MODELING AND SIMULATION OF A BACTERIAL WATER FLOW IN POROUS WALLED MICROCHANNELS

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Abstract - A computer model based on Ansys Fluent v18 software is developed to explain the experimental data of bacterial growth in a water flow through metal-carbon-polymer nanocomposite-based microchannels. Batch growth rate tests were performed on Gram-negative Escherichia coli (E. coli) bacteria. Kinetic tests for the bacterial killing were performed using the silver (Ag) nanoparticles (NPs)-grown carbon nanofibers (CNFs) in polyvinyl acetate (PVAc) nanocomposite film, dispersed in the bacterial solution. Geometrical models for microchannels containing nanocomposite (Ag-ACF/CNF-PVAc) film were developed using the Autodesk inventor. Bacterial control was simulated assuming Ag imprinted porous walls. An adsorption mechanism was used in the model to simulate killing of the E. coli bacteria. The exponential growth of E. coli at inlet to the microchannel was assumed. The simulated results fitted the experimental data reasonably well.

Keywords - computer model; microchannels; bacterial flow; polymer nanocomposite; bacterial growth rate.

I. INTRODUCTION

The demand for potable water has been constantly increasing globally. Therefore, there is an urgent need for an efficient and economical water filtering technique. At present, there are many types of commercially available water filters. However, these are relatively expensive and not affordable to common people. Recently, a novel contactor was developed to remove microorganisms from water. To remove such contaminations, there are technologies such as ultraviolet (UV) disinfection and reverse osmosis (RO) membrane. The UV exposure kills bacteria and virus to certain extent. However, it is not effective considering that suspended solid, organic matter or color reacts with UV radiation, resulting in the decreasing antibacterial characteristics of UV radiation. The RO membrane-based system is a pressure driven process, in which semi-permeable membrane rejects dissolved solids and microbes present in organisms such as yeast are complex in structure and show strong resistance to the disinfection agents. Disinfectants such as chlorine can also not remove total coliforms and fecal coliforms. A new disinfectant is, therefore, required that not only have broad microbial effects but also reduces the generation of disinfection by-product to a minimum level.

The metallic ions of silver (Ag), copper, tin, mercury, lead, bismuth, cadmium, and thallium are known for showing anti-microbial properties. In recent studies, experiments have been performed using Ag as a microbicidal agent against indicator organisms that are pathogenic with respect to human health. Recently, the antibacterial properties of Ag have been revisited with the advent of nanotechnology. Maximum concentration of Ag in water is up to 0.1 mg/L (a concentration that gives a total dose over 70 years of half the human no-observed-adverse-effect-level (NOAEL) of 10 gm), which could be tolerated without risk to health.

Microchannels have been used in various applications such as separation and chemical reactions. The surface area to volume ratio of microchannels is high (~1:1000), which allows high mass and heat transfer rates. Therefore, use of microchannels has potentially increased in bio-applications where the amounts of handled fluid is less. Examples of such applications are diagnostics (immune sensor), electrophoresis separation, drug delivery, separation of proteins and DNA, antimicrobial susceptibility test and cell culture. Traditional filters usually occupy a good amount of space or power (electricity), whereas a microchannel-based device is portable and should consume less electricity.

Microchannels are proposed to remove virus, E. coli or S. aureus. Briefly, the Ag NPs are dispersed in an ACF/CNF-PVAc, using calcination, reduction and chemical vapor decomposition. The Ag nanoparticles-dispersed ACF are then uniformly mixed in the polymer. Microchannels are fabricated in the polymer-based nanocomposite because of cost-effectiveness, good adhesion property, high elasticity and biocompatibility. The substrate provides a long-term stability to the NPs by preventing them from oxidizing and agglomerating in liquid. It also strongly binds with Ag, which decreases the leached-out Ag concentrations in water flow.

