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Computational Fluid Dynamics Study on Particle Rejection in Microfiltration

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ABSTRACT

Computational fluid dynamics (CFD) was applied to modeling particle dynamics in microfiltration (MF). The rejection properties of poly methylmethacrylate (PMMA) and polystyrene (PS) were calculated. Calculated rejection (*R*) of PMMA was independent with the porosity of the membrane, and the *R* was constant in the range of volume flux between 1 x 10^{-4} – 1 x 10^{-2} m/s. These observations were in quantity agreement with our experimental observations. The dependence of PMMA and PS rejection on the ratio of particle diameter and pore diameter were good agreement with the experimental values, which suggesting that the validity of CFD simulation to evaluate rejection of particle in MF membranes. Change of rejection of PMMA as a function of time was molded based on the CFD result which explained well the experimental observation.

INTRODUCTION

We have been investigated rejection properties of dilute concentration of poly (methyl methacrylate) (PMMA) particles in a microfilitration [1]. A dead-end constant flow rate filtration using Nuclepore membranes was employed in the condition; the flow rate was 10^{-4} - 10^{-3} $m^3/(m^2\ s)$, porosity was 0.06 – 0.16, and pore size of membranes was 0.6 – 3.0 μm. Observed rejection did no change in the early stage of filtration but it suddenly increased after a certain time. In the beginning of filtration, the observed rejection properties would be strongly affected by the size parameters of particle and membrane pore as well as surface properties of membranes. Observed period in which the rejection was constant suggests the possible application of MF for particle classification based on size parameter of the particle and membrane pore. We also demonstrated that the period was independent with the flow rate and porosity of the membrane. However, these observations has not been clearly explained yet theoretically .

In this paper, we carried out CFD for evaluating the particle rejection properties using a MF membranes, which modeled a dead-end constant flow rate filtration of diluted solution containing non-charged or charged particle. The comparison with our previous experimental results was made related to the rejection as a function of flux, porosity and the ratio of particle diameter to pore diameter. The correlation between the ratio and calculated rejection was also compared with the theoretical values estimated by a pore model [2] and a steric-hindrance pore model [3] to test the validation of CFD in the estimation of rejection in MF. Time dependence of rejection was also evaluated based on the CFD results.

METHOD

A dead-end filtration of diluted particle solution keeping a flow rate constant by a MF membrane is modeled. Schematic figure of used cell is shown in Figure 1. Trajectory of particle coming the top of the cell (inlet) to the membrane pore was calculated. A flow is evaluated by solving the dispersed equation using a finite volume method. The various sized unit cell were prepared, and flux J was changed in 1 - 10^{-4} m^3/m^2s. The particle density was 1.07 g/cm^3, the particle diameter, d_s, was changed between 0.2 to 0.8 times to the pore size. The porosity and pore diameter of the cell were determined based on those of Nuclepore membranes (Nuclepore. Inc.) that used in the experiment [1]. Nuclepore are non-hygroscopic polycarbonate membranes punctuated by circular pores (0.6 - 3.0 µm) normal to the surface and their porosity is between 0.063 - 0.158. The gravity, buoyancy, and viscous forces were taken into consideration, and the electrostatic interaction and van der Waals interaction based on DLVO theory were considered as an interaction between particle and membrane. The rejection in a KCL electrolyte solution was examined where the concentration of KCl were changed from 1 mM to 10 mM.

