

Interactive comment on “Prediction of RO/NF membrane rejections of PhACs and organic compounds: a statistical analysis” by V. Yangali-Quintanilla et al.

Anonymous Referee #1

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1) Does the paper address relevant scientific questions within the scope of DWES? The manuscript reports on statistical approaches to delineate the rejection mechanisms of organic solutes during NF and RO treatment. The presence of organic trace compounds in wastewater and surface water is of increasing interest and developing approaches to assess the performance of advanced treatment processes to remove these compounds is timely and in line with the scope of DWES.

2) Does the paper present novel concepts, ideas, tools, or data? The paper presents the adaptation of principal component analysis to delineate factors that influence solute rejection in high-pressure membrane. This work is novel and original. The findings of

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the study, however, confirm previous knowledge on the key properties affecting rejection.

3) Are substantial conclusions reached? The study is reporting on an interesting statistical approach that has merit in solute rejection modeling. The study suffers from a limited database (15 compounds), which lacks to provide proof of statistical significance. The objective of the study as stated on p. 23, line 22 is to 'defining the importance of each descriptor'; is not met in providing a comprehensive assessments of individual descriptors or solute properties on rejection.

4) Are the scientific methods and assumptions valid and clearly outlined? Most methods are properly described. However, a couple of important experimental conditions are not stated: - was the membrane pre-compacted - were spacers used to maintain cross-flow conditions? - the hydrodynamic regime during experiments is not clear. P. 27, line 15 suggests 'changes in pressure'; whereas line 21 suggests a constant J/k (constant flux) regime? Please clarify (constant pressure, declining flux or constant flux, increasing pressure?). For comparison, it might be helpful to state the permeate flux (LMH) of the experiment. - the authors didn't address the issue of fouling. While it is acknowledged that the proposed approach is applicable to virgin or fouled membranes, rejection modeling under fouled conditions might require different descriptors; - p. 28, last line, Why 48 hrs? Was steady-state rejection reached after 48 hrs? Provide reasoning, please. - p. 29, line 11. The authors should acknowledge that a 'hydrophobicity'; definition using log Kow of 2 is not a distinct classification. Why 2 and not 2.5 or 3.0? Also, it remains unclear whether log Kow for ionic solutes was used in the statistical approach or log Kow values for the pH of the experiment (log Kow will change as ionic solutes dissociate!). This is also important how compounds were classified using 'HP';. Figure 2 seems to imply that log Kow values have been used for ionic compounds (IBU, CFA, NPX or DCF, which wouldn't be correct?

5) Are the results sufficient to support the interpretations and conclusions? - while the

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paper talks about prediction; at various places, what really is provided is a model for solute rejection. Prediction is not validated anywhere in the study. - While the statistical approach has merit, the database seems way too limited to derive clear conclusions on the role of individual descriptors on rejection. What is difficult to understand are the examples of the model presented in Table 5. Why is the model changing for the same type of compounds between the LE440 and the NF-90 implying that sometimes MV and dipole is important whereas for other membranes HP is more important and MV and dipole moment don't play a role. This seems highly membrane type dependent and clearly might be a result of a lack of statistical robustness.

6) Is the description of experiments and calculations sufficiently complete and precise to allow their reproduction by fellow scientists (traceability of results)? - see comments above.

7) Do the authors give proper credit to related work and clearly indicate their own new/original contribution? - yes

8) Does the title clearly reflect the contents of the paper? The term prediction; in the title as well as in the abstract is an over-statement. What is presented in the paper is a rejection modeling exercise.

9) Does the abstract provide a concise and complete summary? Yes.

10) Is the overall presentation well structured and clear? - yes

11) Is the language fluent and precise? - yes

12) Are mathematical formulae, symbols, abbreviations, and units correctly defined and used? - see comments above

13) Should any parts of the paper (text, formulae, figures, tables) be clarified, reduced, combined, or eliminated? - see comments above

14) Are the number and quality of references appropriate?

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15) Is the amount and quality of supplementary material appropriate? N/A

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