Simplified Model Based Design for T-shaped Microreactors with Secondary Flow

1. Introduction

T-shaped microreactors are the simplest passive microreactors with two horizontal arms as the inlets and one vertical arm as the mixing channels. They have been attracted to industrial application because of secondary flow regime in the mixing channel. At higher Reynolds number (Re) of mixing channels where the flow is in the engulfment flow regime [1], i.e. secondary flow regime, the mixing performance is improved.

Most of the former researches on T-shaped microreactors are executed by Computational Fluid Dynamics (CFD) simulations. However, when optimum size or operation optimization runs need to be performed in the microreactors, the repetitive computational burden related to CFD model is usually much too large. Therefore, effective models are needed to allow for a fast evaluation of design variants.

In this work, a reduced-order model, which combines CFD model and multi-resolution lamellar model, is developed to simulate the reaction, diffusion and advection in T-shaped microreactors. An optimization of reaction product concentration is carried out by the proposed model. The optimization results have a good agreement with CFD simulation results. Meanwhile, a considerable saving in computational effort of CFD simulation can be realized.

2. Efficient design for T-shaped microreactors basing the lamellar models

In the research, some alternately arrayed thin laminas at the entrance of the mixing channel, as shown in Fig. 1, are used to describe the three-dimensional concentration distributions.

![Fig. 1 A schematic diagram of T-shaped microreactor.](image)

The multi-resolution lamellar model is constructed by the N kinds of models with single thickness ($y_m$) of laminas. In each model, the $y_m$ is different. The laminas are located in the center along the flow direction (as Fig. 1 shows). The model is a two-dimensional (x,y) mass conservation model because the diffusion in z direction is assumed to be neglected [2], as described by the following equation,

$$ u \frac{\partial C}{\partial x} = D \frac{\partial^2 C}{\partial y^2} - r_j $$

(1)

where $C_i$ is the mass concentration of the component i, $r_j$ is the reaction rate of the jth reaction. $D_j$ is the diffusivity and u is the average velocity at the outlet of the mixing channel.

The two times of CFD calculations with $Re_1$ and $Re_2$ are first executed. In the two multi-resolution lamellar models, the $y_{m, k}$ ($Re_1$, $Re_2$ ($k=1, 2, ... N$) and the corresponding weighting coefficient $a_k$ in Eq. (2) are estimated by fitting the CFD results of product concentration, as described by Eq. (2). For a different $Re$ ($Re_1 < Re < Re_2$), the $C_{m, k}$ can be calculated by $C_{m, \text{lam}}$ and $C_{m, \text{CFD}}$ with the interpolation method.

$$ \min J = \sqrt{\sum_{i=1}^{n} (C_i(\text{CFD}) - \sum_{k=1}^{N} a_k C_i(y_{m,k}))^2} \quad \text{s.t.} \quad \sum_{k=1}^{N} a_k = 1 $$

(2)

In the design problem, the objective function is to maximize the reaction product concentration, u and hydraulic diameter $D_H$ of mixing channel are selected as optimization variables. Table 1 and Fig. 2 show the optimization results, which have a good agreement to the CFD simulation results.

![Fig. 2 Optimization results compared to the CFD results.](image)

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Objective</th>
<th>$A + B \rightarrow R$</th>
<th>$B + R \rightarrow S$</th>
<th>$\max C_R$</th>
<th>$157.5 &lt; Re &lt; 420$</th>
<th>$\Delta P &lt; 4.0 \times 10^5 \text{ Pa}$</th>
<th>Main product concentration</th>
<th>Pressure loss of mixing channel</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_R$</td>
<td>$\Delta P$</td>
<td>$C_R$</td>
<td>$\Delta P$</td>
<td>$C_R$</td>
<td>$\Delta P$</td>
<td>$C_R$</td>
<td>$\Delta P$</td>
<td>$C_R$</td>
</tr>
</tbody>
</table>

Table 1 Optimization results

<table>
<thead>
<tr>
<th>Optimization results</th>
<th>Non-Optimization results</th>
</tr>
</thead>
<tbody>
<tr>
<td>$u$ [m/s]</td>
<td>4.14</td>
</tr>
<tr>
<td>$D_H$ [μm]</td>
<td>102</td>
</tr>
<tr>
<td>$C_R$ (same retention time)</td>
<td>0.254</td>
</tr>
</tbody>
</table>

3. Conclusion

In this study, a simplified reduced-order model of T-shaped microreactors is proposed. In engulfment regime, based on the limited times of CFD simulation results, the model can easily calculate the optimum product concentration along the mixing channel. Moreover, the model can be applied to the optimization of reshaping for microreactors in the future work.

*e-mail: wang@cheme.kyoto-u.ac.jp*