Identification of transport and clogging parameters of porous media

ICMM

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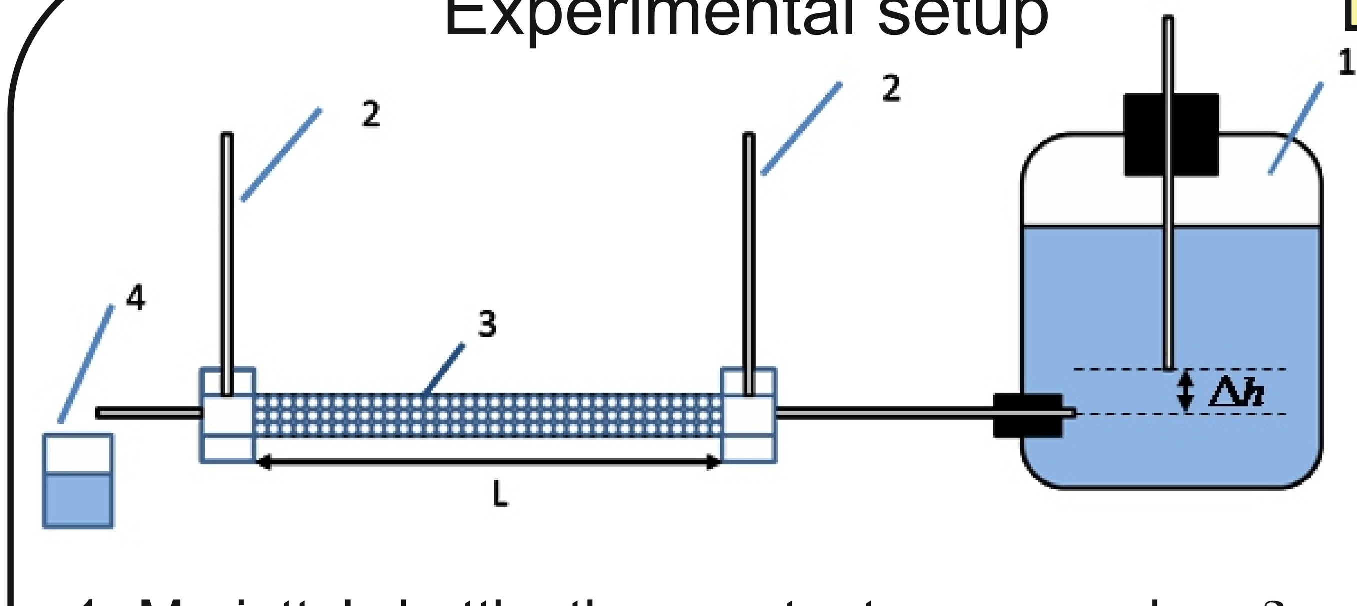
Abstract: In this work, the process of solute transport through a porous medium is experimentally studied. The experimental setup is constructed from a copper tube filled with a porous medium. Glass balls are used as porous filler. Distilled water is pumped through the tube, pumping is carried out with a initial constant pressure drop between the inlet and outlet. A pumping of constant concentration NaCl solution starts in initial time moment. Simultaneously, the measurement of NaCl concentration and mixture flow rate at the outlet begins. The measurement is carried out continuously until the registration zero concentration and constant flow rate. To estimate the transport parameters of the medium, a one-dimensional problem of the solute transport was solved numerically. It was assumed that the permeability is an unambiguous function of the porosity of the medium. To model this dependence, the Kozeny-Karman relation was used. The solute transport was modeled within the MIM approach. It was assumed that in this case the porosity of the medium decreases in proportion to the volume concentration of the adsorbed solute. Based on the comparison of the experimental data with the data obtained in the course of numerical simulation, we solve inverse problem of identifying the transport parameters of the medium. The work was supported by the Russian Science Foundation (Grant No. 20-11-20125)

