Interactive comment on “Polar organic compounds in rural PM$_{2.5}$ aerosols from K-puszta, Hungary, during a 2003 summer field campaign: sources and diurnal variations” by A. C. Ion et al.

Anonymous Referee #1

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The aim of this study was to identify the source and/or the mechanism of production of several polar oxygenated organic compounds which were previously observed in the PM$_{2.5}$ fraction of ambient aerosol matter. To identify the relevance of photochemical processes, separate day-time (D) and night-time (N) samples were collected at a rural site in Hungary. It was found that several of the analysed organic compounds exhibit much larger concentrations in the D samples than in the N samples. The differences are considered as evidence that photochemical oxidation is a very important production mechanism. A distinctly different behaviour, with (very) high concentrations in the N samples, was observed with levoglucosan, a tracer for wood burning. As far
as one can tell from the described details, the data are of good quality and may fi-
nally be worth publication in ACP. In the present form, however, publication cannot be
recommended because the text and the data presentation suffer from several major
deficiencies. These may be summarised as follows.

The main text contains a large number of repetitions and unessential statements. In
the Abstract, for example, the method of analysis needs not be described; the specific
compounds should be named only once. The Introduction can be reduced to the first
sentences of the first and second paragraph. All the relevant information is summarised
(again) on pp. 1870–2. Once is enough. The section Experimental contains a lot
of details which should be shortened wherever possible. On the other hand, some
aspects of the experimental approach are missing. Why were the quartz filters baked
only at 550°C? Why was only 1/16 of the high-volume filter used? How was WSOC
determined? What is OC, just the C in OM? It is very irritating to see that the description
of experimental details is continued in sect 3.1. This part must be integrated in sect
2.2, shortened and put into perspective, better than in the present form. The section
Results and Discussion should start with an overview on the quantitative details, in
the form of the data in Table 1. However, the table should contain separate columns
for N and D data. Table 2 must be cancelled (no problem for the reader to calculate
fractions by him/herself). The text on pages 1872, 1873 and 1875 must be condensed
significantly. In its present form, the section Conclusions merely constitutes a second
abstract, a waste of paper. A new section Conclusions should (i) briefly describe the
improvement in understanding that has been achieved by the present study and (ii)
address consequences as well as desirable future work. In total, the 13 pages of the
main text should be reduced to about 9 or even less.

As to the figures, the reviewer has the impression that the authors spent by far too little
time on data evaluation and optimum data presentation. The information contained
in several of the figures is hard, sometimes impossible to read. More specifically, the
following comments and suggestions should be considered.
Fig. 1. To be cancelled; reference should be made to other papers where the molecular structure has already been shown.

Fig. 2. The labels should be enlarged by about 30% to make them easily readable in print (all figures one-column wide). Fructose and glucose should either not be mentioned specifically (there are other unlabelled small peaks), or should also be labelled by number. Which are the three peaks for fructose?

Fig. 3. All labels, notably those for N and D at the abscissa would be unreadable in print (one-column wide figure). Dates at the abscissa should only be shown in two- or three-day intervals. The figure caption should state that points reflect alternating N/D data. To illustrate the relevant differences in N/D behaviour only one example for a photosensitive compound should be shown, e.g. Mannitol (use x instead of * to indicate multiplication factor).

Fig. 4. “% XYZ” is not a physical quantity; an appropriate notation would be XYZ Fraction of OC (%). Why fraction of OC and not mass concentration? Remove upper inset. The caption should state that the line is the result of a linear regression.

Figs. 5 and 6. These two figure must be redesigned completely to make the data transparent and to identify a correlation with meteorological parameters. The differences between D and N become much more evident if they are identified by different symbols and if each set of N and D data is connected by a separate line. Data for two typical examples (compounds) plus one for levoglucosan should be shown in individual panels, log scale (same scale in decades/cm). Data for other compounds should be described by comparison to these graphs. In doing so, it will become clear that most of the time the D/N ratios were large, but there were several days/night on which the ratios were around or even below unity. Interpretation of the data in terms of efficient photochemical oxidation makes sense only if the times with high D/N ratio exhibited much higher intensity of sunshine than those on which D/N was around unity. The correlation with meteorological parameters must be included in a revised manuscript.
Again, the authors should provide a good argument for presenting the data for the organic compounds as fractions of OC and not as mass concentrations.

Fig. 7. Scatter plot for malic acid vs OC. Using the terms “OC” and “Malic acid” to indicate mass concentrations (MC) is laboratory slang. More importantly, the statement (p. 1874) that “malic acid can serve as a reasonably good general indicator compound for the organic carbon mass in the PM$_{2.5}$ aerosol” cannot be accepted. First of all, to substantiate such a statement, one would have to consider a scatter plot of MC$_{OC}$ vs MC$_{MA}$ (subscript MA for Malic Acid), as shown in the attached Figs. 1a and b. A linear regression of the data in a lin-lin presentation, Fig. 1a, clearly results in a large offset on the OC scale ($2.3$ $\mu$g/m$^3$ for MC$_{OC}$ vs MC$_{MA}$). In other words, if MA were to serve as an indicator for OC, we would find OC even if there is no MA. A better fit to the data, with $R^2 \approx 0.60$, is obtained using a third order polynomial fit in the lin-lin presentation or a linear regression in a log-log presentation, see Fig. 1b. The latter presentation implies that MC$_{OC} \approx 0.75MC_{MA}^{0.46}$, i.e. MC$_{OC}$ varies roughly as the square root of MC$_{MA}$. Formally, this is the best one can get out of the data, but what is the interpretation? The authors should either spend more time on data evaluation to identify true correlations or should limit themselves to merely presenting the data without adding unjustified interpretations.

In summary, the manuscript needs major revisions and should be passed through a second review.

Interactive comment on Atmos. Chem. Phys. Discuss., 5, 1863, 2005.
Figure 1: Scatter plots for the mass concentrations of malic acid vs organic carbon. (a) Double linear, (b) double logarithmic data presentation. The lines reflect different methods of data regression, as specified in the insets.