Prediction of SOC breakthrough in Granular Activated Carbon(GAC) Adsorption

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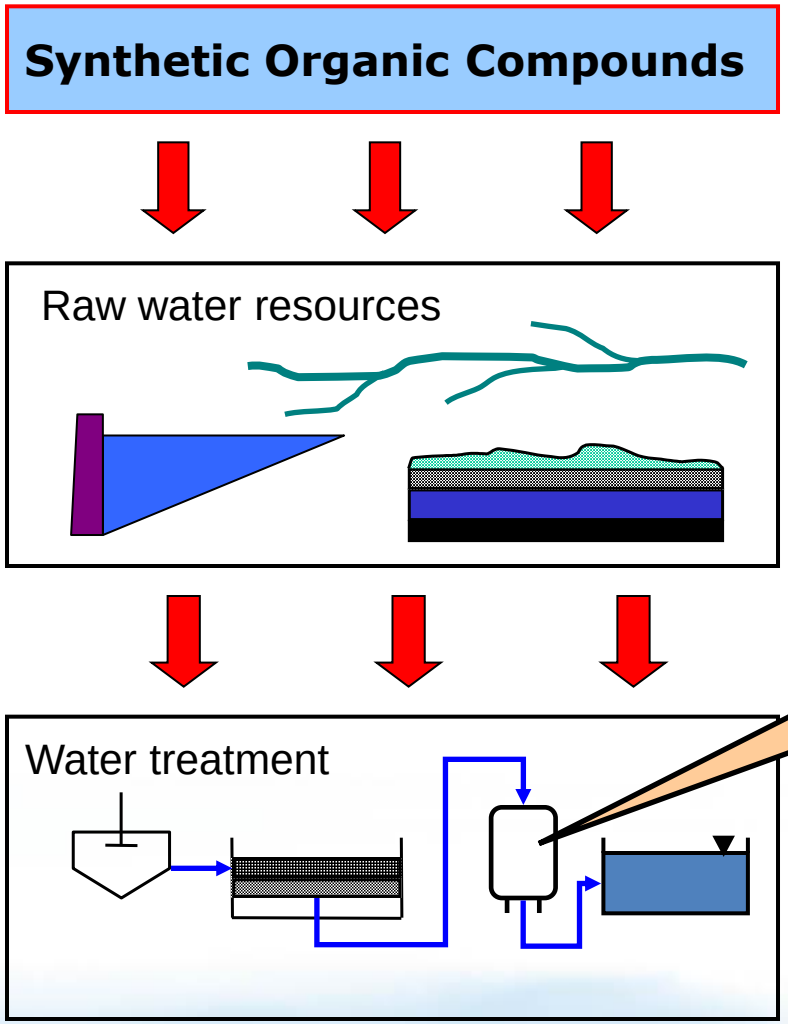
Chair of Water Supply Engineering

