



Mainz Convective Transport and Scavenging (MCTS version 1.0) – Introduction and Evaluation of the new Column Model for Convection-Chemistry-Interactions

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Abstract. Convective systems can rapidly redistribute atmospheric trace gases. For soluble species, not only does convective transport play a key role, but also the interactions with cloud hydrometeors, i.e. scavenging. Global chemistry-climate models have difficulties reproducing observed vertical profiles of soluble trace gases under convective influence. One example is the model EMAC (ECHAM MESSy Atmospheric Chemistry). There are two possible reasons for this issue: (1) the lack of retention and multi-phase transport in the model and (2) the subsequent treatment of the convective transport and the convective scavenging. We present the new column model Mainz Convective Transport and Scavenging (MCTS), which overcomes these shortcomings. MCTS considers transport of trace substances and their scavenging via the ice and liquid hydrometeors quasi-simultaneously. Furthermore, the new model takes retention and multi-phase transport into account. MCTS is evaluated against aircraft observations from the NASA SEAC⁴RS campaign. WRF-Chem cloud-resolving output was used as meteorological input data for MCTS to accurately represent the convective storm. The new column model performs reasonably well given that it was originally designed for the application in a global model and not for the inter-comparison with a single convective storm. Additionally, MCTS is compared to the convective transport and scavenging in the chemistry-climate model EMAC. Both models affect insoluble species similarly, but have a different effect on the soluble species. Sensitivity simulations with MCTS demonstrate that the time scales of convective transport and the dissociation reactions within the droplet have a major effect on the simulated tracer profiles. MCTS can represent the competition between these two process types, which is a benefit for the calculation of vertical profiles of soluble tracer profiles compared to EMAC. MCTS opens the path for a wide range of future studies, for example, sensitivity studies regarding the ice phase scavenging, which is fraught with high uncertainty. In the long run, we aim to improve the representation of convective transport and convective scavenging in global chemistry-climate models with MCTS.



20 1 Introduction

Moist convective systems can be thought of as the roller-coasters for atmospheric trace species. For example, convection is of high importance for the water (vapour) transport in the upper troposphere (Sassi et al., 2001; Luo et al., 2007; Jain et al., 2013; Singh and Ahrens, 2025).

Convection might also cause a moistening of the lower stratosphere (Hegglin et al., 2004), and even have a direct impact on the lower stratospheric water vapour concentration via tropopause overshooting in combination with gravity wave breaking as observed by Konjari et al. (2025) in the extra-tropics during the TPEX (TropoPause composition gradients and mixing Experiment) campaign (Bozem et al., 2025). Also, Homeyer et al. (2014) found evidence for connectively induced water vapour in the lower stratosphere during the DC3 (Deep Convective Clouds and Chemistry, Barth et al., 2015) field experiments. Variations in the water vapour concentration in the upper troposphere/lower stratosphere are highly relevant for the energy budget (Riese et al., 2012). However, convection does not only redistribute water vapour and condensate but influences atmospheric tracers in general (e.g. Dickerson et al., 1987; Hegglin et al., 2004; Bechara et al., 2010; Li et al., 2017), for example, biomass burning tracers and aerosols (Ray et al., 2004; Barth et al., 2026), hydrogen peroxide (H_2O_2 , e.g. Barth et al., 2016; Bozem et al., 2017), and ozone (e.g. Dickerson et al., 1987; Lawrence et al., 2003).

Lawrence et al. (2003) found that the convective transport would lead to a reduction of the column ozone, but that the transport of ozone precursors counteracts this decrease. In total, Lawrence et al. (2003) derived an increase in ozone burden in polluted regions. These results contradict with the findings of Doherty et al. (2005) who also took the transport of ozone itself and its precursors into account and determined an overall reduction of ozone due to convective transport. However, these two studies agree that the ozone transport alone (without considering precursors) would lead to a decrease of the total ozone and especially of the upper tropospheric ozone. Frey et al. (2015) and Tinney and Homeyer (2021) further argue that the lower stratospheric ozone is reduced due to convectively driven downwelling.

Recently, Curtius et al. (2024) found observational evidence for a pathway for the formation of aerosols in the upper troposphere over the Amazonian rain forest, which is enabled by convective transport of precursor gases. Volatile organic compounds (VOCs) are transported to the upper troposphere by convective updrafts as suggested by aircraft observations (Tripathi et al., 2025) and from model simulations (Bardakov et al., 2021, 2022). In the upper troposphere, these VOCs can form new particles (Bardakov et al., 2024; Curtius et al., 2024). It is widely assumed that the aerosol loading influences the convective cloud properties (i.e. see Wang, 2005; Lebo and Seinfeld, 2011). Further, the impact of the newly formed aerosols could lead to a feedback on convective systems as suggested by Desouza (2023).

It is highly important to include convective transport in models to represent the impacts of convective transport on the composition and chemistry. Already in the 80s and 90s, efforts were made to model convective transport and to evaluate its effect (Gidel, 1983; Feichter and Crutzen, 1990; Strand and Hov, 1993; Mahowald et al., 1995, 1997). Furthermore, moist convection is not only associated with gas phase transport but also with wet removal (for example, see Gidel, 1983; Mari et al., 2000; Bozem et al., 2017). Especially the importance of SO_2 aqueous phase chemistry is already known for several decades (see, for example, the review by Hobbs, 1986). Model studies targeting the aqueous SO_2 chemistry were performed,



for example by Baboolal et al. (1981). More complex cloud chemistry models were developed, coupled to gas-phase chemistry mechanisms, and implemented in three-dimensional models in the following decades, for example by Leriche et al. (2000); Tost et al. (2006a); Leriche et al. (2013).

Already, Gidel (1983) considered scavenging while modelling the impact of convection on vertical trace gas profiles. Cho et al. (1989) included the aqueous phase SO_2 oxidation within their model of convective transport and scavenging. Later, Mari et al. (2000) developed a column model considering convective transport and scavenging as well, highlighting the importance of different scavenging processes, i.e. Mari et al. (2000) showed that the H_2O_2 concentrations in the outflow are increased compared to the background, while HNO_3 is efficiently scavenged, indicating the impact of retention. Barth et al. (2007) discovered large deviations of soluble tracer profiles derived from different models, which might result, inter alia, from the ice process representation. Aerosol particles are influenced by the convective transport and scavenging as well; they are also considered, for example, in the submodel SCAV (Tost et al., 2006a). A comprehensive description of aerosol scavenging has a huge impact on the aerosol optical depth in global simulations (see, e.g. Croft et al., 2012). The results by Barth et al. (2026) indicate that cloud chemistry might increase organic aerosol mass in the outflow and mask partially the effect of aerosol scavenging.

Several studies were performed using the model Weather Research and Forecasting model coupled with Chemistry (WRF-Chem, Grell et al., 2005; Fast et al., 2006) to investigate the impact of convective transport and scavenging (Fried et al., 2016; Bela et al., 2016, 2018; Li et al., 2018, 2019; Cuchiara et al., 2020, 2023). For example, Li et al. (2019) tested different retention coefficients (the portion of a species that stays within a freezing droplet) to fit the simulated tracer profiles with observations. Also Cuchiara et al. (2023) tried to overcome the uncertainties arising from the ice phase. The modelling results were compared with aircraft measurements to give an estimate for the retention factor (Cuchiara et al., 2023).

