HWRS 505: Vadose Zone Hydrology

Lecture 23

11/19/2024

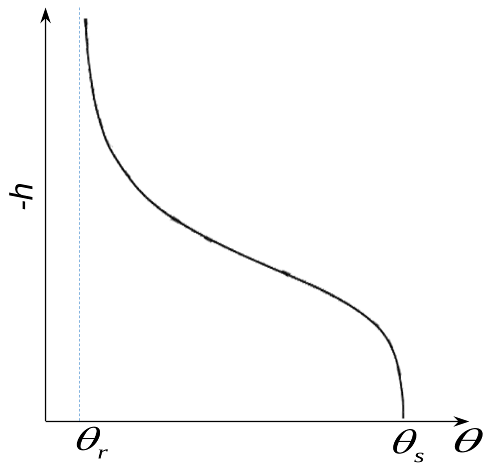
Review of Lecture 22

- PFAS is a large family of compounds (> 12,000)
- Unique properties of PFAS
- Occurrences in the environment
- Regulation (PFAS vs. other contaminants)
- Conceptual and physical model for PFAS transport in the vadose zone

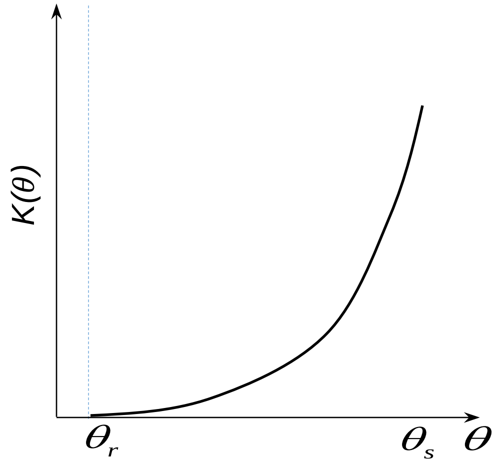
Modeling PFAS Transport in the Vadose Zone

Variably saturated flow in the vadose zone

$$\frac{\partial\theta}{\partial t} - \frac{\partial}{\partial z}\left[K\left(\frac{\partial h}{\partial z} - 1\right)\right] = 0,$$



SWC



$K-\theta$

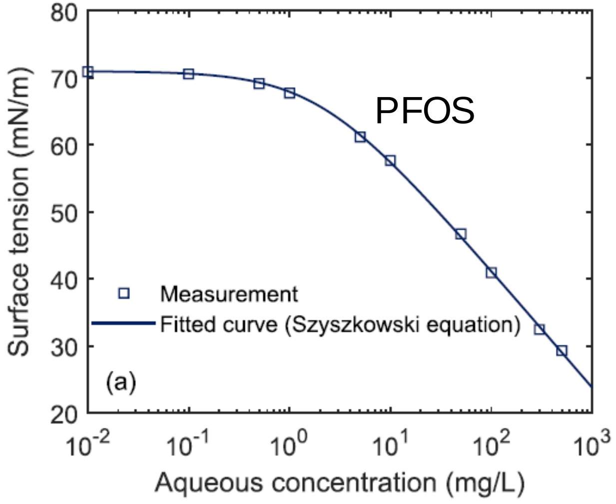
PFAS dissolving in water changes surface tension

$$\sigma = \sigma_0[1 - b\ln(1 + \frac{C}{a})]$$

PFAS concentration

Surface tension of water w/o PFAS

Fitting parameters



Question: Will the SWC and $K-\theta$ change in the presence of PFAS? If so, how?