Motivation

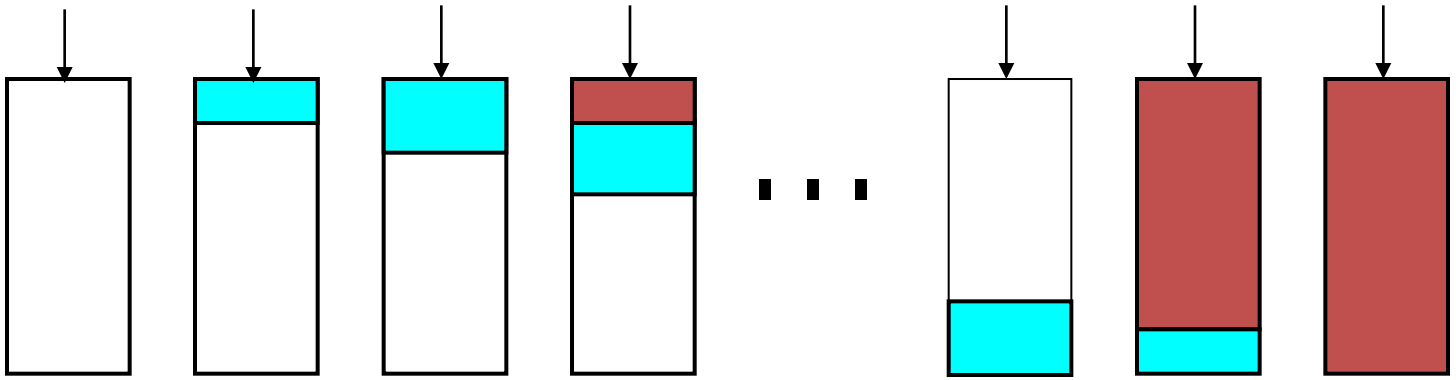


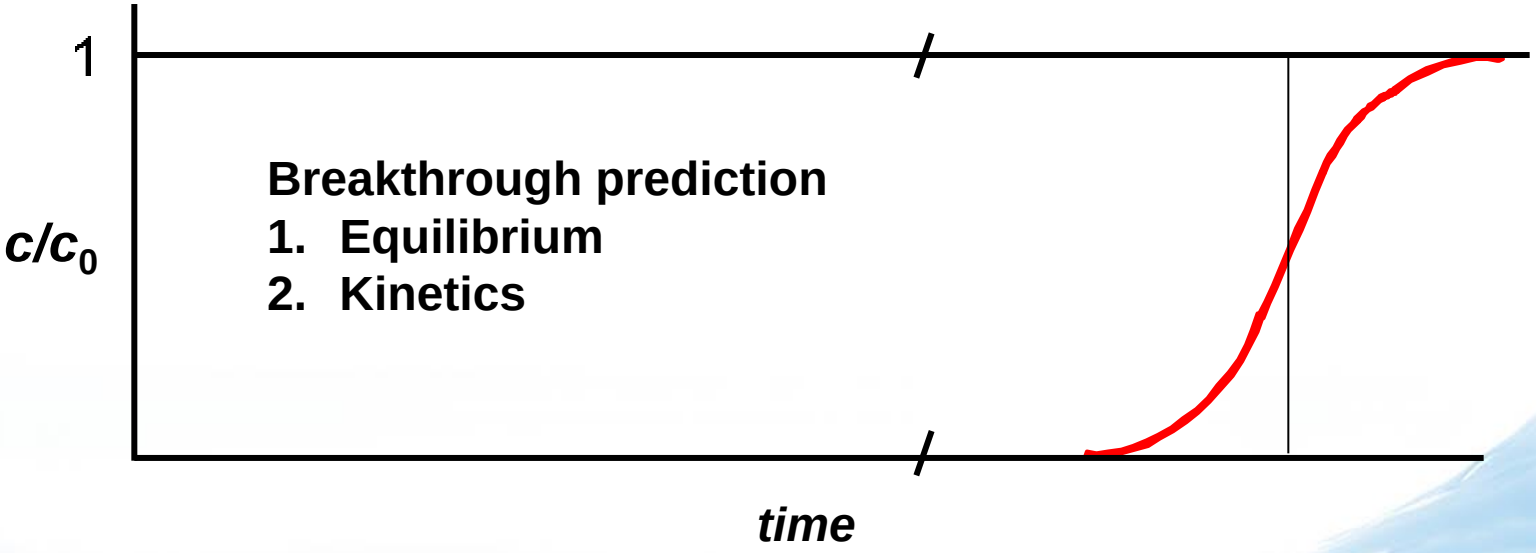
Prediction of break-through behavior of SOCs during granular activated carbon filtration?

Removal of SOCs during drinking water treatment by activated carbon filtration?

