Liquid Filtration Modeling of Fibrous Filters with Polydisperse Fibers under Unfavorable Conditions

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Introduction

- Liquid filtration by fibrous filters is one of the most widely used techniques to separate contaminants in liquids.
- The performance (efficiency) of liquid filtration is hard to predict due to complex interactions between solid surfaces in liquid.
- In liquid filtration, particle detachment can easily occur due to high viscosity flow and repulsion energy between surfaces (unfavorable condition).
- Typical fibrous filters consist of polydisperse fibers with a broad fiber size distribution.
- Different fiber sizes may result in different particle attachment behaviors due to the flow characteristic around fibers.

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Objectives

- The main objective is to predict the filtration performance of polydisperse fibrous filters.

1. Validation of CFD simulations using single collectors
   - ✓ Contact efficiency (no detachment: Favorable)
   - ✓ Collision efficiency (possible detachment: Unfavorable)

2. Modeling of fibrous filters
   - ✓ Applying the developed CFD simulations to polydisperse fibers
   - ✓ Comparing simulation results with experiments

Air and Liquid Filtration

- Deposition process
  1) TRANSPORT: Contact efficiency (air and liquid filtration)
  2) ADHESION: Interaction energy (liquid filtration)
  3) TORQUE: Detachment (liquid filtration)

Collision Efficiency (successful attachment)

$$\boldsymbol{\alpha = \frac{E_{unfavorable}}{E_{favorable}} = \frac{E_{final}}{E_{contact}} \leq 1}$$

Flow Simulation and Particle Tracking Methods

- Solve continuity, momentum and energy equations using ANSYS Fluent
- Track particles in a Lagrangian reference frame using discrete phase model (DPM)

✓ $$\frac{d\vec{v}_p}{dt} = \frac{1}{m_p}\sum \boxed{\vec{F}}$$: Gravitational, Brownian and Stokes drag forces

✓ Trap by impaction, Brownian diffusion and interception

✓ User Defined Function (UDF) to model interception and to calculate interaction energy between particle and filter surfaces

✓ UDF to implement adhesion and drag torques for detachment criteria

Through DPM process ...

TRANSPORT → ADHESION → TORQUE

ESOTA

DLVO Theory and Torque Analysis

- DLVO theory describes the force between charged surfaces interacting through a liquid medium.

Van der Waals energy (VDW) $\Phi^{VDW}(H) = -\frac{Aa_p}{6H}\left(\frac{1}{1+14H/\lambda}\right)$

Double layer energy (DL) $\Phi^{DL}(H) = \pi\varepsilon\varepsilon_0 a_p\left\{2\psi_p\psi_s \ln\left[\frac{1+\exp(-\kappa H)}{1-\exp(-\kappa H)}\right] + \left(\psi_p{}^2 + \psi_s{}^2\right)\ln\left[1-\exp(-2\kappa H)\right]\right\}$

Born energy $\Phi^{BR}(H) = \frac{A\sigma^6}{7560}\left[\frac{8a_p + H}{(2a_p + H)^7} + \frac{6a_p - H}{H^7}\right]$

- Depending on particle kinetic energy, the particle location is determined (either primary or secondary minimum distance).
- Depending on particle deposition location, adhesion torque is calculated.
- From flow simulation, flow field information, e.g., velocity, is obtained and hydrodynamic drag torque is calculated.

DLVO Theory and Torque Analysis

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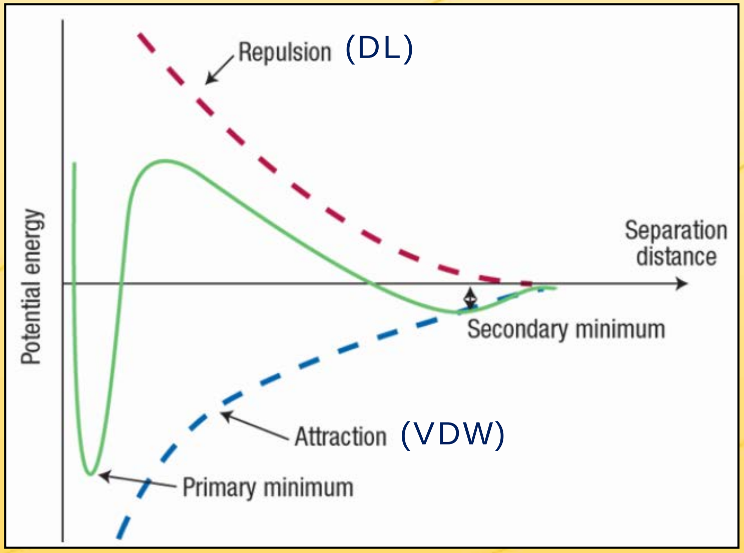
Van der Waals energy (VDW)

+

Double layer energy (DL)