Modeling PFAS Transport in the Vadose Zone

Let's employ the capillary tube model to think about the problem

w/o PFAS

$$-h_0 = \frac{2\sigma_0 \cos\gamma_0}{\rho g r}$$

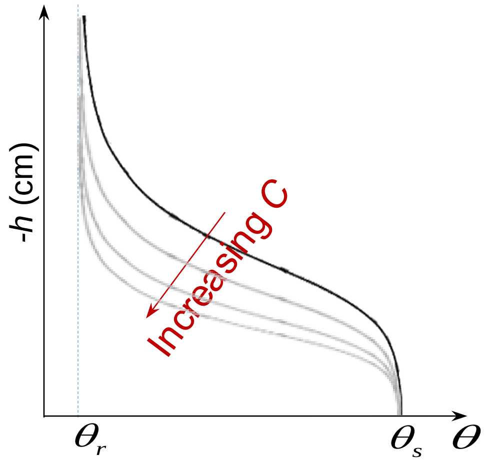
w/ PFAS

$$-h = \frac{2\sigma \cos\gamma}{\rho g r}$$

$$\Rightarrow h = \frac{\sigma \cos\gamma}{\sigma_0 \cos\gamma_0} h_0$$

$$\Rightarrow \theta = \begin{cases} \theta_r + \dfrac{\theta_s - \theta_r}{\left[1 + \left(\dfrac{\sigma_0 \cos\gamma_0}{\sigma \cos\gamma} \alpha |h|\right)^n\right]^m}, h < 0 \\ \theta_s, h \geq 0 \end{cases}$$

Scaling factor



Insights:

(1) We can think of this as PFAS modifies the α in the V-G model.

$$\alpha_{\text{modified}} = \frac{\sigma_0 \cos\gamma_0}{\sigma \cos\gamma} \alpha$$

(2) Now, the variably saturated flow depends on PFAS transport.

Modeling PFAS Transport in the Vadose Zone

PFAS transport in variably unsaturated flow (neglecting the interactions among PFAS)

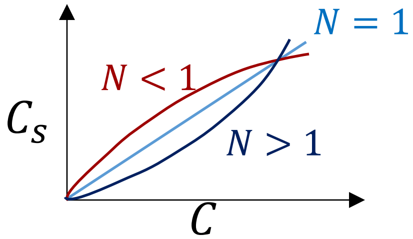
Advection Dispersion

$$\frac{\partial(\theta C)}{\partial t} + \rho_b \frac{\partial C_s}{\partial t} + \frac{\partial C_{aw}}{\partial t} + \frac{\partial}{\partial z}(\theta v C) - \frac{\partial}{\partial z}\left(\theta D \frac{\partial C}{\partial z}\right) = 0,$$

Storage in the aqueous phase

Storage in the solid-phase adsorption

Storage in the air-water interfacial adsorption



Solid-phase adsorption

$$C_s = K_f C^N$$

Air-water interfacial area

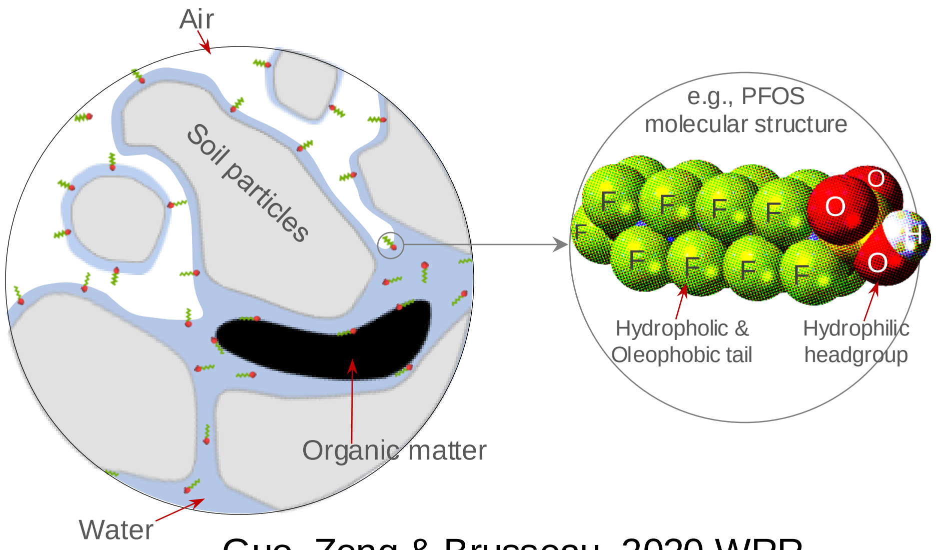
Air-water interfacial adsorption

$$C_{aw} = \Gamma A_{aw} = K_{aw} C A_{aw} \qquad \sigma = \sigma(C)$$

Szyszkowski equation

$$K_{aw} = \frac{\Gamma}{C} = -\frac{1}{RTC}\left(\frac{\partial \sigma}{\partial \ln C}\right)_T$$