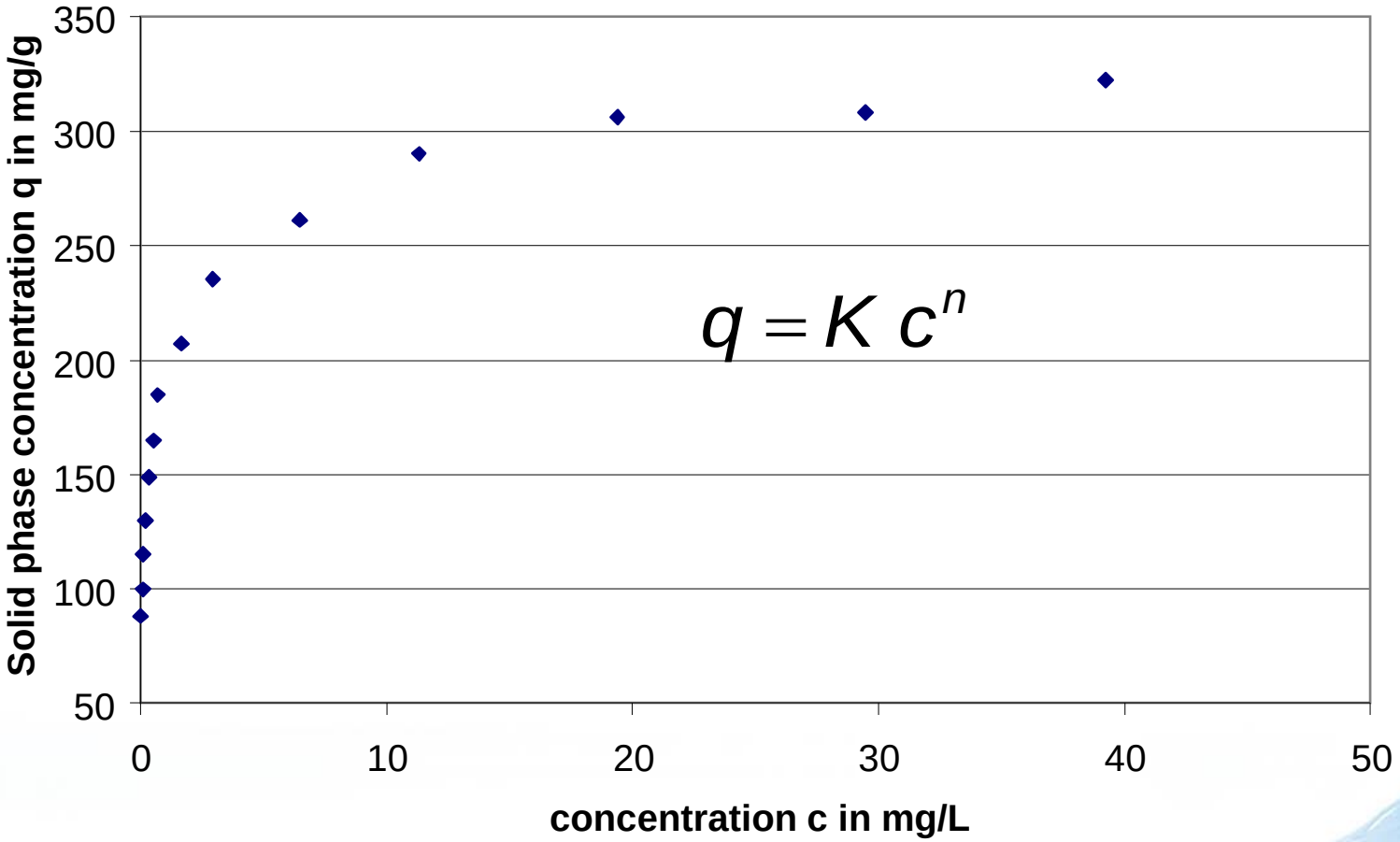
Water treatment using GAC

Breakthrough

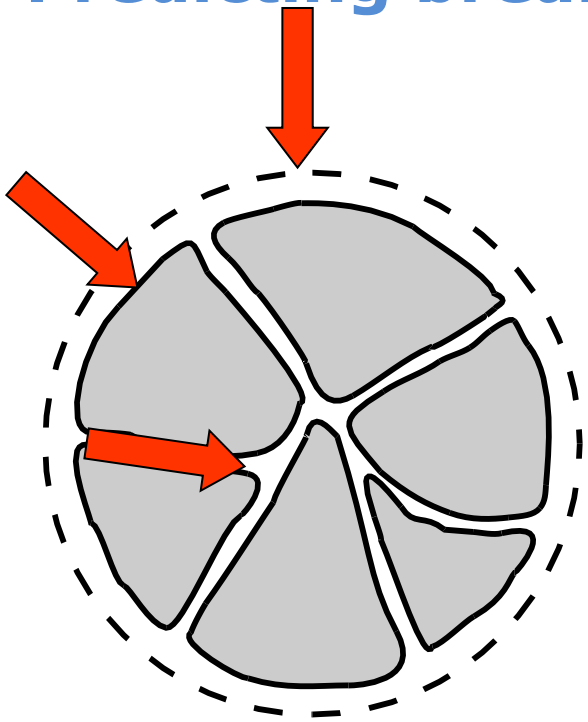




Predicting breakthrough: equilibrium



Predicting breakthrough: kinetics



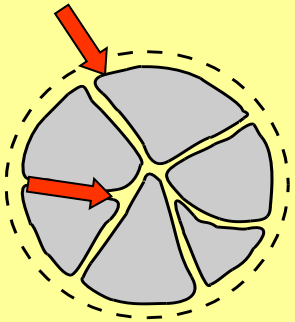
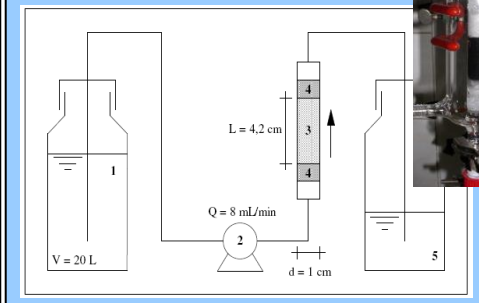
Filmdiffusion to the grain surface

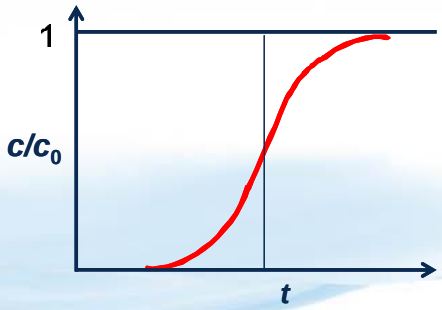
$$\dot{n}_F = k_F \cdot (c - c_S)$$

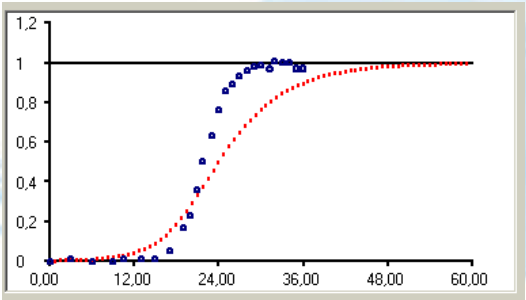
Surface diffusion inside the grain

$$\dot{n}_S = \rho_K \cdot k_S \cdot (q_S - \bar{q})$$

Two ways to predict breakthrough of new substances

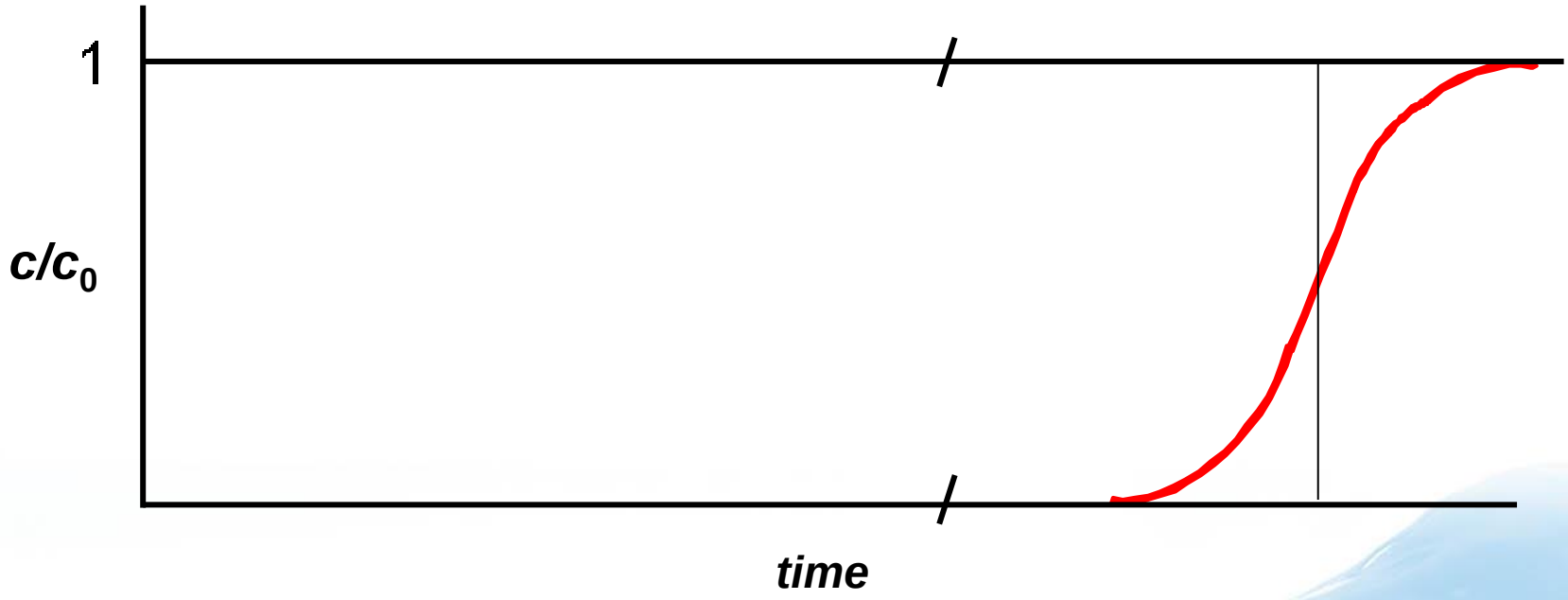
Simulation			Lab-scale filter test
Equilibrium (Freundlich-parameters)		**Kinetics**	• e.g. rapid small scale column tests (RSSCTs)
Models: • Polanyi-theory • LSER • normalized Freundlich-equation	Experiment: 	Model: 	 





