High fidelity simulation of ultrafine PM filtration by multiscale fibrous media characterized by a combination of X-ray CT and FIB-SEM

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This "Supporting information" includes: Text S1, S2, Figure S1 to S5 and Table S1.

Text S1. Creation of virtual substrate from geometric parameters

FiberGeo (Math2Market, Germany) was used here for the generation of parametric substrates. As the component information provided by the manufacturer, the substrate was made of polyethylene terephthalate (PET) fibers and two types of cellulose fibers, and the mass ratio was 5:35:60. The input geometric parameters were summarized in Table S1, which were mainly obtained by using the SEM and fiber analyzer (the detailed information can be found in our previous work). The PET fibers were assumed straight, the curls of cellulose fibers were described by the sinusoidal curves defined as equation $y = \sin x$.[1] The sine length 1, 2 were half of wavelength in horizontal and vertical direction, respectively. The sine amplitude described the oscillation of fibers. As the cross-sectional shape of cellulose fibers were assumed as ellipse, the aspect ratio was used to depict the minor diameter of an ellipse. The inner diameter fraction was the factor used to describe the hollow structures of cellulose fibers, which was determined by fitting the pressure drop / face velocity curves with experimental results. Specially, the orientation of fibers in the substrate were obtained by analyzing the fiber orientation of virtual substrate from CT slices using the Star Length Distribution (SLD) algorithm.[2] The orientation tensor of fibers in *x, y, z* directions of the substrate were 0.35, 0.54 and 0.10, respectively.

Text S2. Validation of slip model used on the surface of solid phase

Before applying to cases studied in this paper, the Maxwell first order slip model was firstly verified by comparing the simulated velocity profile in 2-D Poiseuille flow to an analytic solution.[3] The analytic solution for velocity distribution in 2-D Poiseuille flow using first-order boundary was given by

$$u(x)_y = 6\bar{u}\left(-\frac{x^2}{W^2}+\frac{x}{W}+2\frac{2-\sigma_v}{\sigma_v}Kn\right)/\left(1+12\frac{2-\sigma_v}{\sigma_v}Kn\right) \tag{1}$$

where $u(x)_y$ was the air flow velocity in x direction, W was width of the pipe. The ratio of pipe length to width was configured as 5, and the periodic boundary condition in flow direction was used.

Simulated velocity filed for Poiseuille flow at three Knudsen number were shown in **Figure S4a**. With the increasement of Knudsen number, the flow velocity along the wall was increased. As shown in **Figure S4b**, velocity profiles from numerical simulations agreed well with results from analytical calculations.

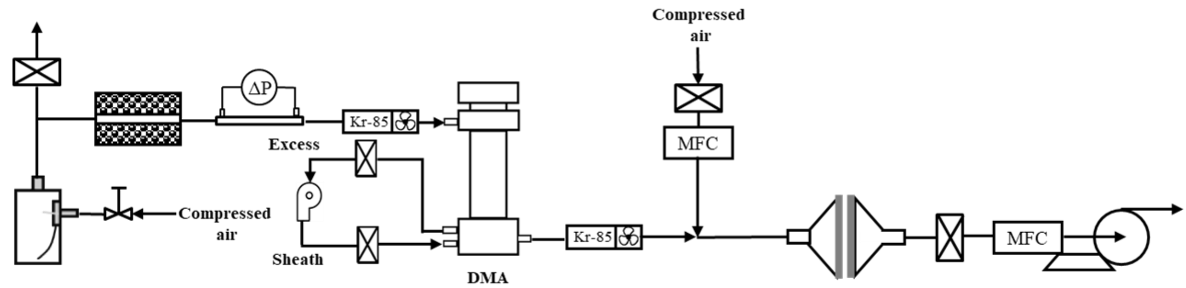

Figure S1. Schematic of experimental set up for fraction filtration efficiency test.

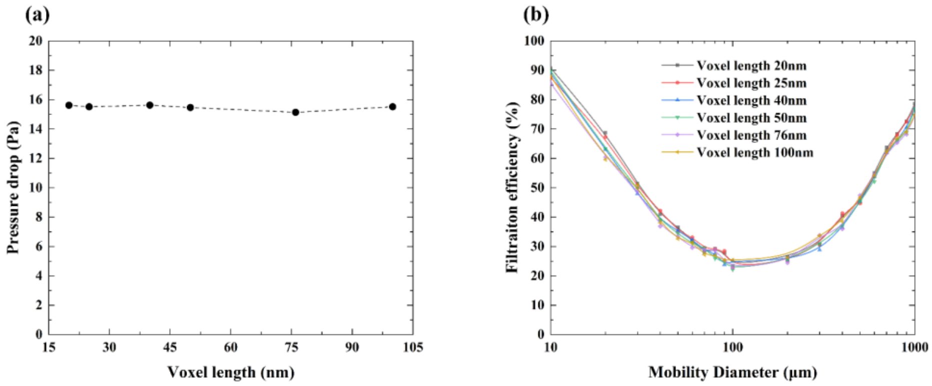

Figure S2. Voxel length effect on a) pressure drop and b) particle filtration efficiency.