$$\Rightarrow K_{aw} = \frac{1}{RT}\frac{\sigma_0 b}{a + C}$$



Guo, Zeng & Brusseau. 2020 WRR

Modeling PFAS Transport in the Vadose Zone

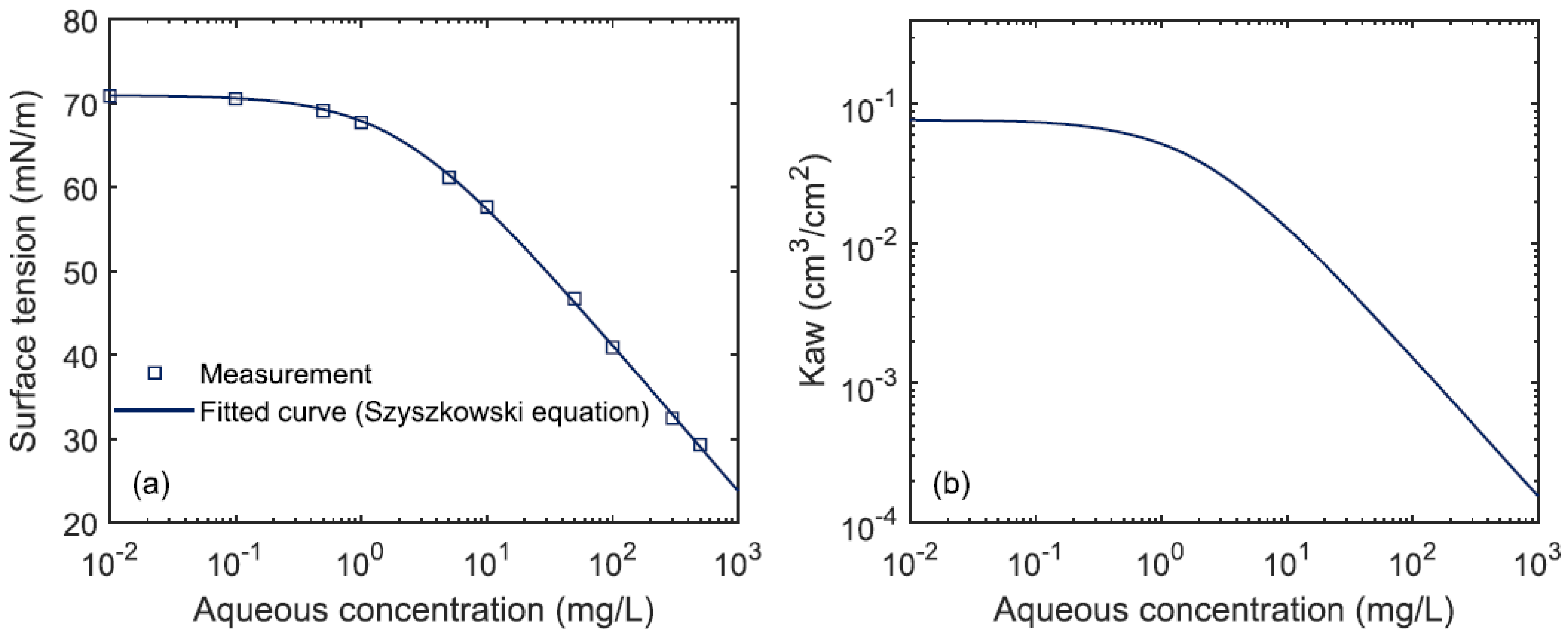


Figure 3. (a) Measured surface tension as a function of the aqueous concentration of PFOS. The solid line is a fitted curve using the Szyszkowski equation. (b) The computed air-water interfacial adsorption coefficient (K_{aw}) as a function of the aqueous concentration of PFOS.

Guo, Zeng & Brusseau. 2020 WRR