The experiment

Experimental setup

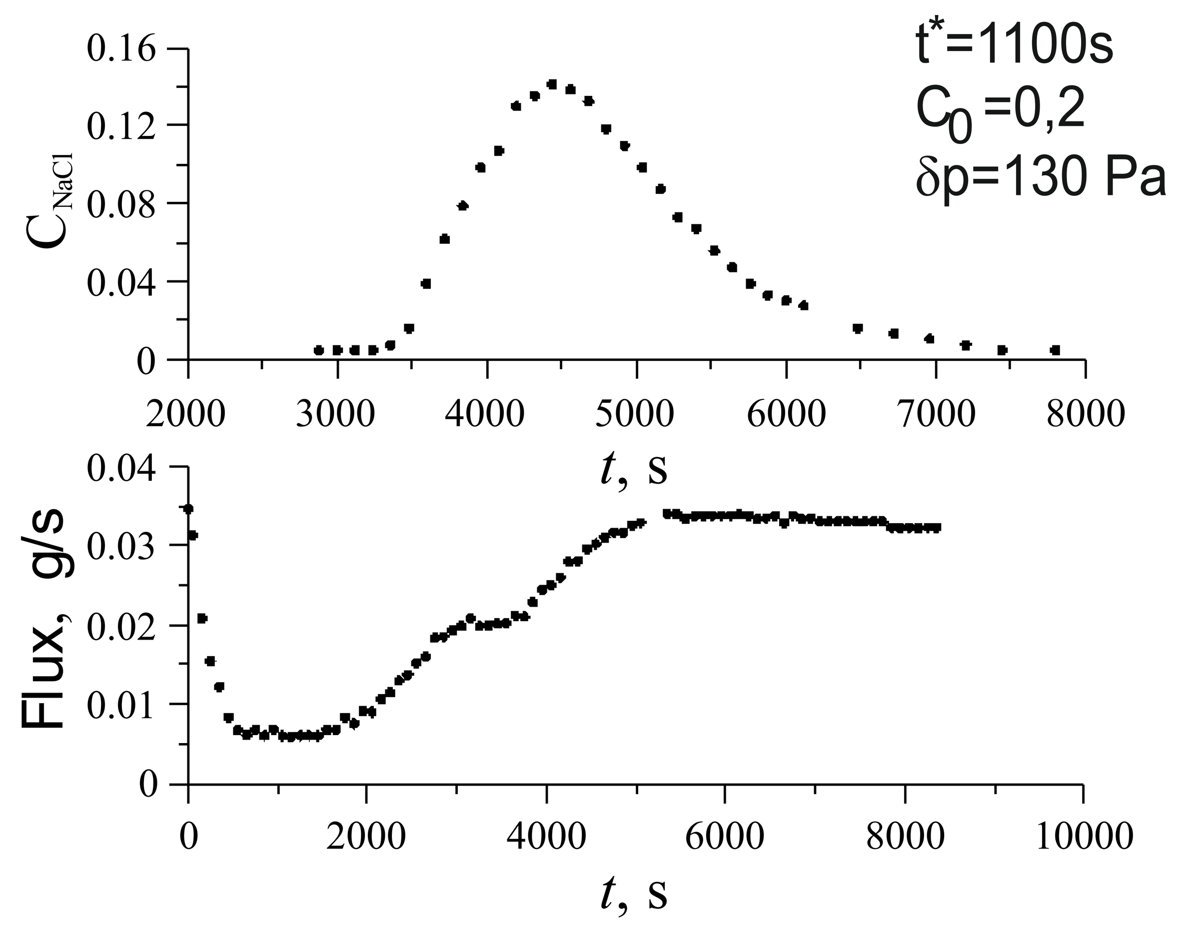


1- Mariotte's bottle, the constant pressure drop $\delta p=\rho g \Delta h$
2- Manometric tubes
3- Working domain with porous media, porosity 0.365, length L=392 mm, diametr 15.6mm
4- The outlet container

Description

The salt water with mass m=27g and salt concentration C_0 is injected to saturated porous media during the time t^*. After time t^* the concetration of salt becomes 0. The salt concentration and mass flux is mesured at outlet.

Resulted plots



The modelling of experiment

MIM approach with clogging

$$\operatorname{div}\mathbf{u}=0,\quad \mathbf{u}=-\frac{\kappa(\varphi)}{\eta}\nabla p,$$

$$\frac{\partial(\varphi c+q)}{\partial t}=-\mathbf{u}\cdot\nabla c+D\nabla(\varphi\nabla c),$$

$$\frac{\partial q}{\partial t}=a(q_0-q)c-bq.$$

$$\varphi=\varphi_0-q,\quad \kappa(\varphi)=K\frac{\varphi^3}{(1-\varphi)^2},$$

φ — porosity, φ_0 — porosity of clean media,
K — Carman-Kozeny constant,
$\mathbf{u}$ — filtration velocity, p — pressure
c,q — mobile and immobile concentrations,
κ — permeability, D — diffusivity,
a,b — adsorption and desorption rates,
q_0 — saturation of immobile concentration.