The cloud resolving simulations as from Cuchiara et al. (2020, 2023) provide the most comprehensive setup to study convective transport and scavenging simulations, but in global chemistry climate simulation, the computing power is a limiting factor up to today. Therefore, it is not yet feasible to go to cloud resolving scale for interactive, long-term global-chemistry simulations. These simulations still depend on convection parametrisations.

Bardakov et al. (2020) developed a less computationally expensive framework to model convective transport and scavenging. The scavenging and mixing is calculated along trajectories which were derived from large eddy simulations beforehand (Bardakov et al., 2020). However, applying trajectories in global simulations is very expensive. In EMAC (ECHAM/MESSy Atmospheric Chemistry Jöckel et al., 2006, 2010, 2016), the submodel ATTILA (Atmospheric Tracer Transport in a Lagrangian model) by Brinkop and Jöckel (2019) calculates the Lagrangian advection and convective transport of passive tracers. The number of trajectories is limited due to the computational constraints, three are typically initialised in one grid box (Brinkop and Jöckel, 2019). Bardakov et al. (2020) used 500 trajectories to describe the upward transport of one convective system; it would take an enormous amount of computing resources to archive this number of trajectories in global simulations.

Tost et al. (2010) developed a convective transport routine for tracers, CVTRANS, for EMAC, which is coupled with the basemodel ECHAM5 (European Centre Hamburg general circulation model version 5 Roeckner et al., 2006) via MESSy (Modular Earth Submodel System version 2, Jöckel et al., 2005, 2010). (The Eulerian) CVTRANS can be used for long term



simulations. The submodel makes use of the bulk approach as described in Lawrence and Rasch (2005). Ouwersloot et al. (2015) included an option to apply adaptive time stepping in CVTRANS. Later, Jeske and Tost (2025) revisited the closure formulation in CVTRANS and implemented the convective exchange matrix, which can be used to diagnose convective transport properties. CVTRANS does not directly include scavenging processes. The scavenging is calculated by the SCAV submodel (Tost et al., 2006a), which is called separately. Tost et al. (2010) evaluated the convective tracer transport and scavenging in EMAC using different convection parametrisations via CONVECT (Tost et al., 2006b) against aircraft observations. For ozone (O_3) and carbon monoxide (CO), CVTRANS and SCAV mostly do a fairly reasonable job. However, the simulations cannot reproduce the measured upper tropospheric sulphur dioxide (SO_2) mixing ratios (see Fig. 6c of Tost et al., 2010). This does not depend on the choice of convection parameterisation; all simulations perform equally poor. The wash out of SO_2 is too strong as the mixing ratios are significantly underestimated according to Tost et al. (2010). SO_2 is not only partitioning between the aqueous phase and the gas-phase according to Henry's law, but also dissociates fast in the cloud droplets. The dissociation products are further oxidised (Tost et al., 2006a). Therefore, there is a rapid SO_2 loss within the aqueous phase.

The underestimation of the mid to upper tropospheric SO_2 can have multiple reasons. As already discussed in several studies (e.g. Mari et al., 2000; Bela et al., 2016) the vertical profiles of soluble species can be sensitive to the treatment of the retention. As Tost et al. (2010) does not take the retention into account, this might cause the underestimation of SO_2 . However, Li et al. (2019) found that the upper tropospheric mixing ratios of HCHO were underestimated in their simulations regardless of the chosen retention factor and that the SO_2 mixing ratios in the upper troposphere are not sensitive to the retention factor at all. This indicates that the retention might not be the (only) issue. The transport and the scavenging are calculated subsequently in EMAC, i.e. the numerical integration is performed subsequently. This subsequent treatment is referred to as operator splitting. The usage of operator splitting might lead to errors if the convective scavenging and the convective transport take place at similar time scales.

We developed a new column model, Mainz Convective Transport and Scavenging (MCTS), to overcome the misrepresentation of soluble tracers affected by convection. With MCTS, we aim to improve the simulations of trace gas mixing ratios across the troposphere and especially of the impact of convection on the upper tropospheric composition to enable more accurate predictions of upper tropospheric chemistry, new particle formation and radiative effects. MCTS includes tracer transport in the gas phase, droplet uptake, ice surface uptake and a simple aqueous phase chemistry. Furthermore, MCTS does take the multi-phase transport and retention into account. All these processes are quasi-simultaneously taken into account, i.e. MCTS does not use operator splitting. Therefore, MCTS overcomes both issues EMAC suffers from, i.e. the above mentioned problems of ice phase interactions and operator splitting.

MCTS is currently a stand-alone column model, which requires data about the convective system, the temperature, pressure and background tracer profiles as input. Based on these quantities, MCTS calculates the convective influence on the trace gases, i.e. the new tracer profiles after the convective cloud vanishes.

MCTS is presented in this study. For the evaluation, two tests were performed.

1. MCTS is applied to input data from cloud-resolving simulations from WRF-Chem which were performed by Cuchiara et al. (2020) for comparison with the observations from the SEAC⁴RS field campaign. The MCTS output is evaluated



using WRF-Chem output and the measurement data to ensure that MCTS can realistically reproduce the measured tracer profiles.

2. MCTS is run with input data from EMAC. This is done to check whether the process representation is comprehensive, and whether MCTS produces reasonable profiles when it is applied on typical spatial and temporal scales of a chemistry-climate model. This test is crucial as MCTS is designed to be implemented in those models. The analysis also gives a first hint whether MCTS might perform better as the submodels incorporated in EMAC for convective transport and scavenging.

The long term goal of MCTS is to improve the representation of convection-chemistry-interactions in large scale chemistry-climate and composition models. Further, the column model MCTS can be used for different process studies.

In Section 2 the models and observational data are briefly described which were used to perform the comparisons. MCTS is introduced in Sec. 3. The meteorological cases used to perform the evaluation are discussed in Sec. 4. The evaluation of MCTS (Sec. 5) is followed by a discussion in Sec. 6 and the conclusions in Sec. 7.

2 Models and Data

MCTS is evaluated in a case study utilising three different data sources for input and for comparison, which are described in the following subsections:

- DC-8 data from the SEAC⁴RS campaign,
- WRF-Chem high resolution data, and
- low resolution EMAC output.

2.1 SEAC⁴RS

The Studies of Emissions and Atmospheric Composition, Clouds and Climate Coupling by Regional Surveys (SEAC⁴RS) campaign took place in August and September 2013 (Toon et al., 2016). Toon et al. (2016) stated that one goals of this campaign was to investigate aerosols and gases in the convective outflows and the convective redistribution of emissions. On September 2nd, several pre-frontal, deep convective cells occurred (Cuchiara et al., 2020). The DC-8 aircraft from NASA sampled in the outflow of different storm cores (Toon et al., 2016; Cuchiara et al., 2020). Two of these cores, an isolated airmass storm and the other a multicellular storm, were studied in greater detail by Cuchiara et al. (2020). Cuchiara et al. (2020) performed cloud resolving simulations with WRF-Chem to study the convective transport and scavenging efficiency. Convective outflow and inflow observations with accompanying cloud-resolving simulations are the best possible prerequisites to test the newly developed column model MCTS.



