

***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 #2

Thank you for your thorough review and in-depth comments on our article. My point-by-point reaction on your comments:

1. relation pKa, pH The Henderson-Hasselbalch equation has been added to the paper, and in table 1, the charged fraction is indicated at the 3 pH values for all solutes.
2. and 4. absolute charge vs dissociation It is true that the charge factor is a simplification which does not take partial dissociation/protonation into account. This is especially

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relevant for the negatively charged solutes at pH 4, as their charged fraction may vary between 12% and 81%. At other pH values, charged fractions are >97%. The charged fraction of positively charged solutes is >88% at all pH values. To account for partial dissociation/protonation, the fictive charge parameter (-1, 0, +1) has been multiplied by the charged solute fraction for all solutes.

A subquestion involves the low pH of the ultrapure water (pH 4). We think this is caused by the low buffering capacity of ultrapure water. The produced ultrapure water is collected in a storage vessel which is not completely air-tight. As a result, CO<sub>2</sub> uptake can result in a lowering of the pH.

3. pKa neutral solutes Agreed, a pKa value of 0 is clearly wrong. I meant to put n/a there; the sources I used do not give a pKa value for these solutes, so I understood that there is no dissociation or protonation of these solutes. At the moment, they have been adjusted to n/a, with the exception of Carbamazepine. Could you please mention the source where you found this pKa value of Carbamazepine, so I can check if the other neutral solutes have a pKa value or not.

5. parameter independance The pKa is used for log Kow correction (log D), and to determine solute charge. As both log D and charge are corrected by the same parameter, they are most likely not independant of each other. However, this is only valid when considering a single solute! When considering the total dataset, cross-correlation coefficients are under 0.14. Furthermore, it is essential to consider charge interaction separately from log D. In log D, the effect of solute charge on hydrophobic partitioning and hydrophobic bonding is considered. However, electrostatic interaction between carbon and solute is not considered when using log D alone. The need for a charge parameter becomes clear from figure 1. Here, negatively charged solutes show lower removal than neutral or positively charged solutes on preloaded carbon, while their log D values are significantly higher.

6. pH(pzc) value Unfortunately, we did not measure the pH<sub>pzc</sub> on fresh or preloaded

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carbon, and did not find it in the literature. However, it is very likely that the fresh carbon surface is positively charged in ultrapure water, at pH 4, as this is significantly lower than the typical  $pH_{pzc}$  for carbon. In the case of surface water (pH 8), the carbon is preloaded with NOM, which is negatively charged. According to Newcombe et al. 1994, effective surface charge could be determined by summing the carbon charge and the NOM charge. At pH 8, NOM is strongly negatively charged and it is not to be expected that the carbon is strongly charged, as the pH is close to typical  $pH_{pzc}$  values. For preloaded carbon at pH 4, fresh carbon positive charge can potentially overrule NOM negative charge. However, the results in figure 1 suggest that this is not the case, as positively charged solutes show higher removal on fresh carbon, and negatively charged solutes lower.

7. dispersion interactions The suggested addition has been made.

8. initial solute concentration vs removal If I understand this correctly, only the surface water/preloaded NOM model can then also be used for other initial concentrations. The ultrapure models are both specific for an initial concentration of 2 ug/l. At the moment, I removed the sentence in question.

9. Model accuracy Indeed, I meant absolute deviations; the differences in removal-%. I think it is not fair to work with numeric deviation percentages, as this would "punish" deviation from small values of  $C_e/C_0$  (i.e. high removal) more than deviation from larger values. Moreover, I think that absolute deviations have more practical value. In fact, I'm giving a confidence interval here, without being specific on the level of confidence.

10. formal errors corrected

Please also note the Supplement to this comment.

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