Advanced Materials for Selective Nitrate/Chloride Separation (Anchor)

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Motivation

The selective removal or recovery of elements from a multicomponent stream plays a key role in many industrial and agricultural applications. For instance, nitrate needs to be removed from industrial brines. In closed horticulture systems however the aim is to retain the nitrate in the recirculating water but to selectively remove the chloride, a requirement also mandatory in the production process of fertilizers. Currently used electrochemical and biological methods deal with safety issues, season-dependent environmental factors, time-consuming process steps and/or high capital costs. For all these reasons, alternative approaches have to be explored.

Technological challenge

The separation of nitrate and chloride is particularly challenging. The reason is that these two equally charged ions are similar in size, resulting in a rather similar (de)hydration energy as well [1]. Apart from these similarities, a clear difference between the two ion species is related to their (hydrated) structure. Whereas nitrate is a rather planar molecule, chloride is relatively symmetrical in three dimensions [2]. This structure difference can be exploited by new materials possessing chemical moieties that allow discrimination between the two ion species. Together with differences in hydrophobicity, the structural difference between the (solvated) nitrate and chloride will be the starting point for Anchor.

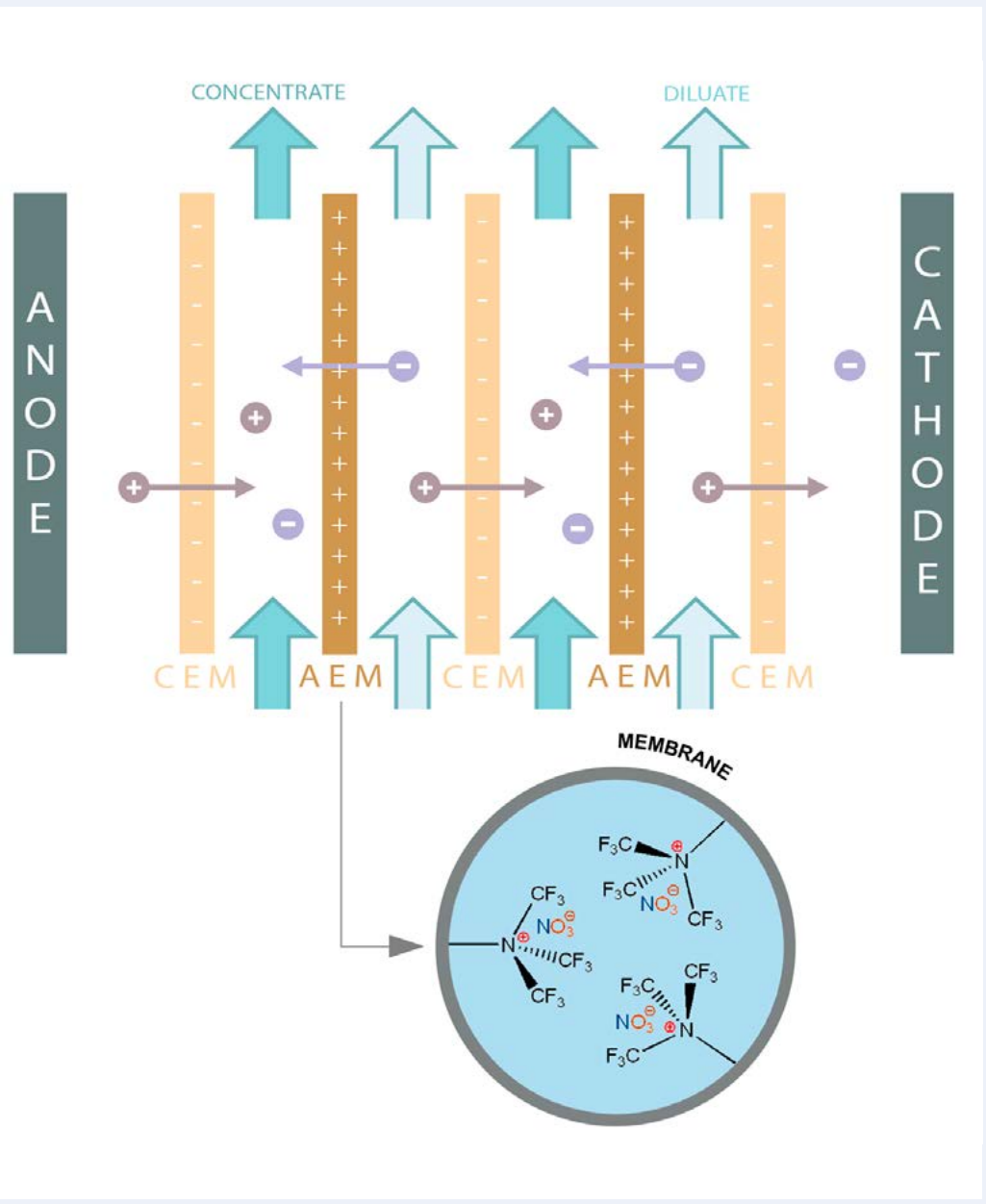