+

Born energy



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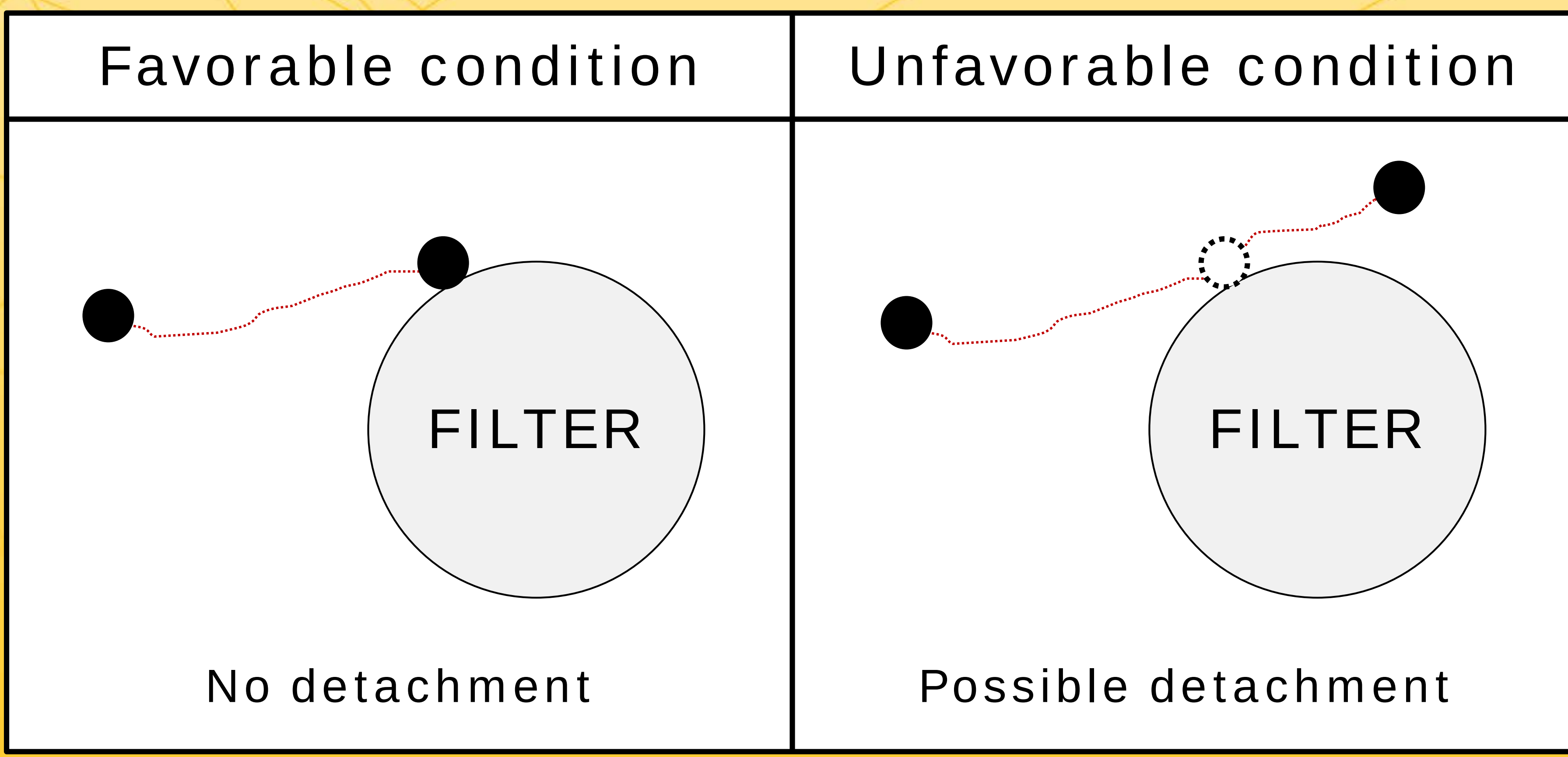
Single Collector Simulations

- Validation of CFD simulations
  - ✓ Obtaining contact efficiency of single collector under favorable condition
  - ✓ Predicting collision efficiency of single collector under unfavorable condition



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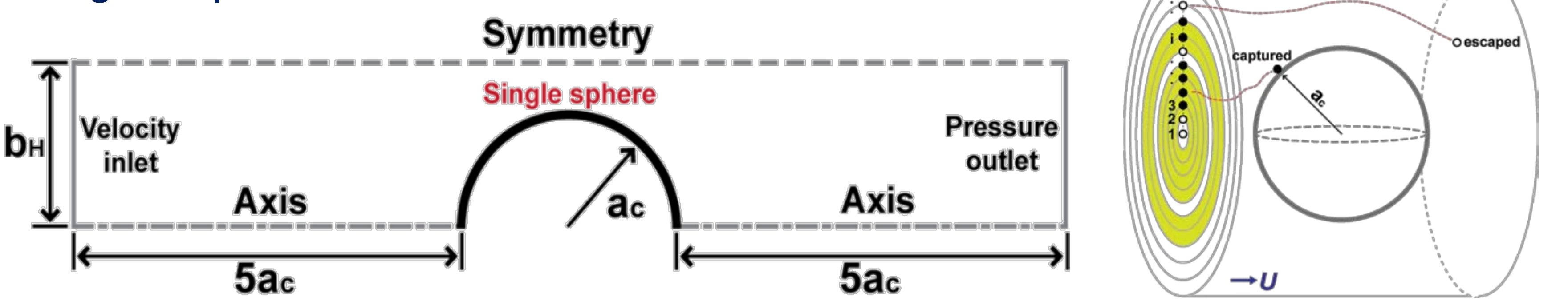
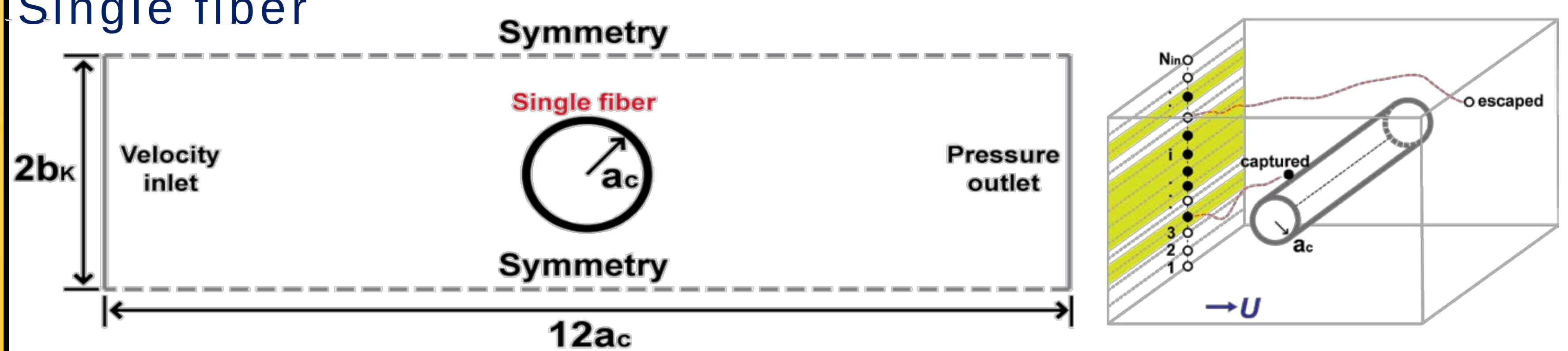
Single sphere



Single fiber



Single Collectors (Contact efficiency)

- Single sphere efficiency (Tufenkji and Elimelech, 2004)

$$\eta_{favor} = \underbrace{2.4A_S^{1/3}N_R^{-0.081}N_{Pe}^{-0.715}N_{vdW}^{0.052}}_{\text{Diffusion}} + \underbrace{0.55A_SN_R^{1.675}N_A^{0.125}}_{\text{Interception}} + \underbrace{0.22N_R^{-0.24}N_G^{1.11}N_{vdW}^{0.053}}_{\text{Gravity}}$$

- Single fiber efficiency (Choo and Tien, 1992)

$$\eta_{favor} = \frac{\pi d_f}{4(1-\varepsilon_0)} \times (\lambda_0 + \lambda_{BM})$$

Interception / gravitation / London-van der Waals

$$\lambda_0 = \left(\frac{6}{\pi}\right)\frac{1-\varepsilon_0}{d_f}A_S\left[0.216 \times 10^{-0.41\varepsilon_0}N_R^{1.55}N_{LO}^{0.1542} + 2.99 \times 10^{-4} \times 10^{3\varepsilon_0}N_G^{1.1}N_R^{-0.3}\right]$$

