Modeling surface active solute transport with HYDRUS

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Surface Active Solute

Surface Active Agent – Surfactant

Substance which reduces surface/interfacial tension between two phases

http://www.attension.com/critical-micelle-concentration

Young–Dupré equation

\[ \gamma_{LV} \cos \omega = \gamma_{SV} - \gamma_{SL} \]

Young–Laplace equation

\[ \Psi = \frac{2 \gamma \cos \omega}{\rho g r} \]

\[ \frac{\Psi_1}{\gamma_1 \cos \theta_1 r_1} = \frac{\Psi_0}{\gamma_0 \cos \theta_0 r_0} \]

\[ \Psi_1 = \Psi_0 \left( \frac{\gamma_1}{\gamma_0} \right) \left( \frac{\cos \theta_1}{\cos \theta_0} \right) \]
Capillary pressure vs. Surface tension/contact angle

\[ \Psi = \Psi_0 \left( \gamma \left( \cos \theta_0 \right) \right) \cdot \frac{1}{a_0} \left[ \frac{1}{S^{m_1 - 1}} \right] \]

Capillary pressure vs. contact angle

\[ \Psi = \Psi_0 \left( \gamma \left( \cos \theta_0 \right) \right) \cdot \frac{1}{a_0} \left[ \frac{1}{S^{m_1 - 1}} \right] \]

Surface tension vs. surfactant concentration

\[ \frac{\gamma}{\gamma_0} = 1 - b \ln \left( \frac{c}{a} + 1 \right) \]

Unsaturated Transient Water Flow and Solute Transport

[Images and graphs related to water flow and surfactant concentration]
**Viscosity vs. surfactant concentration**

![Graph showing viscosity vs. surfactant concentration](Image)

\[ \frac{D_1}{D_0} = 1 - B_1 \ln \left( \frac{C}{B_2} + 1 \right) \]

(Read and Gregory, 1997)

**Solute transport dependent hydraulic properties**

![Graph showing solute transport dependent hydraulic properties](Image)

\[ \frac{\partial \psi}{\partial t} + \frac{\partial \psi}{\partial x} \left[ k \left( \frac{\partial \psi}{\partial x} + \cos \omega \right) \right] = -S \]

\[ S = \frac{\partial \psi}{\partial t} + \frac{\partial \psi}{\partial x} \left( 1 + \frac{\partial \psi}{\partial x} \right) \]

\[ K(S) = K_0 S^2 \left( 1 - \left( 1 - S^{1/4} \right)^2 \right) \]

\[ \psi_i = \psi_0 \left[ \left( \frac{C_i}{C_0} \right)^{\frac{1}{\gamma_i}} \left( \cos \theta_i \right) \right]^{1} \left[ \frac{1}{S_i - 1} \right] \]

\[ T_0 = 0, \quad T_1 = 0.0007, \quad T_2 = 0.05, \quad T_3 = 4.05, \quad T_4 = 300 \text{ sec} \]

**Profile Information:**

- **Pressure Head:**
  - T0: -10
  - T1: -5
  - T2: 0
  - T3: 15
  - T4: 30

- **Water Content:**
  - T0: 0
  - T1: 0.2
  - T2: 0.4
  - T3: 0.6
  - T4: 0.8

- **Hydraulic Conductivity:**
  - T0: 0
  - T1: 0.1
  - T2: 0.2
  - T3: 0.3
  - T4: 0.4

- **Concentration:**
  - T0: 0
  - T1: 0.1
  - T2: 0.2
  - T3: 0.3
  - T4: 0.4

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**Smith and Gillham (1994)**
Future work:
- Incorporating additional empirical and/or physically-based equations to HYDRUS 1D
- Modification of HYDRUS 2D/3D

Implications:
- Root exudates, humic substances, DOM and commercial surfactants
- Rhizosphere
- Soil amendment with recycled biosolids
- Organic soilless media
- Drip irrigation
- Evaporation and/or transpiration

Thank you for your attention