Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supplementary Information

Transport of Microorganisms into Cellulose Nanofiber Mats

Katrina A. Rieger, Raghuram Thyagarajan, Maureen E. Hoen, Hiu Yeung,

David M. Ford, and Jessica D. Schiffman *

Department of Chemical Engineering

University of Massachusetts Amherst, Amherst, Massachusetts 01003-9303

* Corresponding author: Jessica D. Schiffman

Email: schiffman@ecs.umass.edu; Phone: (413) 545-6143

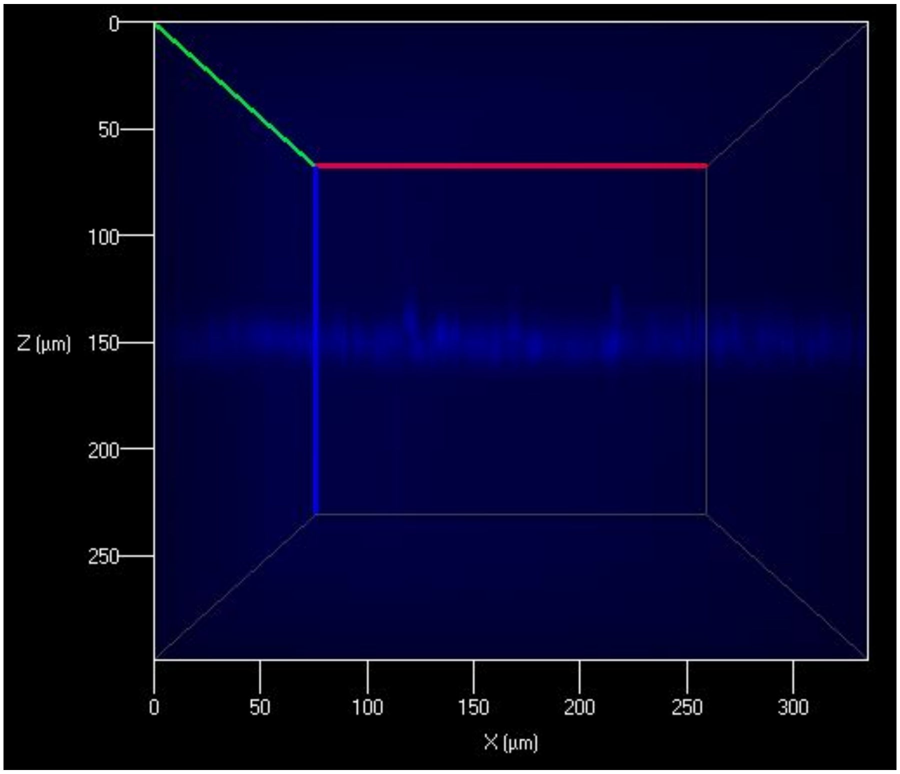


Figure S1. Representative z-stack composite image displays the cross-section of a nanofiber mat. Measurements were utilized to obtain the average thickness of the nanofiber mats, 50 measurements were obtained using 5 different nanofiber mats stained with calcofluor white.

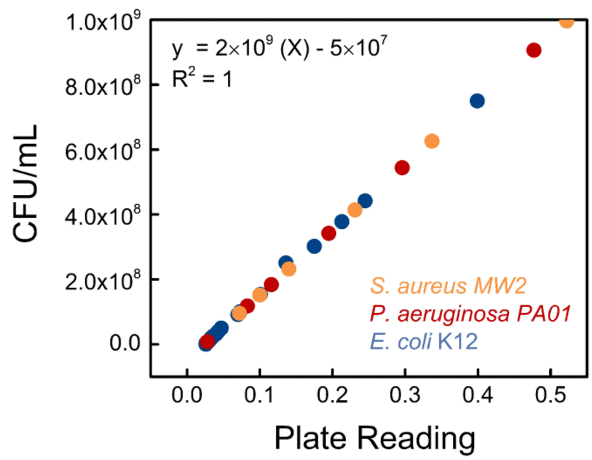


Figure S2. Calibration curve used to convert plate readings (600 nm) to CFU/mL for *S. aureus* MW2, *P. aeruginosa* PA01, and *E. coli* K12.