Objectives

Appropriate prediction of breakthrough behavior possible?



Approach

Prediction of breakthrough behavior

Simulation

Equilibrium (Freundlich-parameters)

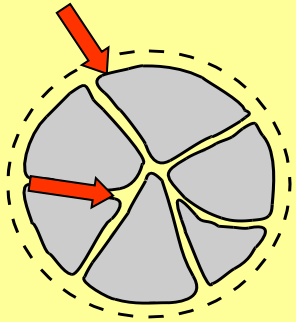
Models:

- Polanyi-theory
- LSER
- normalized Freundlich-equation

Experiment:

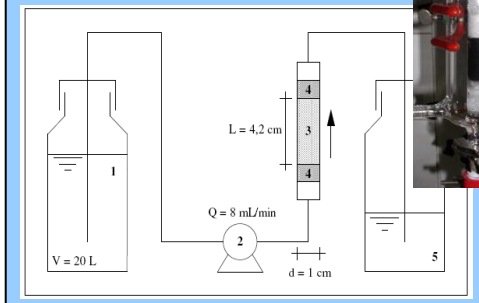
Kinetics

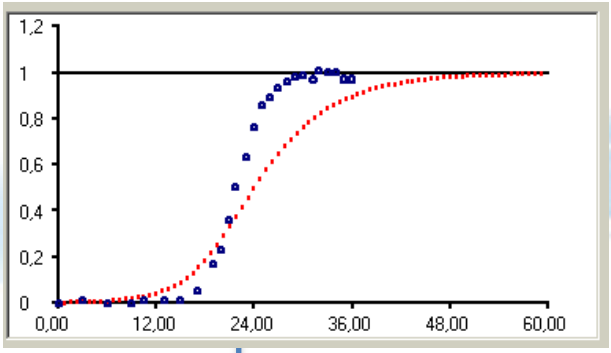
Model:



Lab-scale filter test

- e.g. rapid small scale column tests (RSSCTs)





