UNIVERSITEIT GENT

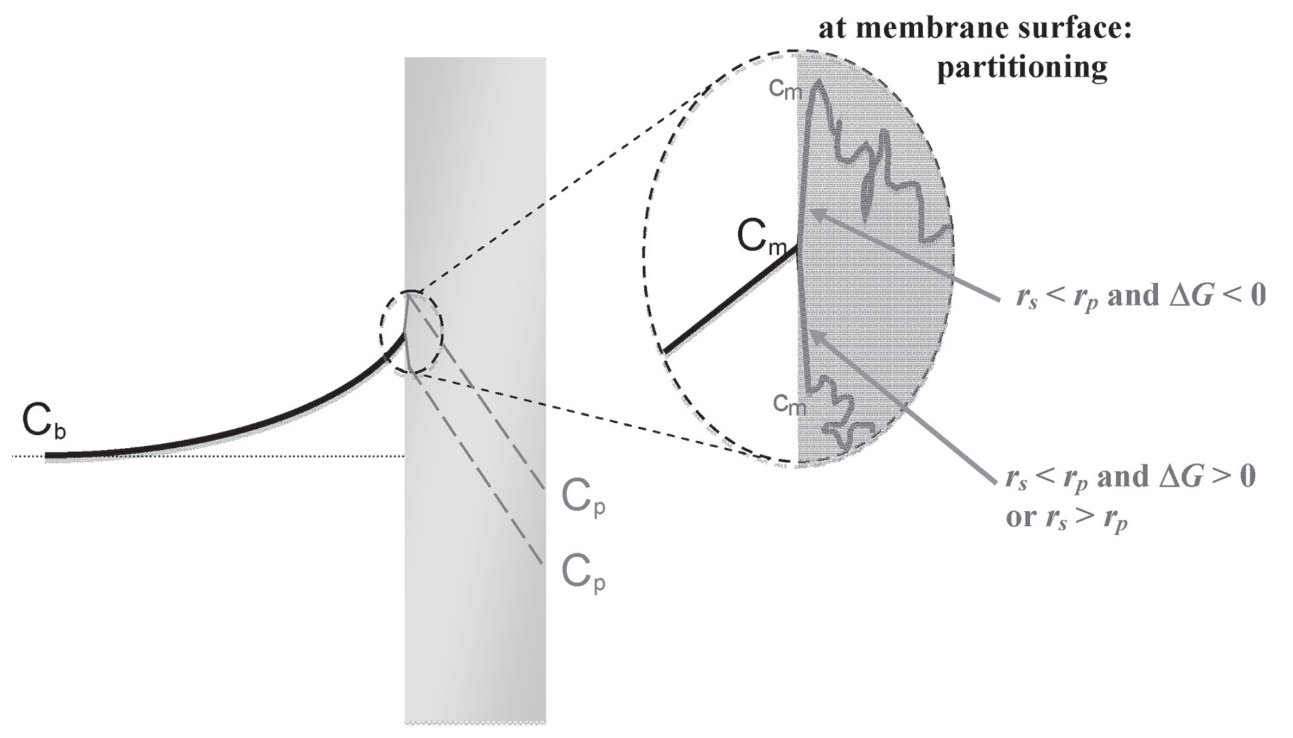
Trace organics rejection in NF/RO and FO: model development and influence of fouling

A. D'Haese, M. M. Mxolisi, T. O. Mahlangu, E. R. Cornelissen, P. Van der Meeren and A.R.D. Verliefde

Particle and Interfacial technology group, Department of Applied and Analytical Physical Chemistry
Coupure Links 653, B-9000 Gent, Belgium
arnout.dhaese@ugent.be

Problem statement:

- Occurrence of trace organics in environment with possible health consequences
- Removal by NF/RO and FO widely investigated, need for reliable predictive models
- Influence of membrane fouling not clear



Objective:

- Develop (predictive) rejection models for NF/RO and FO, incorporating fouling effects

Model development: Transport in NF/RO and FO: convection-diffusion: $< J_s > = < J_w > \cdot C_{s,p} = -D_{m,s} \cdot \frac{dc_s}{dx} + < J_w > \cdot K_{c,s} \cdot c_s$