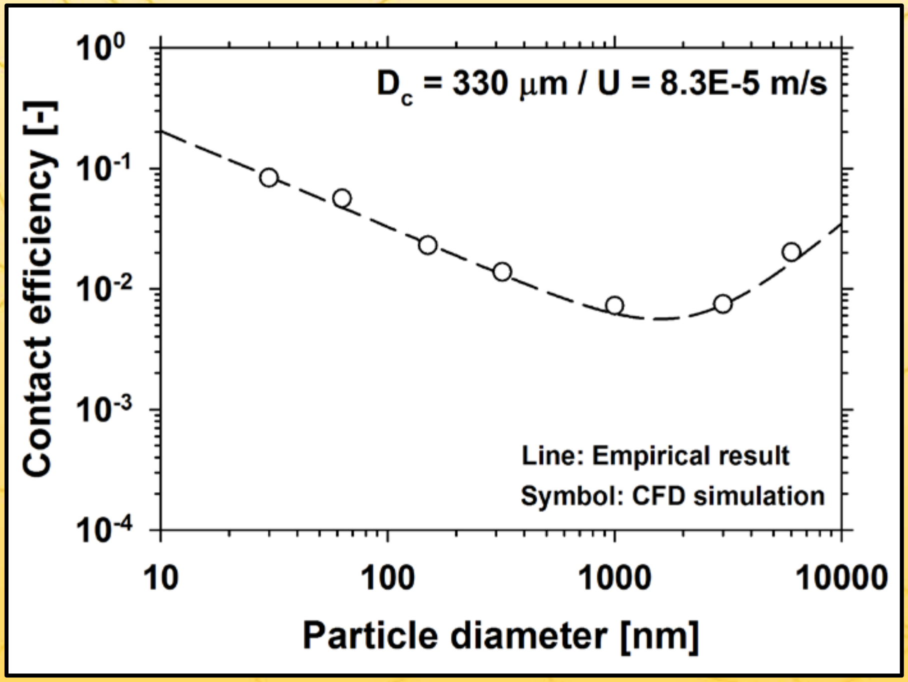
Diffusion

$$\lambda_{BM} = \left(\frac{9.2}{\pi}\right)(c_1 + c_2)^{1/3}\left[(1-\varepsilon_0)/d_f\right]N_{Pe}^{-2/3}$$

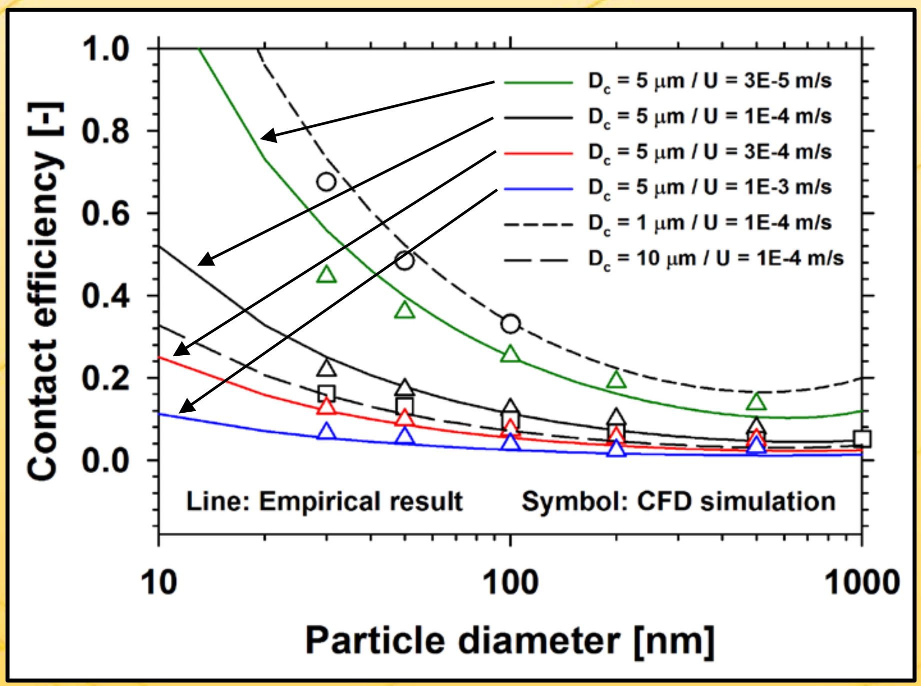
*$\boldsymbol{\lambda}$ (Filter coefficient): Probability of particle capture

Contact Efficiency (Favorable)

Single sphere efficiency



Single fiber efficiency



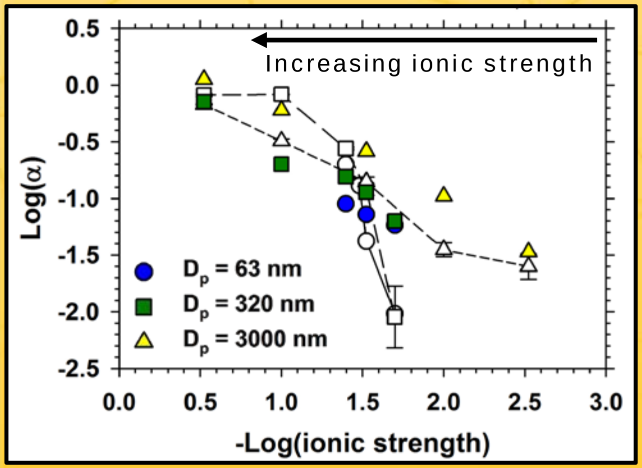
- Contact efficiencies obtained by empirical equations and CFD simulations were compared.
- Good agreement between CFD and empirical results of both single sphere and single fiber theory in liquid medium under favorable (no detachment) condition.