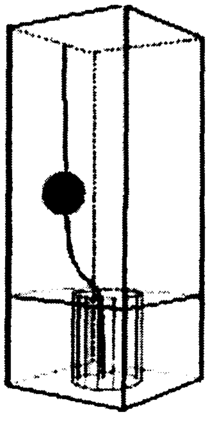

Fig.1 Schematic figure of used cell

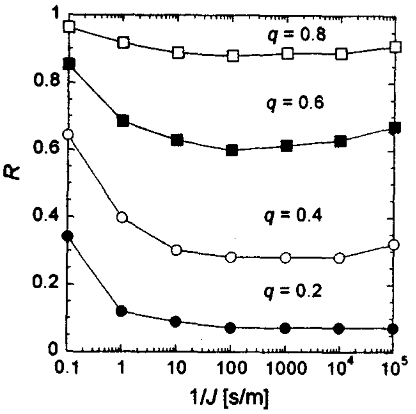

Fig.2 ***R*** **vs. 1/*J*** **of PMMA**

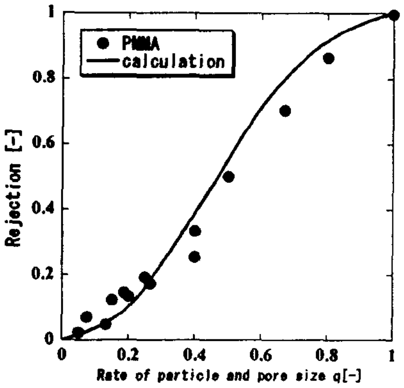

Fig.3 ***R*** **vs. *q*** **of PMMA**

Since an interaction between particles can be neglected in a dilute solution, we calculated trajectory of one particle in the cell. A rejection was evaluated from a ratio of a number of rejected particles to a number of permeated particles. The area of the inlet was divided to the 200 x 200 squares (sub-cell) and a trajectory of particle coming from each of the sub-cell was calculated. A rejection was estimated from a trajectory of particles; the particle was judged to be rejected when the particle collided to the membrane wall. Rejection, R, is calculated as follows:

$$R = 1 - \frac{N}{N_c} \qquad (1)$$

where N is the number of trajectory which permeated through the membrane pore without collision to the membrane surface, and N_c is the number of the sub-cell. A symmetric part of 1/8 of the sub-cell was considered as initial flowing position to deduce the computing cost.

RESULT AND DISCUSSION

1) Rejection of PMMA

Figure 2 indicate calculated rejection (R) for the models having different porosity as a function of $1/J$. As shown in these figures, the R values increased as increase in the ratio of particle diameter to pore diameter (q), and R against $1/J$ changed concave. All R decreased as increase in $1/J$, and turned to increase slightly when $1/J$ were significantly large. It is noted that there is a range of J where R did not changed. The range became wider as increase in porosity (P). The R dependence on J has been investigated in experimentally and reported that R were constant in the investigated flux range; 1.65 x 10^{-4} – 3.30 x 10^{-3} m/s [2]. This range is consistent with that observed in this study, which was about 1 x 10^{-4} – 1 x 10^{-2} m/s. In this study the motion of equation of particle includes three forces; the inertia force, the viscous force, and the gravity force. Thus, supposing that the viscous force dominates the particle dynamics, the particle moves along the streamlines and flows without collision with membrane surface resulting in no rejection. In such condition the rejection is independent with the flow rate and porosity. However, when the flow rate is vary large or small, the dominated force of particles will change to the inertia force or the gravity force. In such conditions, the particle movement is apart from the streamlines and results in the increase of rejection.

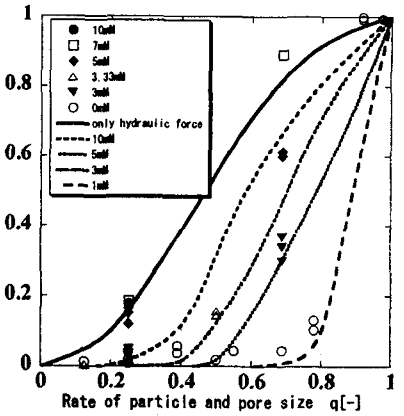

Fig.4 R vs. q of PS particle.

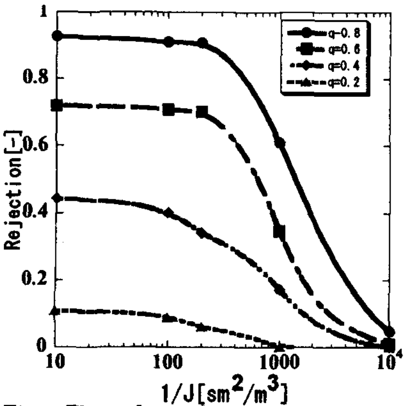

Fig.5 The relationship between flux and

Figure 3 shows the relationship of R with q. Experimental result [1] and the theoretical results obtained from a pore model [2] and a steric hindrance- pore model [3] are also indicated. The experiment has been done for the same condition in the calculation. The calculated change of R is in good agreement with the experiment. This validates our calculation for the estimation of rejection in microfiltration.