Fig.1 Scheme of an electrodialysis system, identifying the repeating unit (cell pair); in the outer circle is represent the exemplary and generalized structure of the ion-exchange polymer membranes that will be studied.

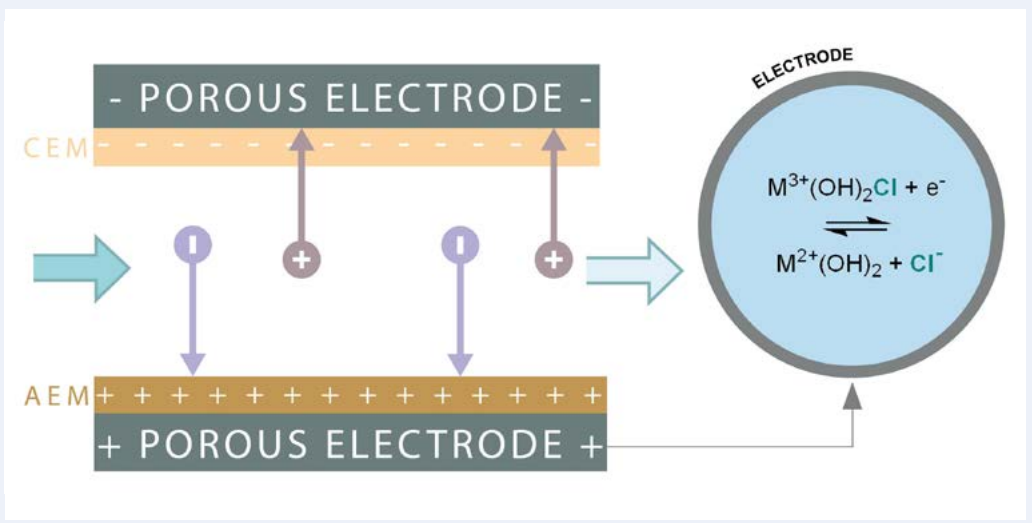

Fig.2 Schematic design of a cell for Membrane Capacitive Deionization (MCDI); in the outer circle is represent the exemplary and generalized mechanism of the electro-adsorb ions materials that will be studied.

Research goals

- The design and engineering of nitrate or chloride selective materials based on the physico-chemical properties of the two ion species.
- The functionalization of membranes by fine-tuning their hydrophobicity. Assessing the nitrate and chloride membrane permeation by using Electrodialysis (ED) *(Fig. 1)*.
- The functionalization of adsorption materials (electrodes) by including chemical moieties that can distinguish between nitrate and chloride. Characterizing the adsorption (and desorption) of nitrate and chloride by using Membrane Capacitive Deionization (MCDI) *(Fig. 2)*.

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[1] Luo, L.; Abdu, S.; Wessling, M. Selectivity of Ion Exchange Membranes: a Review. *J. Memb. Sci.* **2018**, 555, 429–454.
[2] Hawks, S. A.; Ceron, M. R.; Oyarzun, D. I.; Pham, T. A.; Zhan, C.; Loeb, C. K.; Mew, D.; Deinhart, A.; Wood, B. C.; Santiago, J. G., Stadermann, M.; Campbell, P. G. Using Ultramicroporous Carbon for the Selective Removal of Nitrate with Capacitive Deionization. *Environ. Sci. Technol.* **2019**, 53, 10863-10870.

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