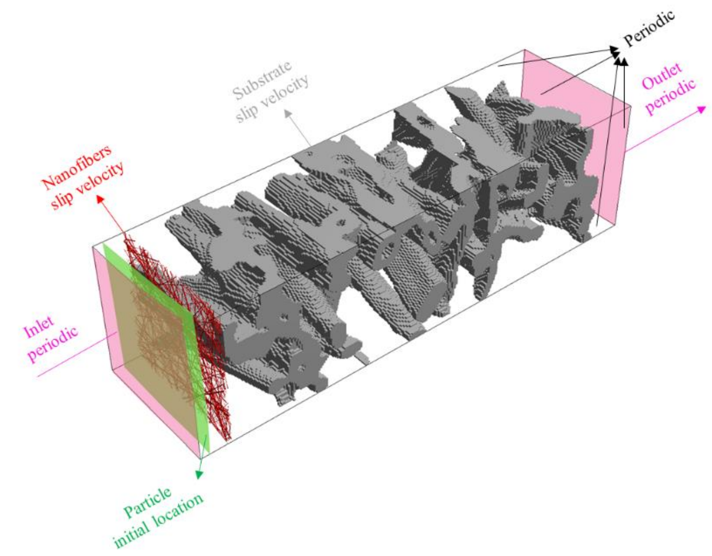

Figure S3. Schematic drawing of the computation domain and boundary conditions.

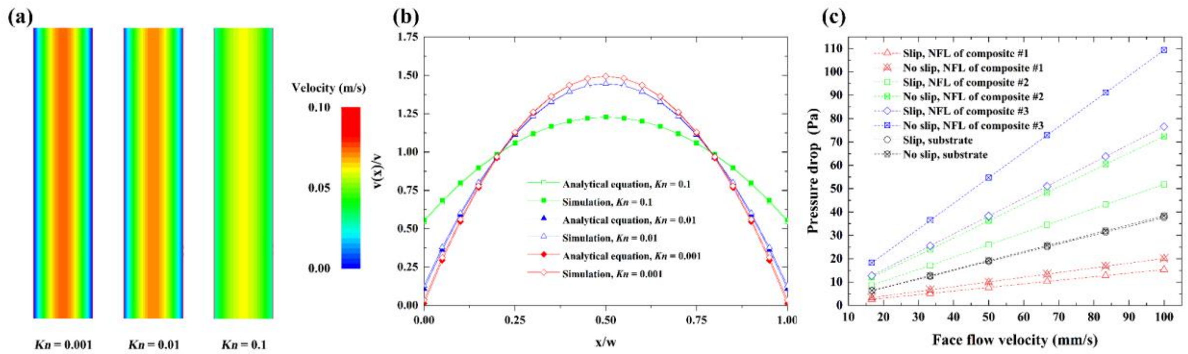

Figure S4. Validation of slip model used on the surface of solid phase. a) Simulated velocity field for Poiseuille flow at three Knudsen number. b) Comparison of velocity profiles for Poiseuille flow from numerical simulations and analytical calculations. c) Comparison of pressure drop across filter media at different face velocities with different boundary condition on the surface of the fibers.

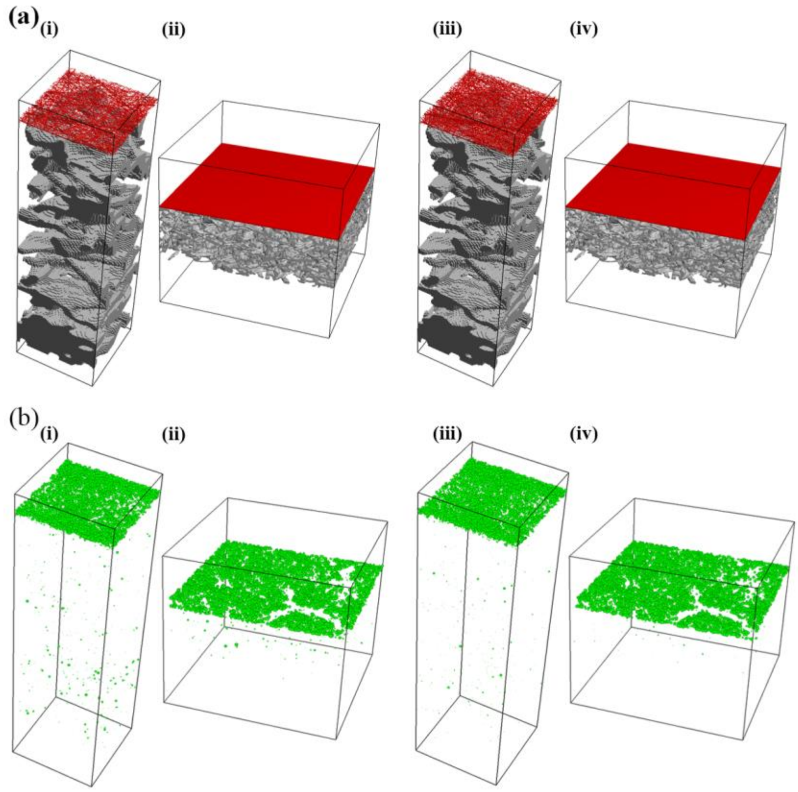

Figure S5. Visualization of captured particles in the composites. Deposited particles in the a(i) resolved model of composite #2, a(ii) unresolved model of composites #2, resolved model of composite #3 and a(iv) unresolved model of composite #3. b(i-iv) Captured particles in the computation domain without filter media corresponding to a(i-iv).

Table S1. Geometric parameters for creation of parametric substrate.

Parameter	Cellulose 1	Cellulose 2	PET
Diameter (μm)	29.3± 8.0	32.9± 5.9	11.06
Aspect ration	0.396	0.406	-
Inner diameter fraction	0.45	0.45	-
Length (μm)	2000	2000	5000
Density (g/m^3)	1.5	1.5	1.38
Sine length 1, 2 (μm)	1015, 250	1015, 250	-
Sine Amplitude 1, 2 (μm)	123, 5	123, 5	
Mass ratio (%)	35	60	5

References

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