In this study, the Ag-ACFs/CNFs are used as an antibacterial agent. The material was in situ mixed into the reaction mixture used for synthesizing polyvinyl alcohol (PVA). Microchannels (7.5 mm long x 150 µm wide x 100 µm deep) were fabricated in the polymer using laser-ablation for increasing the exposure of Ag-ACF/CNF to water flowing in the passages (channels). The CNF has multiple roles. It

tightly holds the Ag NPs and increases the tensile strength of the nanocomposite film. An efficient microchannel-based contactor device was developed to remove bacteria from water solution using Ag-ACF/CNF.

In this study, the model assumption takes into consideration the replication time of E. coli, i.e., population of E. coli grows exponentially with time.

Mathematical model will help to scale up the proposed process and also, understand the bacterial disinfection process. The Fluent-based model developed in this study is used to explain the experimental data. The inlet concentration of E. coli is assumed to increase exponentially with time. E. coli is assumed to get adsorbed on the Ag-ACF/CNFs dispersed in the nanocomposite via diffusion through the porous walls. The results from the modeling is compared to the experimental results.

II. EXPERIMENTAL SET-UP

A schematic diagram of the water purification system used in this study is shown in Figure 1. Approximately 50 ml volume of the prepared E. coli solution was taken as the inlet solution at room temperature. A peristaltic pump was used to transfer the E. coli solution to microchannel nanocomposite. E. coli was adsorbed on Ag-ACF/CNFs dispersed in the walls of the channels. Purified water was collected at the outlet. The experimental data were used for validating the computational model.

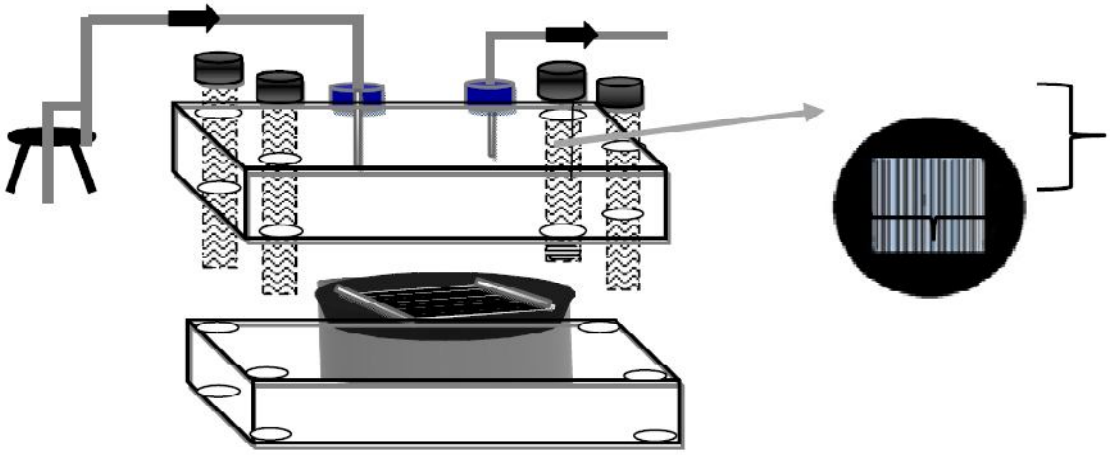


Figure 1: Experimental set-up used for performing the antibacterial tests

III. MODEL GOVERNING EQUATIONS

Flow is described by continuity equation 1 and Naiver Stoke equation 2. Species balance is governed by the diffusion-convection-generation equation 3.

$$\frac{\partial \rho}{\partial t} + \nabla.(\rho v) = 0 \quad \ldots\ldots\ldots\ldots\ldots \quad (1)$$

where ρ is the density of fluid and v is the velocity of fluid.

$$\frac{\partial(\rho v)}{\partial t} + v.\nabla(\rho v) = \nabla(-P + \mu\nabla v) + \rho g \quad \ldots\ldots\ldots\ldots \quad (2)$$

, where P is the pressure, μ is the viscosity, and g is the gravitational constant. Equations (3) and (2) are used for determining pressure and velocity profiles.

$$\frac{\partial(c)}{\partial t} + v.\nabla(c) = \nabla.(D\nabla c) + R \quad \ldots\ldots\ldots\ldots\ldots\ldots (4)$$

