, based on CFD simulations.

2. Methods

Three different microreactor geometries were tested (Figure 1), with reaction volumes varying from 3.5 to 6 mL. The meshes associated with the geometries were obtained by the Ansys Mesh software (version 2023 R2), while the CFD simulations were performed in the Ansys Fluent software (version 2023 R2).

An aqueous solution of the peroxidase enzyme was employed in the simulations, considering flow rates that led to a 10-minute space-time. The solution of peroxidase was inserted in the reactor by a pulse of 0.5 s, simulating a typical experimental procedure. The following conditions were applied: transient formulation, multiphase Eulerian model, Population Balance Model, laminar flow, pressure-velocity coupling by Phase Coupled SIMPLE.

Similar tests were employed to analyze the RTD of guaiacol, a pollutant model, with the following conditions: transient formulation, laminar flow, pressure-velocity coupling by Phase Coupled SIMPLE.

3. Results and discussion

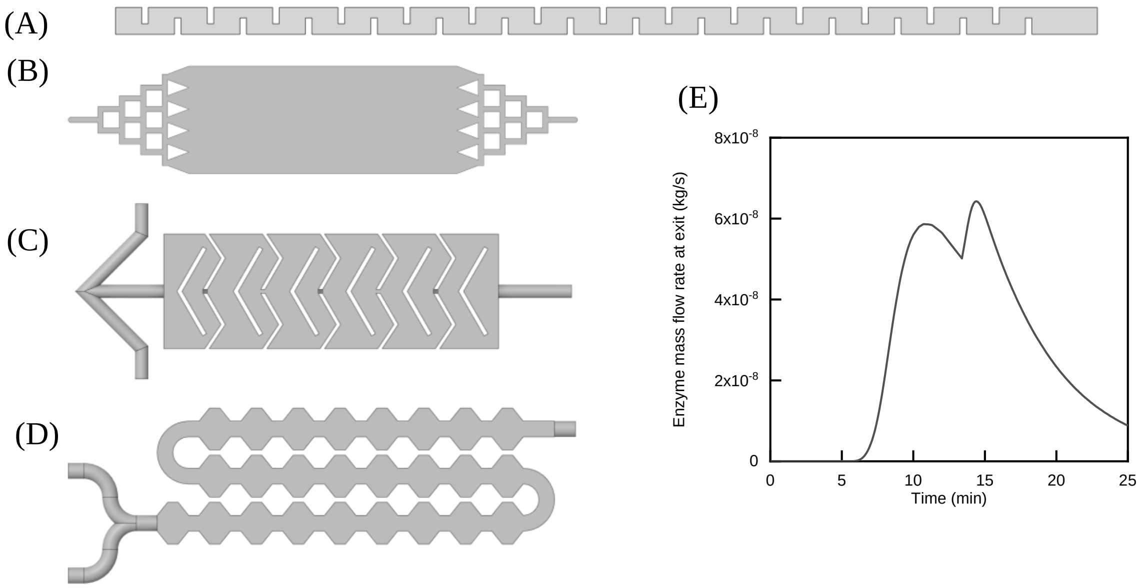

Figure 1. (A), (B), (C), (D): Geometries of the microreactors tested; (E) RTD for peroxidase in geometry A.

Geometry A consists of one inlet and one outlet with perpendicular barriers to promote the micromixing. Geometry B was considered for tests based on previous applications in photocatalysis in our research group [6], and it consists of only one inlet and one outlet, with subdivisions that enable micro mixing near the inlet and outlet. Geometry C considers two inlets, one outlet, and micro barriers that lead to a wave motion of the system that enables the mixture. Geometry D also includes two inlets and one outlet but with expansion and contraction of the cross-section area that aims to promote micromixing with lower energy expenditure than geometry C.

The CFD simulations provided asymmetric RTD curves shifted toward high residence times, in comparison to the stipulated space-time of 10 min, for both peroxidase and guaiacol. The guaiacol flow resulted in RTD curves that were less impacted by the microstructure type than the peroxidase curves. Considering the peroxidase curves, the mean residence time increased in the following order of reactor geometries: A < B < C < D. Possible explanations derive from diffusivity effects, considering that the enzyme presents a much higher molar mass than the guaiacol (around 40000 g/mol for peroxidase, in contrast to 124 g/mol for guaiacol).

4. Conclusions

Preliminary RTD tests were obtained through a CFD procedure, considering the flow of the enzyme peroxidase and the substrate guaiacol. The results will be useful for understanding the reaction limitations in microreactors and proposing better geometries and conditions to increase the reaction efficiency.

References

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Keywords

Enzymes; Microreactor; Computational Fluid Dynamics; Residence Time Distribution.