Bacterial Interactions and Transport in Unsaturated Porous Media

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Potential groundwater contamination with pathogens

Wastewater reclamation for irrigation

- In California, 60% of recycled wastewater used for irrigation

Animal waste applications

- In US, approximately 1.3 billion tons of animal manure generated annually
- Land applications
St Mark River

Fecal Coliform
16 ~ 100/100 ml
Vision of Animal Waste Management

• Challenged with finding a balance between land applications and environmental protection

• Provide education and training in growth biology, efficient nutrient management and environmental protection

• Solid theoretical background in Agricultural Engineering, Biological System Engineering and Environmental Science & Engineering, etc., focusing on applications
Objectives

• Bacterial interaction quantification

• Bacterial transport model structures and formulations

• Surface thermodynamic characterization applications
**Bacterial Strain**

**E. Coli HB101**

A plasmidless non-fimbriated bacterium, obtained from ATCC (33694)
Bacterial Strain

*P. fluorescens*  
*B. subtilis*

Obtained from ATCC (17559 and 6051a)
Bacterial Surface Property Quantification

\( \gamma_{\text{LW}} \) – Liftshitz-van der Waals component surface tension (mJ/m\(^2\))
\( \gamma^+ \) – Electron-acceptor parameter of Lewis acid/base component surface tension (mJ/m\(^2\))
\( \gamma^- \) – Electron-donor parameter of Lewis acid/base component surface tension (mJ/m\(^2\))
\( \zeta \) – Zeta potential (mV)
van Oss-Chaudhury-Good Equation

Solve for $\gamma_{S}^{LW}$, $\gamma_{S}^{+}$ and $\gamma_{S}^{-}$

\[
(1 + \cos \theta)\gamma_{L} = 2\left(\sqrt{\gamma_{S}^{LW}\gamma_{L}^{LW}} + \sqrt{\gamma_{S}^{+}\gamma_{L}^{-}} + \sqrt{\gamma_{S}^{-}\gamma_{L}^{+}}\right)
\]

\[
\begin{align*}
(1 + \cos \theta_{1})\gamma_{1} &= 2\left(\sqrt{\gamma_{S}^{LW}\gamma_{1}^{LW}} + \sqrt{\gamma_{S}^{+}\gamma_{1}^{-}} + \sqrt{\gamma_{S}^{-}\gamma_{1}^{+}}\right) \\
(1 + \cos \theta_{2})\gamma_{2} &= 2\left(\sqrt{\gamma_{S}^{LW}\gamma_{2}^{LW}} + \sqrt{\gamma_{S}^{+}\gamma_{2}^{-}} + \sqrt{\gamma_{S}^{-}\gamma_{2}^{+}}\right) \\
(1 + \cos \theta_{3})\gamma_{3} &= 2\left(\sqrt{\gamma_{S}^{LW}\gamma_{3}^{LW}} + \sqrt{\gamma_{S}^{+}\gamma_{3}^{-}} + \sqrt{\gamma_{S}^{-}\gamma_{3}^{+}}\right)
\end{align*}
\]
Interaction Free Energy Calculation

\[ \Delta G_{132}^{\text{TOT}} = \Delta G_{132}^{\text{LW}} + \Delta G_{132}^{\text{AB}} + \Delta G_{132}^{\text{EL}} \]

\[ \Delta G(y)_{132}^{\text{LW}} = -4\pi \frac{y_0^2}{y} R[(\sqrt{\gamma_3^{\text{LW}}} - \sqrt{\gamma_2^{\text{LW}}})(\sqrt{\gamma_3^{\text{LW}}} - \sqrt{\gamma_1^{\text{LW}}})] \]

\[ \Delta G(y)_{132}^{\text{AB}} = 4\pi R y_0 e^{(y-y_0)/\lambda} [(\sqrt{\gamma_1^{+}} - \sqrt{\gamma_2^{+}})(\sqrt{\gamma_1^{-}} - \sqrt{\gamma_2^{-}}) - (\sqrt{\gamma_1^{+}} - \sqrt{\gamma_3^{+}})(\sqrt{\gamma_1^{-}} - \sqrt{\gamma_3^{-}}) - (\sqrt{\gamma_2^{+}} - \sqrt{\gamma_3^{+}})(\sqrt{\gamma_2^{-}} - \sqrt{\gamma_3^{-}})] \]

\[ \Delta G(y)_{132}^{\text{EL}} = \pi\varepsilon\varepsilon_0 R[2\psi_1\psi_2 \ln\left(\frac{1+e^{-\kappa y}}{1-e^{-\kappa y}}\right) + (\psi_1^2 + \psi_2^2) \ln(1-e^{-2\kappa y})] \]
Contact Angle Measurement