Weak clogging assumption (1D problem)

$$\operatorname{div}\mathbf{u}=0=-\frac{\kappa}{\eta}\frac{\partial^2 p}{\partial x^2}+\frac{1}{\eta}\frac{\partial\kappa}{\partial\varphi}\frac{\partial q}{\partial x}\frac{\partial p}{\partial x},\quad \frac{\partial q}{\partial t}=a(q_0-q)c-bq,$$

$$\varphi\frac{\partial c}{\partial t}+(1-c)\frac{\partial q}{\partial t}=\frac{\kappa}{\eta}\frac{\partial p}{\partial x}\frac{\partial c}{\partial x}+D\frac{\partial q}{\partial x}\frac{\partial c}{\partial x}+\varphi D\frac{\partial^2 c}{\partial x^2},$$

$$q\to q_0 q,\quad c\to c_0 c,\quad z=\frac{q_0}{\varphi_0},\quad \varphi=\varphi_0(1-zq)\Rightarrow$$

$$\frac{\partial^2 p}{\partial x^2}=\left[\frac{1}{\kappa}\frac{\partial\kappa}{\partial\varphi}\frac{\partial q}{\partial x}\right]\frac{\partial p}{\partial x},\quad \frac{\partial q}{\partial t}=ac_0(1-q)c-bq,$$

$$(1-zq)\frac{\partial c}{\partial t}+z\left(\frac{1}{c_0}-c\right)\frac{\partial q}{\partial t}=\frac{\kappa}{\varphi_0\eta}\frac{\partial p}{\partial x}\frac{\partial c}{\partial x}+Dz\frac{\partial q}{\partial x}\frac{\partial c}{\partial x}+(1-zq)D\frac{\partial^2 c}{\partial x^2};$$

weak clogging: $\varsigma=\frac{q_0}{\varphi_0}=\ 1,\quad \varphi_0 c_0\sim q_0\Rightarrow c_0\sim\varsigma;$

$$\frac{\kappa}{\varphi_0}\approx\frac{\kappa(\varphi_0)}{\varphi_0}-\frac{\partial\kappa}{\partial\varphi}\frac{z}{\varphi_0}=\kappa(\varphi_0)\left(\frac{1}{\varphi_0}-\frac{\partial\kappa}{\partial\varphi}\frac{1}{\kappa(\varphi_0)\varphi_0}z\right)=$$

$$=\kappa(\varphi_0)\left(\frac{1}{\varphi_0}-F(\varphi_0)z\right),\quad F(\varphi_0)\geq 10\Rightarrow\frac{\kappa}{\varphi_0}\sim 1$$

$$\boxed{\begin{aligned}&\frac{\partial^2 p}{\partial x^2}=\left[\frac{1}{\kappa}\frac{\partial\kappa}{\partial\varphi}\frac{\partial q}{\partial x}\right]\frac{\partial p}{\partial x},\quad \frac{\partial q}{\partial t}=ac_0(1-q)c-bq,\\&\frac{\partial c}{\partial t}+\frac{z}{c_0}\frac{\partial q}{\partial t}=\frac{\kappa}{\varphi_0\eta}\frac{\partial p}{\partial x}\frac{\partial c}{\partial x}+D\frac{\partial^2 c}{\partial x^2};\end{aligned}}$$

the modelling of 1D transport and inverce problem

$$\begin{cases}\frac{\partial}{\partial t}\left(c+\frac{zq}{c_0}\right)=-\frac{u}{\varphi_0}\frac{\partial c}{\partial x}+D\frac{\partial^2 c}{\partial x^2},\quad u=-\frac{K}{\eta}\frac{\varphi^3}{(1-\varphi)^2}\frac{\partial p}{\partial x}\\ \frac{\partial q}{\partial t}=ac_0(1-q)c-bq\\ \frac{\partial^2 p}{\partial x^2}-\frac{1}{\varphi}\frac{(3-\varphi)}{(1-\varphi)}\frac{\partial q}{\partial x}\frac{\partial p}{\partial x}=0\end{cases}$$

$$\varphi=\varphi_0(1-zq),\quad p|_{x=0}=p_1,\quad p|_{x=L}=p_2,$$

$$u|_{x=0}\,c|_{x=0}-\varphi_0 D\left(1-z\,q|_{x=0}\right)\frac{\partial c}{\partial x}\bigg|_{x=0}=u|_{x=0}\,f(t),$$