2.2 WRF-Chem

The Weather Research and Forecasting with Chemistry model (WRF-Chem) enables the use of a variety of chemistry and physics processes (Grell et al., 2005). Cuchiara et al. (2020) performed WRF-Chem (version 3.9.1) simulations to reproduce the storms and their impact on the outflow mixing ratios observed during the SEAC⁴RS field mission on September 2nd, 2013. Cuchiara et al. (2020) used 74 vertical levels and a horizontal grid of $12.15 \times 12.15 \text{ km}^2$ for the outer domain with two embedded nests. The innermost nest has a grid resolution of $1.35 \times 1.35 \text{ km}^2$ with explicitly resolved convection (Cuchiara et al., 2020). The simulation output from the innermost domain is used as input data in this study. The WRF-Chem simulation domain top is located at 100 hPa. Please see the publication by Cuchiara et al. (2020) for further information about the WRF-Chem simulations.

2.3 EMAC

EMAC (version 2.55.2, Jöckel et al., 2010, 2016) is a chemistry-climate model based on the global circulation model ECHAM version 5 (Roeckner et al., 2006) which is combined with the Modular Earth Submodel System (MESSy, Jöckel et al., 2005, 2006) version 2 (Jöckel et al., 2010). MESSy is used to couple the base-model ECHAM with process submodels. These submodels take care of different physical and chemical processes. For example, the convection parametrisation can be chosen via the submodel CONVECT (Tost et al., 2006b). For this study, the Tiedtke scheme with Nordeng closure (Tiedtke, 1989; Nordeng, 1994) was utilised. The submodel SCAV takes care of the scavenging in convective and large scale clouds (Tost et al., 2006a) and the submodel CVTRANS calculates the convective transport (Tost et al., 2010). The spectral dynamical core of the model was run at a T42 resolution, which corresponds to a horizontal resolution of $\sim 2.8^\circ$ (128 times 64 horizontal grid boxes) and with 90 vertical levels up to 0.01 Pa. More information about the simulation setup can be found in the supplement.

3 Model description: Mainz convective transport and scavenging

MCTS is an one-dimensional column model with 31 vertical levels. The model level at the top of the domain is labelled as 1 and the level closest to the surface is the level 31. MCTS treats the convective transport and the related scavenging together, i.e. quasi-simultaneously. In total, more than 20000 ordinary differential equations (ODEs) are used to describe all considered processes. In this section, the MCTS (version 1.0) is briefly described. Please see the documentation (supplement) for further details.

3.1 Input and output

It is necessary to provide the background profile of the trace gases and the convective properties as input for MCTS. All input variables are listed in Table 1. MCTS is designed for the usage in combination with EMAC, but it is also possible to use MCTS with other models. For this study, the input data was taken from EMAC and from WRF-Chem output.



Based on these input data, MCTS calculates the redistributed vertical profiles of the trace species, i.e. the vertical tracer profiles after the convective event occurred. It is also possible to investigate the partition of species between different reservoirs (i.e. gas phase, dissolved in cloud droplets, attached to the ice crystal surface, etc.). The default output consists of the new gas phase profiles. The included species and processes are described briefly in the following.

Table 1. Input quantities for MCTS.

Variable	Unit
Background profile	mol mol^{-1}
Updraft mass flux	$\text{kg m}^{-2} \text{s}^{-1}$
Downdraft mass flux	$\text{kg m}^{-2} \text{s}^{-1}$
Updraft entrainment mass flux	$\text{kg m}^{-2} \text{s}^{-1}$
Updraft detrainment mass flux	$\text{kg m}^{-2} \text{s}^{-1}$
Downdraft entrainment mass flux	$\text{kg m}^{-2} \text{s}^{-1}$
Downdraft detrainment mass flux	$\text{kg m}^{-2} \text{s}^{-1}$
Temperature	K
Surface pressure	Pa
Pressure	Pa
Hybrid coefficients	-
Liquid water content	kg kg^{-1}
Ice water content	kg kg^{-1}
Liquid precipitation flux	$\text{kg m}^{-2} \text{s}^{-1}$
Snow precipitation flux	$\text{kg m}^{-2} \text{s}^{-1}$
Convective cloud cover	-

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3.2 Considered species

Only a limited number of trace gases is embedded in MCTS due to computational restrictions. The selection of soluble tracers and the considered reactions was made according to the so-called SCM mechanism considered in SCAV (see Tost et al. (2007) and supplementary material to Jöckel et al. (2006): "The Chemical Mechanism of SCAV" by H. Tost, R. Sander and
 190 A. Kerkweg, 2006.) All considered species are listed in Table 2. This selection can be considered as the bare minimum that should be taken into account to establish reasonable pH values within the droplets, see also the results by Tost et al. (2007) who investigated the impact of using different scavenging mechanisms on the global composition.

CO and C₅H₈ are not soluble. The insoluble trace gases are considered in this study to test the transport mechanism in
 195 MCTS. MCTS is rather large and computationally not as efficient as a pure transport routine (without quasi-instantaneous



Table 2. Considered species and their characteristics. N_2O_5 is a special case because it directly produces HNO_3 in contact with water or ice.

Species	Soluble	Aqueous chemistry	Retention	Ice uptake
SO_2	yes	yes	yes	no
H_2SO_4	yes	yes	yes	yes
O_3	yes	yes	yes	no
H_2O_2	yes	yes	yes	yes
NH_3	yes	yes	yes	no
HNO_3	yes	yes	yes	yes
CO_2	yes	yes	yes	no
HCHO	yes	no	yes	no
HCOOH	yes	yes	yes	no
CH_3OOH	yes	no	yes	no
CH_3COOH	yes	yes	yes	no
HCl	yes	yes	yes	yes
N_2O_5	HNO_3	HNO_3	no	HNO_3
CO	no	no	no	no
C_5H_8	no	no	no	no

chemistry). Therefore, it might be favourable to exclude these two species from the MCTS framework and use MCTS only for soluble species in the future.

3.3 Overview of the processes

Convection-chemistry-interactions are determined by a highly complex interplay of dynamical and chemical multi-phase processes. An illustration of (most) transport and phase partitioning processes is given in Fig. 1. The key players can be categorised as follows:

1. Aqueous scavenging:

(a) Liquid phase uptake: Soluble tracers are partitioned between droplets and the surrounding air (Sander, 1999; Tost et al., 2006a; Jöckel et al., 2016), see (6), (7), (17), and (18) in Fig. 1.

(b) Aqueous phase chemistry: Acids and alkaline species dissociate inside the droplets and several other chemical reactions take place, e.g. oxidation processes (Tost et al., 2006a, 2007; Jöckel et al., 2016; Barth et al., 2021). The chemical reactions are illustrated in Fig. 2.

(c) Rain: Rain droplets wash out the species trapped inside them (process (19) in Fig. 1).

