wetsus
european centre of **excellence**
for sustainable **water technology**

# Multi-component mass transport modeling of water desalination with reverse osmosis

**Edward Kimani**
edward.kimani@wetsus.nl

## Motivation

Reverse osmosis (RO) is a membrane-based technology for the desalination of seawater and brackish water, where under pressure water is pushed through the ultra-thin polyamide (PA) top-layer (≤ 200 nm) of the thin film composite (TFC) membrane, while the undesired ions are retained, see Fig 1 [1-4].

To develop an optimal RO-process, we need accurate theoretical models to describe energy consumption and the composition of the product water. These models help in understanding the transport and separation processes better, the development of more suitable membranes and module designs, and in the design of an improved process layout for a given objective. Accurate models help to predict the exact retention of key undesired ions, such as boron or arsenic.

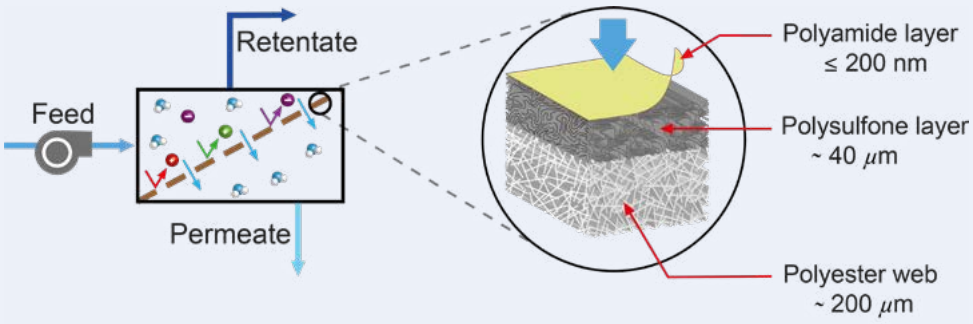


*Fig 1. Overview of the RO process and a detailed view of the arrangement of the layers of a TFC – RO membrane [4].*

## Technological challenge

Despite the technological advances in understanding RO membrane transport and separation, precise models based on a detailed physico-chemical description of the processes that take place in and around the membrane are not yet developed to make the desired design possible. The existing models neglect the various intricate couplings between the transport fluxes of the various ions when the feed water contains a large number of species (multicomponent mixtures). These couplings originate from the constraints of zero total current and local electroneutrality at each position in the membrane, while ions also interact via acid-base reactions [5-8].

With the inclusion of all the chemical equilibria into the extended Donnan-Steric Partitioning (ext-DSP) pore model, we are able to predict profiles of concentration, flux, and reaction rates of species. Fig 2 shows an example case involving carbonic acid (neutral), carbonate and bicarbonate (anions), with the involvement of a hydronium ion.

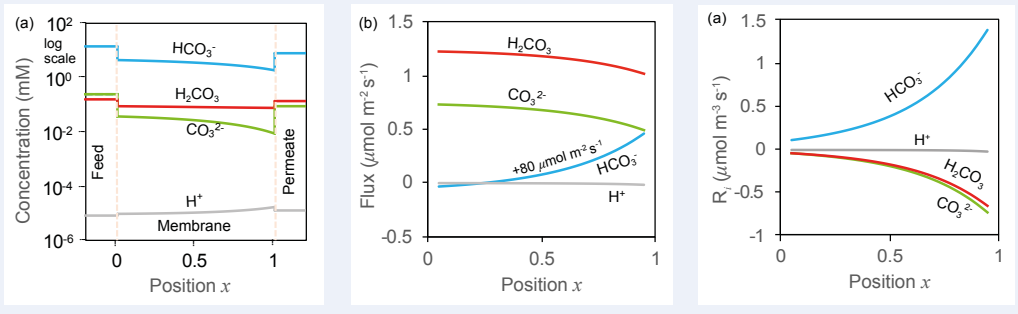


*Fig 2. Profiles across the PA top-layer of a TFC – RO membrane of a) ion concentration, b) ion flux, and c) acid-base reaction rates, as function of dimensionless position.*