, where c is the concentration of E. coli in bulk, and D is the diffusivity constant. R denotes generation term and surface concentration is governed by equation (5)

$$R = \frac{a.(1-\varepsilon)*\partial(cs)}{\varepsilon*\partial t} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (5)$$

$$\frac{\partial(cs)}{\partial t} = k_a c\theta \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (6)$$

where

k_a is the death rate constant of E. coli, c_s is surface site density and Θ is the surface coverage factor which can be defined from equation 5. The numerical values for other variables were assumed as follows: $\mu = 1$, $\varepsilon = 0$ and $\eta = 0$.

IV. INITIAL AND BOUNDARY CONDITIONS:

Initial condition:

At t = 0, C(x, y, z, t) = 0 …… (7)

Boundary conditions:

(1)

At inlet, C(x, y, z)

- $C_0 * \exp(kt)$, $C \geq C_{max}$
- C_{max}, $C \leq C_{max}$

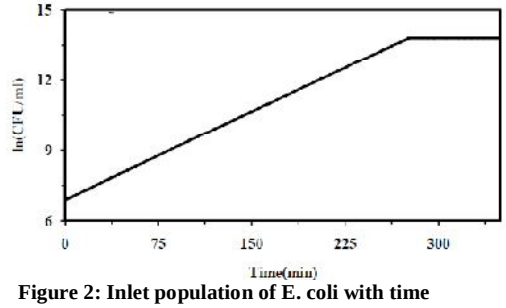


Figure 2: Inlet population of E. coli with time

(2) V (inlet) = V_0 ..... (8)

At t = 0, concentration of E. coli was assumed to be zero everywhere. At t = 0^+, inlet population of E. coli was assumed to exponentially grow with time. After some time, the E. coli population was assumed to be constant at 10^6 CFU/ml.
(3) Outflow: dc/dz = 0; (t > 0)

V. VALIDATING EXPERIMENTAL DATA

Simulations were performed for different inlet volumetric flow rates (60, 120, 150 µL/min), initial concentrations of E. coli (10^3, 10^4, 10^5 CFU/ml), widths of the channel (150, 200, 250 µm) and depths of the channel (30, 50, 100 µm). Adsorption of E. coli in Ag-ACF/CNF increasing exponentially with the inlet concentrations of E. coli was assumed in the model simulations. The model predicted results were found to be in reasonably good agreement with the experimental data. Error bars (± 20%) were added to the data.

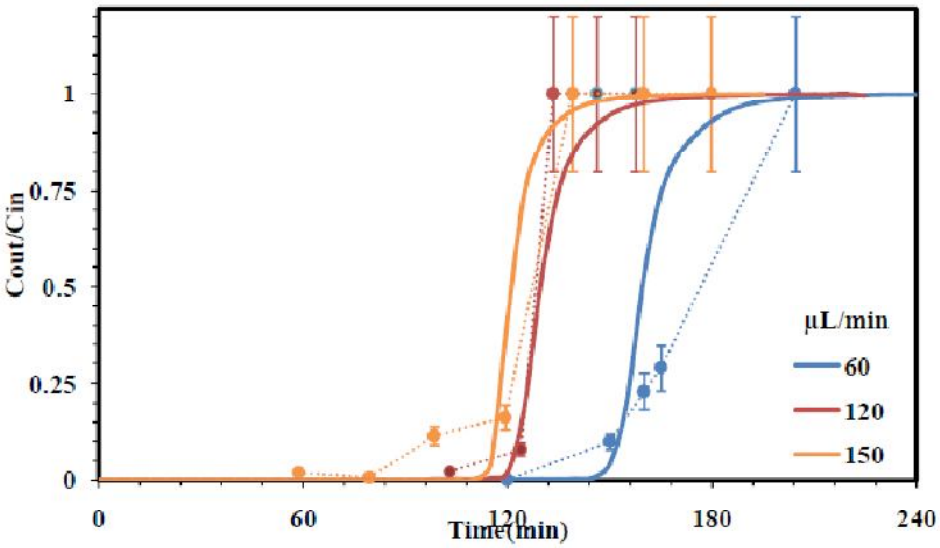


Figure 3: Effect of variation in the volumetric flow rates on the breakthrough concentrations