2. Ice phase scavenging:



- 210 (a) Retention: Cloud droplets freeze, when they are transported upward to altitudes with sufficiently low temperature. Thereby, some components remain (partially) in the freezing droplets, i.e. are retained. The other portion is expelled to the gas phase (compare Jost et al., 2017, and see process (11) in Fig. 1).
- (b) Uptake upon ice: Snow and ice crystals take up some tracers from the surrounding environment upon their surface (von Kuhlmann and Lawrence, 2006; Bardakov et al., 2020; Seymore et al., 2025, and see for illustration the
 215 processes (14), (16), (20), and (21) in Fig. 1).
- (c) Ice precipitation: Precipitating ice might form from the small ice crystals ((15) in Fig. 1) and wash out the contained species ((22) and (23) in Fig. 1).
3. Transport: The species are transported due to the high vertical wind velocities and the large scale subsidence (see processes (1), (2) and (3) in Fig. 1). The gas phase compounds are transported based on the work by Lawrence and Rasch
 220 (2005) and Tost et al. (2010). Specifically, the gas-phase transport is treated according to the convective transport sub-model CVTRANS (Tost et al., 2010; Ouwersloot et al., 2015) version 3.0 (Jeske and Tost, 2025) in MCTS. Furthermore, the species in the hydrometeors (within droplets or ice crystals) are transported in MCTS as well, because the hydrometeors are redistributed by the convection (see, for example, process (9) in Fig. 1). In contrast, CVTRANS takes only the transport within the gas phase into account.
- 225 This classification makes no claim to be complete, but summarises the processes included in the column model MCTS. All processes are treated quasi-simultaneously to comprehensively represent the convection-chemistry-interactions in MCTS. To achieve this goal, all processes are described as (pseudo-)chemical reactions. The transport is given by first order loss reactions representing exchanges between individual reservoirs. This formulation leads to a large system of coupled ordinary differential equations, which is solved with the Kinetic PreProcessor version 2 (KPP, Damian et al., 2002; Sandu et al., 2003; Daescu et al.,
 230 2003; Sander et al., 2019). The Rodas integrator (Harier and Wanner, 1991) 4th order is used with adaptive time stepping.

In the following, we briefly discuss the implementation of the most important processes in MCTS. All reactions are listed in the accompanying documentation.

3.3.1 Gas phase

Transport

- 235 The transport scheme is based on Tost et al. (2010) including the adaptations by (Jeske and Tost, 2025). Therefore, updraft and downdraft mass fluxes are taken from a convection parameterisation, which drive the convective transport in MCTS. As in Tost et al. (2010), it is presumed that the mass transport is closed in the sense that an equally distributed tracer field stays equally distributed under convective influence (in a model column). We will use the term homogeneous tracer field in the following. To avoid a mass imbalance in the column (i.e. an accumulation of mass at the top) the grid-scale subsidence is included. The
 240 subsidence balances the updraft mass flux as the downdraft is usually weaker than the updraft.

As in Fig. 1, the notation is used that level $n+1$ is located below level n , i.e. level $n+1$ has a higher pressure as level n . MCTS calculates the detrainment and entrainment regarding the updraft mass flux (MD_{up} and ME_{up}) and downdraft mass

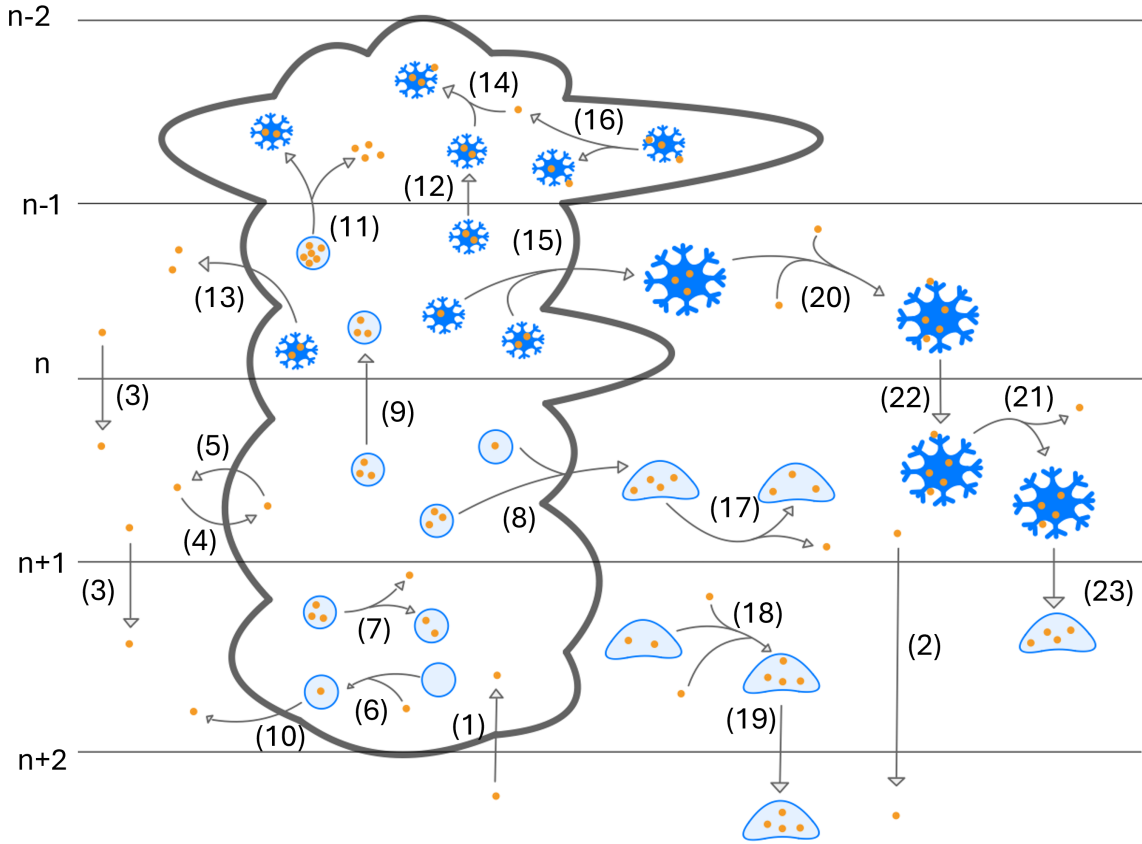


Figure 1. Sketch of most of the considered transport and transition processes in MCTS. The orange points illustrate the trace species. The different blue symbols refer to the four types of hydrometeors considered in MCTS: cloud droplets, rain droplets, ice crystals/cloud ice and snow/precipitating ice. The thin black lines indicate the level structure, whereby n denotes the model level number. The processes are: (1) Updraft transport, (2) downdraft transport, (3) mass-balancing subsidence, (4) entrainment, (5) detrainment, (6) and (7) gas and cloud droplet partitioning, (8) formation of rain drops, (9) upward transport of cloud droplets, (10) detrainment of cloud droplets and instantaneous evaporation, (11) retention, (12) upward transport of cloud ice, (13) detrainment of cloud ice and instantaneous sublimation, (14) surface uptake at cloud ice, (15) snow formation, (16) desorption from the cloud ice surface, (17) and (18) gas and rain droplet partitioning, (19) liquid precipitation, (20) and (21) adsorption and desorption at snow, (22) solid precipitation and (23) solid precipitation melting.

flux (MD_{do} and ME_{do}) based on the closure

$$MF_{up}^n = MF_{up}^{n+1} + ME_{up}^n - MD_{up}^n \quad (1)$$

$$245 \quad MF_{do}^{n+1} = MF_{do}^n + ME_{do}^n - MD_{do}^n \quad (2)$$



(see Tost et al., 2010) to ensure the conservation of a homogeneous tracer field. MF_{up}^n is the updraft mass flux out of level n and MF_{do}^n the downdraft mass flux out of the same level.

