

Mechanistic Modeling of Non-Spherical Bacterial Attachment on Plant Surface Structures

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Abstract

Introduction: Bacterial attachment to the surface and passive internalization to fresh produce is the first step in contamination of food. Understanding the mechanism of attachment and internalization could lead to the prevention of future outbreaks on fresh fruits and vegetables (Figure 1). The goals of this model were to use a Lagrangian particle tracking simulation of a spherocylinder shaped bacteria, *Escherichia coli*, to simulate and validate rotational motion (Figure 2) and to determine the dominant forces and the effect plant surface structures have on attachment.

Use of COMSOL Multiphysics® software: The Particle Tracing Module with laminar flow and the wall distance physics were used to simulate bacterial movement in microfluidic devices created in COMSOL. The wall distance is necessary for calculating the relative position of particle to the wall for surface forces (such as DLVO). COMSOL only simulates spherical particles and so the movement of non-spherical was simulated by coding in the additional equations of motion and plotting done in MATLAB®.

Results: Bacterial rotation was first validated versus Jeffrey periods for rotation of non-spherical particles in a constant shear flow. Results showed excellent agreement with less than 1% difference between theoretical and model predictions. Next, rotation was validated versus experimentally tracked bacteria (Figure 2) in a complex shaped microfluidic device. Figure 3 shows a qualitative agreement with the experiment. The simulation showed that small perturbations in the initial cell position greatly influenced the rotational motion of the cells. With the translational and rotational motion of cells validated, the attachment was studied. Preliminary results show excellent agreement with experimental results that obstacles increase attachment while the majority of cells deposit laterally to the flow direction.

Conclusion: Implications of this research are that the model will determine the primary forces acting on cells and geometrical plant features that lead to cell attachment and internalization on plant surfaces. The understanding of physical mechanisms that lead to cell attachment and deposition will improve our understanding and help in developing mitigation strategies. Broader implications is that this model will help researchers in other fields develop understandings in particle, colloidal, and cell attachment, deposition, and internalization in non planar geometries with non-spherical particles.

Reference

Zeming, K.K., et. al. Rotational separation of non-spherical bioparticles using i-shaped pillar arrays in a microfluidic device. Nature communications 4;16:25(2013).

Figures used in the abstract

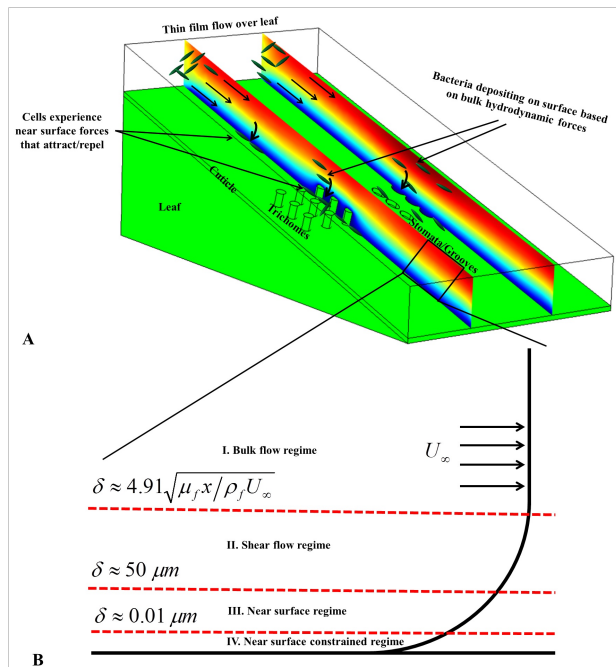


Figure 1: A) Schematic overview of bacteria flowing over a surface and attaching to trichomes and in grooves. B) Fluid flow regimes where cells experience various forces relative to the bulk and surface

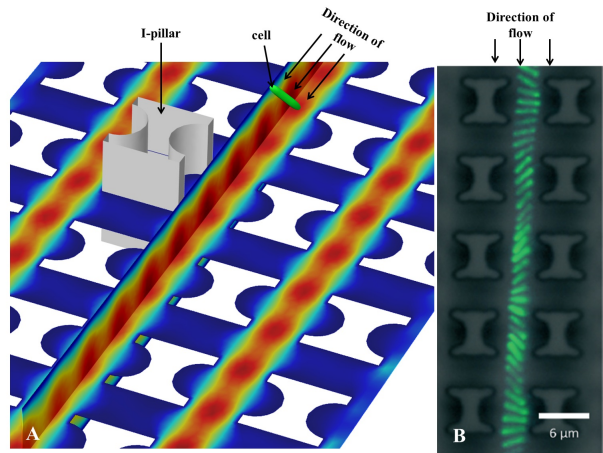


Figure 2: A) Model schematic of bacterial flow in I-pillar microfluidic device B) Experimental observations of bacterial rotation from (Zeming et al., 2013)

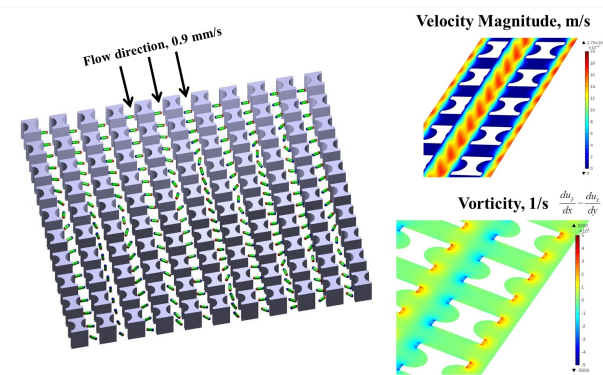


Figure 3: Validation of spherocylinder cells in a microfluidic device. a) Cells with the same orientation were randomly released from a 1 m cubic box. The initial cell velocity was 0.9 mm/s and each cell represents 1 ms in time. The results show how small perturbations in the initial position change the rotation of the cell. The cells show similar rotation to that of the experiment (Zeming et al., 2013). Unlike the experiment, the cells complete a revolution instead of reversing halfway through. Three possible explanations for this is the experimental geometry might have had defects, such as the rounded corners on the I-pillars (Zeming et al., 2013) b) or the magnitude of the repellant force on the surface not being uniform (Zeming et al., 2013). The velocity (b) and vorticity (c) show the high intensity flow in the center of the channel and high rate of shear near the corners of the pillars. The third possible explanation is that the cell in the model experiences the velocity and shear at its center while in the experiment, the cell experiences different velocities and shear along its axes. The cell is nearly the same size of the channel and the vorticity varies significantly from the center to the ends of the pillars likely creating non-uniform vorticity that could explain the discrepancy.

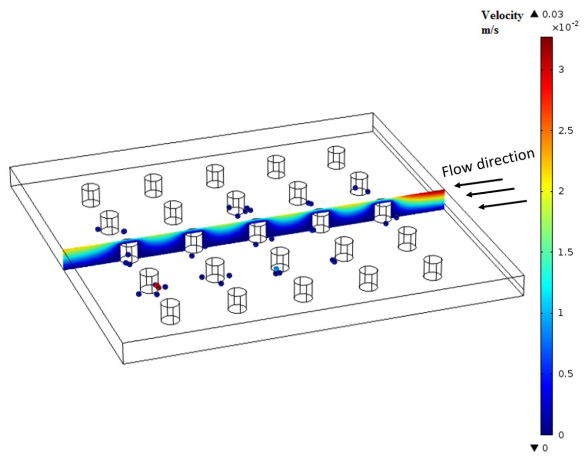


Figure 4: Preliminary results of cell attachment to trichomes. Legend is velocity magnitude