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Simulation of aerosol chemical compositions in the Western Mediterranean Sea

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This work aims at evaluating the chemical transport model (CTM) Polair3d of the air-quality modelling platform Polyphemus during the ChArMex summer campaigns of 2013, using ground-based measurements performed at ERSA (Cape Corsica, France), and at determining the processes controlling organic aerosol concentrations at ERSA. Simulations are compared to measurements for concentrations of both organic and inorganic species, as well as the ratio of biogenic versus anthropogenic particles, and organic aerosol properties (oxidation state).

For inorganics, the concentrations of sulphate, sodium, chloride, ammonium and nitrate are compared to measurements. Non-sea-salt sulphate and ammonium concentrations are well reproduced by the model. However, because of the geographic location of the measurement station at Cape Corsica which undergoes strong wind velocities and sea effects, sea-salt sulphate, sodium, chloride and nitrate concentrations are strongly influenced by the parameterizations used for sea-salt emissions. Different parameterizations are compared and a parameterization is chosen after comparison to sodium measurements.

For organics, the concentrations are well modelled when compared to experimental values. Anthropogenic particles are influenced by emission of semi-volatile organic compounds (SVOC). Measurements allow us to refine the estimation of those emissions, which are currently missing in emission inventories. Although concentrations of biogenic particles are well simulated, the organic chemical compounds are not enough oxidised in the model. The observed oxidation state of organics shows that the oligomerisation of pinonaldehyde was over-estimated in Polyphemus. To improve the oxidation property of organics, the formation of extremely low volatile organic compounds from autoxidation of monoterpenes is added to Polyphemus, using recently published data from chamber experiments. These chemical compounds are highly oxygenated and are formed rapidly, as first-generation products.