2) Rejection of PS

In experiment, PS particle shows lower rejection than that of PMMA, because of electrostatic repulsion between a charged PS particle and a membrane that usually behaves to have a negative charge. Calculated rejection of PS in the solution of various electrolyte concentration of KCl are shown in Figure 4. Calculated results are in good agreement with our experimental results. There was the electrostatic double layer between the PS particle and membrane surface, which originated from the gathering ions which has a opposite charge to that of the membrane surface and particle. The width of double layer depends on the electrolyte concentration. The smaller electrolyte concentration results in the wider electric double layer and the strong electrostatic repulsion. Large electrostatic repulsion prevents the collision of particle with the membrane surface, which decrease the rejection.

Fig.5 represents the relationship between 1/*J* and *R*. *R* values decreased with increase of *q*. In the range 10 – 100 s/m of 1/*J*, *R* were constant regardless of *q* values. After that range, *R* turned to decrease as increase in the 1/*J*. In the constant *R* region, since all particles were carried along with the streamline of fluid, *R* would be decided by the size of a pore and a particle. In the large 1/*J* region, at near membrane surface, the electrostatic force prevents the particle from approaching to the membranes surface. At such situation, *R* no longer correlates the size of a pore and a particle.

3) Evaluation of change of rejection in the early stage of filtration

In a filtration of dilute solution, observed *R* did not change in the early stage of filtration [1]. After some period, the pores were blocked by the deposited particles resulting in the increase of *R*. This period would depend on the particle dynamics near the surface. We modeled the dynamics of pore blocking of PMMA based on the CFD results. Figure 6 showed the change of *R* of PMMA as a function of time of filtration. In experiment, *R* did not changed during the indicated period as shown in this figure. The theoretical lines estimated from the CFD result are almost constant during this period but slightly increase. These discrepancy are within the experimental error.

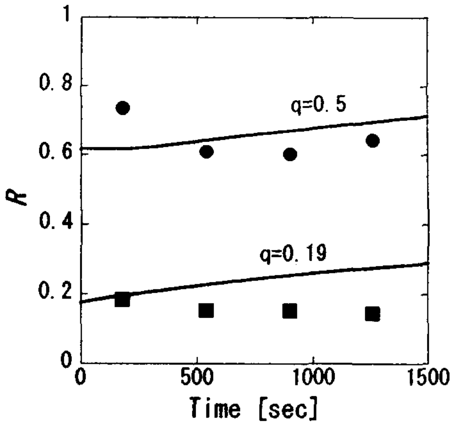

Fig.6 The change of *R* as a function of filtering time. Keys are from experiment and the solid lines are estimated from the CFD results.

CONCLUSION

CFD was applied to modeling particle dynamics in MF membranes. The particle rejection of PMMA and PS was calculated from the trajectory of particles in the permeating fluid through the MF membrane. The observed *R* of PMMA did not change in the range of *J* between 1 x 10^{-4} – 1 x 10^{-2} m/s although in other ranges *R* gradually increased. These observations were in quantity agreement with our experimental observations. The relationship of the calculated *R* with *q* was also in good agreement with the experimental values, which suggesting that the validity of CFD simulation to evaluate the rejection of particle in MF membranes. In the case of PS particle, *R* of PS was much lower than that of PMMA. This is because *R* were significantly influenced by the electrostatic interaction with the membrane surface. The time dependence of *R* was evaluated by the model based on the CFD results, which was consistent with the experimental observations. These consistency of CFD result with the experimental observations validates the use of CFD for the analysis of MF filtration, and the technique will be useful to insight the filtration dynamics in MF from a microscopic level.

REFERENCES

[1] S. Ichimura, Ph.D. Thesis, The University of Tokyo (2001)
[2] A. Verniory et al., *J. Gen. Physiol.*, 62 (1973) 489.
[3] S. Nakao et al., *J. Chem. Eng. Jpn.*, 15 (1982) 200.