



Electrostatic potential on anti-scalants modified CaCO_3 (104) surface: A molecular simulation study

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Abstract

Molecular dynamics simulation and Density Functional Theory were used to investigate the adsorption of two kinds of anti-scalant, ethane diphosphonic acid (EDPA) and polyether polyamino methylene phosphonate (PAPEMP), on the calcite (104) surface in order to increase the level of understanding of the anti-scaling mechanism in membrane processes for water desalination. Calculation results show that the performance of an anti-scalant is mainly determined by the negative electrostatic potential presented on the anti-scalant modified scale surface. A negative electrostatic potential on the scale surface can prevent not only the agglomeration of scale nuclei in the concentrate but also the precipitation of scale nuclei on the membrane surface. Phosphonate groups in 1,1-EDPA are bifunctional since they simultaneously satisfy the requirements for the electrostatic potential distribution and for the adsorption stability on the scale surface. As concerns PAPEMP, the above requirements are fulfilled respectively by different functional groups, i.e. ether groups and phosphonate groups. To simplify the role of functional groups in the anti-scaling mechanism means that the performance of an anti-scalant can be optimized by the combination of specific functional groups; furthermore, these functional groups can also be adjusted with respect to different scale surfaces.

Keywords: Molecular simulation; Anti-scaling mechanism; Electrostatic potential; Calcite

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1. Introduction

Supersaturation in concentrate is inevitable due to the permeate withdrawal and concentration polarization in membrane applications involved in the desalination of sea water or brackish water. Scaling of some sparingly soluble salts (CaCO_3 , BaSO_4 , CaF_2) occurs especially at high permeate fluxes and at low cross-flow velocities, which may cause permanent damage to the membrane. While the scale in the bulk solution can be removed from membrane modules by applying cross-flow operation mode, it is physically and chemically difficult to clean the scale precipitated on the membrane surface. Although some approaches, including anti-scalant addition, back-flushing and chemical cleaning, have already been developed to prevent or mitigate the scaling on the membrane [1–9], such a problem is far from being satisfactorily solved.

The supersaturated concentrate is thermodynamically unstable. When scale nuclei appear in a concentrate due to the increase in salt concentration, they may either stay in the bulk solution or precipitate onto the membrane surface. The scale nuclei on the membrane surface grow into scale which results in an irreversible membrane blockage. It is believed that preventing the nucleation in the concentrate and the nuclei precipitation on the membrane surface should be the key factors to extend the operation period of a membrane module. Many anti-scalants have been developed for this purpose.

Scaling in a membrane involved water process can be partly suppressed by introducing a small quantity of anti-scalants. Some commonly used anti-scalants include ethane diphosphonic acid, polyether polyamino methylene phosphonate, acrylic acid-maleic acid copolymer (AA-MA) and so on. Several metal ions also have a certain inhibiting effect on the scaling potential among which Zn^{2+} was experimentally proved superior to any other applied ion species [10]. As a whole, the anti-scaling performance of polymers men-

tioned above is usually better than that of metal ions.

Up to now, the understanding of anti-scaling mechanism remains semi-empirical. Many anti-scalants developed in the laboratory are far less effective than expected when they are used in industrial applications. Some generally accepted anti-scaling mechanisms are as follows:

- Formation of complexes between the anti-scalant and ions makes the concentrate stable at a higher supersaturated level.
- Adsorption of anti-scalants on the scale surface causes defects during the growth of scale nuclei, which weakens the mechanical strength of the scale.
- A certain electrostatic potential is presented on the anti-scalant modified nuclei surface, and the agglomeration among crystal nuclei is therefore suppressed by electrostatic repulsion.

The above concepts are subject to some limitations. Since the formation of complexes should satisfy a certain stoichiometric ratio, a common dosage of anti-scalants at the ppm level can hardly reduce the degree of supersaturation of concentrate dramatically. Besides, instead of considering the interaction between the membrane and anti-scalant modified scale, the available mechanisms only deal with the situation in the bulk phase of the concentrate.

Apparently, study on the anti-scaling mechanism at the molecular level might be more instructive; unfortunately, only very limited work in this aspect can be found [11–15]. Most of it was focused on the adsorption behavior of anti-scalants on the scale surface, and the authors came to nearly the same conclusions. It was suggested that the matching between the functional groups of an anti-scalant and the ion spacing on the scale surface should favor a strong docking of anti-scalants on the specific positions by electrostatic force and hydrogen bonding. Furthermore, the adsorption heat of anti-scalants on the scale surface was considered vital to their performance.

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