$$f(t)=\begin{cases}\tilde{N}_0,\ t\leq t^*\\ 0,\ t>t^*\end{cases},\quad \frac{\partial c}{\partial x}\bigg|_{x=L}=0,$$

$$c(x,t=0)=0,\quad q(x,t=0)=0.$$

$$E=\sum_{k=1}^{M}\left(\frac{\left(c(x=L,t_k)-C_e(x=L,t_k)\right)^2}{C_e^{\,2}(x=L,t_k)}+\frac{\left(Q(x=L,t_k)-Flux(x=L,t_k)\right)^2}{Flux^2(x=L,t_k)}\right),$$

$$Q(x=L,t)=S\,u|_{x=L}\left[c|_{x=L}\,\rho_{NaCl}+\left(1-c|_{x=L}\right)\rho_{H_2O}\right],$$

$$C_e=\frac{C_{NaCl}\rho_{H_2O}}{\rho_{NaCl}(1-C_{NaCl})-C_{NaCl}\rho_{H_2O}},\quad \boxed{\min E\to\mathbf{h}=(a,b,D,z)\text{—inverce problem}};$$

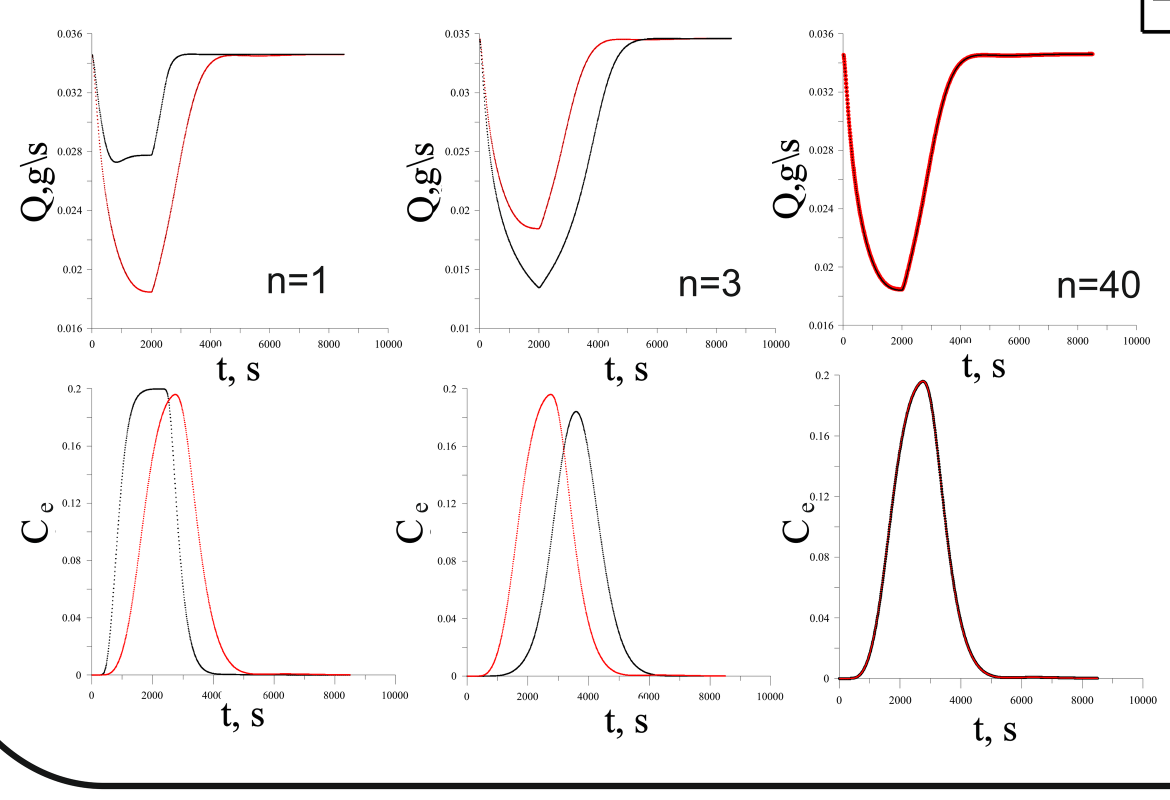
Inverce problem

Test of inverce problem

min E obtained by BFGS method [1]

where $\nabla_{\mathbf{h}}E=\left(\frac{\partial E}{\partial a},\frac{\partial E}{\partial b},\frac{\partial E}{\partial D},\frac{\partial E}{\partial z}\right)$ is calculated by adjoint state [2]

test of inverse algorithm is presented in plot
red curve - generated data (instead of experimental) black curve - data calculated for n-th iteration of BFGS method