All mass fluxes (MF in $kg\ m^{-2}\ s^{-1}$) must be reformulated as first order reaction rates r (in s^{-1}) to describe the transport as loss reaction with the equation

$$k = MF * g / \Delta p \quad (3)$$

with g the gravitational acceleration and Δp the pressure difference between the model interfaces. The rates can then be used in a chemical reaction setups. For example, the updraft transport of SO_2 is described with



The upward transport is illustrated also by process (1) in Fig. 1. In MCTS, it is considered that the updraft, downdraft and environment are at different locations. The updraft can only influence the trace gas molecules within the updraft location. These locations are called reservoirs. The updraft reservoir is indicated by using the subscript $_{up}$. The downdraft affects the molecules within the downdraft reservoir ($_{do}$, see process (2) in Fig. 1) and the subsidence trace gases which are located in the environment ($_{env}$, see process (3) in Fig. 1). Detrainment and entrainment lead to an exchange of the molecules between the environment reservoir and the up- or downdraft reservoir, which is illustrated by processes (4) and (5) in Fig. 1. For simplicity, the reservoirs for updraft and downdraft are not directly connected and do not mix in MCTS, even though in reality updraft and downdraft regions might be adjacent to each other.

Chemistry

Gas phase chemistry is not included in the column model. To take the gas phase chemistry into account a box model, e.g. CAABA/MECCA (Chemistry As A Boxmodel Application/Module Efficiently Calculating the Chemistry of the Atmosphere, Sander et al., 2019) must be coupled to MCTS. This coupling goes far beyond the scope of this study. MCTS takes only care of the multi-phase chemistry within the convective clouds.

3.3.2 Aqueous phase processes

Trace species are partitioned between the air (gas phase) and droplets according to Henry's law (Sander, 1999). This partitioning is indicated in Fig. 1 by (6), (7), (17), and (18). Dissolved in the aqueous phase, these species can undergo a variety of chemical reactions, i.e. dissociation and oxidation (see, for example the review by Tilgner et al., 2021). The multi-phase chemistry introduces a large uncertainty in model simulations (Barth et al., 2021) and plays a crucial rule in Earth system modelling because it can lead to acid rain (Barth et al., 2007). Bozem et al. (2017) measured that the ratio of insoluble tracers in the inflow of convective systems and their outflow is nearly one, but a smaller fraction of soluble tracers reaches the upper troposphere due to scavenging. The reduction of the soluble gases in the outflow compared to the inflow highlights the importance of the consideration of washout to represent the upper tropospheric mixing ratios of soluble tracers correctly. In MCTS, the aqueous phase processes are formulated analogously to SCAV (see Tost et al. (2006a, 2007) and the supplements to Tost et al. (2007)).

Aqueous and gas phase partitioning

The gas-aqueous reaction system is divided by Schwartz (1986) into eight subprocesses, covering the partition and the aqueous



chemical reactions. Sander (1999) put the partitioning in focus and subdivided it into three processes: (1) the diffusion in the
 280 gas phase (towards the droplet), (2) the transport across the droplet surface and (3) the diffusion inside the droplet. MCTS
 considers only (1) and (2) for the calculation of the rates for the partitioning (as it is also done in SCAV by Tost et al., 2006a).
 Analogous to SCAV, the process (3) is neglected, and an instantaneous mixture in the droplets is assumed, as convection is
 highly turbulent. Detailed information about the calculation of the partitioning rates can be found in Tost et al. (2006a).

Aqueous phase chemistry

285 Many of the considered species are acids and form an anion and a proton in dependence of the H^+ concentration in the droplet.
 Further, NH_3 is forming NH_4^+ . The chemical reactions are illustrated for MCTS in Fig. 2 (a). Besides the dissociation, the
 oxidation of sulphur(IV) with O_3 and H_2O_2 are considered, see light grey lines in Fig. 2 (b). In MCTS the so-called "Scm"
 mechanism is implemented, see supplements of Tost et al. (2007).

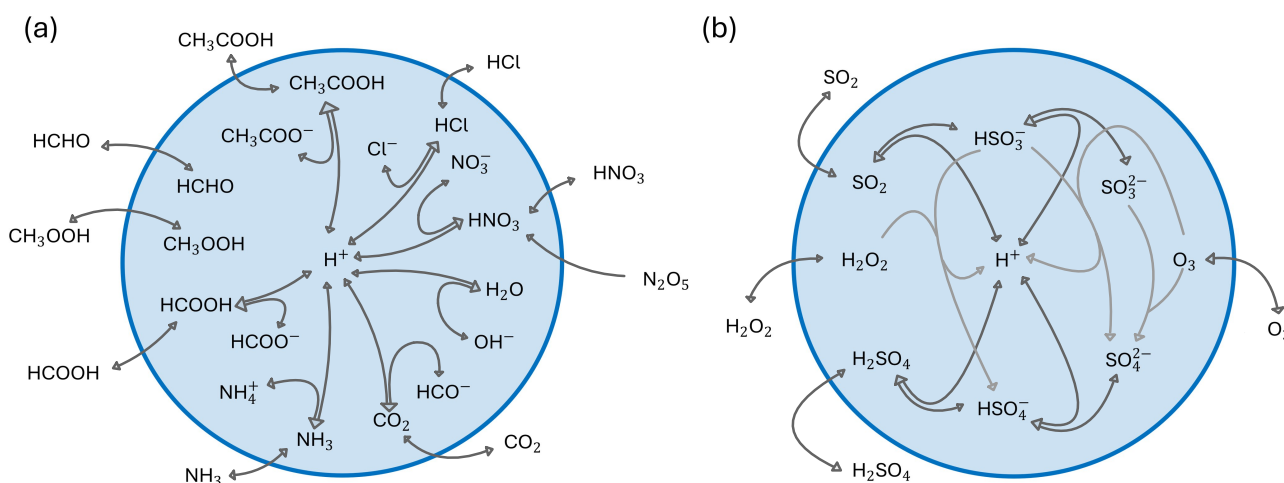


Figure 2. Sketch of the considered chemical processes and liquid-gas partitioning in MCTS. The blue circles represent droplets and the white background the surrounding air. (a) shows the partitioning and the dissociation for all species not involved in further reactions in MCTS. (b) illustrates with the dark gray lines the phase transition and the dissociation and the gray lines represent the oxidations.

