Development of Filter Modeling with Polydispersed Fibers

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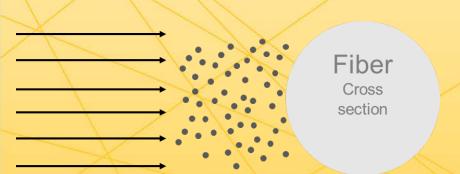


Outline

- Introduction
- Objectives
- Experimental methods
 - Filter properties
 - Experimental method and setup
- Numerical simulation methods
 - Filter generation
 - Flow field calculation
 - Particle trajectory
- Results
 - Collection efficiency comparison
 - Effect of polydispersity

Single Fiber Efficiency (SFE) theory

For the estimation of fibrous filter capture efficiency,
 SFE theory is generally applied



$$P = 1 - E = \exp(\frac{-4\alpha E_{\Sigma}t}{\pi d_f(1 - \alpha)})$$

t: filter thickness, α : solidity d_f : fiber diameter, E_{Σ} : single fiber efficiency

$$E_{\Sigma} = 1 - (1 - E_R)(1 - E_I)(1 - E_D)(1 - E_{DR})(1 - E_G)$$

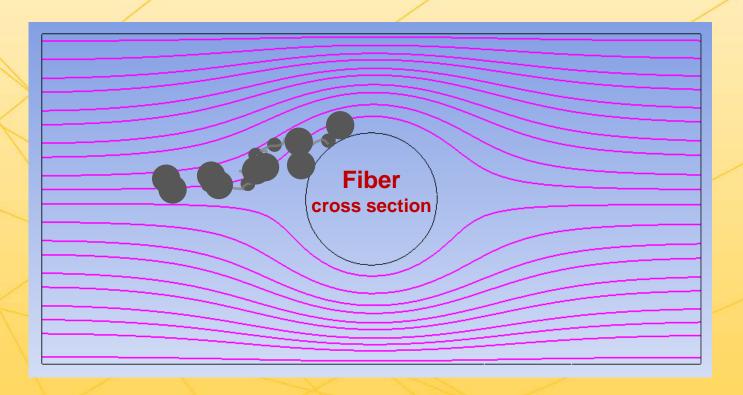
 E_R : Efficiency for interception

 E_I : Efficiency for impaction E_D : Efficiency for diffusion

 E_{DR} : Efficiency for interception of particles with diffusion

 E_G : Efficiency for gravitational setting

Particle deposition mechanism



Deposition mechanism:

- Diffusion
- Interception
- Impaction
- Gravitational settling
- Electrostatic attraction

Analytical expressions for each capture mechanism

SFE Diffusion	ED
Pich (1965)	$2.27Ku^{-1/3}Pe^{-2/3}(1+0.62Kn_fPe^{1/3}Ku^{-1/3})$
Stechkina (1966)	$2.9Ku^{-1/3}Pe^{-2/3} + 0.624Pe^{-1}$
Lee and Liu (1982)	$1.6\left(\frac{1-\alpha}{Ku}\right)^{1/3}Pe^{-2/3}$
Liu and Rubow (1990)	$1.6 \left(\frac{1-\alpha}{K_{H}}\right)^{1/3} Pe^{-2/3} C_{d}$
Payet et al. (1992)	$1.6\left(\frac{1-\alpha}{Ku}\right)^{1/3} Pe^{-2/3}C_dC_{d'}$
Kirsch and Fuchs (1968)	$2.7Pe^{-2/3}$

$$Kn_f = \frac{2\lambda}{d_f}$$

$$Ku = -0.15ln\alpha - \frac{3}{4} - \frac{\alpha^2}{4} + \alpha$$

$$C_{d} = 1 + 0.388Kn_{f} \left[\frac{(1 - \alpha)Pe}{Ku} \right]^{1/3}$$

$$C_{d'} = \left[1 + 1.6 \left[\frac{1 - \alpha}{Ku} \right]^{1/3} Pe^{-2/3} C_{d} \right]^{-1}$$

