Proceedings of the 12th International Conference on Fluid Flow, Heat and Mass Transfer (FFHMT 2025)
July 15, 2025 - July 17, 2025 | Imperial College London Conference, London, United Kingdom
Paper No. 195
DOI: 10.11159/ffhmt25.195

CFD-driven Topology Optimization for Design of Isothermal Catalytic Planar Microreactors

Yuna Yamanishi, Osamu Tonomura*, Ken-Ichiro Sotowa
Department of Chemical Engineering, Kyoto University
Nishikyo, Kyoto 615-8510, Japan
*tonomura@cheme.kyoto-u.ac.jp

Abstract **-** Research on catalytic microreactors has been attracting attention. According to related reports, heterogeneous catalysts are often immobilized on the vessel wall or on packed particles or monoliths due to the ease of separation of reaction components and catalysts. Numerical modelling methods such as computational fluid dynamics (CFD) are often used to analyze and design catalytic microreactors, since their performance depends not only on the catalyst itself but also on the hydrodynamic properties inside the reactor. In particular, it is important to note that the assumed catalyst layer distribution is highly dependent on the reactor performance. In this study, an isothermal catalytic planar microreactor was designed by combining topology optimization with CFD. The effect of the objective function and constraints on the design results was evaluated, and it was shown that the pressure loss was minimized when the initial design domain was elliptical.

Keywords**:** Design, Modelling, Microreactor, Catalyst, Topology optimization, CFD

1. Introduction

Today, the shift from batch to flow production methods is accelerating, mainly in the pharmaceutical and fine chemical fields. One of the key technologies for this is chemical process technology using microdevices with channels of less than a several millimeter (called micro chemical process technology), and research and development into this technology has been actively carried out for nearly 25 years. Many synthetic reactions have been reported using various microdevices, such as Grignard reagent exchange reaction [1], radical polymerization [2], halogen-lithium exchange reaction [3], Swan oxidation [4], condensation polymerization [5], hydrogen peroxide oxidation [6], and fine particle synthesis [7]. The success of these synthetic reaction examples is due to the excellent functions of microdevices, such as efficient mass and heat transfer, rapid mixing, and precise flow control, which are derived from the characteristics of microdevices, such as large surface area per volume, narrow channel width, and small internal device volume. In order to make the most of these excellent features of microdevices in various processes, the design of the microdevices is very important. It is necessary to control the flow and diffusion of materials, which greatly affect the functions of microdevices, and not only the channel size but also the channel structure and geometry are important design variables. Therefore, when formulating a microdevice design problem, rather than assuming perfect mixing or plug flow, it is necessary to use models that can describe the concentration and velocity distributions within the device, which differ depending on the channel structure and geometry. Fortunately, because the flow inside the microdevice is laminar, it is possible to incorporate chemical reactions into commercially available fluid simulation technology, and there are many reports of the analysis of microdevices using computational fluid dynamics (CFD). Recently, there has been an increase in research into microdevice design through the integration of CFD models and optimization techniques. Our group has reported, for example, on the design of an external heat exchanger type multi-tubular reactor [8], the design of a plate-type mixer [9], and the shape optimization of the U-shaped microchannel [10].

Research on microreactors for catalytic reactions has attracted attention in recent years, and in the case of heterogeneous catalytic reactions, there are examples in which the catalyst is immobilized on the channel walls or on packed particles or monoliths [11]. The performance of such fixed-bed reactors depends not only on the catalyst but also on fluid dynamics. Therefore, although design using numerical modelling and simulation such as CFD has been considered, the design results depend on the catalyst layer distribution assumed in advance, which results in limited improvement of the reactor performance. In this study, topology optimization is used as a structural optimization method, and by combining it with CFD, an isothermal catalytic planar microreactor is designed to derive the optimal catalyst layer structure.

2. Design Problem and Solution Method

The design problem for catalytic microreactors is formulated, and its solution method is outlined.

2.1. Desing Problem Setting and Formulation

A catalytic microreactor to be designed is shown in Fig. 1. The reactor consists of three sections, namely, the inlet channel, the fixed bed section, and the outlet channel. The fixed bed section is the design domain in this study. It was assumed that a single isothermal first-order reaction between the porous catalyst and the liquid-phase raw material proceeds in the fixed bed section. The fluid properties were equal to water (298 K), the inlet concentration of reactant A was fixed at 1 mol/m^3, the reaction rate coefficient k_a was fixed at 0.25 s^{-1}, and the local reaction rate r [$mol/m^3/s$] was given by $k_a(1- \theta)c$, where c is the reactant concentration and θ ($0 \leqq \theta \leqq 1$) is porosity, which means the volume fraction of the solid catalyst. A two-dimensional model was constructed using COMSOL Multiphysics® version 6, taking into account vertical symmetry, based on the Navier-Stokes (N-S) equations, the continuity equation, and the transport equations of chemical species [12].