3.3.3 Ice phase scavenging

290 In literature, it is assumed that the ice phase processes play a crucial rule for the tracer mixing ratios in convective systems (for
 example, Bozem et al., 2017; Cuchiara et al., 2020), but these processes are highly uncertain (Barth et al., 2007). In MCTS,
 only retention and uptake into the ice shell layers are considered (process (11), (14) and (16) in Fig. 1). Two different ice
 phase reservoirs are considered for both processes. The molecules induced in the ice phase by retention belong to the bulk ice,
 whereas the molecules taken up at the ice surface are within the surface ice. A transfer between these two reservoirs is not
 295 considered because it is assumed that the diffusion inside the ice is very small (if there is any at all).



Retention

The retention coefficient describes to portion of a species which remains in a freezing droplet. The value is between 0 and 1. For example, Jost et al. (2017); Borchers et al. (2024) put effort in determining the retention coefficients during riming in the Mainz vertical wind tunnel. Gautam et al. (2025) conducted acoustic levitator experiments to discover the retention coefficients during direct freezing of rain droplets. The laboratory experiments by Gautam et al. (2025) indicate that nearly all material is retained in freezing rain droplets due to their size and freezing mechanism (shell formation). In contrast, when the much smaller cloud droplets freeze due to riming, the retention coefficient can be derived from the effective Henry's law coefficient (H, Jost et al., 2017). Jost et al. (2017) derived the following function for the retention coefficient

$$RC = (1 + (a/H)^b)^{-1} \quad (5)$$

with $a = 1.69 \times 10^5$ and $b = 0.26$. This parameterisation is implemented in MCTS. For some trace species the parameterisation did not perform well. For this trace species a fixed retention coefficient was used. The values were taken from Jost et al. (2017) (their Table 4). The new findings of Gautam et al. (2025) are not applied at this point because only the freezing of cloud droplets is considered in MCTS for simplicity and not the freezing of rain droplets. The adapted fit parameters by Borchers et al. (2024) are not yet implemented and tested. It is planed to investigate the sensitivity of MCTS to different treatments of the ice phase processes in the future.

Ice uptake

In MCTS, a rather heuristic approach is used to represent the uptake of tracers at the ice crystals. As the results from the experiment by Seymore et al. (2025) suggest, there is some kind of bulk uptake taking place. We therefore apply the Henry's law approach analogues to the liquid phase but extrapolated to lower temperatures to describe the uptake at the ice surface into the some kind of surface layers. This strong simplification is done due to the lack of validated alternatives. Similar treatments of the ice uptake are common in modelling approaches, i.e. see von Kuhlmann et al. (2003); von Kuhlmann and Lawrence (2006) and Bardakov et al. (2020).

3.3.4 Multi-phase transport

In MCTS, it is considered that the updraft and downdraft redistribute hydrometers. The idea of considering multi-phase transport is not new; already, Gidel (1983) considered the redistribution of trace species within the hydrometeors. However, this multi-phase transport is currently not included in EMAC. In MCTS, the cloud and precipitation hydrometers are treated separatly and independently:

- Cloud droplets and cloud ice and the incorporated species can be transported upward with the updraft rate as sketched by process (9) and (12) in Fig. 1. Cloud droplets and ice crystals can be detrained with the updraft detrainment rate; they evaporate/sublimate directly in the environment due to the lower relative humidity (process (13) in Fig. 1).
- Rain droplets and snow crystals fall down with the precipitation rate (process (19) and (22) in Fig. 1). The ice crystals can melt if they fall into warmer regions (Fig. 1 (23)). If the rain/snow falls out of the lowest box and hits the ground (not shown in Fig. 1), the species are rained out accordingly.



The cloud hydrometeor reservoirs and reservoirs for precipitation are connected via the formation of rain/ice precipitation from cloud droplets/ice. Thereby, ice precipitation is always formed from cloud ice, and rain only forms from cloud droplets and melted snow. This is a simplification due to the fact that only very limited information about the microphysics is available from the convection parameterisations (in EMAC). The coupling of convection and microphysics as proposed by Lohmann (2008) has not prevailed in the development of convection schemes. Thus, the missing representation of cloud microphysics is most unfortunate for the representation of convective scavenging in global models, because (the representation of) the microphysic properties can affect the scavenging efficiency (Leriche et al., 2013; Barth et al., 2016).

4 MCTS setups

Two different sets of input data were used for MCTS, see Table 3. The first one is S(DC8) which makes use of the meteorological input from the cloud resolving WRF-Chem simulations from the multicell storm (core 7) performed by Cuchiara et al. (2020). Background tracer profiles are the clear air DC-8 measurements of H_2O_2 , HCHO , SO_2 , O_3 , C_5H_8 , CO_2 , HCl , HNO_3 and CO . These profiles were influenced by other convective events (Cuchiara et al., 2020). The other species needed as input for MCTS were taken from EMAC simulations. This simulation is compared with the measurements from convective core 7 which matches the simulated WRF-Chem convective storm core A well. S(DC8) is used to validate the performance of MCTS.

Table 3. Simulation setups for the evaluation of MCTS.

Simulation set	tracer input	meteorological input	cloud core
S(DC8)	DC-8 observations and EMAC	WRF	7
S(EMAC)	EMAC	EMAC	-

The second set of input data consists purely of the EMAC output. S(EMAC) indicates, how MCTS will behave in a global model. Further, MCTS is compared to simulation results of the EMAC process submodels CONVECT and SCAV. The second simulation S(EMAC) enables the direct comparison of the different treatments of the convection-chemistry-interactions in the two models. Further information about the EMAC simulation setup can be found in the supplements of this study (Table S1) and about the WRF-Chem simulations in the supplements to Cuchiara et al. (2020) (Table S2). The model top is not the same in both simulations (S(EMAC) and S(DC8)). The model top was chosen to represent the vertical extent of the convective cloud in S(DC8). Accordingly, the input data were interpolated to the chosen grid. For the S(EMAC) simulations, the 31 EMAC levels closest to the surface were used, most of which are located in the troposphere.

4.1 Meteorological input based on WRF-Chem

The storm Core A based on the WRF-Simulations by Cuchiara et al. (2020) represents the multicell storm. The simulation output of this convective event is used to create meteorological input for MCTS. The WRF-Chem output is sampled for the



355 updraft (updraft wind $\geq 2 \text{ m s}^{-2}$) and downdraft (downdraft wind $\leq -0.5 \text{ m s}^{-2}$) area. The sampled values were then used to provide the conditions in the reservoirs, i.e. updraft, downdraft and environment reservoir. The sampling has an effect on the representation of the convection. For example, the convective event in MCTS has a lower cloud top than the real event which is a possible source of uncertainties when MCTS is compared to the observations. However, the derived input profiles should capture the most important features of the multi-cell storm simulated by WRF-Chem.

360 Figure 3 shows the core temperature, the water contents, the updraft, and the downdraft. MCTS uses these profiles to perform the calculations. The temperature decreases with height from 304 K at 986 hPa to 238 K at 281 hPa within the convective core area (Fig. 3(a)). All hydrometeors in the updraft reservoir are considered to be cloud hydrometeors despite their size, because MCTS only allows for the interactions of cloud hydrometeors in the updraft reservoir and of precipitation hydrometeors in the downdraft. This separation of the droplets is a simplification to reduce the number of reactions and the computational efforts. The cloud is purely liquid up to 700 hPa. Above/at lower pressures, the cloud is considered a mixed phase cloud. In the uppermost two levels, the cloud only consists of ice. The maximum of the total water content of nearly 8 g kg^{-1} is reached at 322 hPa. The liquid water content is much smaller than the ice water content. Its maximum reaches nearly 3.4 g kg^{-1} at 646 hPa, showing that there is an efficient transport of water to higher altitude leading to efficient ice formation.