SFE Interception	Er
Lee and Gieseke (1980)	$\left(\frac{1-\alpha}{Ku}\right)R^2(1+R)^{\frac{-2}{3(1-\alpha)}}$
	$(1+R)^{-1} - (1+R) + 2(1+1.996Kn_f)(1+R)ln(1+R)$
Pich (1966)	$2(-0.75 - 0.5ln\alpha) + 1.996Kn_f(-0.5 - ln\alpha)$
Lee and Liu (1982)	$0.6\left(\frac{1-\alpha}{Ku}\right)\frac{R^2}{1+R}$
Liu and Rubow (1990)	$0.6\left(\frac{1-\alpha}{Ku}\right)\frac{R^2}{1+R}C_r$

$$R = \frac{d_p}{d_f}$$

$$C_r = 1 + \frac{1.996Kn}{R}$$

SFE Impaction EI

Yeh and Liu (1974)
$$\left(\frac{stk}{2Ku^2}\right)J$$

$$Stk = \frac{\rho_p d_p^2 C_c U_0}{18\mu d_f} \qquad J = (29.6 - 28\alpha^{0.62})R^2 - 27.5R^{2.8}$$

Equivalent fiber diameter (for SFE theory)

An equivalent fiber diameter is applied to SFE to obtain collection efficiency of filter media

Equivalent fiber diameter

Different concepts of mean: +

Fiber Cross section *Arithmetic mean: $\sum_{n=1}^{n}$

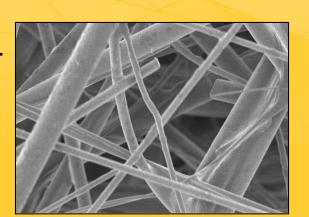
*Geometric mean: $\sqrt[n]{D_{f1}D_{f2}\cdots D_{fn}}$

*Volume-surface average fiber diameter: $\frac{\sum nD_f^2}{\sum nD_f}$

Effective fiber diameter: -

*Davies:
$$D_f = \sqrt{U_{\infty}\mu t(\frac{64\alpha^{\frac{3}{2}}(1+56\alpha^3)}{\Delta P})}$$

 However, real fibrous filter is composed of a wide range of fibers



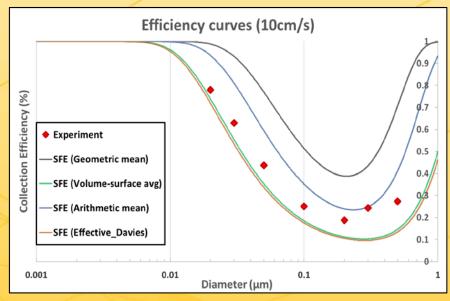
Direct measurement of fiber size (e.g. SEM)

Empirical expression:
Approximation based on the pressure drop measurement (\(\Delta P\), t, \(\alpha\) are required)

Issues with using an equiv. fiber diameter

Podgorski (2009) pointed out that
 "it is impossible to select any one universal mean fiber diameter to describe penetration of nanoparticles with different sizes."

 Different equivalent fiber diameter definitions affect the efficiency curve



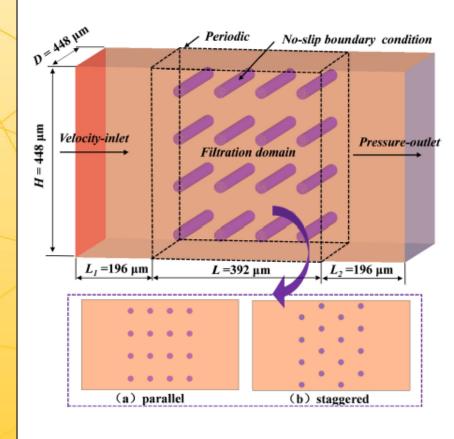
HF-0012 (Hollingsworth & Vose)

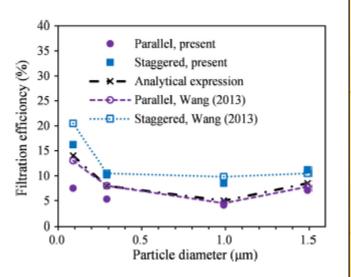
 However, an equivalent fiber diameter is still widely applied to the numerical modeling and SFE theory

Podgorski (2009). Journal of Nanoparticle Research 11: 197-207.

