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A simplified representation of the water soluble organic fraction for modelling the aerosol hygroscopic behaviour over the Amazon Basin.

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A comprehensive aerosol characterisation experiment have been carried out at a pasture site in Rondonia (Brazil) in the period 10 Sept - 14 Nov 2001, i.e. from the middle of the dry season to the on-set of the rainy season in the framework of SMOCC project. The samples were subjected to an extensive chemical analysis for both inorganic and organic components and a particular effort was dedicated to characterise the most polar fraction of the organic aerosol, defined by its extractability in water (WSOC, "water-soluble organic compounds"). WSOC represented 57 to 76% of organic carbon in fine particles, and their mass concentrations were 3 - 6 times higher than those of the inorganic salts, suggesting that they contributed significantly to the aerosol hygroscopicity. The complex organic chemical composition obtained by an extensive analytical set up and analyses, was reduced to simplified representations which can be exploited as observational basis for thermodynamic models predicting water uptake and CCN properties of organic aerosol. The molecular composition of WSOC determined by GCMS and IC methods was linked to the functional group composition provided by 1HNMR analysis. The resulting WSOC composition can be characterised as a mixture of low-molecular weight polar compounds, mainly C2-C6 carboxylic acids and polyhydroxylated compounds, and medium-to-high molecular weight less polar compounds which could not be speciated at the molecular level.

Such a mixture encompasses a wide range of water-solubilities, leading to the conclusions that the water-extraction was effective for classes of compounds of very different polarity/solubility, and that the WSOC mixture cannot be correctly represented by a single organic compound. To provide a more realistic scenario, a series of model compounds was derived from either lumping of the identified species or by introducing hypothetical compounds which reproduce the functional group composition of the WSOC fraction not speciated at the molecular level. Different sets of model compounds were evaluated to represent the average organic compositions for the different periods of the SMOCC campaign. Finally, a simplified representation was derived by further reducing the list of model compounds to four simple categories selected on the basis of different water solubility and according to the neutral/acidic character, useful for modelling the aerosol water uptake and the aerosol/cloud interaction.