Computational fluid dynamics simulation on the effect of pillar shapes on chitosan-coated zinc oxide nanoparticles flows in pillar-based microfilter

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Abstract. The computational fluid dynamics (CFD) simulation on the effect of pillar shapes on chitosan-ZnO nanoparticles flows in pillar-based microfilter was considered using ANSYS Fluent in the laminar flow condition. Three shapes of the pillar were studied: cylindrical, cuboid, and rotated cuboid pillar. The volume of fluid (VOF) method was performed under a certain set of considerations and assumptions in order to validate the microfilter design to have the same flow patterns based on the literature. The discrete phase model (DPM) was carried out in order to simulate and analyze the chitosan-ZnO nanoparticles flow behaviour and separation efficiency performance in pillar-based microfilter. The DPM was carried out in 200, 300, and 400 streams to track the position of the nanoparticles in order to analyze the separation performance for each pillar shape. The simulation involved a different number of streams that were observed on the impact of nanoparticle Reynolds number and the total number of nanoparticles. It was observed that microfilter-C (rotated cuboid pillar) has the best separation efficiency of chitosan-ZnO nanoparticles compared to microfilter-A (cylindrical pillar) and microfilter-B (cuboid pillar) based on the particle position from the outlet of microfilter which was 2.5 mm, 0.08 mm, and 2.1 mm respectively. The shape of the pillar is a critical parameter that plays a significant role in the separation performance of nanoparticles in pillar-based microfilter.

1. Introduction

Microfluidics is the science that studies about the process or manipulation of fluids in a channel with the range of small volumes from microliters (10⁻⁶) to picoliters (10⁻¹²) and the dimension of the channel from 100 nanometers to 500 micrometers [1]. Microfluidics technologies offer many useful applications such as analysis of blood-cell separation, nanoparticle synthesis, micro-thermal technologies, cell encapsulation in microdroplets and analysis of individual cells from a population.

Microfluidic system provides the scale of a perfect interface for the manipulation of single cells and accesses these forces in a various way. They also may reduce reagent volume and cost and are potentially portable. Moreover, microfluidic systems are good alternatives in the future for high throughput sorting systems of cells. Based on the study by Gossett et al. [2], microfluidic systems have various separation techniques to achieve cell separation and sorting. This study focuses on microfluidics filter separation
technique. In this technique, it has the advantage to adjust the filter pore size to increase separation efficiency. However, this method also encounters many common issues such as clogging and fouling.

Numerous experiments have been done to synthesize chitosan-zinc oxide hybrid composite for many applications such as zinc oxide nanoparticles-chitosan composite film for cholesterol biosensor [3], chitosan-zinc oxide hybrid composite for enhanced dye degradation and antibacterial activity [4], chitosan-zinc oxide nanoparticles for imparting antimicrobial and UV protection to cotton fabric [5].

Many designs of microfilters such as membrane, weir, pillar, and crossflow type of microfilter have been investigated and analyzed for cell separation and sorting [6]. Moreover, the performance of each design has been compared to investigate the separation efficiency for many applications.

This study focuses on the pillar-based microfilter as it is known for its great separation efficiency performance among those designs [6]. Critical parameters such as pillar arrangement, pillar spacing, and pillar shape are significant to the separation efficiency performance. Likewise, pillar-based microfilter is capable to separate particle over a wide dynamic range that involves rapid separation in a variety of environmental, medical, or manufacturing applications [6]. Fabrication of microfilters can be a complicated task and high cost by using various techniques such as micromilling, soft lithography and laser ablation processing. Numerical investigations using CFD software able to provide a good prediction of fluid flow in the various design of pillar-based microfilter prior to the fabrication process. The best design of pillar-based microfilter with the high separation efficiency can be identified to proceed for fabrication work, hence saving costs. There is still a lack of study on various shapes of pillar for pillar-based microfilter toward the nanoparticle flows, therefore three types of pillar designs were considered in this simulation work. The main objective of this study is to numerically investigate the potential problems and separation efficiency of chitosan-coated ZnO nanoparticles in the various designs of pillar-based microfilter including cylindrical, cuboid and rotated cuboid pillars using ANSYS Fluent software.