Unfavorable Condition (Repulsion)

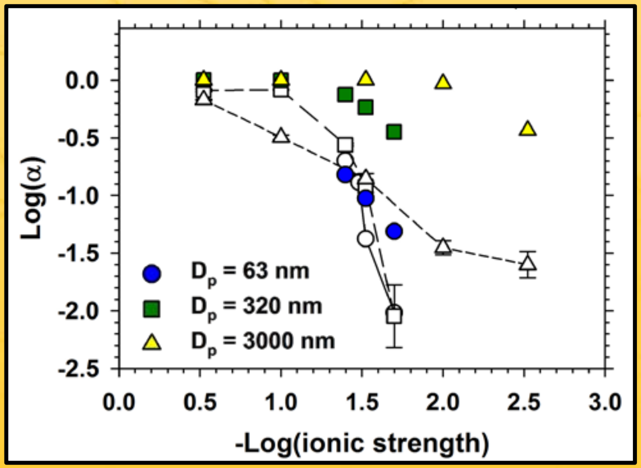
- Bai and Tien [1999] and Shen et al. [2007] suggested empirical equations and theory to evaluate the collision efficiency for granular (spherical) collectors.
- Collision efficiency (**α**) is the rate of successful collisions resulting in attachment of colloidal particles.

$$\alpha = \frac{E_{unfavorable}}{E_{favorable}} \leq 1$$

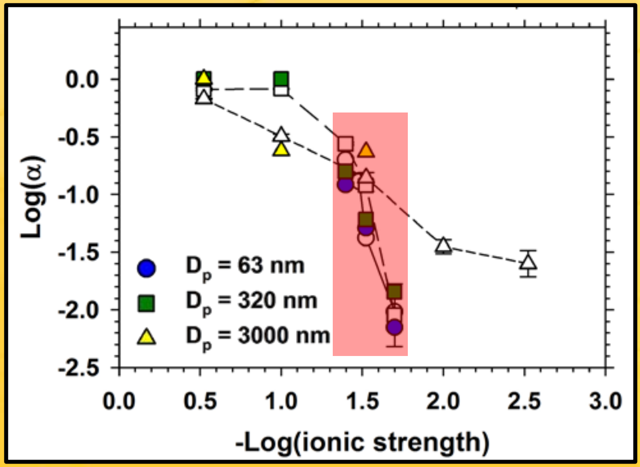
Bai and Tien and Exp.



Shen et al. and Exp.



CFD simulation and Exp.



*Experiment data was obtained from Tufenkji and Elimelech [2005]

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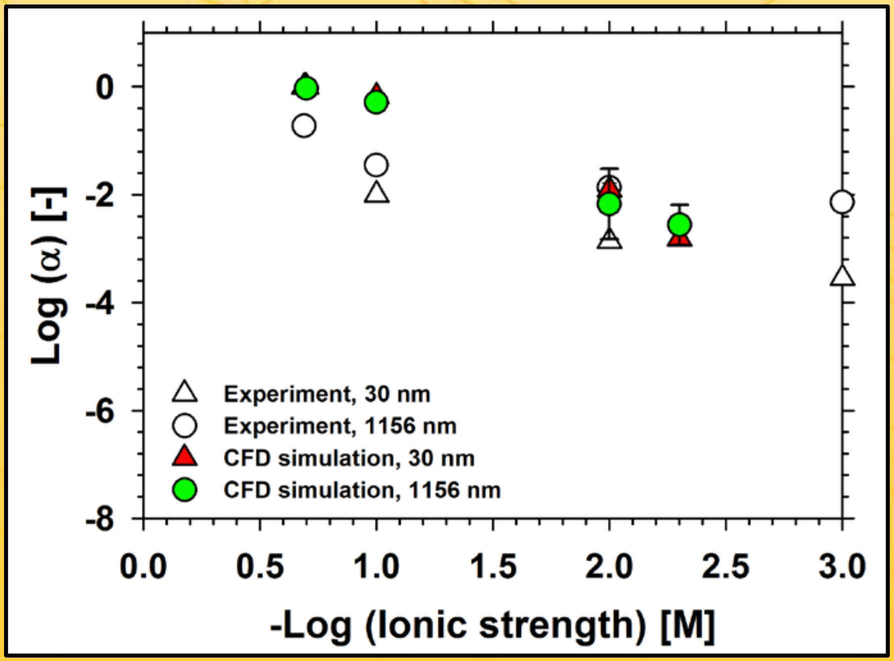

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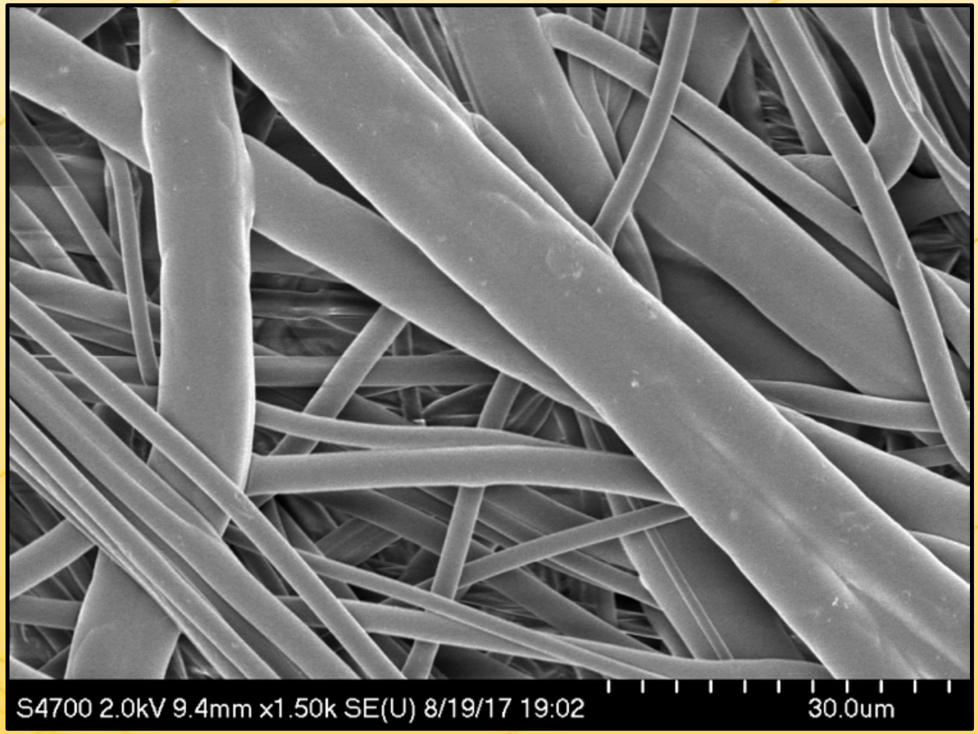
Polydisperse Fibrous Filter Modeling

Filtration Experiment



- Stirred cell filtration system
- Membrane: Polypropylene (PP) filters
- Nominal pore size: 0.1 and 0.2 µm
- Colloidal particle: 100 nm PSL (5×10^{8} #/ml)
- Fluid face velocity: around 2×10^{-4} m/s
- Ionic strength: 0.01 ~ 0.1 M (NaCl)