Isotherm Freundlich coefficients from SOC's properties

Models

- Polanyi-theory
- LSER
- normalized Freundlich-equation

to derive Freundlich-parameters

Data

- Literature data
- Own isotherm measurements

prediction of breakthrough

- Freundlich-parameters from models
- Kinetic models

Compounds investigated

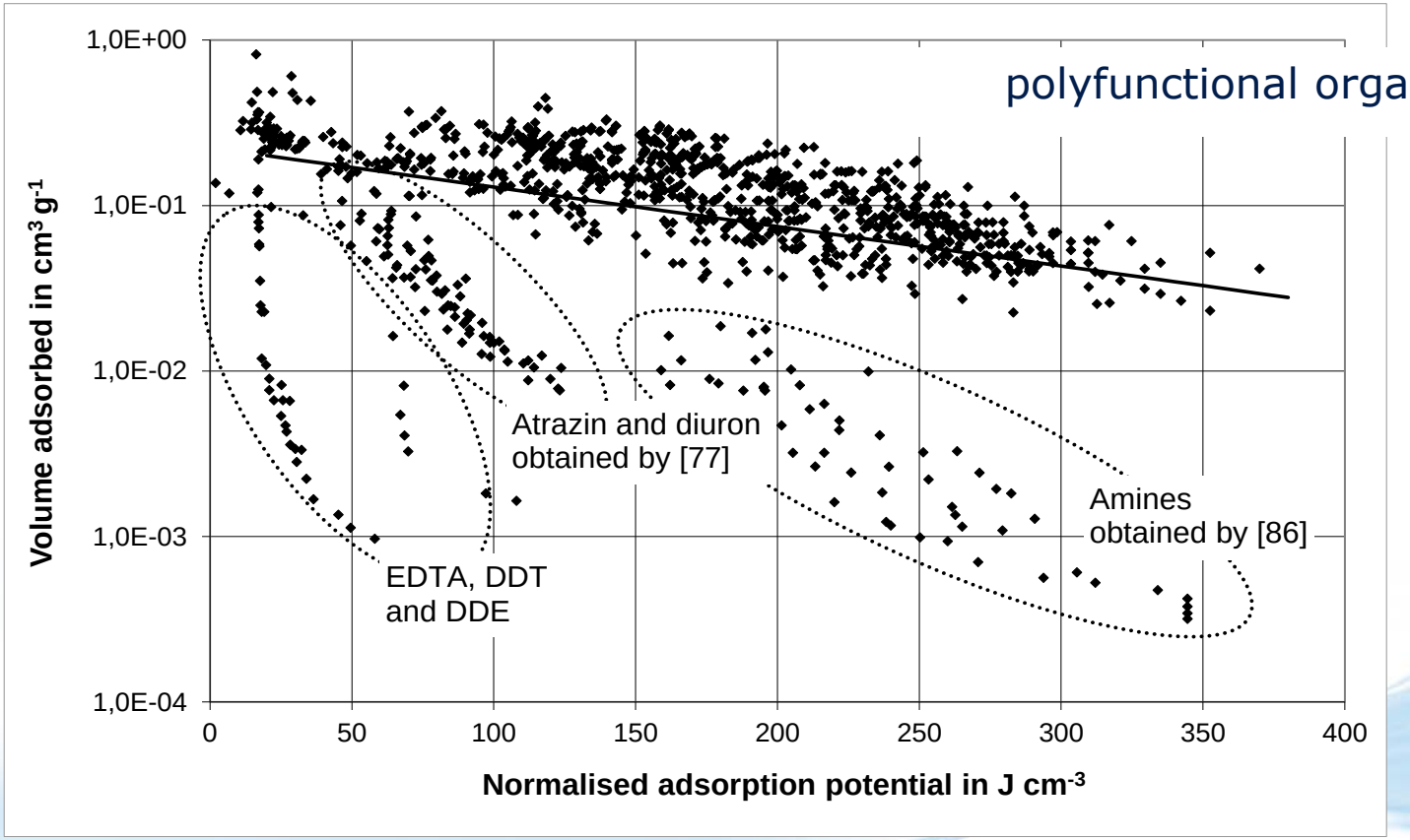
Group of compounds	Alipha-X	Ar / Ar-X	Poly-FG	Ar-Sul	Amines	Phenols	Pesticides	All
Number of compounds	26	24	51	14	15	35	7	112

Correlation of isotherm data using the Polanyi-model

$$\ln V_{ads} = \ln \frac{q_{eq}}{\rho} = \ln V_0 - A \cdot \left(\frac{RT \ln(S / c_{eq})}{V_m} \right)$$

$$K = \rho \cdot V_0 \cdot \exp\left(- \frac{A \cdot R \cdot T}{V_m} \cdot \ln S \right)$$

$$n = \frac{A \cdot R \cdot T}{V_m}$$



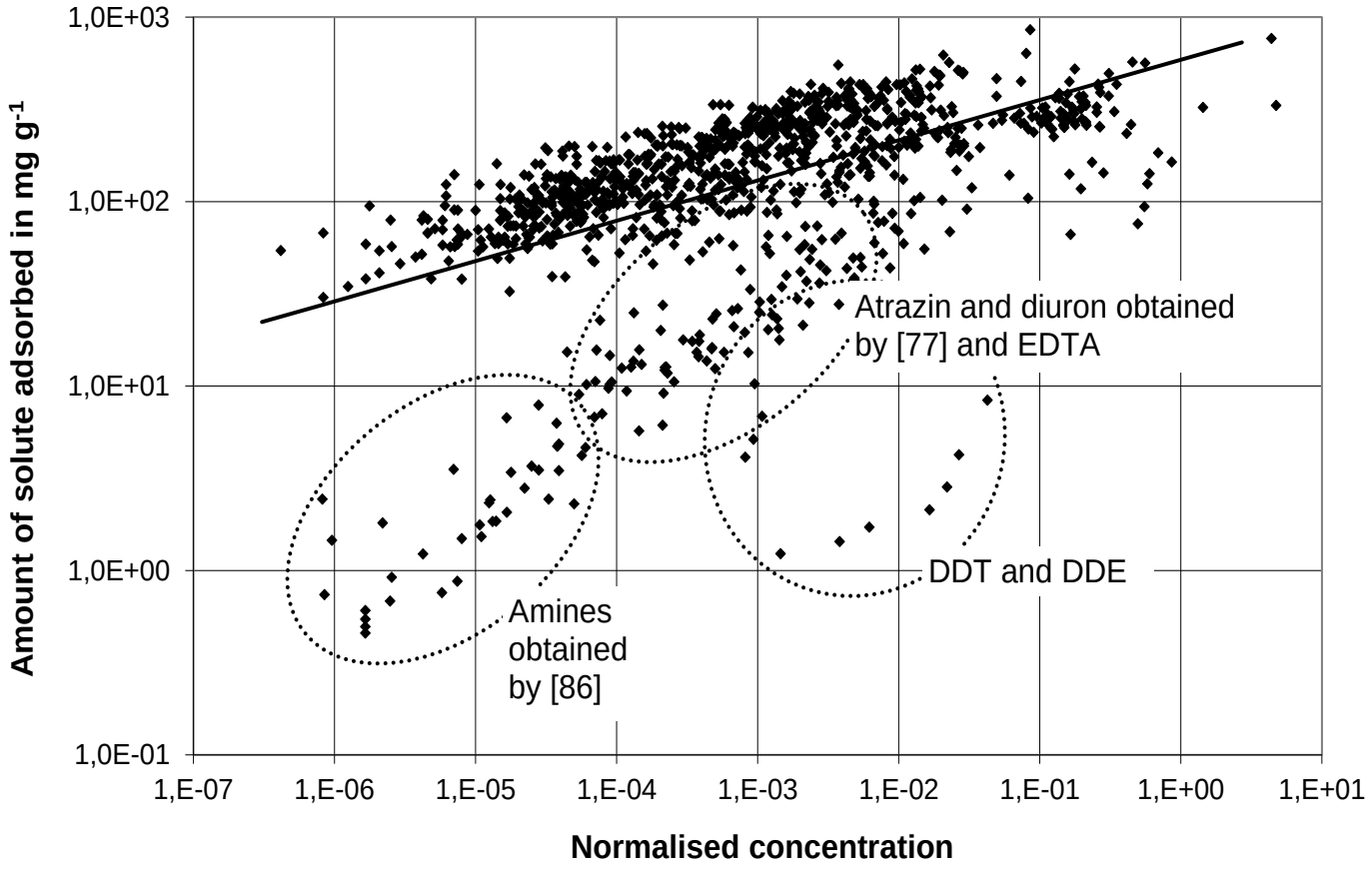
Correlation of isotherm data using the normalized Freundlich-equation

