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Exploration of the seasonal variation of organic aerosol composition using an explicit modeling approach

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Organic compounds account for a major fraction of fine aerosols in the atmosphere. This organic fraction is dominated by secondary organic aerosol (SOA). Processes leading to SOA formation are however still uncertain and SOA composition is far from being fully characterized. The goals of this study are to evaluate our current understanding of SOA formation and explore its composition. For this purpose, a box-model that describes explicitly processes involved in SOA formation has been developed. This model includes the emission of 183 gaseous and particulate organic compounds. The oxidation of these emitted organic compounds is described using the Generator of Explicit Chemistry and Kinetics of Organics in the Atmosphere (GECKO-A). Gas/particle partitioning has been implemented considering an ideal homogeneous condensed phase. The generated chemical scheme contains 500,000 species and the gas/particle partitioning is performed for 90,000 of them. Simulations have been performed for summer and winter scenarios representative of continental and urban conditions. NO_x and ozone simulated concentrations reproduce the expected winter and summer diurnal evolutions. The predicted organic aerosol composition is a mixture of primary and secondary organic aerosols during the winter and is largely dominated by SOA during the summer.