CFD Simulation of Single-phase Flow Characteristics and Pressure Drop in SiC Hollow-strut Foam Microchannel Reactors

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Abstract. Microchannel reactors (MCR) have received considerable attention by researchers in recent years. A novel hollow-strut ceramic foam microchannel reactor (HSCF-MCR) taking the material and structural advantages of SiC foam was proposed. The reactor could be used as a structural scaffold for continuous gas or liquid phase flow and reaction because all of its struts are hollow and interconnected with each other. The three-dimensional (3-D) microstructure of the SiC foam was characterized by SEM and micro-CT method. Based on the tetrakaidecahedron cell model, computational fluid dynamics (CFD) method was utilized to analyze the single-phase flow characteristics and pressure drop of HSCF-MCR. The 3-D interconnected structure can form the static mixing effect of the flow fields inside the foam microchannel and strengthen the mass transfer process. Both channel diameter $D$ and cell size $L$ of the foam play a vital role in the pressure drop gradient $\delta$ of the fluid flowing through HSCF-MCR. When the ratio of $D$ to $L$ is controlled as 0.1, $\delta$ is minimized. The CFD simulation results contribute to the structural optimization and energy saving of HSCF-MCR for its applications in the future.

1. Introduction

Microchannel reactors (MCR), also well known as microstructure reactors, are devices carrying channels or similar fluid paths with dimensions under a millimeter, and more specifically between ten and several hundred micrometers\[1-3\]. Due to their small dimensions, MCR could provide rapid response times for reactions and safe operation with highly reactive products\[4\]. The short transport paths and high surface-to-volume ratio of MCR can efficiently enhance the heat and mass transfer rates, optimize the process of complex reactions as well as improve the reaction efficiency\[5, 6\]. Numerous applications based on MCR have been reported in the past few decades: catalysis\[7\], organic synthesis\[8\], liquid phase micro-extraction and separation\[9\], steam methane reforming\[10\], and so on.

Reticulated ceramic foams are a class of important inorganic materials composed of 3-D network of ceramic struts\[11\]. These materials especially SiC foams have attracted more and more attention mainly due to their high porosity, low density, high specific surface area, excellent corrosion and thermal resistance, high mechanical strength, controlled permeability and so on\[11-13\].

In this manuscript, we report a novel hollow-strut ceramic foam microchannel reactor (HSCF-MCR) taking the material and structural advantages of SiC foams. This reactor could be used as a structural
scaffold for continuous gas or liquid phase flow and reaction because all the SiC struts are hollow and interconnected with each other. Unlike common transparent T-type or Y-type glass flat MCR made by etching technology, it is difficult to observe the flow characteristics in HSCF-MCR because of their opaque ceramic materials and complex 3-D structures. With the rapid improvement of computing power, simulation by computational fluid dynamics (CFD) method has become an attractive and efficient approach for recovering the transport properties of the medium, especially when it refers to turbulence, mixing and reaction[14, 15]. The accuracy and practicability of CFD method have been confirmed in a large number of previous studies[14-17].

The aim of this study is to analyze the flow characteristics and pressure drop of HSCF-MCR to optimize its structural design and provide theoretical support for its applications in the future.

2. Materials

![Figure 1. Structural characterization: (a) macro-morphology of the foam; (b) photo of the foam cross-section; (c) SEM image of the foam skeleton; (d) Micro-CT image of the foam strut; (e) Micro-CT image of the foam strut cross-section; (f) Micro-CT section view of the foam strut.](image)

The reticulated SiC hollow-strut foam in this study was prepared by the active liquid silicon infiltration method in Shenyang National Laboratory for Materials Science, and its macro-morphology and microstructure were characterized in figure 1.

The cylindrical SiC hollow-strut foam with the size of a diameter 50 mm, height 60 mm is shown in figure 1(a) and figure 1(b). The microchannel reactor can be made by sealing the two ends of the SiC foam reasonably. A typical cube was cut off from the internal region of the SiC foam in order to observe its skeleton structure under the scanning electron microscope (SEM), as shown in figure 1(c). SiC hollow struts are interconnected in the form of 3-D mesh. To obtain comprehensive structural information, a short strut of the foam was scanned and reconstructed by X-ray micro computed tomography (Micro-CT)[18]. From the micro-CT images presented in figure 1(d), figure 1(e) and figure 1(f), the outer diameter, the inner diameter and the wall thickness of the SiC hollow strut were measured as 1 mm, 600 μm, and 200 μm respectively. Taking the advantages of high strength and excellent corrosion resistance of SiC materials, the stable structure and long service life of HSCF-MCR could be obtained.
3. CFD analysis
In order to study the flow fields characteristics and pressure drop of HSCF-MCR, CFD analysis was carried out based on the simplified cell model of SiC hollow-strut foam.

