Detailed multiphase chemistry in the regional 3-D chemistry transport model COSMO-MUSCAT: Application for the field experiment HCCT-2010.

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Summary
The 3D-chemistry transport model COSMO-MUSCAT consisting of MUSCAT [WOLKE ET AL., 2004] and the forecast model of the German Weather Service (DWD) COSMO [SCHÄTTLER ET AL., 2014] was extended to consider size-resolved cloud-chemical processes (chemical aqueous phase reactions and phase transfer processes). The advanced model system was applied for the measurement period of the field experiment HCCT-2010 (Hill Cap Cloud Thuringia 2010, [VAN PINXTEREN ET AL., 2012]). The model output using aqueous phase chemical mechanisms of different complexity was compared to available measurements.

Introduction
Clouds play a major role in the atmosphere due to their influence on the Earth's radiative budget, on the hydrologic cycle and on the tropospheric chemical composition. Cloud lifetime is driven by the dynamics of the atmosphere at the synoptic scale and, in close interaction, by microphysical processes on the small scale.
These processes depend on the chemical composition of particles and cloud droplets. In addition, microphysical processes redistribute chemicals among the various reservoirs: gaseous, particulate, liquid and ice phases. Clouds favor the development of "multiphase chemistry" since they are an ideal reaction medium for this. The evaluation of multiphase chemistry versus overall tropospheric chemistry and its role in the Earth's radiative budget is challenging since microphysical and chemical processes occurring at different time scales within clouds are still poorly known.

Methodology and Results
Increasing kinetic and mechanistic knowledge on chemical aqueous phase reactions lead to the development of advanced aqueous phase chemical mechanisms such as the Chemical Aqueous Phase Radical Mechanism (CAPRAM) [TILGNER AND HERRMANN, 2010]. CAPRAM is an almost explicit mechanism, which describes relevant chemical aqueous-phase conversions of both inorganic and organic compounds. For this study, it a reduced version of CAPRAM was applied [DEGUILLAUME ET AL., 2009].

Conclusions
The 3-D model was applied in a regional domain around Mt. Schmücke, Germany. The comparison of CAPRAM with a simpler mechanism showed differences in e.g. in the modeled multiphase HOx budget and pH whereas. The difference in pH leads consequently to different regimes for e.g. the S(IV)-oxidation and organic partitioning in the droplet bins. A comparison to the point measurements is difficult due to the spatial variability of the modeled concentration fields as well as mechanistic and measurement uncertainties.

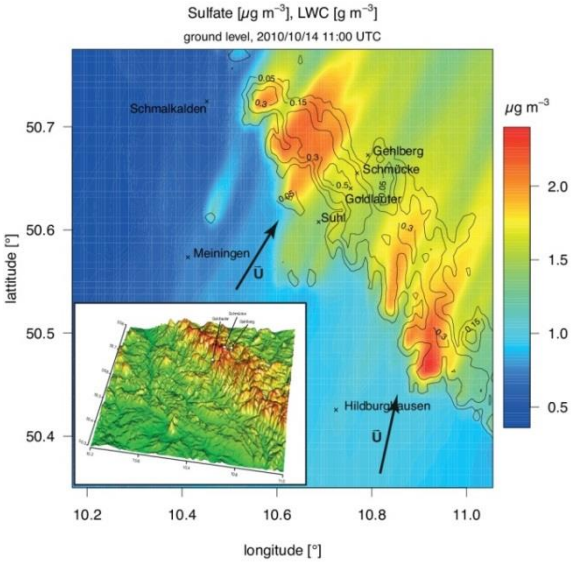

Figure 1: Large: Sulfate formation and LWC at Mt. Schmücke. Small: Orography of the model domain.

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