Fig. 3 shows plots for the model predicted curves (solid lines) and experimental data (dotted lines) for different flow rates (60,120,150 µL/min), inlet concentrations of 10^3 CFU/ml and channel dimensions of 50-D x 150-W $(\mu m)^2$. the breakthrough time decreased with increasing flowrates. The model predictions may be considered to be reasonably fitting well the data. At high volumetric flow rate, residence time is low. However, the contact time to kill E. coli is in micro-seconds. Therefore, the experiments should be performed at high volumetric flow rates.

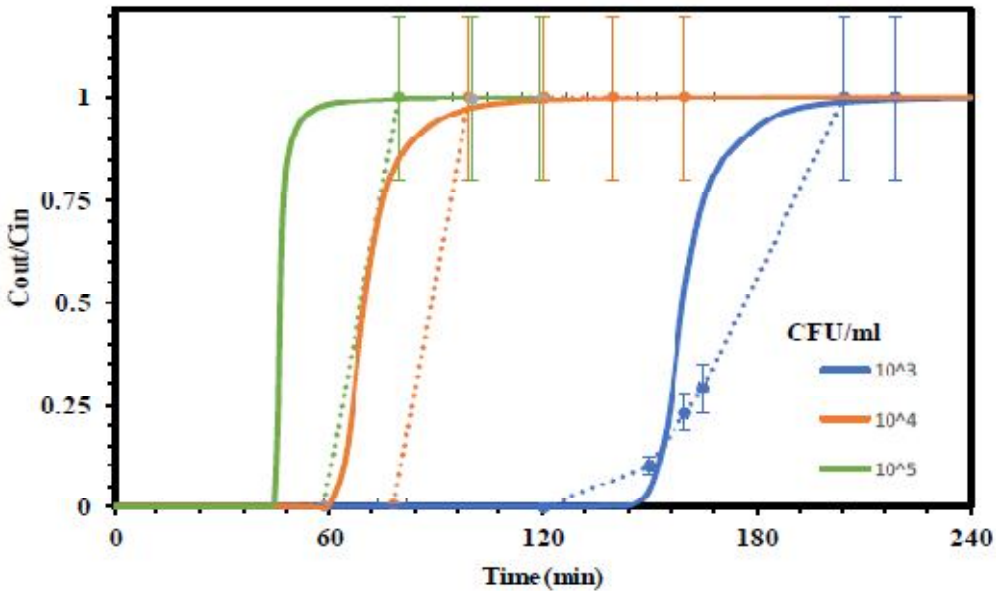


Figure 4: Effect of variation in the inlet bacterial concentrations on the breakthrough concentrations

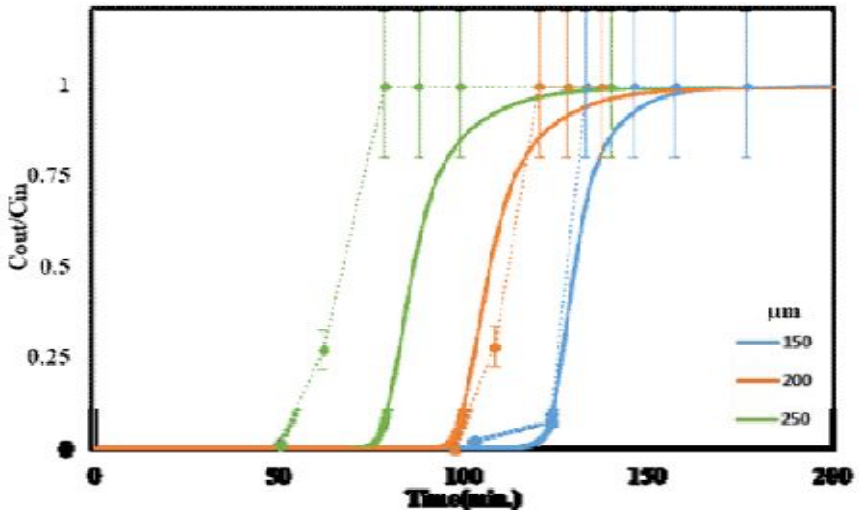


Figure 5: Effect of variation in the channel widths on the breakthrough concentrations at 120 µL/min flowrate

