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Modeling of RO/NF membrane rejections of PhACs and organic compounds: a statistical analysis

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Abstract. Rejections of pharmaceutical compounds (Ibuprofen, Diclofenac, Clofibric acid, Naproxen, Primidone, Phenacetin) and organic compounds (Dichloroacetic acid, Trichloroacetic acid, Chloroform, Bromoform, Trichloroethene, Perchloroethene, Carbontetrachloride, Carbontetrabromide) by NF (Filmtec, Saehan) and RO (Filmtec, Saehan, Toray, Koch) membranes were studied. Chloroform presented the lowest rejection due to small molar volume, equivalent width and length. Diclofenac and Primidone showed high rejections related to high molar volume and length. Dichloroacetic acid and Trichloroacetic acid presented good rejections caused by charge exclusion instead of steric hindrance mechanism influencing rejection. Bromoform and Trichloroethene showed low rejections due to small length and equivalent width. Carbontetrabromide, Perchloroethene and Carbontetrachloride with higher equivalent width than BF and TCE presented better rejections. A qualitative analysis of variables using Principal Component Analysis was successfully implemented for reduction of physical-chemical compound properties that influence membrane rejection of PhACs and organic compounds. Properties such as dipole moment, molar volume, hydrophobicity/hydrophilicity, molecular length and equivalent width were found to be important descriptors for simulation of membrane rejection. For membranes used in the experiments, we may conclude that charge repulsion was an important mechanism of rejection for ionic compounds. After analysis with Multiple Linear Regression, we also may conclude that membrane rejection of neutral compounds was well predicted by molar volume, length, equivalent width, hydrophobicity/hydrophilicity and dipole moment. Molecular weight was a poor descriptor variable for rejection modelling. We were able to provide acceptable statistical significance for important results.

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