



## Modelling the multiphase chemical processing of Monoethanolamine from industrial CCS processes in tropospheric aqueous particles and clouds

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Using amine based solvent technology is an option to realise CO<sub>2</sub> capture from the exhaust of power plants. Amines such as Monoethanolamine (MEA) may potentially be released in trace amounts during the carbon capture and storage (CCS) process. In order to investigate the tropospheric chemical fate of MEA from CO<sub>2</sub> capturing processes and their oxidation products, multiphase modelling was performed and a reduced mechanism for future 3D model applications was developed in the present study.

Based on former laboratory investigations and mechanism developments, an up-to-date multiphase mechanism describing the gas and aqueous phase chemistry of MEA has been developed in the present study. The developed multiphase phase oxidation scheme of MEA and its oxidation products, incl. nitrosamines, nitramines and amides, was coupled to the existing multiphase chemistry mechanism (RACM-MIM2ext-CAPRAM3.0i-red, Deguillaume et al. 2010) and the CAPRAM Halogen Module 2.0. Overall, the multiphase mechanism comprises 1276 chemical processes including 668 gas and 518 aqueous phase reactions as well as 90 phase transfers. The multiphase amine module contains in total 138 processes. The final mechanism was used in the Lagrangian parcel model SPACCIM (Wolke et al., 2005) to investigate e.g. the main oxidation pathways, the formation of hazardous oxidation products and seasonal differences. Simulations were performed using a meteorological scenario with non-permanent clouds, different environmental trajectories and seasonal conditions.

The simulations revealed the importance of both cloud droplets and deliquescent particles to be an important compartment for the multiphase processing of MEA and its products. Due to the shifted partitioning of MEA towards the aqueous phase, the model investigations implicated that aqueous phase oxidation by OH radicals represents the main sink for MEA under daytime cloud summer conditions. Reaction flux analyses have shown that under deliquescent particle conditions, the Cl radical represents an important oxidant. Moreover, the simulations showed that MEA oxidations are quite restricted under low photochemical winter conditions leading to much longer tropospheric residence times. Additionally, the model simulations implicated that the aqueous phase reduces substantially the formation of harmful compounds such as MEA-nitramine in the gas phase. Furthermore, simulations revealed that the aqueous formation of N-nitrosoamines is not a relevant process under tropospheric conditions.

In order to provide a condensed mechanism applicable for regional scale dispersion modelling, a mechanism reduction was performed based on comprehensive reaction flux investigations. The developed reduced mechanism contains just 303 gas and 112 aqueous phase reactions and 32 phase transfers. The reduced mechanism describes adequately the multiphase chemistry of MEA and its key oxidation products. The required computational costs are reduced by about 45 % compared to the full MEA mechanism. Thus, the reduced mechanism provides the basis for further regional dispersion model studies.

### References

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