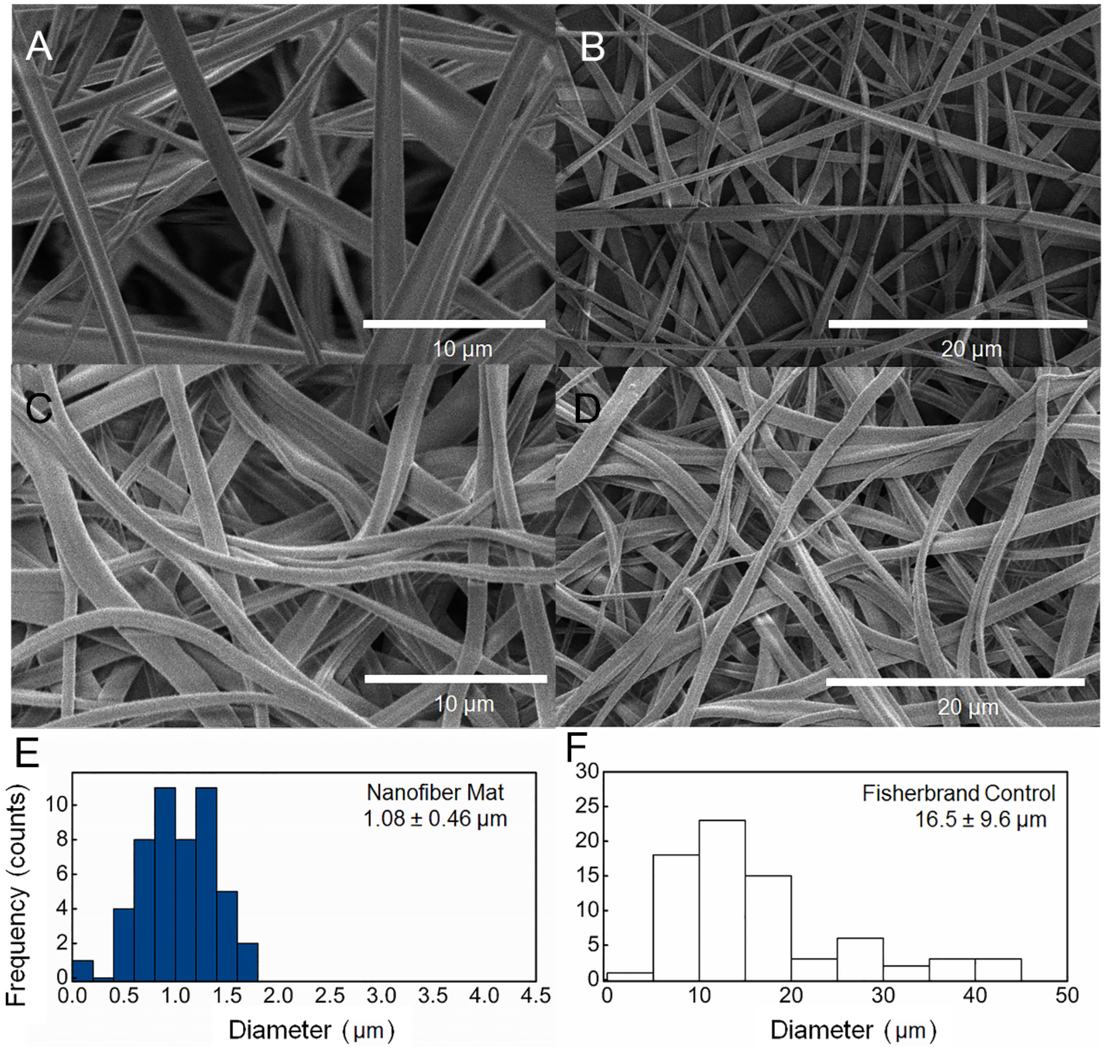
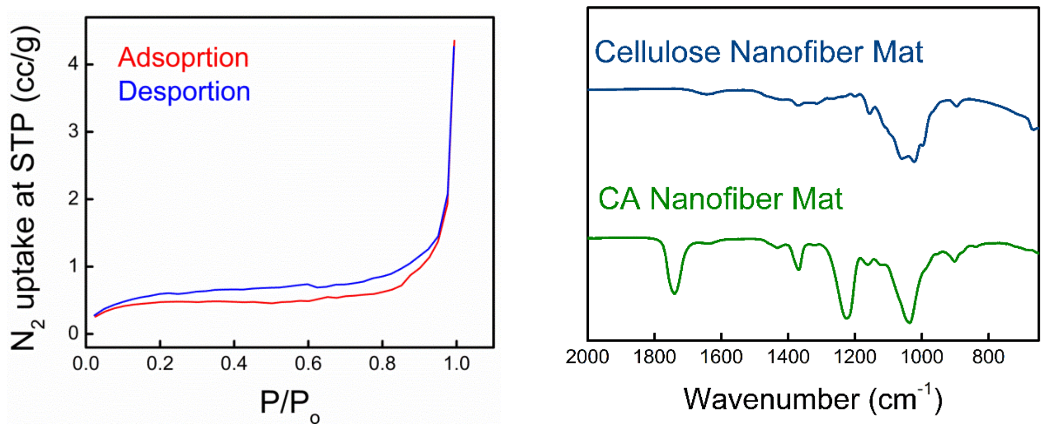