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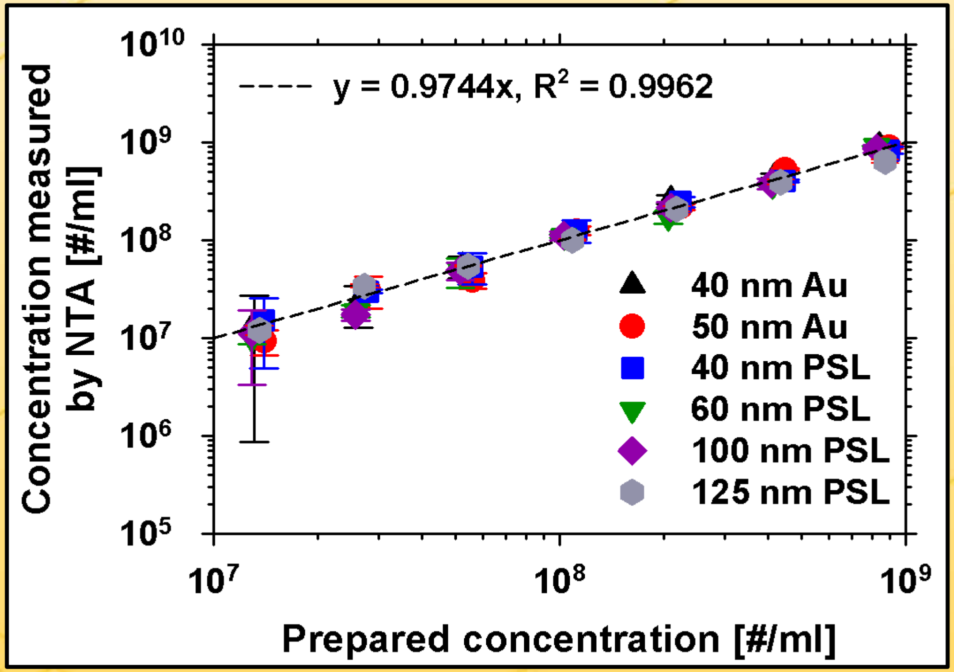
Concentration Measurement

100 nm PSL



- Particle size and number concentration were measured using Nanoparticle Tracking Analysis (NTA).
- NTA calibration results show very clear linearity between prepared and measured concentrations.
- No aggregation was observed in all cases.

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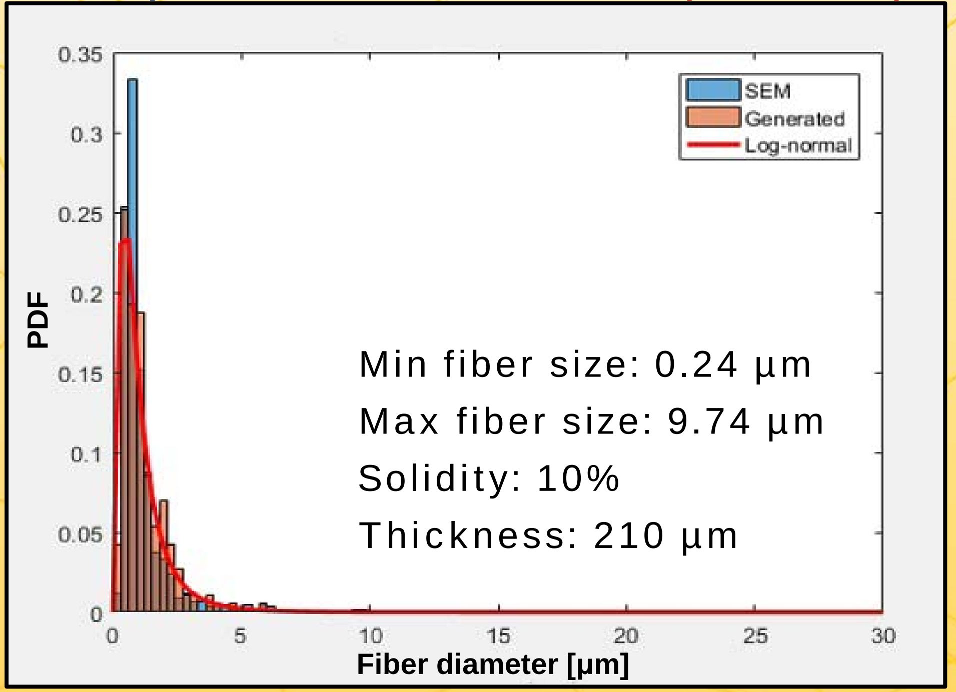
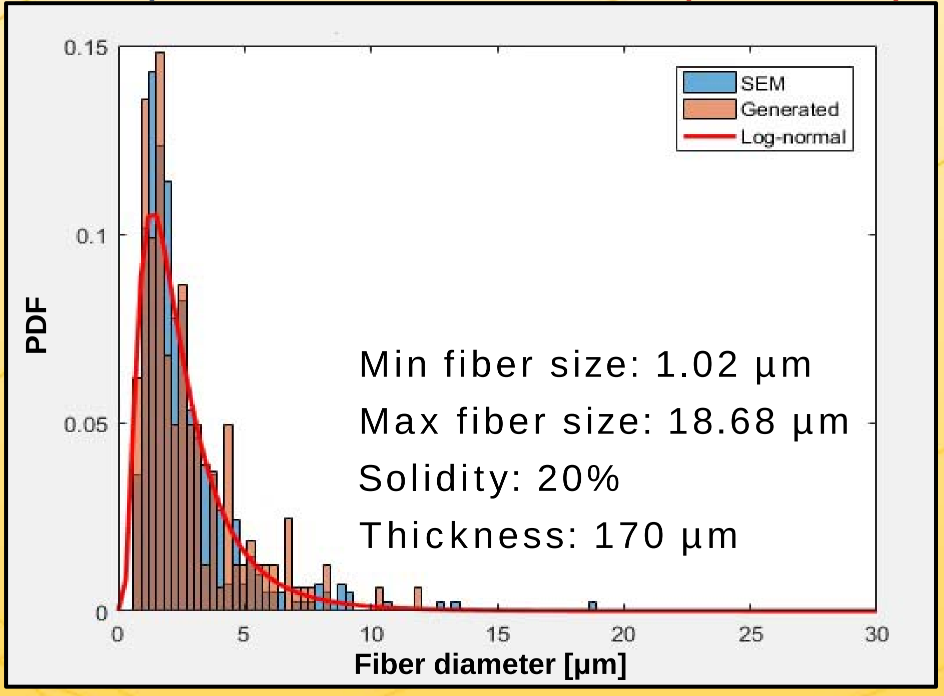
H. Lee, S.-C. Chen, C. Kim, E. Westenburg, S.I. Moon, D.Y.H. Pui, Sep. Purif. Technol. 184 (2017) 34–42.

