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Cluster analysis of the Atlantic aerosol particles by combining particle chemical composition and number concentration

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The marine aerosol plays an important role in global climate regulation and marine biogenic system. However, aerosol particles in the marine boundary layer (MBL) are seldom from exclusively marine origins. Complex sources and atmospheric processes determine the chemical and physical properties of aerosol particles. In this study, chemically distinct groups are identified by k-means clustering, in an exploratory way, on chemical composition (provided by a High Resolution Time of Flight Aerosol Mass Spectrometer, HR-ToF-AMS) and particle number concentration (PNC) of MBL aerosol particle, and linked to the air mass origins. The analysis is based on physical and chemical measurements performed on board the German research vessel Polarstern during 4 research cruises over the Atlantic Ocean in 2011 and 2012, covering spatial range from 53°S to 53°N in two seasons (spring and autumn). In total 12 variables were used for clustering, including PNC of aerosol particles and 11 chemical components (ammonium, nitrate, chloride and BC directly provided by instruments, plus 5 organic components and 2 sulfate components with identified sources given by source apportionment models). With this algorithm, a total of 4 clusters was identified based on the distinct chemical composition corresponding to 2 marine types and 2 continental types. Moreover, when compared to air mass back trajectories, each cluster can be attributed to a specific air mass type and/or influenced by location. Specifically, the marine 1 cluster was characterized by dominating contribution of dimethyl sulphide (DMS) oxidation products, coincidently with air masses from the ocean. The marine 2 cluster containing significant nitrogen products, which could be attributed to biogenic amines sources, was found mainly in autumn (especially over the Southern Atlantic) within marine air masses. The continental cluster appeared only in the Northern Hemisphere, in most case associated with air masses from the Europe. The combustion cluster occupied a wide area between 15 °S and 15 °N in autumn (November), influenced by the seasonal continental outflow (e.g. biomass burning). The resulting clusters are repeatable in the same season along the similar ship tracks, which makes the method helpful for modelization on predicting physicochemical properties of MBL aerosol. Also, this approach appears to be particularly useful and convenient for analysis of large mobile measurements in association with various air masses.