Recent papers using single fiber diameter



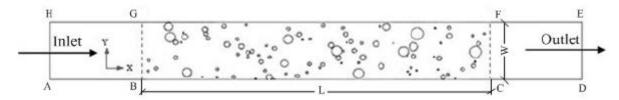


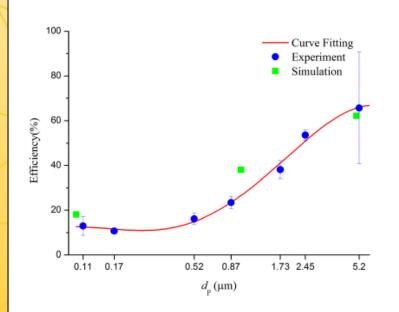


- CFD-DPM (Discrete Phase Modeling)
- Parallel vs staggered
- Collection efficiency of multi-fiber filters is obtained

Papers using polydisperse fibers

Bin et al. (2016). Aerosol and Air Quality Research (Article in press)





- Lattice Boltzmann method
- Randomly located polydisperse fibers

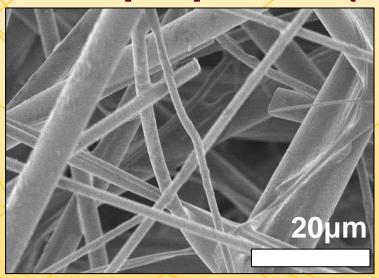
Limitations:

- Smallest particle challenging filter is 100 nm (Capture by diffusion cannot be well understood)
- Only three particle sizes are investigated, and only one of them is submicron

Objectives

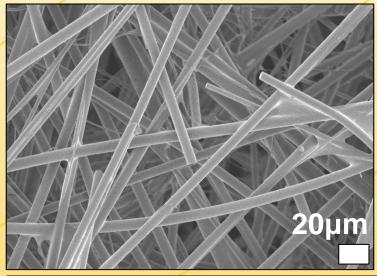
- To develop a method to generate <u>fibrous filter domain</u> composed of <u>polydisperse fibers</u> using commercial filter media (H & V)
- To develop a <u>numerical model</u> of nanoparticle filtration by fibrous filters
- To compare the <u>collection efficiency</u> between numerical model and experimental data with challenging particle diameter from <u>3nm up to 500 nm</u>
- To investigate the effect of <u>equivalent fiber diameters</u> on predicted collection efficiency

Filter properties (Hollingsworth & Vose)



HF-0012				
Fiber distribution	size (μm)			
Arithmetic mean	3.3			
Geometric mean	2.5			
Volume-surface average	5.1			
Effecitve Fiber diameter (Davies)	5.3			

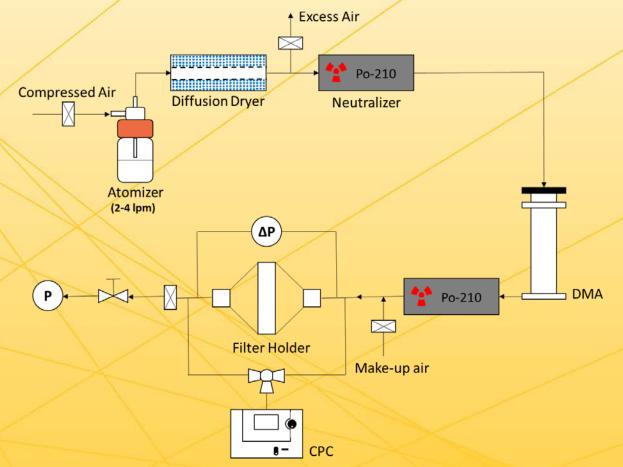
Filter Parameters			
Thickness (mm)	0.74		
Solidity 0.03			
DOP % Penetration	79.9		
(0.3 µm at 5.3 cm/s)	19.9		
Pressure drop (Pa)	13		
@ 5.3 cm/s	13		



HF-0493				
Fiber distribution	size (μm)			
Arithmetic mean	5.7			
Geometric mean	4.5			
Volume-surface average	5.6			
Effecitve Fiber diameter (Davies)	8.3			

Filter Parameters			
Thickness (mm)	0.36		
Solidity	0.076		
DOP % Penetration	88		
(0.3 µm at 5.3 cm/s)	00		
Pressure drop (Pa)	8		
@ 5.3 cm/s	0		