A : Moisture-controlled Chamber
B : Sample platform
C : Syringe holder
D : Camera with imaging lens
E : Light source

Contact Angle > 90°

Contact Angle < 90°
Wicking Method

Washburn Equation

\( h^2 = \left( R_e \cdot t \cdot \gamma_L \cdot \cos \theta \right) \cdot \left( 2 \cdot \mu \right)^{-1} \)

- \( h \) : height of capillary rise (m)
- \( R_e \) : average interstitial pore size (m)
- \( t \) : measuring time (sec)
- \( \gamma_L \) : Measuring liquid surface tension (mJ/m\(^2\))
- \( \mu \) : measuring liquid viscosity (N·s/m\(^2\))

Kruss K100 Tensiometer
Column Experiment

Bacterial Suspension

Luciferin & Luciferase

Syringe Pump

Column

Luminometer
**ATP Measurement**

Luciferin + ATP + O$_2$ $\xrightarrow{\text{Luciferase, Mg}^2+}$ Oxyluciferin + AMP + CO$_2$ + PP$_i$ + Light (560 nm)
$S_e = \left[ 1 + (\alpha h)^n \right]^{(1/n-1)}$

$\alpha$: inverse of the air-entry potential (m$^{-1}$)

$h$: water potential (m-H$_2$O)

$n$: parameter related to pore size distribution (-)

$\alpha = 0.136$ cm$^{-1}$

$n = 4.776$
Bacterial Transport Modeling

\[
\frac{\partial}{\partial t} [\theta_m C] = \frac{\partial}{\partial z} [D_z \theta_m \frac{\partial C}{\partial z}] - \frac{\partial}{\partial z} [qC] - k_1 \theta_m C + k_{\text{des}} \frac{\rho_b S}{S_e} C_r
\]

\[
\frac{\partial C_r}{\partial t} = k_1 \frac{\theta_m S_e}{\rho_b S} C - k_{\text{des}} C_r
\]

C — bacterial concentration in the solution (cells/m\(^3\))
Cr — retained bacterial concentration [cells/(g)(m\(^2\)/m\(^3\))]  
D\(_z\) — apparent dispersion coefficient (m\(^2\)/sec)  
\(\theta_m\) — moisture content (m\(^3\)/m\(^3\))  
q — specific discharge (Darcian fluid flux) (m/sec)  
k\(_1\) — deposition coefficient (sec\(^{-1}\))  
k_{\text{des}} — desorption coefficient (sec\(^{-1}\))  
\(\rho_b\) — bulk density (g/m\(^3\))  
S — air-water interfacial area (m\(^2\)/m\(^3\))
Bacterial Retention Mechanism
Bacterial Retention Mechanism

Liquid-Gas Interface

Attractive Interaction with Liquid-Gas Interface

Flow Direction

Medium Surface

Repulsive Interaction with Medium Surface

c

Liquid

Attractive Interaction with Liquid-Gas Interface

Flow Direction

Medium Surface

Attractive Interactions with Medium Surface

d
### Bacterial Interactions with Porous Media

<table>
<thead>
<tr>
<th></th>
<th>$\Delta G_{132}^{\text{LW}}$ (kT)</th>
<th>$\Delta G_{132}^{\text{AB}}$ (kT)</th>
<th>$\Delta G_{132}^{\text{EL}}$ (kT)</th>
<th>$\Delta G_{132}^{\text{LW+AB+EL}}$ (kT)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>E. coli</strong></td>
<td>-36.3</td>
<td>1234.8</td>
<td>17.8</td>
<td>1216.3</td>
</tr>
<tr>
<td><strong>P. fluorescens</strong></td>
<td>-17.6</td>
<td>649.6</td>
<td>0.48</td>
<td>632.5</td>
</tr>
<tr>
<td><strong>B. subtilis</strong></td>
<td>-119.6</td>
<td>3023.4</td>
<td>467.0</td>
<td>3370.8</td>
</tr>
</tbody>
</table>

