Progressive methods for investigation of migration of pharmaceuticals in soils

M. Klučáková and P. Závodská

Faculty of Chemistry, Brno University of Technology, Purkyňova 118 Brno, 612 00, Czech Republic

(e-mail: klucakova@fch.vutbr.cz)

Introduction

the migration of pharmaceuticals in soils = important role in toxicity and bioavailability

knowledge of transport behaviour essential for the prediction of their biotoxicity

soil "self-cleaning" ability related to the organic matter = immobilization = stable complexes

decrease in concentration of free mobile drugs = decrease in ability to enter into environment

Experimental

humic acids (HA) = representant of organic matter

sulphapyridyne (SPY) = representant of antibiotics

diffusion experiments *in situ* and model hydrogels

agarose hydrogel enriched by HA and HA hydrogels

c = concentration
c_s = concentration at interface
m_t = total diffusion flux in time t
x = distance from interface
D = diffusion coefficient
L = thickness of hadrogel layer
ε = partition coefficient
S = area
n = SPY pulse at interface

Eq. (1)
$$m_t = 2 \cdot c_s \cdot \sqrt{\frac{D \cdot t}{\pi}}$$

Eq. (2)
$$c = c_s \cdot \operatorname{erfc} \frac{x}{2 \cdot \sqrt{D \cdot t}}$$

Eq. (3)
$$\vec{J} = -D \cdot \varepsilon \cdot \frac{\Delta c}{L}$$

Eq. (4)
$$c = \frac{n}{S \cdot \sqrt{\pi \cdot D \cdot t}} \cdot \exp\left(-\frac{x^2}{4 \cdot D \cdot t}\right)$$

Eq. (5)
$$\ln c = \ln \frac{n}{S \cdot \sqrt{\pi \cdot D \cdot t}} - \frac{x^2}{4 \cdot D \cdot t}$$

diffusion from constant source
cuvette filled by hydrogel immersed in saturated solution

diffusion couple
donor SPY hydrogel connected with pure acceptor hydrogel

diffusion cells
hydrogel between donor and acceptor compartments

diffusion from instantaneous planar source
filter paper saturated by SPY as source for hydrogel

in situ
soil column in real conditions (filter paper …)

Results & Discussion

Results obtained for agarose hydrogel allows to differentiate between the effects of porous structure of hydrogel and interactions between HA and SPY.

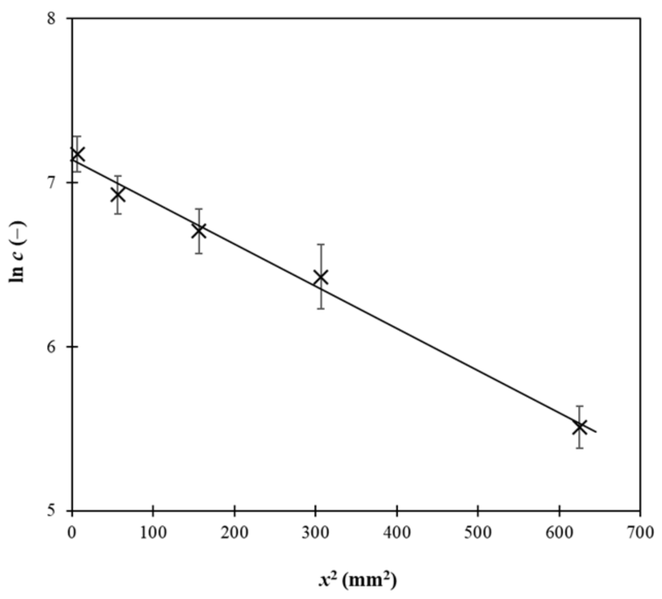
The D values obtained for pure inert hydrogel:

$(1.01 \pm 0.05) \times 10^{-10}$ m^2 s^{-1} (diffusion couple);

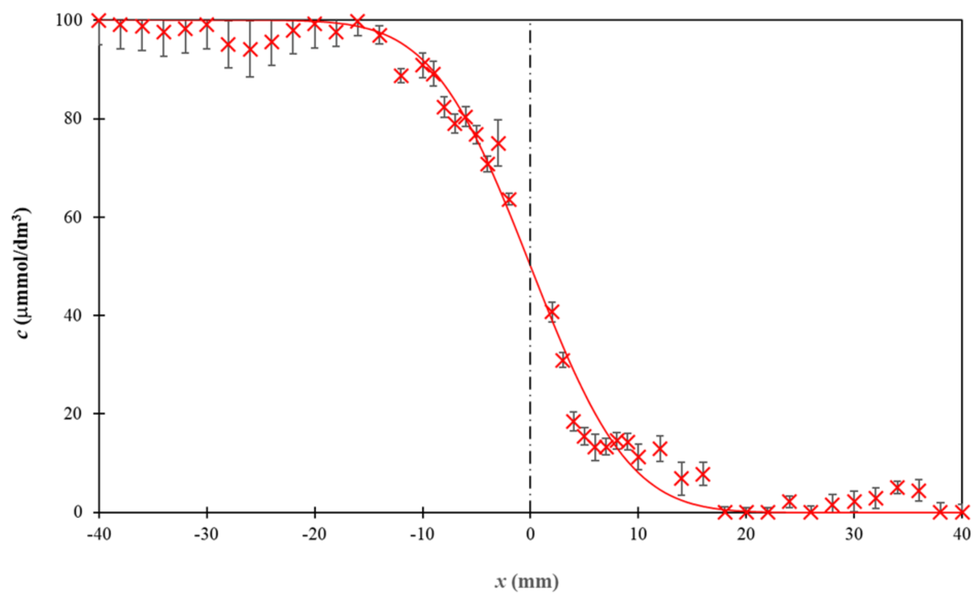
$(4.60 \pm 0.21) \times 10^{-10}$ m^2 s^{-1} (constant source);

$(4.93 \pm 0.38) \times 10^{-10}$ m^2 s^{-1} (diffusion cells).

matrix	method	diffusion coefficient (m^2 s^{-1})
enriched agarose hydrogel	diffusion couple	$(9.85 \pm 0.47) \times 10^{-11}$
	constant source	$(3.40 \pm 0.13) \times 10^{-10}$
	diffusion cells	$(4.49 \pm 0.12) \times 10^{-10}$
humic hydrogel	instantaneous planar source	$(4.38 \pm 0.29) \times 10^{-10}$
soil	*in situ*	$(4.23 \pm 0.27) \times 10^{-10}$



The example of experimental data fitting using Eq. (5).



The example of experimental profiles for diffusion couple after 72 h fitted by Eq. (2).

Comparing with D value (2.03×10^{-9} m^2 s^{-1}) for the diffusion of SPY in aqueous solution (10.1016/j.arabjc.2013.12.009), the decrease caused by the pore structure is observed.

The HA addition in porous hydrogel resulted in the additional decrease in D value caused by the interaction between SPY and HA and immobilization of SPY in hydrogel structure.

Conclusions

Both model mediums (agarose hydrogel enriched by HA and HA hydrogel) can provide practically the same results as *in situ* measurements in soil, if a suitable experimental method is chosen. This finding is very usable for a prediction of the behaviour of SPY and pharmaceuticals (and other pollutants) in soil environments.

This project is supported by: The NATO **Science** for **Peace** and **Security** Programme

https://land-security.org/
Nr. G6296