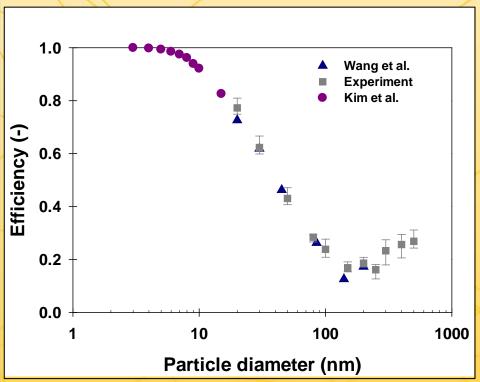
Experimental method and setup



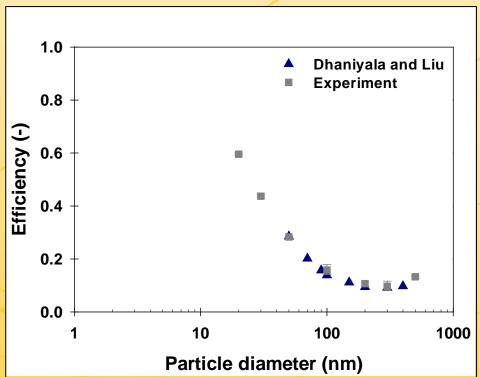
- KCI particles (20, 30, 50, 80, 100, 150, 200, 300, and 500 nm) are used to challenge the filter media (HF-0012 and HF-0493)
- Particle size from 3 to 20nm was obtained from Kim et al. (2008) to be compared with the simulation results
- Kim et al. (2007). Journal of Nanoparticle Research 9: 117-125.

Experimental results comparison

HF-0012 10cm/s



HF-0493 10cm/s

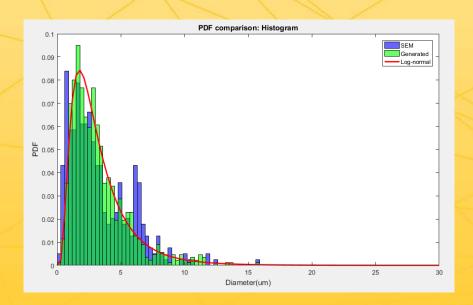


- Kim et al.: Silver particles (3-20nm)
- Wang et al.: NaCl particles (20-200nm)
- Experiment: KCl particles (20 500nm)
- Dhaniyala and Liu: DOS (50-400nm)
- Experiment: KCl particles (20 500nm)

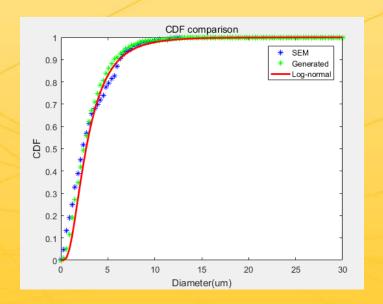
- Dhaniyala and Liu (1999). Journal of the IEST 42(1): 32-40.
- Wang et al. (2007). Journal of Nanoparticle Research 9: 109-115.
- Kim et al. (2007). Journal of Nanoparticle Research 9: 117-125.

Fiber generation

- Fiber size distribution measured by SEM images follows log normal distribution
- Figures shows the fiber size distribution from <u>HF-0012</u> (<u>Blue color Measured by <u>SEM</u>) and from randomly generated one (<u>Orange color Generated by the code developed</u>)
 </u>
- Their distributions are well agreed as shown in the picture