$$q_{eq} = K^* \cdot \left(\frac{c_{eq}}{S} \right)^{n^*}$$

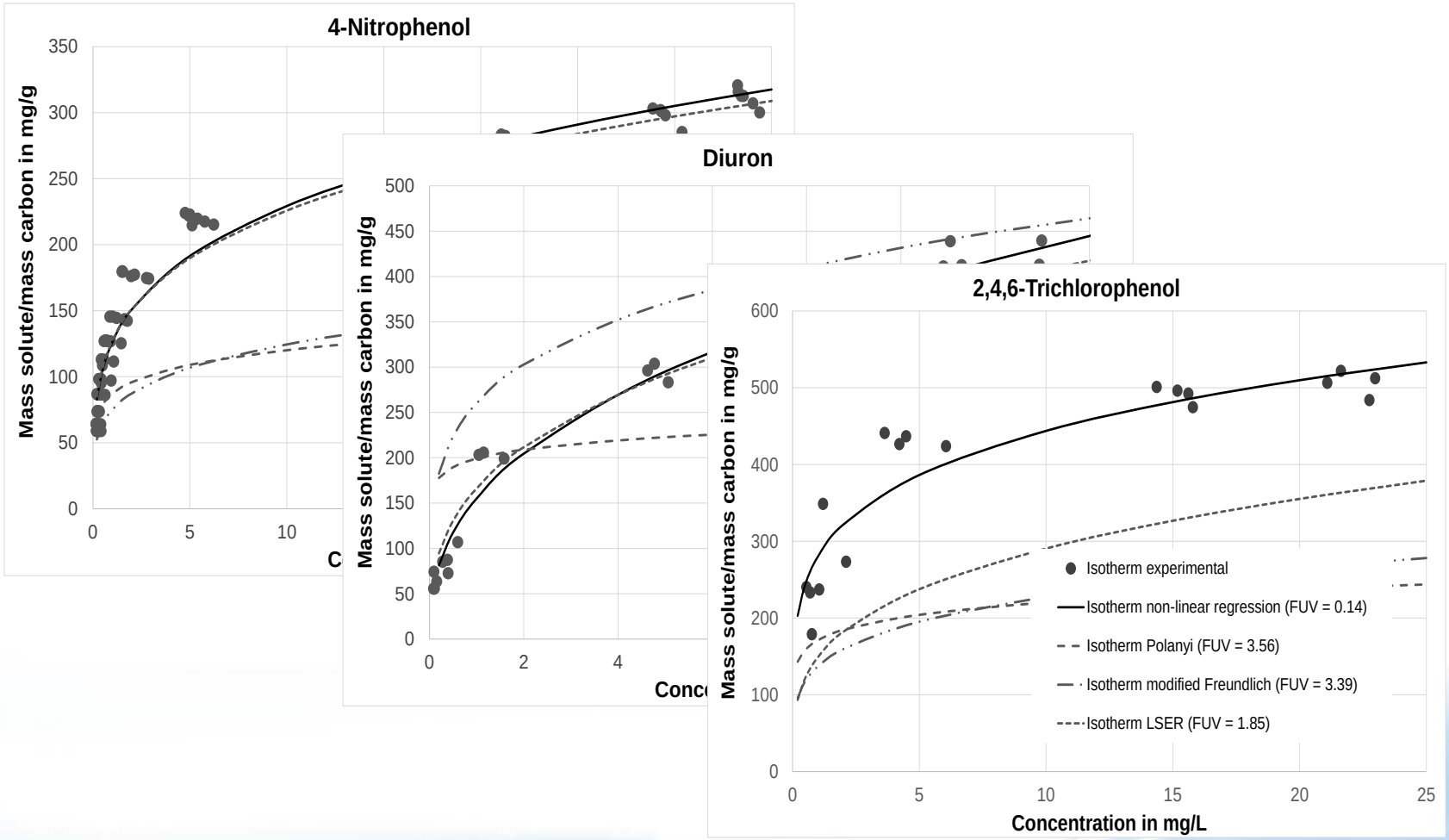
$$K = K^* \cdot \frac{1}{S^{n^*}}$$

$$n = n^*$$

polyfunctional organic compounds



Comparison of adsorption isotherms obtained by theory and experiment

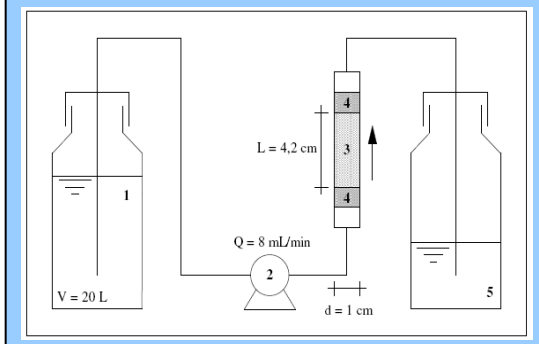


Can breakthrough be described using Freundlich coefficients from compound properties?

