

Interactive comment on “Functional group analysis by H NMR/chemical derivatization for the characterization of organic aerosol from the SMOCC field campaign” by E. Tagliavini et al.

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Answers to Referee2

First of all we wish to emphasize that this paper deals with a NMR spectroscopy/chemical derivatization technique which is conceptually new for the analysis of water-soluble organic aerosol. Thanks to this method we were able to provide reproducible data for concentrations of total carboxylic groups in biomass burning aerosol samples. Despite these advancements, we could not overcome all the technical problems associated with the analysis, which is currently labor-intensive and is accurate only for relatively highly loaded samples. We have prepared a revised version of the

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manuscript for submission to ACP, in which we have detailed the sensitivity and accuracy of the method.

(1) We have calculated the uncertainty deriving from the relatively low sensitivity of the technique employed and we have consequently modified Tables 1 to 9.

(2) A comparison with the amounts of levoglucosan found by other authors (Schkolnik et al., 2005) on the same samples and employing validated chromatographic techniques has been added to Fig. 4, finding a fairly good correlation.

(3) We have estimated the sensitivity of our method for one compound identified for sure (levoglucosan) and we have added a sentence about this in section 2.5.

(4) The good agreement between the concentrations of levoglucosan obtained by our technique and those obtained by chromatographic analysis indicates that a good recovery was obtained for polar non-volatile compounds. On the basis of our data, we cannot exclude that the most volatile fraction of OC was partly lost during the sample preparation, however WSOC on the back-up filters was usually below 10

(5) We believe the hypotheses put forward in the discussion section are the most likely sources of carbon imbalance. Extraction problems cannot be completely ruled out, but, based on the agreement found between our analysis of levoglucosan and its determination by chromatographic methods, they were not major sources of error.

(6) The identity of the few compounds recognized was established from the comparison with the NMR spectra of the pure compounds. We did not recursively search for the possible identification of many compounds, since the aim of our work was different.

(7) On page 9456, l. 22, “relatively less” means that, by looking at the spectra, the area of the signal corresponding to H-C-C= protons in coarse samples is a minor part of the total integrated area of these samples when compared to fine samples. The same is expressed quantitatively in Table 3.

(8) The concentration M of a given (H or C) species in the coarse fraction of the aerosol

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was calculated according to the following equation:

$$M (\text{micro}_{mol}/m3) = (\text{micromol}_c - Fc/Ff * \text{micromol}_f)/(Fc + Ff)$$

where Fc and Ff are the volumes of air passed through the coarse and the fine filters, respectively, and the 61549;molc and 61549;molc are the mass loadings in the coarse and fine filters, respectively. The Referee can easily verify that the above equation allows to correct for the contribution of the fine particles in front filters on the basis of both relative volume and mass loadings.

Interactive comment on Atmos. Chem. Phys. Discuss., 5, 9447, 2005.

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