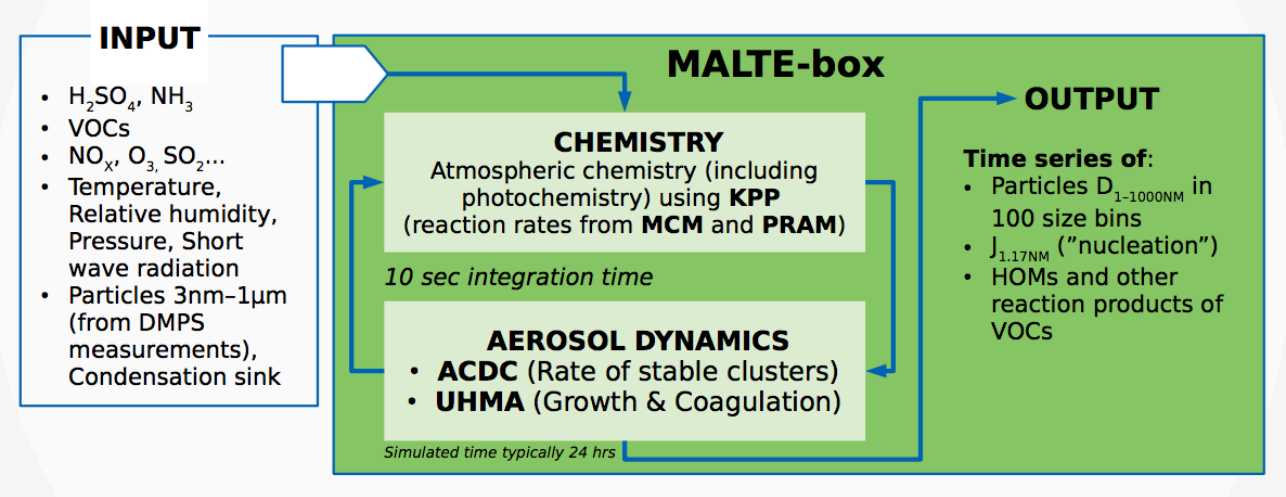
MALTE-box

Model to predict new Aerosol formation in the Lower TropospherE



MALTE–box is a zero–dimensional improved version of the one-dimensional model MALTE (Model to predict new Aerosol formation in the Lower TropospherE) (Boy et al., 2006, Qi et al., 2018). In this model version we either read in the measured parent organic gas concentrations from measurements (anthropogenic and biogenic) or predict biogenic emissions from vegetation with **Model of Emissions of Gases and Aerosols from Nature – MEGAN** (Guenther et al., 2006). The concentrations of inorganic vapours are usually taken from measurements. The further faith of all vapours is calculated using the chemical reaction schemes from the **Master Chemical Mechanism - MCM** (http://mcm.york.ac.uk) and the **Kinetic PreProcessor - KPP** (Damian et al., 2003).

Recently we have implemented the **Peroxy Radical Autoxidation Mechanism - PRAM** (Roldin et al., 2019) and incorporated it alongside MCMv3.3.1. PRAM explicitly describes the formation and evolution of peroxy radicals (RO_2) from the ozonolysis and OH oxidation of monoterpenes, driven by subsequent H-shifts and O_2 additions. The autoxidation is terminated by bimolecular reactions, wherein the RO_2 formed reacts with NO, HO_2 or other peroxy radicals, thereby forming alkoxy radicals, closed shell monomers or dimers (Roldin et al., 2019). The PRAM considers temperature dependent autoxidation reaction rates, which is important when investigating the SOA mass yields at varying temperatures.

Aerosol dynamical processes (nucleation, coagulation, condensation, and evaporation) are calculated using the model **University of Helsinki Multicomponent Aerosol module – UHMA** (Korhonen 2004). The new particle formation through neutral and ion-induced clustering of NH_3 and H_2SO_4 molecules is modelled using the **Atmospheric Cluster Dynamics Code – ACDC** (Olenius, 2013), which is coupled to UHMA module of MALTE-box. In this way we can explicitly simulate time-dependent molecular cluster formation directly. We are thereby able to predict size dependent aerosol number and mass concentration together with the specific composition of atmospheric aerosol particles.

References

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