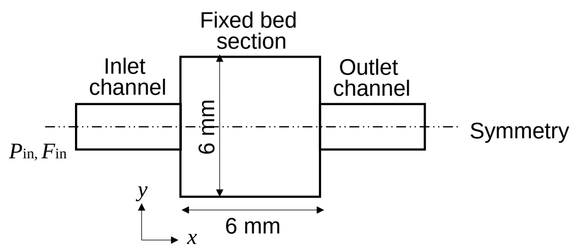


Fig. 1: A catalytic planar microreactor.

In this study, two design problems were formulated, as shown in Table 1. In case 1, the design objective is to maximize the average reaction rate (R) under a given constant inlet pressure (P_{in}), and in case 2, the design objective is to minimize the inlet pressure under a given constant inlet flowrate (F_{in}) and a constraint on reaction conversion rate (X). In both problems, the optimization variable is the porosity θ at each location in the fixed bed.

Table 1: Design problem formulation.

	Case 1	Case 2
Objective function	Average reaction rate R (maximized)	Inlet pressure P_{in} (minimized)
Optimization variable	Porosity $\theta(x, y)$	Porosity $\theta(x, y)$
Main constraint	Constant inlet pressure P_{in}	Constant inlet flowrate F_{in} Conversion rate X of 60% or more

2.2. Density-based Topology Optimization

A density-based topology optimization algorithm [13] was used to solve the design problems presented in the previous section. The catalyst layer distribution in the fixed bed section was expressed by the normalized material density. Based on the idea that the presence of a catalyst layer in the fixed bed brings about resistance to the flow, a term for the fluid resistance proportional to the flow velocity was added to the N-S equation in the model constructed in the previous section, and the proportionality coefficient was given as a function of θ. In this type of CFD-driven topology optimization, the objective function is maximized or minimized by adjusting the porosity θ, which is a continuous variable, in each mesh of the design domain. $\theta = 1$ represents only fluid, and $\theta = 0$ represents only solid catalyst layers. Note that a Helmholtz filter was used to prevent the derived θ from becoming discrete, and hyperbolic tangent projection and Darcy interpolation were introduced to deal with the problem of the occurrence of a region where $0 < \theta < 1$, known as the gray scale. In this study, these optimization algorithms were implemented by COMSOL Multiphysics® ver. 6.

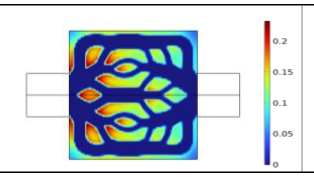
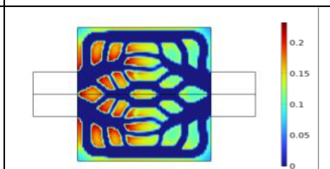
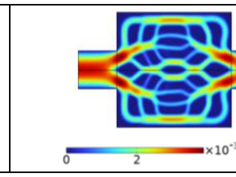
3. Results and Discussion

The design results and discussion of Cases 1 and 2 are presented.

3.1. Case 1

Table 2 shows the design results for Case 1. The local reaction rate distribution was superimposed on the catalyst layer distribution in the fixed bed section derived for different P_{in}, with the dark blue areas corresponding to the channels. The flow velocity distribution was shown only when P_{in} = 0.60 Pa. When P_{in} was increased, the channel width became narrower and the number of channels increased, and R and x became 1.23 times and 0.94 times, respectively. It was suggested that whether it is appropriate to increase P_{in} depends on whether the priority is given to the reaction rate or the conversion rate.

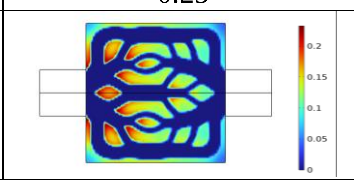
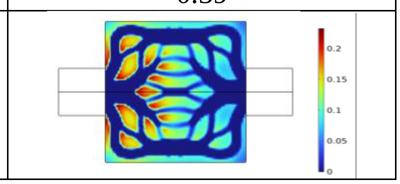
Table 2: Design results for Case 1.

P_{in} [Pa]	0.25	0.60	
r [mol/m^3/s]			 [m/s]
R [mol/m^3/s]	0.050	0.062	
X [-]	0.49	0.46	

3.2. Case 2

In Case 2, the F_{in} was fixed at 1.81×10^{-6} m^2/s, which is the same as in Case 1, and x was restricted to 0.6 or more. The result is shown in Table 3. In Case 2, since the restriction of a higher conversion rate was imposed, the channels (dark blue part in the figure) became narrower overall, and P_{in} was 1.54 times larger.

Table 3: Design results for Case 2.

Case	1 (Same as Table 2)	2
P_{in} [Pa]	0.25	0.39
r [mol/m^3/s]		

In addition, the optimization results when the initial shape of the fixed-bed section is rectangular, diamond, and elliptical, with the area constant, are shown in Fig. 2 (a), (b), and (c), respectively. The P_{in} for the rectangular, diamond, and elliptical shapes were 0.30 Pa, 0.36 Pa, and 0.29 Pa, respectively. In all shapes, P_{in} tended to be lower when the channel structure was closer to a parallel one than a mesh one. This is likely because the mesh-like shape requires repeated split and recombine of flow, which increases the channel resistance. The reason why P_{in} was smallest in the elliptical case is thought to be because there are few sharp bends in the channel and resistance is less likely to occur. P_{in} in the elliptical case was 0.76 times that of Case 1.