2. Numerical simulation

2.1. Geometry of pillar-based microfilter

The geometry of the microfilter model is shown in Figure 1. The microfilter considered here is a three-dimensional rectangular channel shape and consists of 10 × 15 (row × column) array of 350 μm cylindrical pillars (microfilter-A). Furthermore, the similar dimensions of the microfilter model were created for a cuboid pillar (microfilter-B) and rotated cuboid pillar (microfilter-C) designs.

Figure 1 Geometry of the microfilter
2.2. Governing equations and simulation model parameters

The VOF model can model two or more immiscible fluids by solving a single set of momentum equations and tracking the volume fraction of each of the fluids throughout the domain using the Euler-Euler approach. The tracking of the interface between the phases is accomplished by the solution of a continuity equation for the volume fraction of one or more of the phases. Since the VOF model only involved two phases which are air (primary phase) and ethanol (secondary phase) in this study, therefore, the volume fraction equation is written as follows,

\[ \alpha_g + \alpha_l = 1 \]

In this study, the CFD simulation was performed to predict, simulate, compare, and verify the initial fluid flow with Saha et al. [7] study in various pillar-shaped in the microfilter model as the basis for DPM case study. The following assumptions were considered in this study as shown in Table 1.

Table 1 VOF simulation model parameters

| Description                      | Value                      | Comment                      |
|----------------------------------|----------------------------|------------------------------|
| Model                            | -                          | Volume of Fluid (VOF)        |
| Solver                           | -                          | 3D double-precision solver   |
| Liquid density (ethanol)         | 791 kg/m³                  | Adopted from [7]             |
| Gas density (air)                | 1.1614 kg/m³               | Adopted from [7]             |
| Fluids inlet velocity            | 0.25 m/s                   | specified (initial guess)    |
| Solid density (PDMS)             | 965 kg/m³                  | Adopted from [7]             |
| Inlet boundary condition         | -                          | velocity inlet (incompressible flow) |
| Outlet boundary condition        | 101325 Pa                  | pressure outlet              |
| Phase Interaction (surface tension) | 0.0214 N/m       | Adopted from [7]             |
| Wall boundary condition          | -                          | stationary wall              |
| Wall adhesion (contact angle)    | 0°                         | Adopted from [7]             |
| Time-steps                       | 0.345 s                    | Adopted from [7]             |
| Maximum iteration                | 100                        | specified                    |

2.3. Discrete Phase Model (DPM)

DPM follows the standard formulation of the Lagrangian multiphase model which using the general form of the mass and momentum conservation equations:

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = S_{DPM} + S_{other}
\]

\[
\frac{\partial \rho \vec{v}}{\partial t} + \nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla p + \nabla \cdot \tau + \vec{F}_{DPM} + \vec{F}_{other}
\]

The fluid phase is treated as a continuum by solving the time-averaged Navier-Stokes equations, while the dispersed phase is solved by tracking many particles, bubbles, or droplets through the calculated flow field.

In this study, after the VOF models were verified for the prediction of fluid flows, the configurations were implemented to the DPM case studies. The case studies involved particle tracking in order to obtain the particle position and analyze the separation efficiency. The case studies also focused on the particle Reynolds number and the number of particles injected into the microchannel models. Finally, the pillar-based microfilter model that has the best separation efficiency performance was selected to further analysis in order to improve the separation efficiency. Most of the assumptions were taken from VOF model into DPM case studies, however, several assumptions in the particle injection setup were considered as shown in Table 2.
Table 2 DPM simulation model parameters