3.1. Cell modeling

The SiC foam can be considered to be formed by numerous similar cells in series and parallel as displayed in figure 2(a). It is very difficult to generate the large number of grids needed when the entire foam is used for simulation directly. In order to simplify the simulation process, a tetrakaidecahedron structural model composed of six squares and eight hexagons was provided based on the formation of the foam as shown in figure 2(b). This structure is the only polyhedron that can stack the full space and it is in good agreement with the principle of the minimum surface energy[19]. The simplified cell model represents the inner channels of HSCF-MCR because the fluid inside SiC foam struts was the real object of this study. Therefore, the flow fields characteristics and pressure drop of one cell was simulated rather than the entire foam. Edge length L of the outer cube of a cell represents the size of the foam cell, while the cell strut diameter D represents the diameter of the foam channel.

3.2. Governing equations
Kerosene was selected as the liquid phase flowing through HSCF-MCR in present CFD study, and it was considered to be incompressible Newtonian fluid at steady state. The basic governing equations for CFD include the continuity, momentum and energy equations. The energy equation was not taken into account in this simulation because no heat transfer was involved. The simulations were carried out by solving Reynolds-averaged Navier-Stokes (RANS) equations[20], which is an effective and practical means to solve engineering problems. The continuity and momentum equations can be written as follows:

\[
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_i)}{\partial x_i} = 0 \tag{1}
\]

\[
\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_i u_j) = -\frac{\partial p}{\partial x_j} + \frac{\partial \sigma_{ij}}{\partial x_j} + \frac{\partial}{\partial x_j}(\rho u_i' u_j') \tag{2}
\]

where \( u_i \) denotes the Reynolds mean velocity component with the average sign omitted, \( \rho \) densities, \( p \) pressures, \( u_i' \) pulsating velocities, and \( \sigma_{ij} \) stress tensor components.

It needs to be pointed out that the turbulence model rather than the laminar model was applied to this simulation for the reason that turbulence could be caused by the complex 3-D interconnected structure of the SiC hollow-strut foam[19], despite the Reynolds number \( Re \) of the fluid in this study was not large enough. The standard k-\( \varepsilon \) model[21, 22] used in present CFD study is a two-equation turbulence model widely applied in flow fields and heat exchange simulation. The k-equation and \( \varepsilon \)-equation for incompressible fluid can be written as equation (3) and equation (4), respectively:

\[
\frac{\partial (\rho k)}{\partial t} + \frac{\partial (\rho u_i k)}{\partial x_i} = \frac{\partial}{\partial x_j} \left( \mu + \frac{\mu_i}{\sigma_k} \right) \frac{\partial k}{\partial x_j} + \mu_i \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \frac{\partial u_i}{\partial x_j} - \rho \varepsilon + S_k \tag{3}
\]

\[
\frac{\partial (\rho \varepsilon)}{\partial t} + \frac{\partial (\rho \varepsilon u_i)}{\partial x_i} = \frac{\partial}{\partial x_j} \left( \mu + \frac{\mu_i}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} + C_{1\varepsilon} \varepsilon \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \frac{\partial u_i}{\partial x_j} - C_{2\varepsilon} \rho \frac{\varepsilon^2}{k} + S_\varepsilon \tag{4}
\]
The constants in this model are specified as: \((C_\mu, \sigma_K, \sigma_E, C_{1E}, C_{2E}) = (0.09, 1.0, 1.3, 1.44, 1.92)\).

### 3.3. Boundary conditions and numerical details

In this CFD study, all the inner channels of the SiC foam were simplified to cylinders so that the surface of the simulated inner channels was smoother than that of the real ones. The fluid/solid interface was set as ‘wall’ with no-slip boundary conditions and symmetry boundary conditions were applied to other faces. The continuous phase was kerosene with density of \(\rho = 780 \text{ kg/m}^3\) and viscosity of \(\mu = 0.0024 \text{ kg/(m·s)}\). The types of inlet and outlet zone were set as ‘velocity-inlet’ and ‘pressure-outlet’ respectively. The governing equations were solved by using finite volume method.

### 4. Results and discussion

#### 4.1. Flow characteristics

The visual distribution of the velocity and pressure fields inside the tetrakaidecahedron structural cell simulated in this CFD study are displayed in figure 3. As can be seen in figure 3(a), after entering the foam cell with the inlet velocity at 5 mm/s, kerosene flows along foam inner channels. The velocity gradient and direction change at the foam skeleton nodes. This 3-D flow mode leads to the mixing effect of the fluid and facilitates the mass transfer process. Therefore, the reactor is very suitable for the efficient mixing of different fluids as well as the rapid reaction between different chemical components in the fluid. Figure 3(b) shows the pressure drop of kerosene flowing through the foam cell clearly, and it can be seen that the fluid pressure inside the channels decreases uniformly along the axis of the foam. The pressure drop of HSCF-MCR is of great importance for its energy consumption.

