Interactive comment on “Functional characterization of the water-soluble organic carbon of size fractionated aerosol in the Southern Mississippi Valley” by M.-C. G. Chalbot et al.

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Received and published: 10 March 2014

This is Stefano Decesari from the National Research Council of Italy. I am writing this comment because the NMR functional group diagram contained in Figure 6 of the present manuscript probably needs some corrections. The corrections I am proposing here do not impact the main conclusions of the paper, but they can help to remove some discrepancies with the results of the previous field experiments. First of all, the functional group diagram that I proposed in my ES&T paper was meant for submicron aerosol samples only, and it is not surprising that the WSOC constituents of coarse aerosols are misclassified using that approach. Then, when I plotted the...
concentrations of the three submicron samples in Table 2 of the present manuscript into the functional group diagram (see the calculations in the excel file attached), I actually found no mismatch: all three fell either in the “biomass burning” or in the “SOA” regions. A possible reason for such different result with respect to what shown in Figure 6 of this manuscript stands in the concentration units used. In my 2007 paper I specified that “The vertical axis shows the aliphatic CARBON FRACTION accounted for by carbonylic/carboxylic groups(HC-C=O), which is maximum for compounds such as succinic acid, ketoglutaric acid, etc.”. The first figure of my paper clarifies that the HC-C=O groups account for the aliphatic carbonyls/carboxyls with their carbon groups in alpha position (which is the one actually measured by H-NMR). This means that one mole of HC-C=O counts for two carbon atoms. The functional group diagram used in my ES&T paper in fact uses carbon concentration units, not moles of functional groups. I suspect that this ambiguity led to an apparent inconsistency between the results shown in this study and my previous findings in Europe and South America. I would rather conclude that the results presented here are completely in line with those achieved in the past, at least in respect to the fine aerosol composition. Finally, I would like to thank the Authors for the interesting contribution to the application of NMR techniques in the aerosol atmospheric field.

Please also note the supplement to this comment:
http://www.atmos-chem-phys-discuss.net/14/C366/2014/acpd-14-C366-2014-supplement.zip

Interactive comment on Atmos. Chem. Phys. Discuss., 14, 3629, 2014.