| Description                          | Value                  | Comment                  |
|--------------------------------------|------------------------|--------------------------|
| Model                                | -                      | Discrete Phase Model (DPM) |
| Solver                               | -                      | 3D double-precision solver |
| Liquid density (wastewater)          | 1006 kg/m³             | Adopted from [8]         |
| Liquid viscosity (wastewater)        | $3.3 \times 10^{-4}$ Pa.s | Adopted from [8]         |
| Particle density (chitosan-ZnO)      | 4660 kg/m³             | Adopted from [5]         |
| Particle diameter (chitosan-ZnO)     | 5 nm                   | Adopted from [5]         |
| Particle injection X position        | 14.65 mm               | specified                |
| Particle injection Y position        | 2.5-5.5 mm             | specified                |
| Particle injection Z position        | 0.02 mm                | specified                |
| Number of streams (group)            | 200, 300, 400 streams  | specified                |
| Fluids inlet velocity                | 0.25 m/s               | specified                |
| Outlet boundary condition            | 101325 Pa              | pressure outlet          |
| Wall boundary condition              | -                      | stationary wall          |
| Time-steps                           | 0.1 s                  | specified                |
| Maximum iteration                    | 20                     | specified                |

3. Results and discussion

3.1. Base case

The result for microfilter-A is compared with work by Saha et al. [7]. Figure 2 shows the ethanol (red) flow until the 6th row (calculated from right to left) in CFD result at $t = 0.345$ s shows a good agreement with the experimental result by Saha et al. [7] at $t = 0.33$ s. As time increased, the ethanol flow would slowly occupy inside the microchannel. The small discrepancy between the numerical result and experimental result may be caused by the fabrication of PDMS microfilter that leads to geometrical inaccuracies.

![Figure 2 Ethanol (red) – air (blue) fluid flow characteristic from CFD result for microfilter-A at t = 0.345 s](image)

3.2. Hydrodynamics for different designs of the pillar

The fluid flow prediction in microfilter-A, microfilter-B and microfilter-C at 0.345 s were obtained using time step with a step size of 2 and 100 iterations, 50 iterations and 40 iterations respectively. The ethanol flow can be observed clearly hindered at 5th row and the 5th column (distance from the inlet) in microfilter-C (rotated cuboid pillar) as the simulation result shows a high value of volume fraction of
ethanol at the region. At this stage, the rotated cuboid pillar can be considered as a good pillar shape design for a microfilter. Hence, the shape pillar was a critical parameter which gave impact to the fluid flow characteristic inside the microfilter.

The ethanol volume fraction is steadily decreased from 14.65 mm (inlet position) which shows that the ethanol is slowly occupied the air region. Moreover, the volume fraction of ethanol is dramatically dropped to 0 at 6.5 mm (from the outlet) approximately which shows that the air was still occupied the outlet area. Hence, it can be clearly seen that at \( t = 0.345 \) s, the ethanol is slowly moved into the microfilter and occupying the inlet area as it applied for all design pillar shapes.

Figure 3 Contour plot of volume fraction of ethanol in (a) microfilter-A, (b) microfilter-B, and (c) microfilter-C

3.3. DPM results for different designs of pillar

The same DPM configurations were set for microfilter-A, microfilter-B, and microfilter-C for 200 streams case. The results of particle position from the outlet in X-direction of three different designs of the pillar in the microfilter. Based on the simulation results obtained, particle position from the outlet of microfilter-A, microfilter-B, and microfilter-C were 2.10 mm, 0.08 mm, and 2.54 mm respectively. Different geometries of the pillar would give impact to the particle position hence geometry of the pillar was a critical parameter for the separation. Since the particle position of microfilter-C was further from the outlet of microfilter compared to microfilter-A and microfilter-B, thus, microfilter-C can be concluded to have slightly better separation than other designs.

Moreover, it can be clearly observed from the particle traces in microfilter-A, microfilter-B, and microfilter-C in Figure 4. It was observed that microfilter-A has the highest in the number of particles which 340,988 particles were tracked in the microfilter at \( t = 0.1 \) s. However, it was significantly decreased for microfilter-B and microfilter-C which the number of particles was tracked about 232,790 particles and 281,971 particles respectively. This occurrence was due to the number of particles were calculated based on the number of parcels which each parcel was representative of a fraction of the total mass flow released in a time step. Based on the simulation results, the particle Reynolds number obtained
was in the range of $1.12 \times 10^{-7}$ to $1.96 \times 10^{-9}$ hence it was considered as laminar flow in the microfilter as the results of particle Reynolds number was very low.

