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Mechanistic understanding of non-spherical bacterial attachment and deposition on plant surface structures

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HIGHLIGHTS

- Simulation validated for translational and rotational motion.
- Trichomes decrease and stomata increase overall attachment.
- Attachment to trichomes predominately normal to flow.
- Attachment to stomata and grooves upstream and downstream of flow.

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ABSTRACT

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. The goal of this model was to validate and use a Lagrangian particle tracking simulation of a spherocylinder shaped bacteria, *Escherichia coli*, to determine the effect plant surface structures have on attachment. Rotation of the cells was validated versus theoretical and experimental data. Also, simulation results of attachment were validated versus experimentally measured cells to microfabricated plant structures: stomata, trichomes and grooves. The simulation results showed how trichomes decreased attachment by lowering shear stress within the microarray while stomata and grooves enhanced attachment by creating small regions of increased shear stress triggering shear enhanced adhesion. Microstructures affecting the local fluid shear stress, and not residence time, increased attachment.

1. Introduction

Since the 1980s, the consumption and demand for fresh produce has increased with the human population and (STAT, 2012) so too has the number of foodborne outbreaks in European countries, USA, Canada, and Japan (CDC, 2013; Cerroni et al., 2010). Bacterial attachment and internalization of fresh produce is an important problem as a means to begin initial contamination but also the spread from one piece of produce to another. Bacterial transport, attachment/adhesion to a surface, and detachment from a surface crosses many disciplines from engineering, physics, materials science, biology, micro and nanotechnology, and chemistry. Many applications of this important topic include biotechnology for membrane filtration (Picioreanu et al., 2009; Vrouwenvelder et al., 2010), civil engineering for clogging, oil recovery, and bioremediation of porous media such as soil (Durham et al., 2012; Zhang et al., 2010; Valiei et al., 2012; Tang et al., 2013), medicine for disease detection in microfluidic devices (Smith et al., 2014; Ranjan et al., 2014) and food safety (De La Fuente et al., 2007; Sirinutsomboon et al., 2011; Sirinutsomboon and Delwiche, 2013; Zhang et al., 2014). This work specifically focuses on the context of food safety but brings together work from other fields, such as cell capture and separation in microfluidic devices (Ge et al., 2015), to further the understanding of how, why, and where bacteria attach to fresh produce surfaces.

1.1. Organization of this manuscript

This article begins by discussing previous studies on how attachment is influenced by surface characteristics and then by describing how attachment works. The objectives are discussed before developing the Lagrangian particle tracking model. The model is then validated against literature, experimental data for

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Nomenclature

Symbols

$\vec{\vec{A}}$	transformation matrix
A_{ham}	Hamaker constant, J
C	force coefficient
$\vec{C}$	center of bead
d	diameter, m
D_p	diffusivity, $m^2\ s^{-1}$
D_h	hydraulic diameter, m
e	electron charge, C
E	energy, J
f	correction function
F	force, N
$\vec{g}$	gravity, $m\ s^{-2}$
G	shear rate, s^{-1}
ΔG	free energy, J
H	height, m
$\vec{I}$	moment of inertia, kg m^2
$\vec{\vec{I}}$	moment of inertia diagonal matrix, kg m^2
$\vec{\vec{I}}_0$	identity matrix
I_s	ionic strength, mol m^{-3}
k	spring constant, N m^{-1}
K_1,K_2	constant
k_B	Boltzmann constant, J K^{-1}
L	length, m
m	mass, kg
$\vec{n}$	normal vector
N	number of particles
N_A	Avogadro's number, mol^{-1}
P_1 P_2	attachment functions
p	pressure, Pa
Pe	Péclet number
$\vec{q}_i$	particle position vector
r	radius, m
$\vec{r}_{com-b}$	vector from particle center to bead
Re	Reynolds number
S	surface area, m^2
St	Stokes number
t	time, s
Δt	time step, s
T	temperature, K
u	velocity, m s^{-1}
U_∞	bulk velocity, m s^{-1}
V	volume, m^3
W	width, m
x, y, z	coordinate system

Greek Symbols

β	aspect ratio
$\vec{\Omega} = \left[\omega_{x'}, \omega_{y'}, \omega_{z'}\right]$	angular velocity
ϕ, ψ, θ	Euler angles
Φ	spherocity
δ	distance, m
δ	delta function
ρ	density, kg m^{-3}
ϵ	Euler parameters
σ	Eikonal equation smoothing parameter
τ	torque, N m
λ	decay length, m
ε	permittivity, F m^{-1}
μ	viscosity, Pa s
ϑ	wall collision parameter
Θ_c	contact angle, rad
π	constant
γ	interfacial energy, J m^{-2}
ζ	zeta potential, V
κ	Debye length, m^{-1}
ξ	random normal distributed coefficient
α_i	angle of incidence, rad

Subscripts

adh	adhesion
b	bead
$barr$	barrier
$buoy$	buoyancy
$Brown$	brownian
$chan$	channel
cop	center of pressure
$drag$	drag
eff	effective
eb	energy barrier
$elem$	element
eq	equivalent
f	fluid
g	gas
h	hydraulic
i, j, k, l	indice
l	liquid
$lift$	lift
n	normal
com	center of mass
min	minimum
p	particle
pg	pressure gradient
$post-collision$	post-collision
$pre-collision$	pre-collision
r	relative
rot	rotational
s	surface
$tang$	tangential
$trans$	translational
vm	virtual mass
w	wall
x, y, z	inertial coordinate system
x', y', z'	particle principle axis
x'', y'', z''	particle coordinate system
0	initial
1,2	labels
$\parallel$	parallel
$\perp$	perpendicular
∞	maximum, bulk, velocity at infinity

Superscripts

AB	Acid-base
$bulk$	bulk
EDL	electric double layer
$local$	local
VdW	van der Waals