Figure 3(c) shows the updraft mass fluxes. The mass fluxes are always defined regarding the upper edge of the model boxes but are shown in Fig. 3(c) with regard to the box mid point pressure for consistency. The updraft stretches between 959 hPa and 294 hPa, i.e. it reaches into the uppermost model level. The maximum of $6.65 \text{ kg m}^{-2} \text{ s}^{-1}$ is located at 571 hPa. The profile includes two additional local maxima, one at 671 hPa and one at 372 hPa. The considered downdraft starts also in the uppermost level and reaches into the one associated with a pressure of 959 hPa. The mass fluxes are not allowed to reach beyond the column to ensure that the system is closed. The downdraft reaches up to $1.20 \text{ kg m}^{-2} \text{ s}^{-1}$.

375 4.2 Meteorological input based on EMAC

The second set of input data is derived from EMAC simulations. The air mass storm described above and studied by Cuchiara et al. (2020) occurred in the same area as convective event in EMAC and took place early at the same day. Figure 4 (a) shows the vertical profiles of the temperature and (b) the total, liquid and ice water content. These quantities are the mean values of the box which has a size of about $82,213 \text{ km}^2$. The lowest temperature of about 201 K is reached at 106 hPa. The temperature is 305 K in the model level closest to the surface. The cloud hydrometeors are purely liquid up to 590 hPa. The mixed phase is located between 535 hPa and 300 hPa characterised by a linearly decreasing amount and fraction of liquid water with decreasing temperature (pressure). At lower pressures, the cloud purely consists of ice. The convective cloud reaches up to 140 hPa. The liquid water is with up to 5 g kg^{-1} much higher than the ice cloud water content. The later has a maximum of about 1 g kg^{-1} . This is in contrast to the WRF-CHEM simulations, where ice water dominated the hydrometeor content. Of course, both models show a different convective event. However, it seems that EMAC underestimates the convective cloud ice. This issue cannot be overcome by using linear interpolation and needs further investigation in the convection parameterisation itself, going beyond the scope of this work. As indicated already above, the microphysical properties of the convective cloud are not well represented, because the convection scheme does not include an explicit cloud microphysics in EMAC. The total

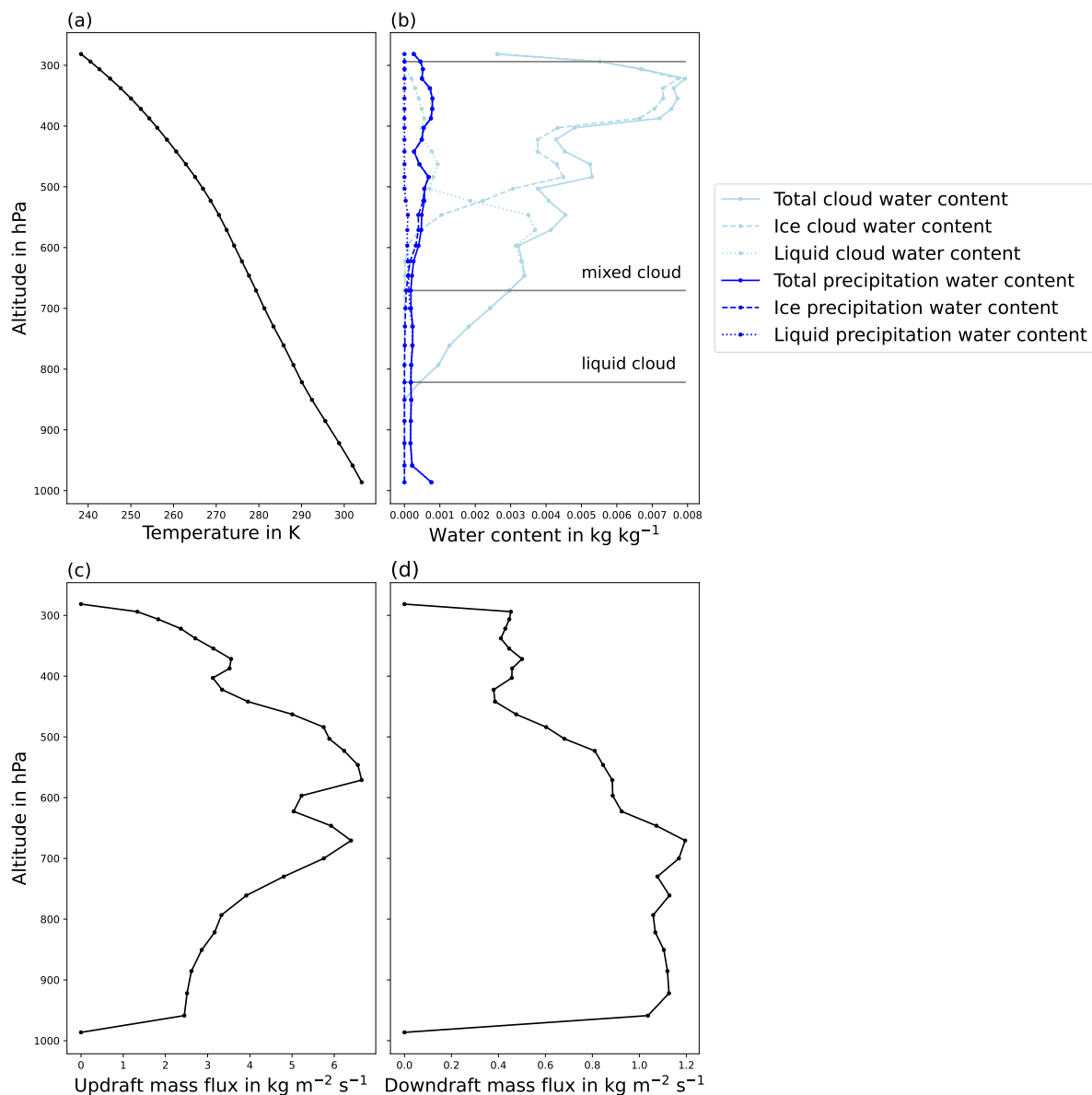


Figure 3. Meteorological properties used for the MCTS simulations of the selected case based on WRF-Chem. The vertical profiles are displayed of (a) the Temperature, (b) the total, liquid and ice water content, (c) the updraft mass flux and (d) the downdraft mass flux for the choose event on September 2nd 2013. The points indicate the grid box mean point pressure. The temperature, the cloud water contents and the updraft are for the cloud core area. Whereas, the downdraft mass flux and the precipitation water contents are shown for the downdraft area. The gray lines in (b) divide the cloud in it's pure liquid, mixed-phase and pure ice part. The ice part is above the uppermost gray line. It is not explicitly mentioned in the Figure due to the limited space.