Polydisperse Fiber Generation

0.1 µm PP membrane (A filter)



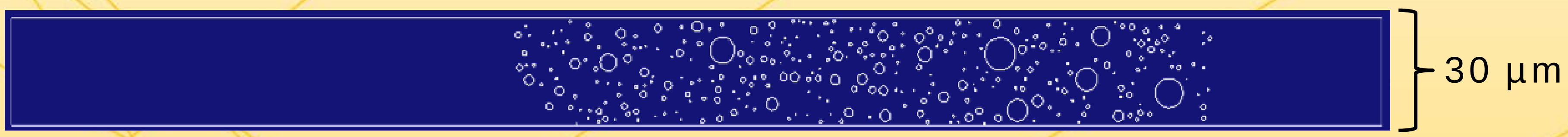
0.2 µm PP membrane (B filter)



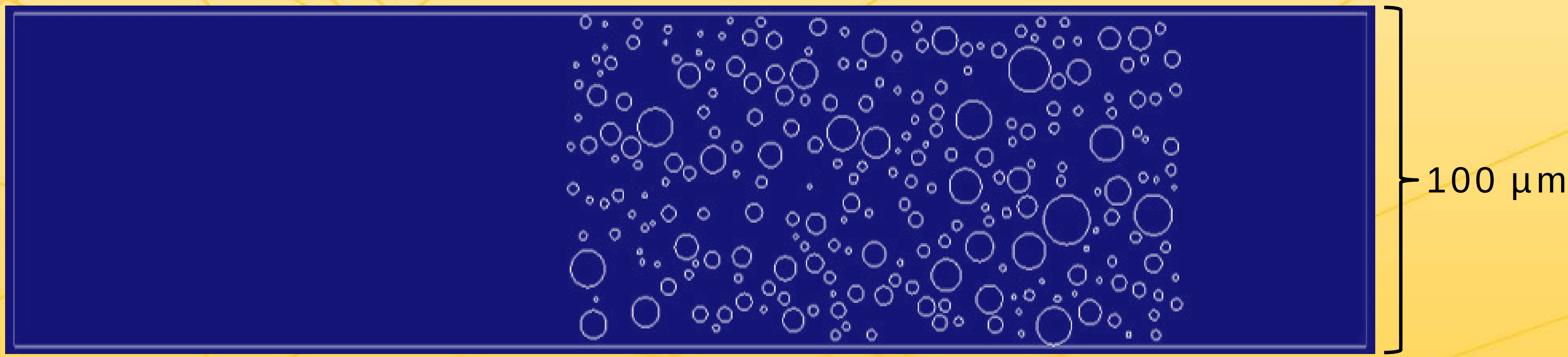
- Measure fiber size from SEM images (total 300 ~ 500 fibers)
- B filter has larger fiber size than A filter and permeability of B filter is higher.
- Generate polydisperse fibers based on fiber size distribution information and the known porosities of filters

Polydisperse Filter domains

0.1 µm PP membrane (305 fibers) – A filter



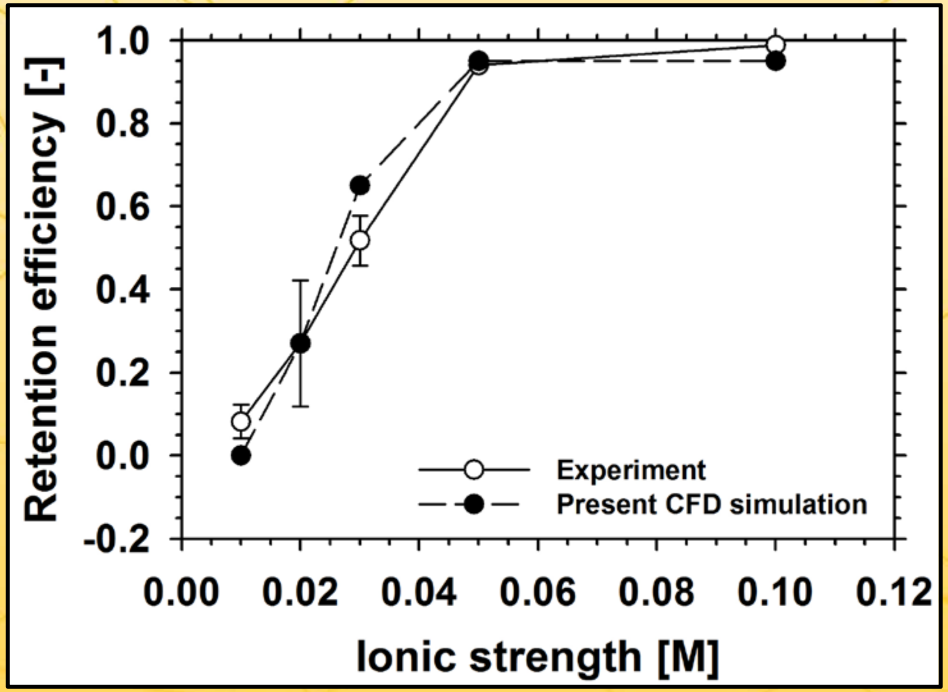
0.2 µm PP membrane (240 fibers) – B filter



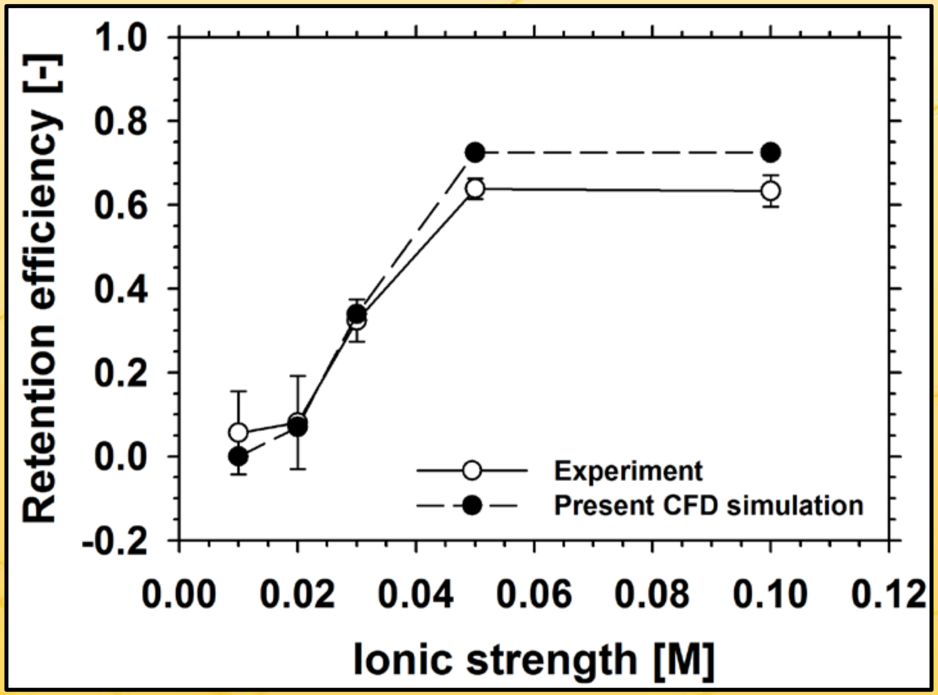
- The domain size (e.g., height) for A filter is smaller than B filter due to the high computational resource consumed by smaller fiber size.
- The effect of height does not affect filtration efficiency as long as there is the sufficient number of fibers.