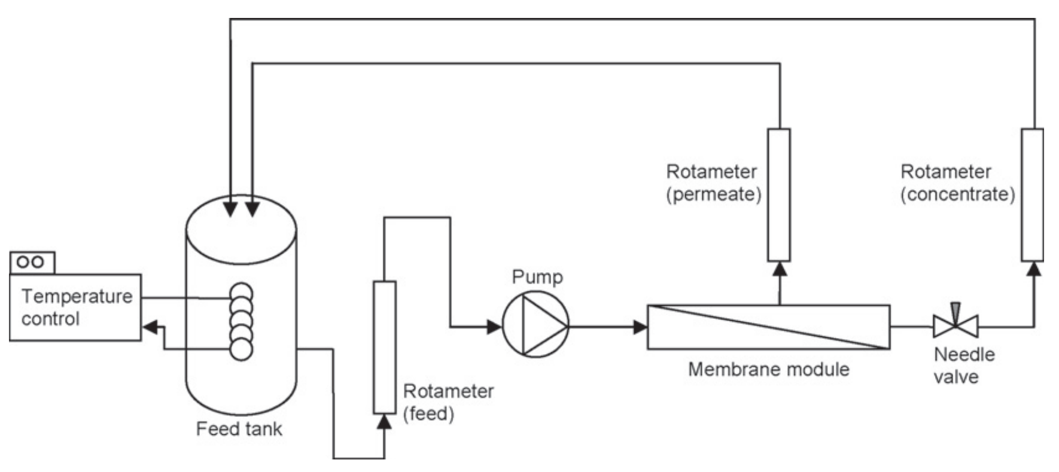
1. Clean membrane:

- Rejection-determining step: partitioning at membrane interphase: $\phi_s = (1-\lambda)^2 \cdot exp\left(-\frac{\Delta G_i}{k \cdot T}\right)$
- Function of ratio solute size/pore size $\left(\lambda = \frac{r_s}{r_p}\right)$ and solute-membrane interaction energy (ΔG_i)
- Rejection: $R = 1 - \frac{\phi_s \cdot K_{c,s}}{1-[(1-\phi_s \cdot K_{c,s}) \cdot exp(-Pe)]}$ with $Pe = \frac{J_w \cdot K_{c,s} \cdot \Delta x}{\varepsilon \cdot K_{d,s} \cdot D_s}$

2. Fouled membrane:

- Membrane-in-series model: the fouling layer behaves as an extra membrane
- Rejection-determining steps: partitioning at fouling layer & membrane interphase, continuous concentration profile
- Rejection: $R = 1 - \frac{\beta_{CECP} \cdot \phi_{mem} \cdot \phi_{foul} \cdot K_{c,mem} \cdot K_{c,foul}}{\left[\phi_{foul} \cdot K_{c,foul} \cdot exp\left(-\frac{K_{c,foul} \cdot \delta_{foul} \cdot Jw}{D\infty \cdot \varepsilon_{foul} \cdot K_{c,foul}}\right) \cdot \left(1-exp\left(-\frac{K_{c,mem} \cdot \Delta x_{mem} \cdot Jw}{D\infty \cdot \varepsilon_{mem} \cdot K_{d,mem}}\right)\right)\right] + \left[\phi_{mem} \cdot K_{c,mem} \cdot \left(1-exp\left(-\frac{\phi_{foul} \cdot \delta_{foul} \cdot Jw}{D\infty \cdot \varepsilon_{foul} \cdot K_{d,foul}}\right)\right)\right] + \left[\phi_{mem} \cdot \phi_{foul} \cdot K_{c,mem} \cdot K_{c,foul} \cdot exp\left(-\frac{K_{c,mem} \cdot \Delta x_{mem} \cdot Jw}{D\infty \cdot \varepsilon_{mem} \cdot K_{c,mem}}\right) \cdot exp\left(-\frac{K_{c,foul} \cdot \delta_{foul} \cdot Jw}{D\infty \cdot \varepsilon_{foul} \cdot K_{c,foul}}\right)\right]}$

Materials and methods:

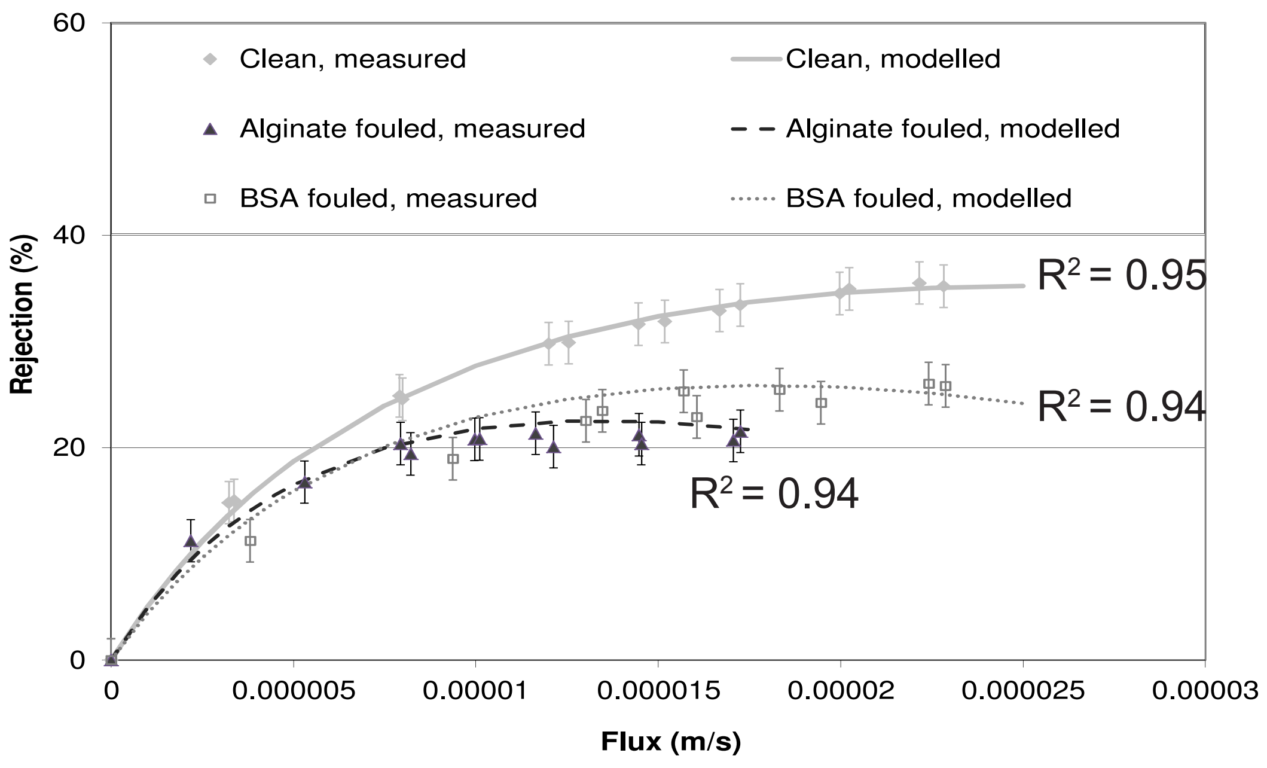


- FO: CTA membrane by HTI, NF: NF270, setup: refer to scheme
- Fouling experiments in single membrane crossflow cell, fouling by BSA and alginate, biofouling due to spiking with AOC
- Contact angles with pure water, glycerol and diiodomethane on a Krüss DSA10-MK2
- Surface tension components of pharmaceuticals: powders were compressed at 1350 bar, after which contact angles were measured on resulting pharmaceutical surface
- Focused on neutral compounds: paracetamol, caffeine, bisphenol-A, carbamazepine, trimethoprim

Results:

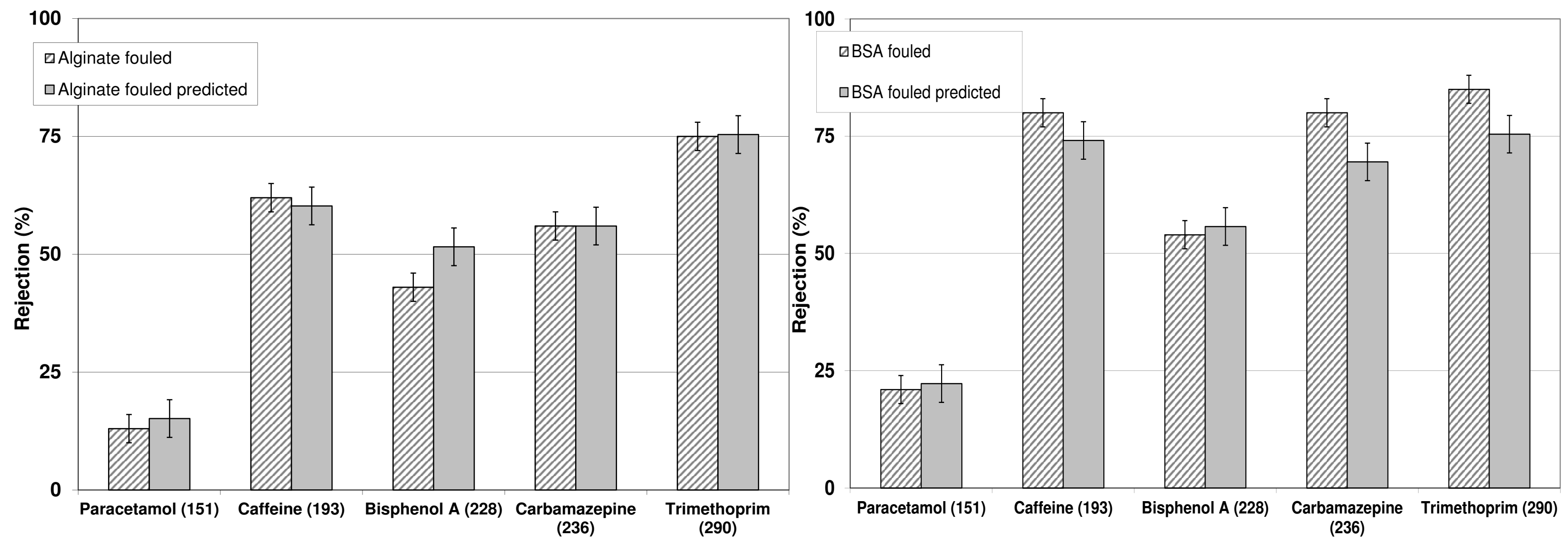
1. NF/RO

- Average pore size and thickness modelled with tracer glycerol for clean and fouled membrane:



- Use fitted porosities & thicknesses for rejection prediction

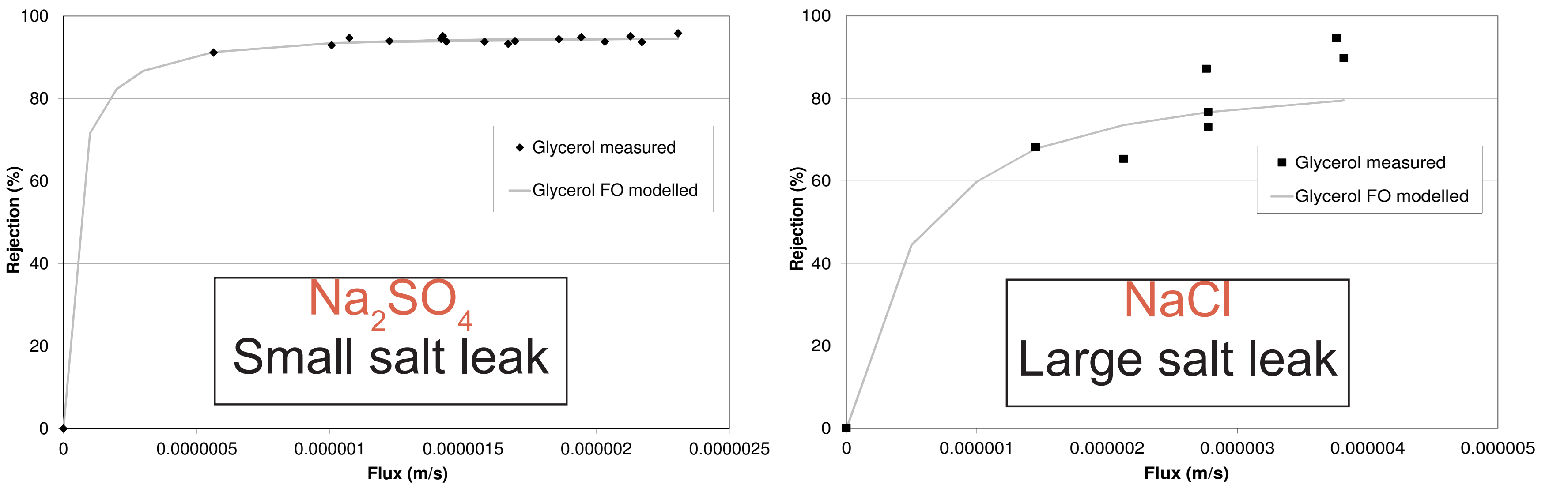
Good results for BSA and alginate:



Worse results for biofouling: difficulty in obtaining representative contact angle measurements of biofilms!

2. FO

Modelling the average pore size and membrane thickness using glycerol as a tracer:



Salt leak	**4.07 ± 1.28**	**24.9 ± 10.1** *10^{-6} mol/(mol·s·m^2)*
Pore size	**0.499 nm** *$R^2 = 0.985$*	**0.598 nm** *$R^2 = 0.794$*
Δx/ε	**20.3 µm**	**13.4 µm**

Glycerol rejection is lowered when the draw solute permeates more through the FO membrane.
Literature: salt leak limits organic solute transport by blocking pores → clearly contradicted by results

HYPOTHESIS: salt leak influences membrane physico-chemical properties and thus ΔG_i