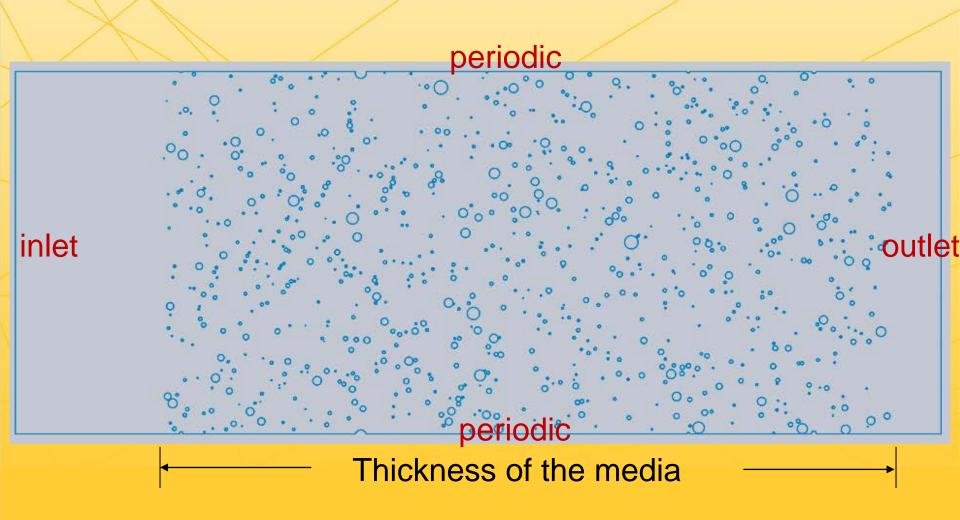
Fiber size distribution (Probability density function)



Fiber size distribution (Cumulative size distribution)

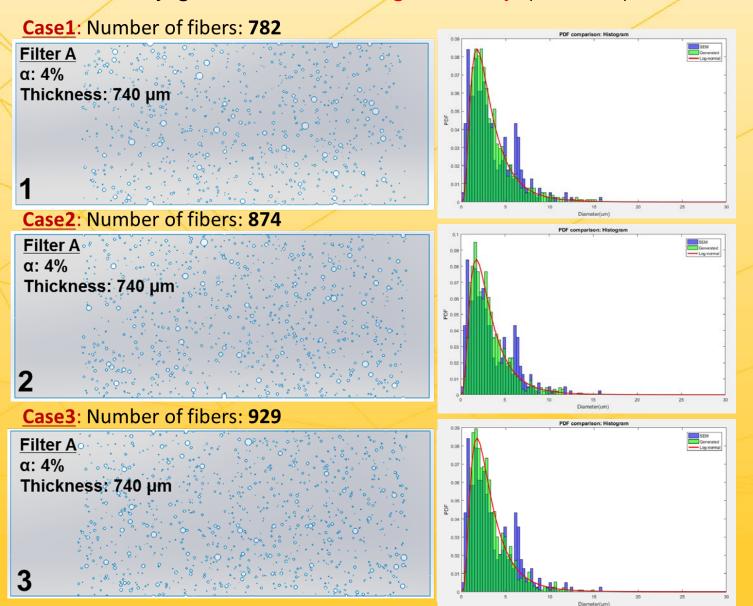
Fiber arrangement and boundary condition

 Fibers are randomly generated and arranged in the real size of the filter domain until the target solidity is achieved



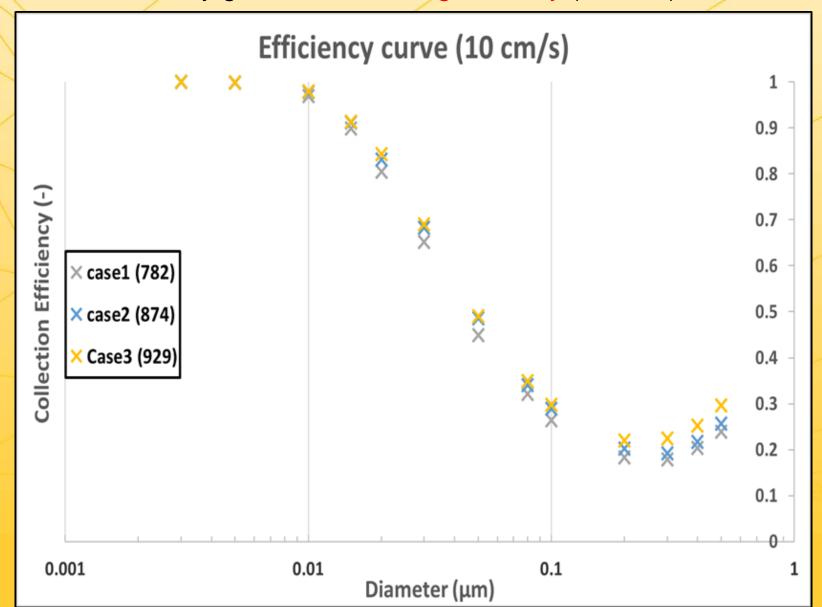
Example of fiber distribution for HF-0012