Filtration Efficiency under Unfavorable Conditions

0.1 µm PP membrane (A filter)



0.2 µm PP membrane (B filter)



- Both filters have a wide range of filtration efficiency (0% to 100% and 0% to 70%) depending on ionic strength due to different interactions.
- Good agreement between CFD simulations and experiments

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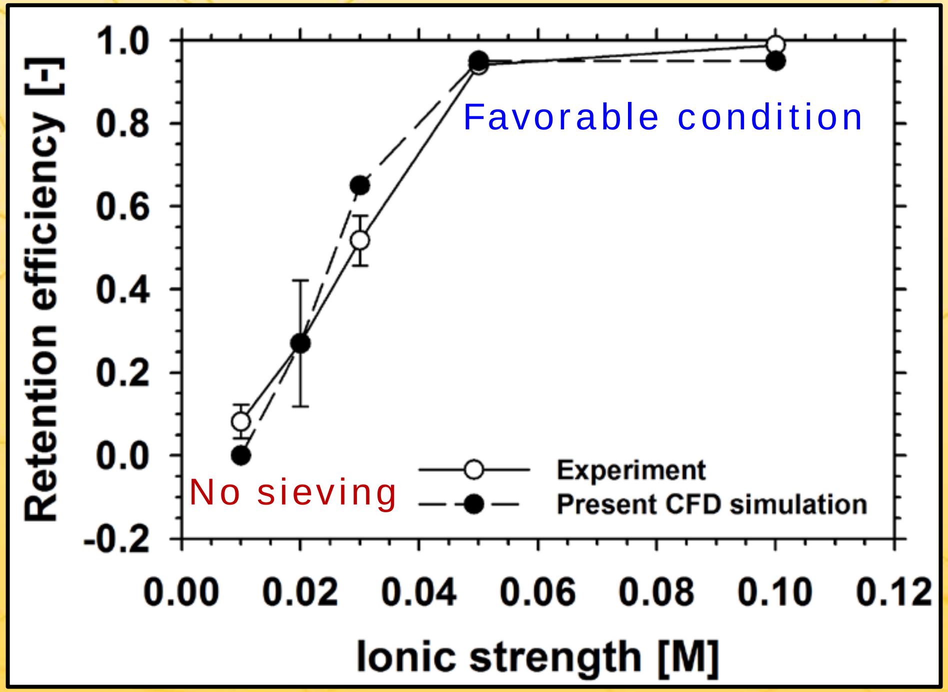
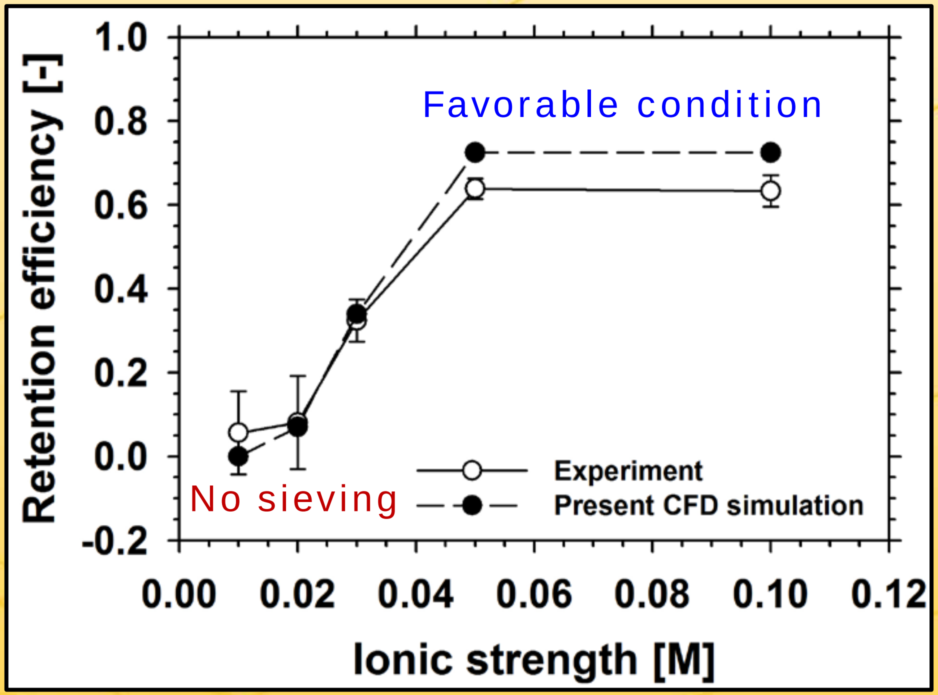
Filtration Efficiency under Unfavorable Conditions

0.1 µm PP membrane (A filter)



0.2 µm PP membrane (B filter)



- Increasing ionic strength results in increasing efficiency.
- Sieving effect of 100 nm PSL was almost negligible for both filters even with the nominal pore size of 0.1 µm (100 nm).
- At ionic strengths of 0.05 M and 0.1 M, similar retention efficiencies were obtained, indicating $E_{favorable}$ (maximum).