![Figure 3. Flow characteristics: (a) the velocity distribution; (b) the pressure distribution.](image)

#### 4.2. Pressure drop

The pressure drop is expressed as \(\Delta P\) while the pressure drop gradient (pressure drop per unit length of a cell) is expressed as \(\delta\) and given by this equation:

\[
\delta = \frac{\Delta P}{L} \tag{5}
\]

The pressure drop of the entire foam can be obtained by multiplying the pressure drop gradient \(\delta\) of one cell with the foam length. The pressure drop of a cell is related to many factors, and the most important factors are its structure parameters. Therefore, the effects of foam structure parameters on pressure drop gradient \(\delta\) were studied.
4.2.1. The effect of channel diameter on pressure drop gradient. For cells with L 5 mm and kerosene inflow rate 5 mm/s, the effect of the foam channel diameter D on pressure drop gradient δ was studied. The simulation results are shown in figure 4(a). As D increases, δ decreases. When D increases from 0.04 mm to 0.1 mm, δ decreases significantly from 120 Pa/mm to 11 Pa/mm. When D increases from 0.1 mm to 0.25 mm, δ decreases gradually from 11 Pa/mm to 3 Pa/mm. This is because when the foam cell size L is constant, the larger the foam channel diameter D is, the smaller the viscous resistance of the fluid in the foam channel is, resulting in the decrease of the pressure drop gradient.

4.2.2. The effect of cell size on pressure drop gradient. For cells with D 0.4 mm and kerosene inflow rate 5 mm/s, the effect of the foam cell size L on pressure drop gradient δ was studied. The simulation results are shown in figure 4(b). As L increases, δ decreases firstly and then it increases. When L increases from 2 mm to 4 mm, δ decreases gradually from 22 Pa/mm to 20 Pa/mm. At this stage of change, L is small, and when D remains unchanged, the proper increase of L makes the flow field more smoothly within the cell, thus reducing the pressure drop gradient δ. When L increases from 4 mm to 10 mm, δ increases gradually from 20 Pa/mm to 37 Pa/mm. At this stage of change, L is larger, and the increase of L leads to a narrower intracellular channel D remains unchanged, resulting in greater viscous effect on the fluid, thus increasing the pressure drop gradient.

4.2.3. The effect of structure parameter λ on pressure drop gradient. From the above simulation results, we can see that both the foam channel diameter D and the foam cell size L have great influence on the pressure drop gradient δ. In order to have a better understanding of the relationship between the foam cell structure and its pressure drop gradient, a parameter λ was defined to characterize the foam cell structure, and it is given by this equation:

$$\lambda = \frac{D}{L}$$

For cells with D 0.2, 0.4, 0.6, 0.8, 1.0 mm, kerosene inflow rate was set as 5 mm/s, and the effect of λ on δ was studied. The simulation results are shown in figure 5.
Figure 5. The effect of $\lambda$ on pressure drop gradient.

On one hand, it can be seen from figure 5 that the foam channel diameter $D$ has a significant effect on the pressure drop gradient $\delta$ when $\lambda$ is constant. When $D$ is 0.2 mm or 0.4 mm, $\delta$ is relatively large. When $D$ is equal to or larger than 0.6mm, $\delta$ decreases significantly. On the other hand, for cells with different inner channel diameters, their changing trends of the pressure drop gradient $\delta$ with the increase of $\lambda$ are approximately the same: $\delta$ decreases firstly and then it increases. When $\lambda$ is controlled as 0.10, the pressure drop gradient $\delta$ is the smallest. These simulation results are of great importance for the design and preparation of hollow-strut foam materials for HSCF-MCR.

5. Conclusion

A new type of SiC hollow-strut ceramic foam microchannel reactor (HSCF-MCR) that combines the material and structural advantages of reticulated ceramic was proposed as a structural scaffold for continuous gas or liquid phase flow and reaction. Based on the tetrakaidecahedron cell model, CFD method was utilized to analyze the single-phase flow characteristics and pressure drop of HSCF-MCR. The 3-D interconnected structure can form the static mixing effect of the flow fields inside the foam microchannel and strengthen the mass transfer process. The relationship between the foam cell structure and its pressure drop gradient $\delta$ was studied. When cell structure parameter $\lambda$ (the ratio of the foam channel diameter $D$ to the foam cell size $L$) is controlled as 0.1, the pressure drop gradient $\delta$ of the fluid flowing through HSCF-MCR is minimized. The CFD simulation results make sense to optimize the structure design of HSCF-MCR and reduce its pressure drop, thus saving the energy consumption for its applications in the future.

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