Data

- Literature data
- Own isotherm measurements

Lab-scale filter test



Models

- Polanyi-theory
- LSER
- normalized Freundlich-equation

to calculate Freundlich-parameters

Plot of breakthrough

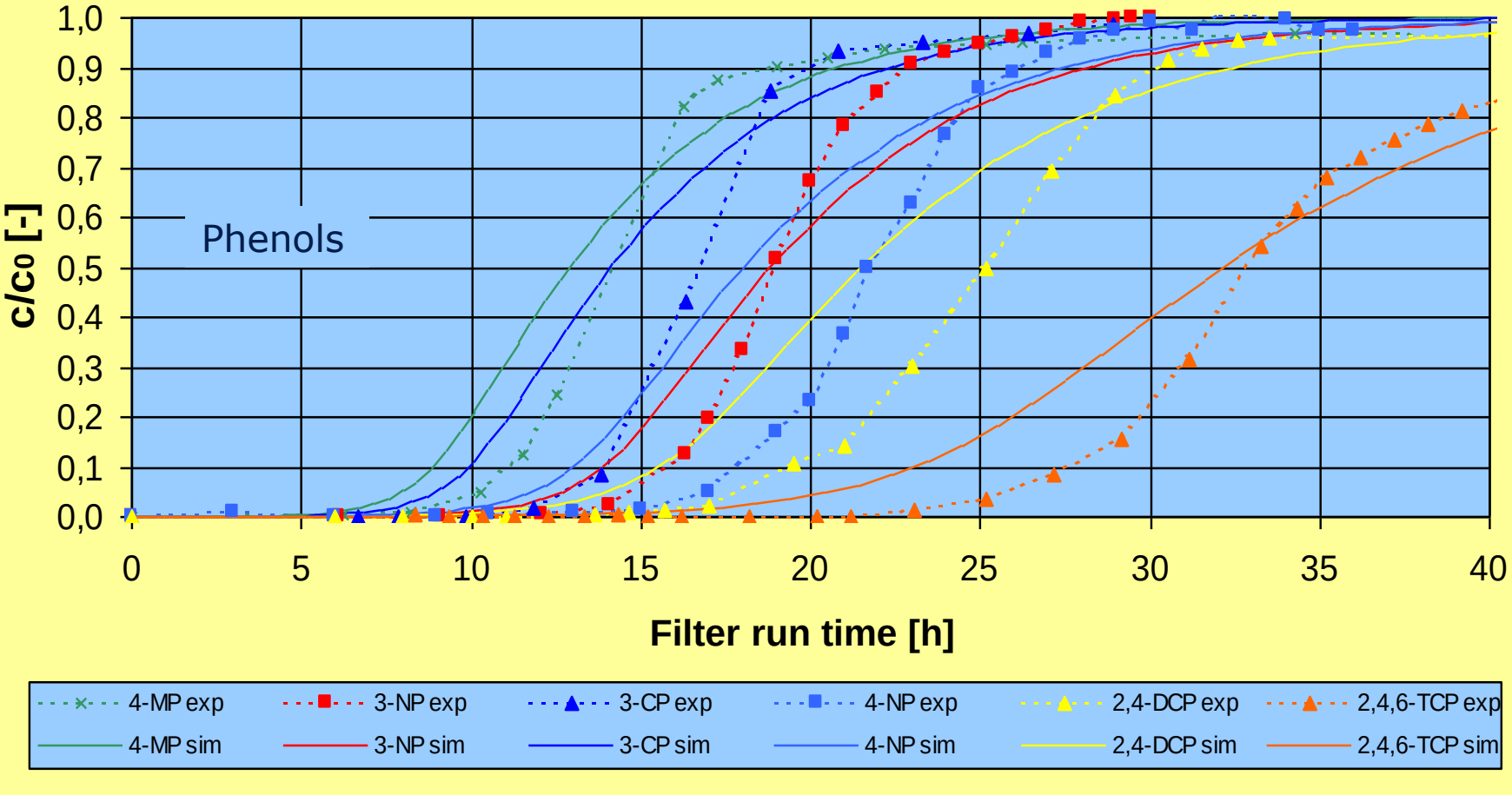
as determined in experiment

Simulation of breakthrough

using calculated Freundlich-parameters

Comparison

Breakthrough in SSCT from experiment and predicted using the normalized Freundlich equation



Results

Comparison of breakthrough at $c/c_0 = 0.1$

Compound	Exp. break-through	Simulated breakthrough					
		Polanyi-model		LSER-model		normalized Freundlich-equation	
	[h]	[h]	[Δh]	[h]	[Δh]	[h]	[Δh]
4-MP	11	7	-36 %	9	-18 %	9	-18 %
3-CP	14	9	-36 %	12	-14 %	10	-29 %
3-NP	16	13	-19 %	14	-13 %	14	-13 %
4-NP	18	12	-33 %	12	-33 %	13	-28 %
2,4-DCP	19	17	-11 %	16	-16 %	16	-16 %
2,4,6-TCP	28	26	-7 %	19	-32 %	23	-18 %
			-24 %		-21 %		-20 %