- Three fiber domains below have the <u>same domain size and solidity</u>
- Fibers are randomly generated until target solidity ($\alpha = 0.04$) is achieved



Example of fiber distribution for HF-0012

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- Fibers are randomly generated until target solidity ($\alpha = 0.04$) is achieved

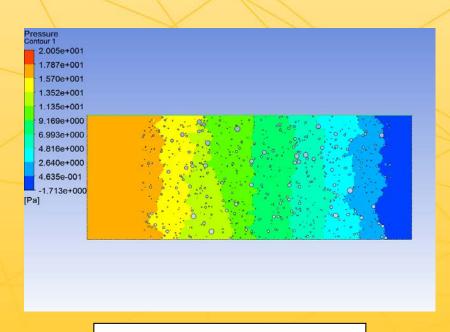


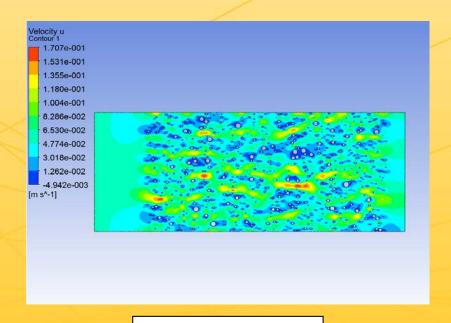
Flow field calculation: CFD

 Continuity and momentum equation in the Stokes regime were numerically solved (Fluent)

$$\nabla \cdot u = 0$$

$$\nabla p - \mu \nabla^2 u = 0$$



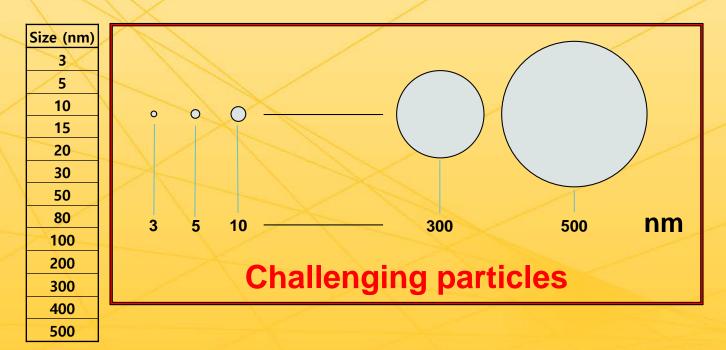


Pressure drop

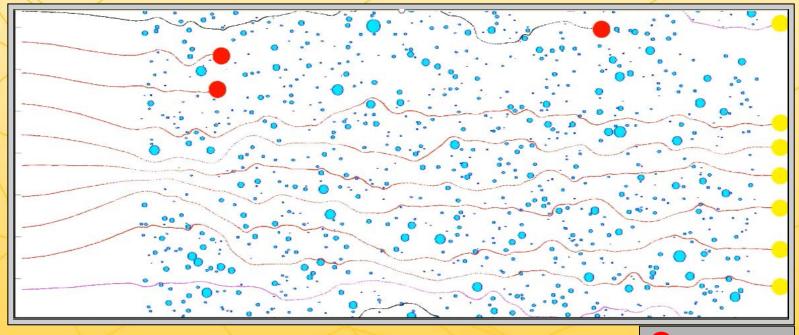
Streamline

Particle trajectory

- In-house JAVA code is applied to solve the Langevin equation
- Collection efficiency is obtained using the particles from 3 nm up to 500 nm