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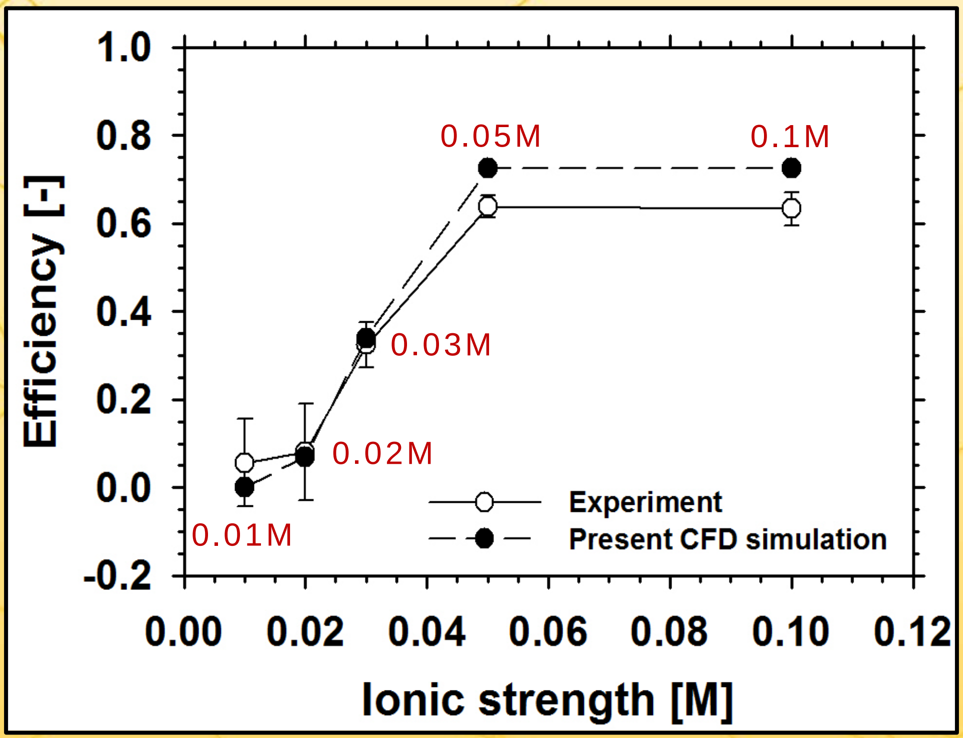
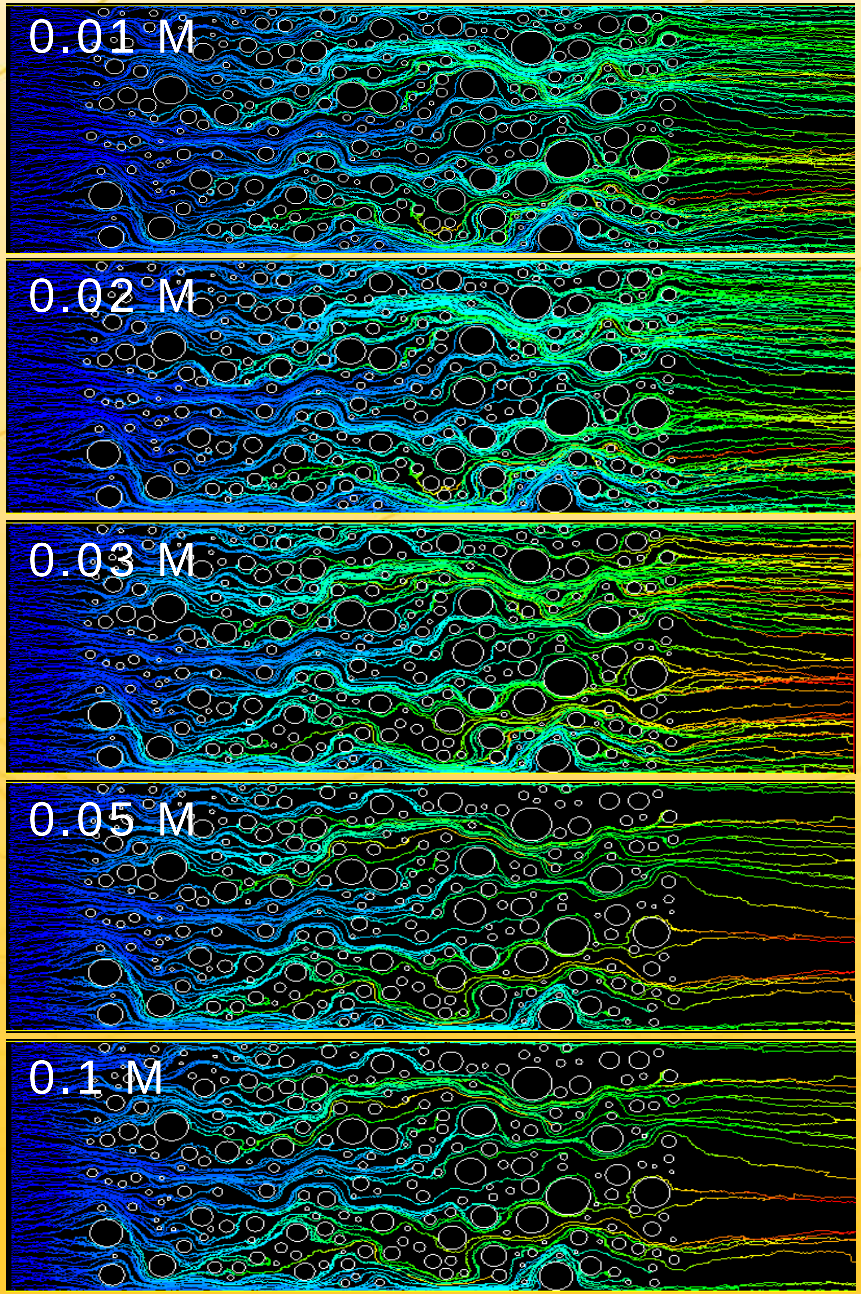
Particle Trajectory (0.2 μm PP Membrane)





- Number of injected particles
  - ✓ Efficiency calculation: 1000 [#]
  - ✓ Particle trajectory: 100 [#]

Conclusion

- CFD simulation using DPM and UDFs can be used to predict the particle deposition behavior under various conditions.
- The simulation method is applicable for granular packed-bed and fibrous membrane filtration systems.
- Performance (quality) of polydisperse fibrous filters may not be characterized by pore size alone and, thus, a proper understanding of surface interactions is required.

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THANK YOU

Q/A

APPENDIX

Single Collector Theory

Single sphere efficiency

$$A_S = \frac{2(1-p^5)}{w}$$

$$w = 2 - 3p + 3p^5 - 2p^6$$

$$p = (1-\varepsilon_0)^{1/3}$$

Single fiber efficiency

$$A_S = \frac{(2/3)(4c_1 + c_4)}{c_1[(1/\varepsilon_s) - 2 + \varepsilon_s] + (c_4/2)(\varepsilon_s - 1 - \ln\varepsilon_s)}$$

$$c_1 = \frac{-\varepsilon_s c_4}{4} \qquad c_3 = c_1 + \frac{c_4}{2}$$

$$c_2 = -c_1 - c_3 \qquad c_4 = \frac{-4}{2\ln\varepsilon_s + 3 - 4\varepsilon_s + \varepsilon_s^2}$$

$$N_R = \frac{d_p}{d_g} \qquad N_{vdW} = \frac{A}{k_B T} \qquad \varepsilon_0\,(porosity) = 1 - \varepsilon_s$$

$$N_{Pe} = \frac{U d_g}{D_{BM}} \qquad N_{LO} = \frac{A}{9\pi\mu a_p^2 U} \qquad d_g\,(or\ d_f)$$

$$N_G = \frac{2(\rho_p - \rho_0)a_p^2 g}{9\mu U}$$