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Computational study of NF membrane removal in rejection of specific NOM compounds

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ABSTRACT

A computational study was conducted to verify natural organic matter removal of two types of nanofiltration (NF) membranes. NF membranes used in this study were fully aromatic polyamide based on trimesoyl chloride and 1,3-benzenediamine (NE90) and semi-aromatic polyamide based on trimesoyl chloride and piperazine with polyvinyl chloride coating (NE70). The solute–membrane interaction was modeled using density functional theory (DFT) to clarify and verify the experiment results of our previous study. The calculations were performed by the calculated highest occupied molecular orbital and lowest unoccupied molecular orbital with frontier orbital gap which reflexed adsorption energy between organic molecules and the membrane surface materials. DFT showed as an effective tool to predict interaction phenomenon between solute and membranes, which is relative to membrane fouling and rejection of particular organic substances. The calculation results showed that carboxylic compound has high-energy gap and tend to adsorb on the membrane surface than the other compounds (phenolic and acetic acid) and it bound higher energy with NE90 than NE70. This is comparable with the experimental results that NE90 is consists of surface material, which is easily to be adsorbed by organic molecule, especially carboxylic type compound.

Keywords: Natural organic matter (NOM); Adsorption; Rejection; Fouling; Polyamide membrane; Density functional theory (DFT)

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