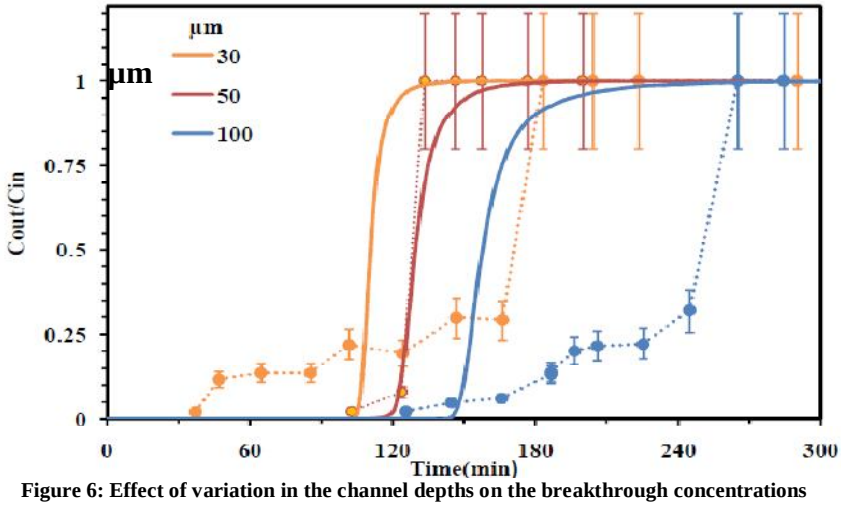


Figure 6: Effect of variation in the channel depths on the breakthrough concentrations

Figure 4 shows the effects of inlet bacterial concentrations. Water volumetric flow rate was set constant at 60µL/min in the channels of 50-D x 150-W $(\mu m)^2$ dimensions. The breakthrough times decreased with increasing inlet concentrations. Figure 5 shows the effects of channel widths for the model simulated inlet volumetric flow rate of 120 µL/min, inlet concentration of 10^3 CFU/ml and channel depth of 50 µm. By increasing width of the channel, total number of channels decreased and the ratio of surface area to volume decreased. Therefore, breakthrough times decreased. Fig. 6 shows the effects of channel depth for the inlet volumetric flow rate of 120 µL/min, inlet concentration of 10^3CFU/mL and channel width of 150 µm. By increasing depth of the channel, the surface area of channel walls increased, implying fluid had increased contact with the walls and diffusion cross-sectional area.

CONCLUSIONS

Microchannels were fabricated in the Ag-ACF/CNF-PVA nanocomposite film using laser ablation technique. Microchannels were used to control bacteria in water flowing in the channels via increased contact between the bacteria and Ag NPs through the porous walls of the microchannels. The microchannel geometry was designed using the Autodesk inventor, for different dimensions and successfully simulated using ANSYS Fluent, to predict RTD, velocity and pressure profiles. Different concentrations of E. coli solution used in the tests showed that the growth rate of E. coli exponentially increased with time. The growth rate (k_g) was calculated to be 0.0336 min^{-1} at 37 ^oC and pH 7.0. The growth rate data showed that the number of E. coli doubled at approximately 20 min intervals. The experiments also showed that the death rate decreased exponentially with time and the numerical value of death rate constant (k_1) was calculated to be 0.028 $mg^{-1}s^{-1}$. The model assumed the control of bacteria by Ag imprinted on the porous walls. It was also assumed that the E. coli concentrations increased with time. The modeled predictions were in qualitative agreement with the experimental measurements.