Results

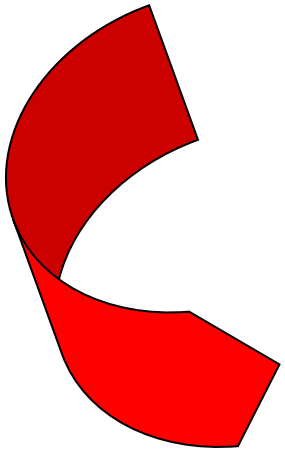
Comparison of breakthrough at $c/c_0 = 0.8$

Compound	Exp. break-through	Simulated breakthrough					
		Polanyi-model		LSER-model		normalized Freundlich-equation	
	[h]	[h]	[Δh]	[h]	[Δh]	[h]	[Δh]
4-MP	16	17	6 %	18	13 %	17	6 %
3-CP	18	19	6 %	22	22 %	18	0 %
3-NP	22	23	5 %	25	14 %	24	9 %
4-NP	24	25	4 %	22	-8 %	24	0 %
2,4-DCP	29	31	7 %	29	0 %	28	-3 %
2,4,6-TCP	39	54	38 %	36	-8 %	41	5 %
			11 %		11 %		4 %

Conclusions

- **Using the huge dataset and the models helps to identify non reliable data**
- **Using Freundlich coefficients derived using compound properties**
  - **breakthrough behavior is best described using Freundlich coefficients using the normalized Freundlich equation**
  - begin of breakthrough (10 %) was predicted about 22 % too early
  - 80 %-breakthrough is predicted well with an average deviation of 8 %

Conclusions



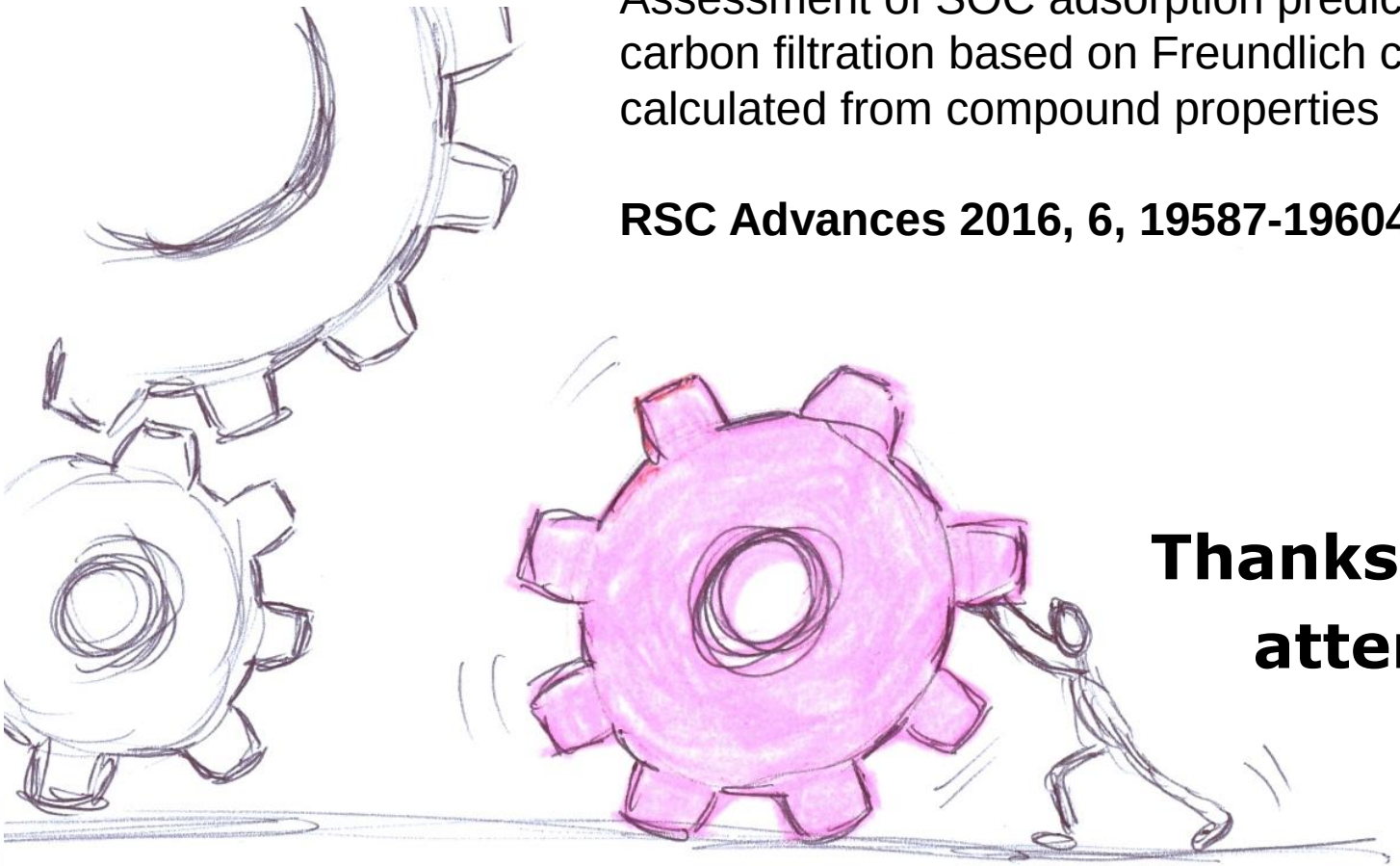
SOC breakthrough prediction

using Freundlich-coefficients determined using compound properties

is appropriate for a conservative risk assessment

Slavik, Uhl, Börnick, Worch
Assessment of SOC adsorption prediction in activated carbon filtration based on Freundlich coefficients calculated from compound properties

RSC Advances 2016, 6, 19587-19604



Thanks for your attention!