Thermo-fluid Design Approach to Microreactors with Uniform Temperature and Residence Time Distribution

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Introduction

Recently, extensive studies have been carried out on micro chemical process technologies (Jensen, 2001; Fletcher et al., 2002). In particular, analysis of chemical reactions and transport phenomena in micro-space has been performed energetically. However, most microreactors are designed and fabricated by trial and error -- there is no systematic procedure for developing microreactors. Therefore, it takes much time and effort to reach the optimal design. Unless this situation is improved, the design period cannot be shortened.

Recent advances in computational fluid dynamics (CFD) enable us to know both flow and temperature distribution in a microreactor precisely without conducting any experiments. Tonomura et al. (2004) proposed the CFD-based optimization method for design of plate-fin microdevices. However, it is not practical to apply CFD simulations directly to the optimal design problem of microreactors, since they require too much computational time and effort.

In this research, a new systematic approach based on simple models is proposed to efficiently design microreactors with constraints related to flow uniformity, temperature distribution, pressure drop, product yield and size boundary conditions. In addition, the validity of the proposed design method is assessed through a case study.

Optimal design problem of microreactors

In general, increasing the throughput of micro chemical plants can be achieved by a large number of parallel microreactors and/or microchannels within the microreactor. The repetition of a microchannel may appear to be simple at first glance, but there are issues that have not been addressed in the design and operation of macro chemical plants.

The commercial standard connections and tubing can be used to connect the individual microdevices in parallel. Accordingly, conventional sensors and actuators may be used to achieve the desirable flow distribution. On the other hand, when many microchannels are stacked and encompassed in a housing, the standard monitoring and control equipment cannot be applied to each microchannel. Therefore, the stacked-type microreactor needs to be designed taking operation and control into consideration. The inadequate design of the microreactor causes poor uniformity in the temperature and residence time distributions among microchannels, which may make product quality worse.

In this paper, we focus on optimal design problem of a plate-fin microreactor. The plate-fin microreactor typically contains the parallel microchannels, inlet and outlet manifolds. Assuming that no reaction occurs in both the manifolds, thermal design and fluid design of microreactors can be separated into independent design problems. Each design problem is summarized as shown in Table 1.

Table 1. Optimal design problem of microreactors

	Thermal design	Fluid design
Objective function	Uniformalization of fluid temperature	Minimization of total residence time
Optimization variables	Microchannel shape Flow rate Coolant temperature	Manifold shape Number of microchannels
Constraints	Maximum pressure drop Reaction temperature Yield / Selectivity	Maximum pressure drop Residence time distribution Throughput

A proposed approach to microreactor design

Figure 1 shows the flowchart of the proposed thermo-fluid design approach to microreactors. The flowchart mainly consists of two parts, i.e. the thermal design and fluid design. In the thermal design stage, a microreactor having parallel channels is divided into a large number of thermal compartments, each of which is modeled as a lamped parameter system. The heat transfer among the compartments is also modeled. Then, microchannel width is optimized as a function of the longitudinal position by taking into account the constraints related to thermal balance, reaction yield, and pressure drop. By changing the channel width of the longitudinal position, the uniform temperature distribution with no hot spot is realized even for a rapid exothermic reaction.

In the fluid design stage, a pressure drop compartment model is used in order to estimate the pressure distribution over a microreactor including inlet and outlet manifolds. In the pressure drop compartment model, the relation between the inlet and outlet pressures is described as a function of the design parameters and flow velocity. Through the fluid design, the shapes of inlet and outlet manifolds and the number of parallel microchannels are determined to optimize a given performance index such as the minimization of the total residence time of the microreactor. Many constraints related to the pressure and mass balances, flow uniformity, and pressure drop are considered in this stage. In the end, the CFD simulations are utilized at the final design stage to optimize the shape rigorously.

