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Drinking Water Engineering and Science Discussions

Interactive comment on "Development of a predictive model to determine micropollutant removal using granular activated carbon" *by* D. J. de Ridder et al.

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Dear reviewer.

Thanks for your critical comments on our paper. Here's my point-by-point reaction on your comments

1. Thanks

2. Too high carbon concentrations The carbon concentrations used were based on a rough estimation, and regrettably the estimated carbon dose was rather high. This could have been prevented by first measuring removal of an indicator solute - such as

a dye - which is easily measured. The problem is that the experiments were carried out with both fresh and preloaded full carbon grains, and as such an equilibrium time of 2 months was taken. Pre-testing would result in a 2-month delay in our experiments

3. data inclusion criteria This was a very relevant comment, as I didn't mention it in the paper and had to delve in the raw data again to find the criteria. The criteria: -only values higher than the LOD were used. This accounts for the highest losses of potential datapoints (surface:65 demi PL:90 demi FR:101) -maximum carbon concentrations were used to prevent bias. At higher carbon concentrations, only data > LOD was found for solutes which are poorly removed (i.e. negatively charged solutes). The data-subset at higher carbon concentrations is excluded if only solutes of similar charge are included in that subset.

As this comment required me to delve into the raw data again, I found that 3 solutes (aminopyrine, pindolol, naproxen) were not included in the demiwater datasets. Probably, they were regarded as outliers and this has not been documented correctly. However, as I cannot explain based on their properties why they are outliers, I included them again in the model. Also the surface water dataset required minor revisions. I included a document which shows the effect of these revisions on the paper. For the surface water model, changes are minimal. For the model with demiwater and fresh carbon, the Q2 value drops, but is still within the QSAR criteria. The demiwater model on preloaded model, however, does no longer meet the QSAR criteria. This shows moreover that r2 and Q2 values are sensitive for the models based on these small datasets. The conclusions based on the graphs on model accuracy (removal predicted against removal measured) still hold. The majority of the datapoints are within 20% deviation in the training set and validation set, with an overprediction of max 40% in the validation set.

4. compound selection validation set We choose to select 20% of the solutes for validation, and 80% for training. That is 4 resp. 17 solutes. The solutes for validation were selected semi-randomly; at least 1 solutes from each charge group was selected

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to prevent a biased validation set and to prevent biasing the training set. However, within the charge groups, the solutes were selected randomly. It would indeed be more convincing to have more solutes for the validation set, but this implies that we have less solutes for the training set, weakining the models that are validated.

Please also note the Supplement to this comment.

Interactive comment on Drink. Water Eng. Sci. Discuss., 2, 189, 2009.