![Figure 4 Particle traces coloured by particle X-direction (from the outlet) of 35,000 scalars in (a) microfilter-A, (b) microfilter-B, and (c) microfilter-C for 200 streams case](image)

The separation efficiency is defined based on the particle position from the outlet in X-direction as the reference to select the best separation performance. Therefore, it can be explained that microfilter-C was selected as the best microfilter design in separation efficiency for 200 streams case. Based on the simulation results, the comparison for the three microfilter designs is summarized in Table 3 to observe the particle position from outlet, particle Reynolds number and a total number of particles in the microfilter. It was observed that microfilter-C has the best separation since the particle position was at 2.5 mm from the outlet (200 streams case) while microfilter-B has the worst separation performance as the particle position was at 0.08 mm nearby the outlet (200 streams case) of the microfilter.

Moreover, it can be clearly observed that microfilter-C maintained a good separation performance for all stream cases as illustrated in Figure 5. Subsequently, the number of streams has a significant role to influence the number of particles which increased as the number of streams increased as well due to the fraction of the total mass flow released in a time step. Furthermore, the particle Reynolds number for all microfilter was considered as laminar flow since it was very low hence the domain was valid as a microfilter.
Table 3 Comparison of microfilter-A (cylindrical pillar), microfilter-B (cuboid pillar), and microfilter-C (rotated cuboid pillar) for all stream’s cases

| Properties                      | Cylindrical pillar | Cuboid pillar | Rotated cuboid pillar |
|---------------------------------|--------------------|---------------|-----------------------|
| Number of streams               | 200                | 300           | 400                   |
| Particle position from outlet (mm) | 2.10               | 0.08          | 2.54                  |
| Particle Reynolds number        | 1.12 x 10^{-7}     | 4.29 x 10^{-8}| 1.96 x 10^{-9}        |
| Total number of particles       | 340,988            | 232,790       | 281,971               |
| Number of streams               |                    |               |                       |
| Particle position from outlet (mm) | 2.15               | 0.01          | 2.53                  |
| Particle Reynolds number        | 4.69 x 10^{-8}     | 2.61 x 10^{-9}| 1.94 x 10^{-9}        |
| Total number of particles       | 504,924            | 350,824       | 419,677               |
| Number of streams               | 400                |               |                       |
| Particle position from outlet (mm) | 2.16               | 0.04          | 2.52                  |
| Particle Reynolds number        | 2.14 x 10^{-8}     | 2.35 x 10^{-8}| 3.94 x 10^{-9}        |
| Total number of particles       | 672,139            | 462,301       | 550,826               |

Figure 5 Graph of particle position from outlet against the number of streams

4. Conclusion
The VOF simulation is obtained a good agreement of flow pattern as work by Saha et al. [7] which the prediction of fluid flow was able to be verified and it was used as the basis for DPM case studies. From DPM case studies results at t = 0.1s, it showed that microfilter-C (rotated cuboid pillar) has the best separation efficiency of chitosan-ZnO nanoparticles compared to microfilter-A (cylindrical pillar) and microfilter-B (cuboid pillar) based on the particle position from the outlet of microfilter which were 2.5 mm, 0.08 mm, and 2.1 mm respectively. Based on simulation the results, it was observed that particle Reynolds number was very low for all pillar designs hence it can be concluded that the flow in the microfilter was laminar flow which can be considered as acceptable. Subsequently, the number of streams would significantly give impact to the total number of particles injected to the microchannel with the increase of approximately 50% for 200 to 300 streams and 32% for 300 to 400 streams. In addition, the simulation results of this study might be not accurate since it lacks experimental validation due to many assumptions were made. Howbeit, this presented CFD simulation can be served as the preliminary study of the design of microfilter prior to complex and laborious microfilter fabrication work.
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