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A QSAR (quantitative structure-activity relationship) approach for modelling and prediction of rejection of emerging contaminants by NF membranes

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ABSTRACT

Principal component analysis (PCA) and multivariate regressions were used to find a quantitative structure-activity relationship (QSAR) model equation that combines interactions between membrane characteristics and solute properties for predicting rejection. An internal experimental database that accounts rejections of contaminants by two nanofiltration membranes (NF-90, NF-200) was used to develop the QSAR model equation. Membrane characteristics related to hydrophobicity (contact angle), salt rejection, and surface charge (zeta potential [ZP]); compound properties describing hydrophobicity (log K_{ow}, log D), polarity (dipole moment), and size (molar volume, molecular length, molecular depth, equivalent width, molecular weight); and operating conditions (flux, pressure, cross flow velocity) were identified and evaluated as candidate variables for rejection prediction. Subsequently, using the QSAR model, rejection predictions were made for an external experimental database. Measured rejections were compared against predicted rejections to determine the best model; an acceptable R^2 (0.93) correlation coefficient was found for the best model with a standard deviation of error of 7% for predicted rejections. In conclusion, a general QSAR model equation was able to model and predict rejections of emerging contaminants during nanofiltration.

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