Figure S3. Micrographs of **(A** and **B)** as-spun cellulose acetate nanofiber mat, as well as the **(C** and **D)** cellulose nanofiber mat used in this study. Fiber diameter distribution for the **(E)** cellulose nanofiber mat and the **(F)** Fisherbrand control as determined using *ImageJ* software on SEM micrographs. The average fiber diameter and standard deviation of 50 random fiber diameters are also provided.



Peak Location (cm^{-1})		Functional Group
Cellulose Acetate (CA)	Cellulose	
895	895	COC, CCO and CCH deformation and stretching
1020	1020	C-C, C-OH, C-H ring and side group vibrations
1046	1046	
1232	-	COH bending at C6
1368	-	In-the-plane CH bending
1750	-	C=O stretching vibration

Figure S4. (**Top Left**) The surface area of the cellulose nanofiber mat was determined to be 4.5 m^2/g using an Autosorb®-iQ system. The surface area of the Fisherbrand and Sartorius controls was too low to be estimated using the Autosorb®-iQ system. (**Top Right**) FTIR spectra of the as-spun cellulose acetate (CA) nanofiber mat and the cellulose nanofiber mat are displayed. Confirmation of the regeneration of cellulose is confirmed by the disappearance of the peak at 1750 cm^{-1} indicating the replacement of acetate groups with hydroxyl groups. (**Bottom**) Characteristic FTIR peaks for CA and cellulose nanofiber mat are summarized in the table.

Modeling of Bacteria Uptake by the Nanofiber Mats. The **dynamic model** defines the driving force for adsorption as the concentration difference between the bulk solution and the nanofiber mat, and assumes that the bacteria are distributed uniformly throughout the nanofiber mat at all stages of the uptake process (i.e., there is no resistance within the nanofiber mat for bacteria transport).

$$\frac{dc_m(t)}{dt} = k_m\left(c_b(t) - \frac{c_m(t)}{K_{eq}}\right); c_m(t=0) = 0 \qquad \text{Equation 1}$$

where c_m is the concentration of bacteria inside the mat, c_b is the concentration of bacteria in the bulk solution, and k_m is a rate constant.

One reasonable hypothesis is that bacterial diffusion through the aqueous medium is controlling uptake, in which case $k_m \sim D_{bulk} / L^2$ where L is a diffusional length scale that depends on both the geometry of the well and the diameter of the nanofiber mat, and D_{bulk} is the effective diffusion coefficient of the bacteria in water through its natural run/tumble movements. At equilibrium ($t \rightarrow \infty$) the rate of uptake vanishes and Equation 1 reduces to the following equilibrium model:

$$c_m = K_{eq} c_b \qquad \text{Equation 2}$$

and therefore is consistent with the equilibrium calculations. To solve Equation 1, a closure relation to eliminate the bulk concentration term $c_b(t)$ is required. For this, the conservation of number of cells shown in Equation 3 was used where V_{sol} is volume of the bulk solution and V_{mat} is the volume of the nanofiber mat.

$$c_{b0} V_{sol} = c_b(t) V_{sol} + c_m(t) V_{mat} \qquad \text{Equation 3}$$

Using Equations 1 and 3, we solve for the fraction of bacteria inside the nanofiber mat as:

$$\frac{c_m(t)}{c_{b0}} = \frac{1}{\phi}\left[1 - e^{-\phi k_m t}\right]; \quad \phi = \frac{1}{K_{eq}}\left(1 + \frac{K_{eq} V_{mat}}{V_{sol}}\right) \qquad \text{Equation 4}$$

Equation 4 was fit to the experimental data (**Figure 3D**) to estimate the rate constant k_m for each of the various nanofiber mat diameters. In this equation, the value of K_{eq} was fixed at 420.3, which was obtained from the equilibrium isotherm calculations above. The ratio of the volume of the nanofiber mat (V_{mat}) to the volume of the bulk solution (V_{sol}) was fixed. V_{mat} was calculated for the various nanofiber mat diameters based on a measured thickness of 42.4 ± 12 μm. V_{sol} was set to 5 mL as used in the experiments. The rate constant k_m was estimated using the curve fitting toolbox in Matlab.