Example particle trajectory



HF-0012 Domain
Face velocity: 10 cm/s
200nm particles

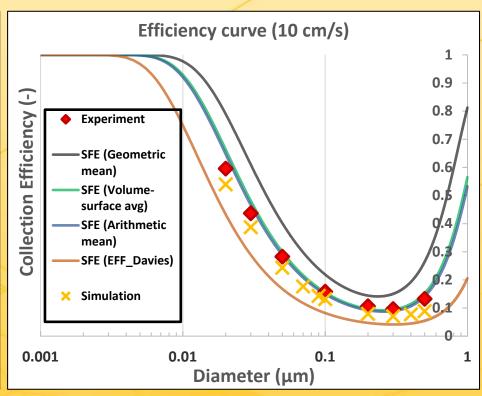


Filtration efficiency comparison

HF-0012 10cm/s

Efficiency curve (10 cm/s) Efficiency (-) Experiment Experiment (Kim et al.) 0.6 SFE (Geometric Collection mean) SFE (Volumesurface avg) SFE (Arithmetic mean) SFE (EFF Davies) Simulation 0.1 0.001 0.01 0.1 Diameter (µm)

HF-0493 10cm/s



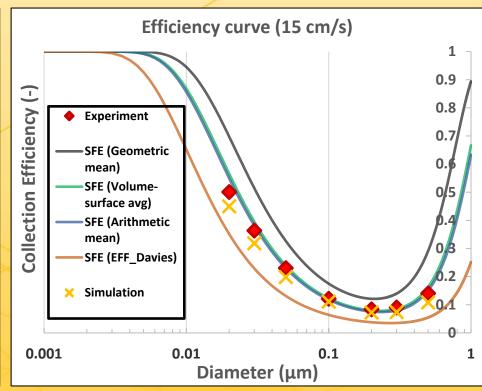
- The relative accuracy of estimated efficiency curve using equivalent fiber diameters varies with the filter media
- Simulation results agree well with experimental data for both filters

Filtration efficiency comparison

HF-0012 15cm/s

Efficiency curve (15 cm/s) Efficiency (-) Experiment 0.7 Experiment (Kim et al.) **0**.6 SFE (Geometric mean) 0.5 Collection SFE (Volume-0.4 surface avg) SFE (Arithmetic mean) SFE (EFF Davies) Simulation 0.1 0.001 0.1 0.01 Diameter (µm)

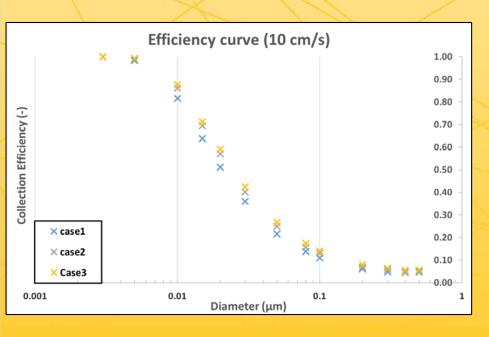
HF-0493 15cm/s

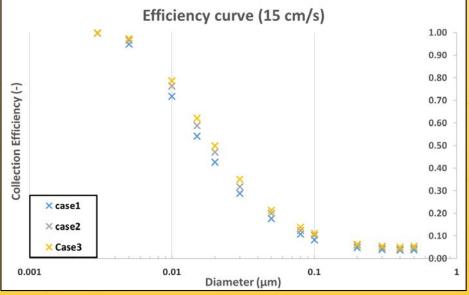




Effect of polydispersity: same average diameter

	Thickness	Solidity	Mean	Min	Max	std		COV
case	(mm)	(-)	(µm)	(μm)	(μm)	(µm)	# fibers	(SD/mean)
1		/	15	3.5	65.0	7	227	0.5
2	1	0.1	15	7.9	30.7	4	269	0.3
3	$\langle \ \rangle$		15	12.5	18.4	1	283	0.1





Applications using the developed method will help us better understand/design filters

- Air/Liquid filtration
- Electret filter
- Particle loading on filter media
- Pleated filter

Summary

- We have developed a numerical simulation of nanoparticle filtration by fibrous filter media
- Collection efficiencies for two different filters were measured experimentally with challenging particles from 3nm up to 500nm, and the efficiencies agree well with those from simulation
- SFE theory is a good method for estimating the trends of collection efficiency for fibrous filters, but the estimated efficiency can deviate depending on the fiber diameter definitions and SFE equations for each capture mechanism
- The relative accuracy of predicted collection efficiency, using an equivalent fiber diameter can be altered for the filter media
- The degrees of polydispersity affect the collection efficiency