

Topology optimization as a tool for designing microbioreactors

Ines Rosinha Grundtvig¹, Anders E. Daugaard², John M. Woodley¹, Krist V. Gernaey¹, Ulrich Krühne¹

¹CAPEC-PROCESS Research Center, Department of Chemical and Biochemical Engineering, Technical University of Denmark, Building 229, 2800 Kongens Lyngby, Denmark

The non-homogeneous concentration profiles inside bioreactors resulting from poor mixing contribute to low product formation. This work is a computational and experimental study of a novel way to discover the best distribution of enzymes inside a microbioreactor in order to improve its yield by accounting for its flow heterogeneities. Topology optimization is the mathematical method used for the optimization of the enzyme spatial distribution.

Topology optimization is a mathematical method applied to optimization of material distribution within a given domain, thus fulfilling a given set of constraints in order to minimize or maximize a predefined objective function.^[1]

The Evolutionary Structural Optimization (ESO) technique is the method used in this investigation. This method is based on the concept of gradually removing elements from inefficient parts of the initial configuration leading to an optimized conformation.^[2] The unneeded elements are removed by using a rejection criterion which identifies the ineffective material.

The innovative contribution of this work is the use of topology optimization to investigate the best configuration of immobilized enzyme in a microreactor, which allows the evaluation of the enzyme spatial distribution in a three dimensional problem. The oxidation of 2,2'-azino-bis(3-ethylbenzthiazoline-6-sulfonic acid) (ABTS) to its radical form by reduction of hydrogen peroxide catalyzed by peroxidase was the reaction chosen for this study.

The computational part of this investigation includes a routine which couples the commercial computational fluid dynamics (CFD) code Ansys CFX[®] to Matlab[®]. Ansys CFX[®] will perform the discretization of the microreactor into finite elements and its analysis taking into account the fluid dynamics and the kinetic models implemented. The Matlab[®] routine consists of the application of an adaptation of the ESO method to the biocatalytic reactor, including evaluation of the objective function and definition and execution of the simulation for each new enzyme configuration. The reaction yield will be the objective function which will be a measure for the system performance.

The experimental part of this investigation includes the determination of kinetic parameters which will be implemented in the CFD simulations for a validation of the computational work, where the performance of the initial case and the optimized configuration will be compared.

This approach will give the opportunity to identify the optimal process conditions, collect information regarding the flow characteristics which influence the reaction yield and even obtain the final optimal enzymatic reactor before performing experimental work.

References

[1] M. P. Bendsoe, O. Sigmund, Topology Optimization: Theory, Methods and Applications, first ed., Springer Science & Business Media, New York, 2003

[2] Y.M. Xie, G.P. Steven, A simple evolutionary procedure for structural optimization, *Comput. Struct.*, 49 (1993) 885-886.