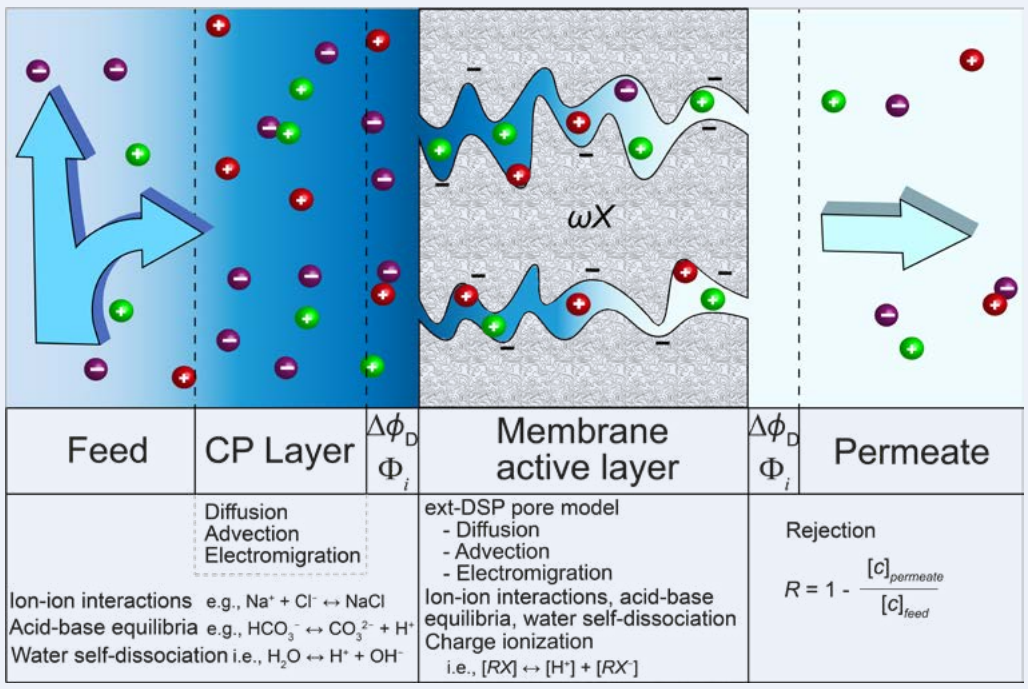


*Fig 3. Scheme of the extended Donnan Steric Partitioning (ext-DSP) pore model with the three factors that contribute to transport together with chemical reactions (ion-ion interaction, acid-base equilibria, and the water self-dissociation).*

## Research goals

In this research we develop and test a continuum transport model for RO which is based on physical principles and chemical information and therefore includes all known interactions between water and ions, which results in more robust predictions outside the (necessarily limited) window of experimental validation. The development and extension of the transport model which is based on the ext-DSP pore model will be done on the level of a full module (two dimensions) and a small RO plant. A physico-chemical model helps in a better understanding of the mechanisms involved in transport and separation (e.g., are ion-ion frictions in the membrane of importance?). Thus, for this research, I will investigate how to:

- Develop a mass transport model based on the ext-DSP pore model for ion-selectivity of RO membranes in multi-component mixtures
- Extend the DSP pore model to include ion-ion interactions, acid-base equilibria, membrane charge ionization and the concentration polarization effect, as represented in Fig 3
- Validate and upgrade the model with experiments
- Develop a two-dimensional model to describe a real RO module
- Use the model for specific cases to investigate the optimal RO operational conditions

### References

[1] R.J. Petersen, J. Membrane Sci. 83 (1993) 81-150
[2] K.P. Lee et al., J. Membrane Sci. 370 (2011) 1-22
[3] C. Fritzmann et al., Desalination 216 (2007) 1-76
[4] S.H. Maruf et al., Polymer 52 (2011) 2643-2649
[5] J.E. Dykstra et al., Phys. Rev. E 90 (2014) 013302
[6] O. Nir et al., Water Research 87 (2015) 328-335
[7] Y.S. Oren and P.M. Biesheuvel, Phys. Rev. Applied 9 (2018) 024034
[8] P.M. Biesheuvel et al., Environ. Sci. Technol. Lett. 7 (2019) 42-47



E.M. Kimani MSc, dr.ir. P.M. Biesheuvel
dr.ir. A.J.B. Kemperman, prof.dr.ir. W.G.J. van der Meer

UNIVERSITY OF TWENTE.