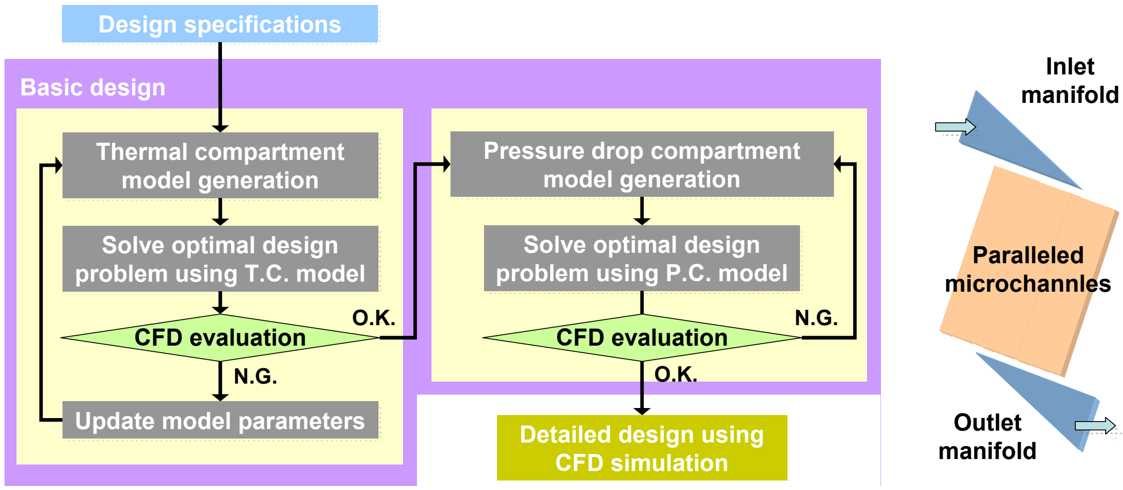

Figure 1. Flowchart of thermo-fluid design approach

Case study

The proposed thermo-fluid design approach is applied to a microreactor design problem with uniform temperature and residence time distributions. An exothermic first-order reaction is taken up in this case study. Keeping temperature in a microreactor uniform at specified reaction temperature is the important design issue. In addition, the perfect flow distribution among parallel microchannels is the key design specification.

Figure 2 illustrates the thermal design results. The solid line in the upper graph shows the optimal channel width along the microchannel and dotted line shows the channel width which is optimized as constant value. As shown in the bottom figure, the optimal shape of microchannel is effective to keep temperature distribution uniform along the microchannel, since narrow channel near inlet shortens residence time for faster reaction rate zone and wide channel near outlet makes residence time longer for slower reaction rate zone. Figure 3 shows the normalized flow distribution among parallel microchannels. The circle points correspond to the optimal design, and the triangle points represents the conventional design. The optimal manifold shape can realize the flow equipartition in all parallel channels, which enhances the conversion and selectivity of reaction products.

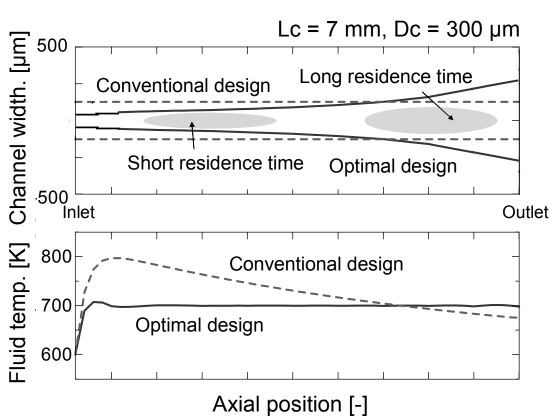

Figure 2. Optimization results of thermal design

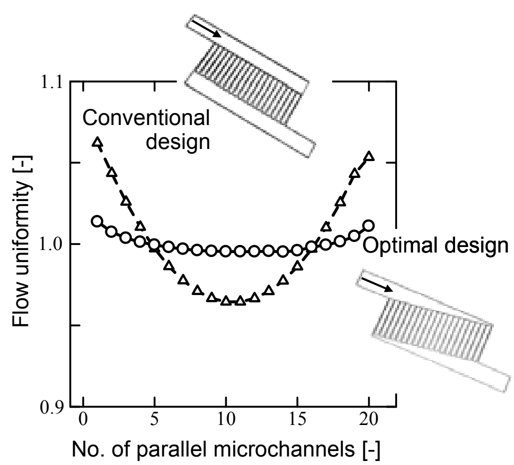

Figure 3. Optimization results of fluid design

Conclusions

The optimal design approach based on the thermal and pressure drop compartment models is developed. The proposed approach is applied to the optimal design problem of a microreactor with uniform temperature and residence time distributions. The validity of the optimal design is confirmed by using CFD simulations. The thermo-fluid compartment model is very simple but powerful tool to shorten the computational time of microreactor design. It can be concluded that the proposed design approach has potential for being widely applied to the optimal design problem of microreactors with various constraints.

Acknowledgements

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