Model Investigations on the Multiphase Chemistry of Biomass Burning Compounds with CAPRAM BBM1.0

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Biomass burning (BB) is an important contributor to air pollution on different time and spatial scales affecting air quality, public health and climate. Anhydrosugars (e.g., levoglucosan) and methoxyphenols (e.g., guaiacol and vanillin,) are key tracer compounds emitted through BB. Emitted BB compounds can undergo complex multiphase chemical processing in tropospheric aerosol particles and fog/cloud droplets contributing to the formation of secondary organic aerosol (SOA) and modification of the primary organic aerosol. However, their chemical multiphase processing is not yet well understood and investigated by atmospheric chemistry models.

The present work aimed at a better understanding of the multiphase chemistry of BB tracers, such as levoglucosan, by process model studies using the chemical multiphase mechanism CAPRAM-BBM1.0. CAPRAM-BBM1.0 is designed to describe the aqueous-phase oxidation of levoglucosan and specific methoxyphenols and their exchange processes with the gas phase. It includes 2881 processes and was coupled with the multiphase chemistry mechanism MCMv3.3.1/CAPRAM4.0 and the extended CAPRAM aromatics module (CAPRAM-AM1.0). Afterwards, CAPRAM-BBM1.0 was applied in simulations with a multiphase chemistry process model for winter and spring residential wood burning scenarios in Europe.

The simulations indicate that levoglucosan and vanillin are effectively oxidized under cloud conditions leading to concentration reductions of 75%/40% and 97%/94% after the third model day under spring/winter conditions. In-cloud oxidations represent the main loss for methoxyphenols but their importance strongly depends on the respective Henry's Law solubilities of the phenolic compounds. The chemistry of BB tracers contributes to the formation of BB-SOA and affects also the aqueous-phase budgets of key radical oxidants such as OH and NO₃. A 38% higher organic mass is modelled for the spring case when CAPRAM-BBM1.0 is coupled to the core mechanism. Especially, the formation of functionalized mono-and dicarboxylic acids was enhanced by a factor of 6.5 and 1.2 in the spring case. Detailed chemical rate analyses revealed that the daytime oxidation by OH acts as the most important sink for BB tracers. Additionally, a reduced levoglucosan oxidation mechanism was derived in the present study based on the performed rate analyses. Overall, the present study implied the potential role of the chemistry of BB compounds for the formation and processing of SOA.