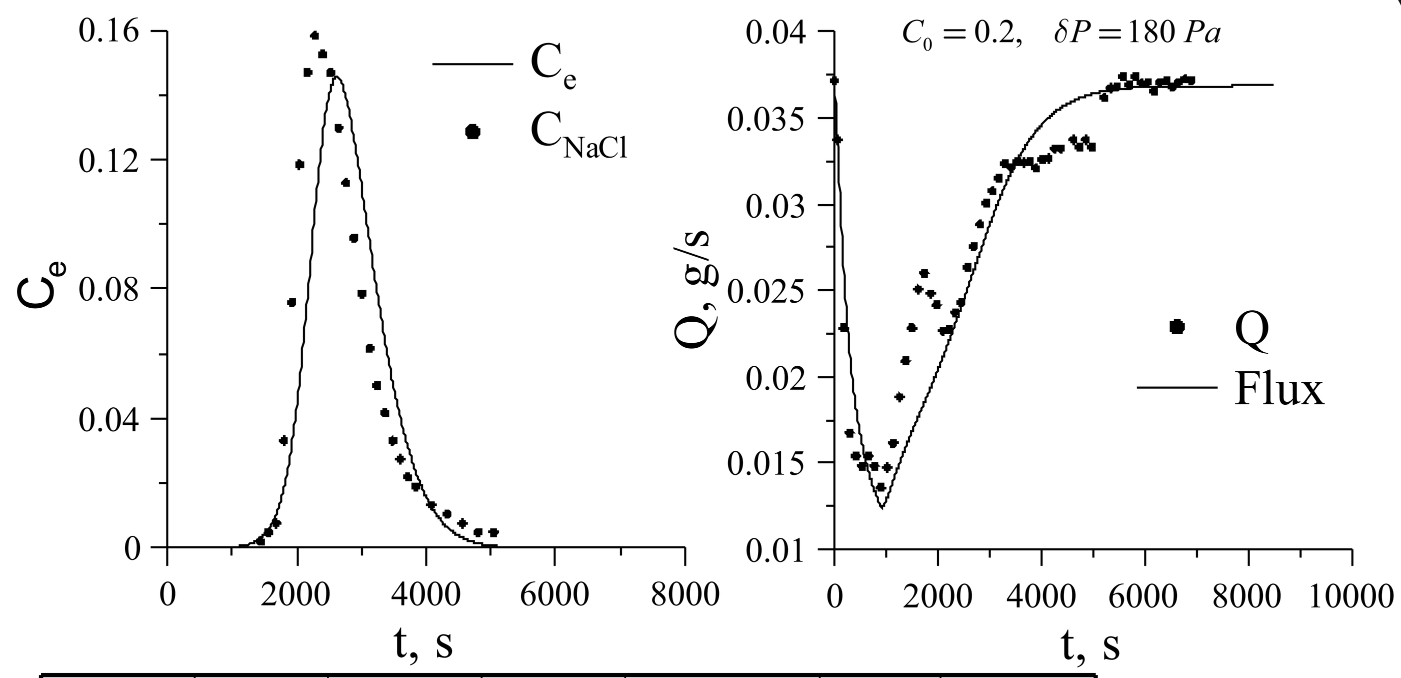
test peremeters

	n=1	n=3	n=40	red
a ,1/h	70	68	79.8	80
b, 1/h	30	28	20.1	20
D, cm²/h	7x10^{-3}	1x10^{-2}	1.02x10^{-3}	1x10^{-2}
z	0.3	0.95	0.41	0.4
E	~252	~217	~3x10^{-4}	-----

results

1) The salt is well sorbed by porous media (a>>b)
2) The flux is greatly decreased because of sorption - clogging
3) The weak clogging assumption works z<<1
4) Not so good accuracy of parameters identification is linked to variation of δp during the experiment - modification of experimental setup

The identification of experiment parameters



δp,Pa	C_0	*a, 1/h*	*b, 1/h*	*D,cm²/h*	*z*	*ε,%*
130	0.2	103.1	16.54	0.293	0.36	8.52
180	0.2	112.8	19.91	0.345	0.32	5.63
240	0.2	123.6	15.52	0.457	0.31	7.86
230	0.05	119.4	14.23	0.428	0.25	10.82
230	0.1	104.3	18.75	0.407	0.29	8.26

$$\varepsilon=\frac{E}{M}\cdot 100\%$$