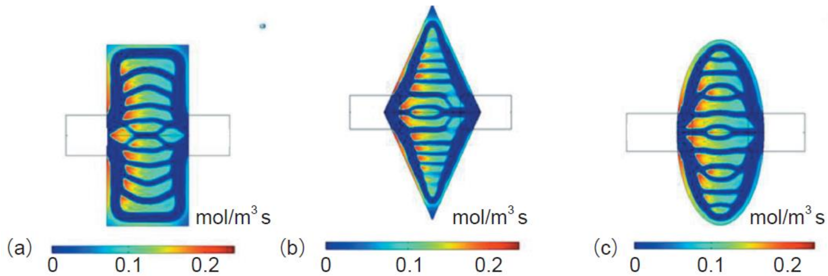


Fig. 2: Optimization results for different initial shapes.

4. Conclusion

The usefulness of the CFD-driven topology optimization method for the catalyst layer distribution design of the fixed-bed section of a catalytic microreactor was demonstrated through a case study. Under a constant fixed-bed section area, three different geometries were compared, and the optimal catalyst layer distribution was derived.

Acknowledgements

This work was partially supported by the Grant-in-Aid for Scientific Research (B) (No. 23H01754), the Grant-in-Aid for Scientific Research (C) (No. 19K05140), and a project, Development of Continuous Production and Process Technologies of Fine Chemicals, commissioned by the New Energy and Industrial Technology Development Organization (NEDO).

References

[1] V. Hessel, C. Hofmann, H. Löwe, A. Meudt, S. Scherer, F. Schönfeld and B. Werner, "Selectivity gains and energy savings for the industrial phenyl boronic acid process using micromixer/tubular reactors," *Org. Process Res. Dev.*, vol. 8, pp. 511-523, 2004.

[2] T. Iwasaki and J. Yoshida, "Free Radical polymerization in microreactors. significant improvement in molecular weight distribution control," *Macromolecules*, vol. 38, no. 4, pp. 1159-1163, 2005.

[3] A. Nagaki, S. Tokuoka, S. Yamada, Y. Tomida, K. Oshiro, H. Amii and J. Yoshida, "Perfluoroalkylation in flow microreactors : generation of perfluoroalkyllithiums in the presence and absence of electrophiles," *J. Org. Biomol. Chem.*, vol. 9, pp. 7559-7563, 2011.

[4] T. Kawaguchi, H. Miyata, K. Ataka, K. Mae and J. Yoshida, "Room-temperature Swern oxidations by using a microscale flow system," *Angew. Chem. Int. Ed.*, vol. 44, no. 16, pp. 2413-2416, 2005.

[5] S. Liu and C.H. Chang, "High rate convergent synthesis and deposition of polyamide dendrimers using a continuous-flow microreactor," *Chem. Eng. Technol.*, vol. 30, no. 3, pp. 334-340, 2007.

[6] K. Yube and K. Mae, "Efficient oxidation of aromatics with peroxides under severe conditions using a microreaction system," *Chem. Eng. Technol.*, vol. 28, no. 3, pp. 331-336, 2005.

[7] R. Schenk, M. Donnet, V. Hessel, C. Hofmann, N. Jongen and H. Löwe, "Suitability of various types of micromixers for the forced precipitation of calcium carbonate," in *Proceedings of the International Conference on Microreaction Technology*, Strasbourg, 2001, pp. 489-498.

[8] Y. Segawa, O. Tonomura and K. Sotowa, "CFD-based design of multi-tube heat exchange type compact reactor," *Chem. Eng. Trans.*, vol. 99, pp. 529-534, 2023.

[9] K. Okamoto, H. Kim and O. Tonomura, "CFD-based design of laminated microdevice with 3D serpentine channel for submillisecond mixing," *Comput. Aided Chem. Eng.*, vol. 53, pp. 1327-1332, 2024.

[10] O. Tonomura, M. Kano and S. Hasebe, "Shape optimization of microchannels using CFD and adjoint method," *Comput. Aided Chem. Eng.*, vol. 28, no. C, pp. 37-42, 2010.

[11] A.Tanimu, S. Jaenicke and K. Alhooshani, "Heterogeneous catalysis in continuous flow microreactors : a review of methods and applications," *Chem. Eng. J.*, vol. 327, pp. 792-821, 2017.

[12] https://www.comsol.jp/model/optimization-ofa-catalytic-microreactor-4401 (2023, Sept. 5).

[13] L.H. Olesen, F. Okkels and H. Bruus, "A high-level programming-language implementation of topology optimization applied to steady-state Navier-Stokes flow," *Int. J. Numer. Meth. Engng.*, vol. 65, pp. 975-1001, 2006.