Modelling ion flotation for the recycling of metals

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Rare-earth metals are crucial in different areas of application, such as magnets, catalysts, metal alloys, batteries, and electronics[1]. These metals are scarce in European soil, so recycling them from end-of-life products may be an important way to obtain them. However, these rare-earth elements are mixed with other elements, making them difficult to isolate and reuse for new applications. Chemical separation methods like ion foam flotation are a resource to separate elements from one another. In ion flotation, a surfactant agent is used to extract ions from the liquid-gas interface [2]. The difference in the ion selectivity with the surfactants is the principle for the separation process.

We performed atomistic simulations to characterize the water-air interface involved in the flotation process, based on previous experiments conducted at our research institute by C.Micheau et al [3,4,5]. In these experiments, they used a commercial carboxyl surfactant (AKYPO RO 90VG) for the ion flotation process. Their findings show that ion flotation using this surfactant can be used to selectively separate mixed ions in solutions, being trivalent ions the ones showing higher selection.

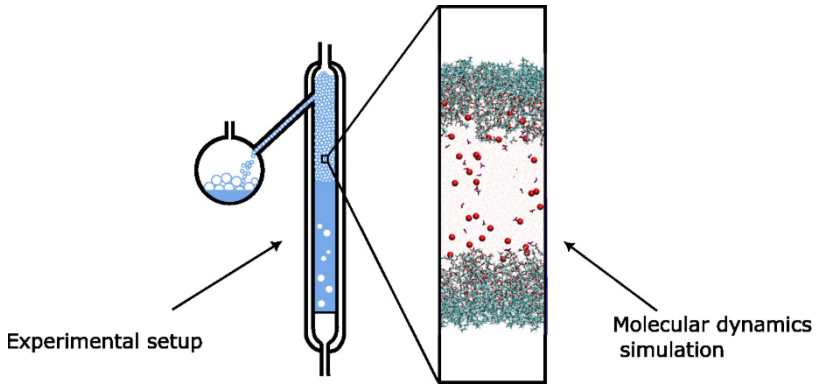
We did molecular dynamics simulations considering different surface excess concentrations of surfactant and calculated the surface tension of the system and its density profile. We then compared the surface tension as a function of the surface excess (obtained from simulations) and the surface tension as a function of bulk concentration (obtained from experiments [3] and simulations). The calculated bulk and surface activity coefficients show that the interactions between the surfactants at the interface are repulsive but attractive in the bulk.

After modelling the water-air interface with a realistic surface excess, we introduced metals to the system, including rare-earth metals. We considered $LiNO_3$, $NaNO_3$, $Ca(NO_3)_2$, $Sr(NO_3)_2$, $Nd(NO_3)_3$ (as in the experiments [4]). We studied two opposite situations: low and high pH. This is, cases in which the carboxyl group of the surfactant is mostly protonated or deprotonated. We observe a significant difference in the selectivity of the ions depending on the pH due to their complexation with the carboxyl group. We also see that calcium and neodymium offer higher selectivity towards the surfactant by calculating the fraction of adsorbed ions and their residence time at the interface.

Overall, this work lays the groundwork for a molecular prediction of the specific effects that govern flotation, a highly significant method for separating elements.

Keywords:

Rare-earth, Ion foam flotation, separation chemistry, molecular modelling



Experimental setup scheme of the ion flotation process and snapshot of the molecular dynamics simulation.

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