$k$ is the Boltzmann constant ($1.38 \times 10^{-23}$ J/K) and $T$ is absolute temperature (K). At $25^\circ C$, $1\, kT = 4.11 \times 10^{-21}$ J.

$\Delta G_{132}^{\text{LW}}$, $\Delta G_{132}^{\text{AB}}$ and $\Delta G_{132}^{\text{EL}}$ evaluated at the equilibrium distance where physical contact between bacteria and media surface and between bacteria and air-water interface occurred.
### Bacterial Interactions with Air-Water Interface

<table>
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<th>(\Delta G_{132}^{\text{LW}}) (kT)</th>
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<th>(\Delta G_{132}^{\text{LW+AB+EL}}) (kT)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>E. coli</strong></td>
<td>-7146.9</td>
<td>-3030.0</td>
<td>1481.1</td>
<td>-8695.8</td>
</tr>
<tr>
<td><strong>P. fluorescens</strong></td>
<td>-4080.2</td>
<td>-1726.5</td>
<td>917.3</td>
<td>-4889.4</td>
</tr>
<tr>
<td><strong>B. subtilis</strong></td>
<td>-19845.9</td>
<td>-6740.9</td>
<td>2611.6</td>
<td>-23975.2</td>
</tr>
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\(k\) is the Boltzmann constant \((1.38 \times 10^{-23} \text{ J/K})\) and \(T\) is absolute temperature (K). At 25\(^\circ\)C, 1 kT = \(4.11 \times 10^{-21} \text{ J}\).

\(\Delta G_{132}^{\text{LW}}, \Delta G_{132}^{\text{AB}}\) and \(\Delta G_{132}^{\text{EL}}\) evaluated at the equilibrium distance where physical contact between bacteria and media surface and between bacteria and air-water interface occurred.
Bacterial Retention Mechanism

Water

Air

Immobile Region

Mass Transfer

Solid medium

$G_{132}^{TOT} \text{ (Air-Water)}$

$G_{132}^{TOT} \text{ (Media)}$

Mobile Region
Bacterial Breakthrough Curve

$S_e = 0.8$
- P. fluorescens
- E. coli
- B. subtilis

$S_e = 0.6$
- P. fluorescens
- E. coli
- B. subtilis

$S_e = 0.4$
- P. fluorescens
- E. coli
- B. subtilis

$C/C_s$ vs Pore Volume
Deposition and Bacterial Interactions

\[ \Delta G_{132}^{\text{TOT}} \text{ (air-water)} + \Delta G_{132}^{\text{TOT}} \text{ (media)} \] (kT)

- P. fluorescens
- E. coli
- B. subtilis
Air-Water Interfacial Area

\[
S = \frac{\rho g}{\alpha \gamma} \int_{\theta_0}^{\theta} \left[ \left( \frac{\theta}{\theta_0} \right)^{1-n} - 1 \right]^n d\theta
\]
Deposition and Interfacial Area

- **P. fluorescens**
- **E. coli**
- **B. subtilis**

**Air-Water Interfacial Area (cm\(^2\)/cm\(^3\))**

- 80
- 90
- 100
- 110
- 120

**\( k_1 \) (min\(^{-1}\))**

- 0
- 1
- 2
- 3
- 4

**Air-Water Interfacial Area (cm\(^2\)/cm\(^3\))**

**\( k_1 \) (min\(^{-1}\))**

- 0
- 1
- 2
- 3
- 4
Desorption and Bacterial Interactions

$\Delta G_{132}^{TOT}$ (media) (kT)

$\text{k}_{\text{des}}$ (min$^{-1}$)

- $P. \text{fluorescens}$
- $E. \text{coli}$
- $B. \text{subtilis}$
Acknowledgements

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Questions?