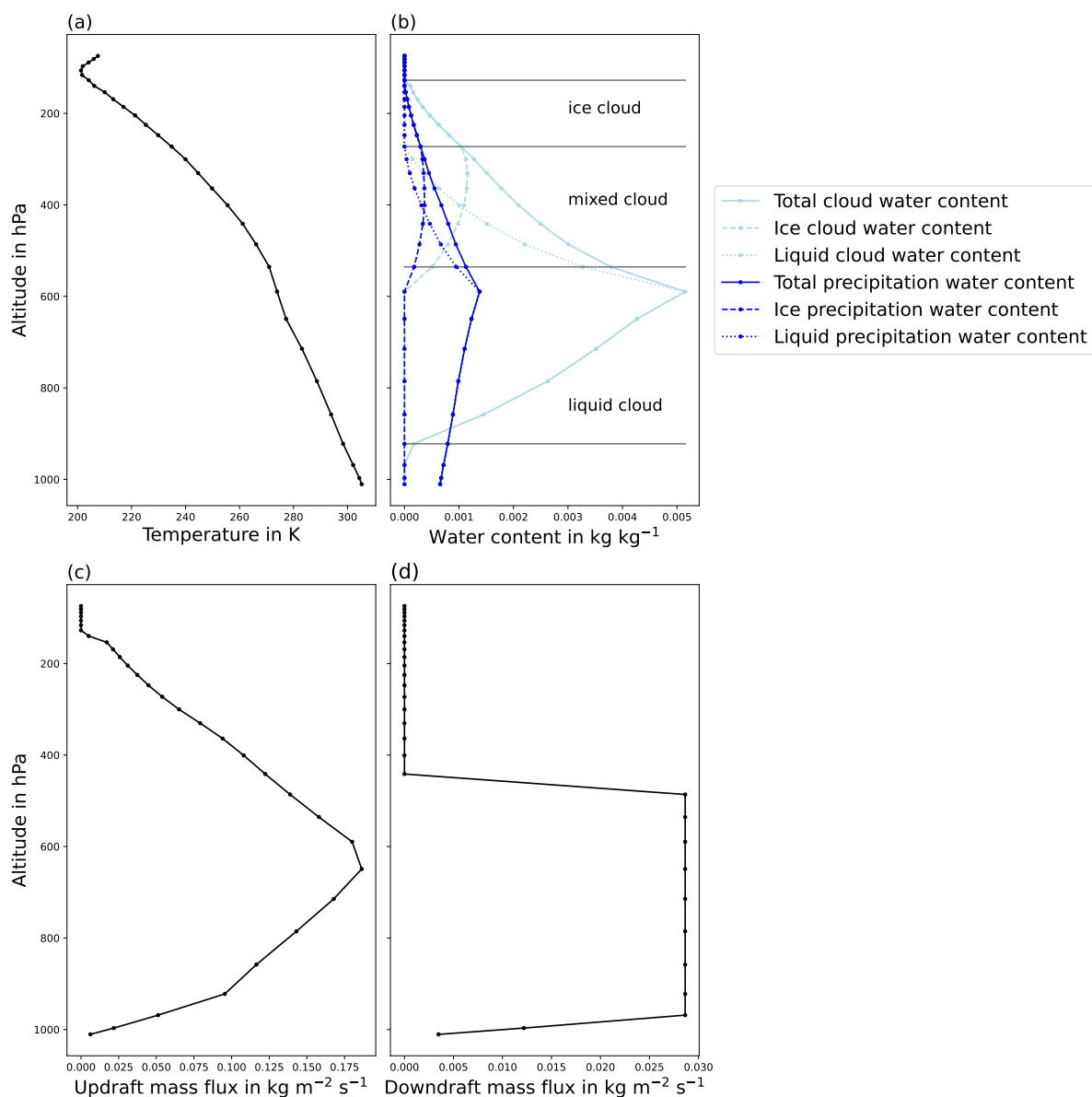


Figure 4. Meteorological properties of the selected case based on EMAC. The vertical profiles are displayed of the Temperature (a), the total, liquid and ice water content (b), the updraft mass flux (c) and the downdraft mass flux (d) for the choose event on September 2nd 2013 23:40 UTC, 90° W 32.1° N. The points indicate the grid box mean point pressure.

precipitation water content is highest at 590 hPa. The maximum of the total precipitation water content is much smaller than
 390 the total cloud water content.



The convective updraft mass flux is located between the level closest to the surface with the midpoint pressure of 1011 hPa and exceeds the level with a pressure of 140 hPa. The maximum of $0.19 \text{ kg m}^{-2} \text{ s}^{-1}$ is reached at 649 hPa. The downdraft mass flux with pressure height is shown in Fig. 4(d). As expected, the downdraft mass flux is weaker than the updraft mass
 395 flux with maximum values of nearly $0.03 \text{ kg m}^{-2} \text{ s}^{-1}$. The downdraft only exists below 441 hPa. The sub-grid subsidence (not shown) ensures the mass balance.

5 Results

MCTS is evaluated for the multicell storm against DC-8 observations and for one convective EMAC case against the EMAC
 400 submodels CVTRANS and SCAV. Both MCTS simulations differ in their setup and the considered scales, and are not comparable to each other for these reasons.

5.1 Performance of MCTS–WRF–Chem vs. observations

MCTS is compared to DC-8 observations of a single convective event. MCTS was slightly adapted to enable a realistic setup for the comparison: The sub-grid scale-subsidence was turned off, and a horizontal advection was introduced. The model results
 405 are compared with outflow measurements for the corresponding convective event. Therefore, much smaller spatial scales are considered than typical GCM grid box sizes. MCTS was adapted for comparison with observations, i.e. the smaller horizontal domain, by considering horizontal advection instead of subgrid-scale subsidence. In the outflow area, air flows away from the convective core. Therefore, molecules leave the domain. Also, air flows into the domain, i.e. towards the convective system, where entrainment takes place.

410 Figure 5 shows the CO , C_5H_8 and O_3 profiles after 10 and 30 min based on MCTS. The time frames of 10 and 30 min were chosen, because the convective transport is supposed to take place on these scales (as well as this is a typical GCM time step length). Additionally, having two profiles at two different times allows to estimate the development of the vertical profiles with time. The real convective system is evolving with time which makes a direct comparison difficult, as MCTS assumes constant meteorological and convective properties. The background profiles/the clear air vertical profiles are displayed in Fig. 5 as well.
 415 The Figure also includes the mean mixing ratios and the standard derivations of the outflow intercept flights of the convective core 7 and boundary layer observations. CO and C_5H_8 are not soluble; they only undergo convective transport because gas-phase chemistry is not considered. O_3 has a low solubility and is mostly affected by the transport as well.

For CO , the background profile is low compared to the measured boundary values (Fig. 5(a)). These differences result from the horizontal variability of CO in the considered domain. The background CO mixing ratios range from 70 ppbv in
 420 the upper troposphere to 125 ppbv in the boundary layer. The background CO increases with decreasing pressure above 372 hPa. This increased CO values in the upper troposphere is a strong indicator of previous convection. In the boundary layer, the values are still a bit higher than in the upper troposphere. After the 10-min simulation with MCTS, the CO mixing ratios are mostly reduced at 500 hPa and at higher pressures despite some distinct peaks. At lower pressures, CO is very similar to

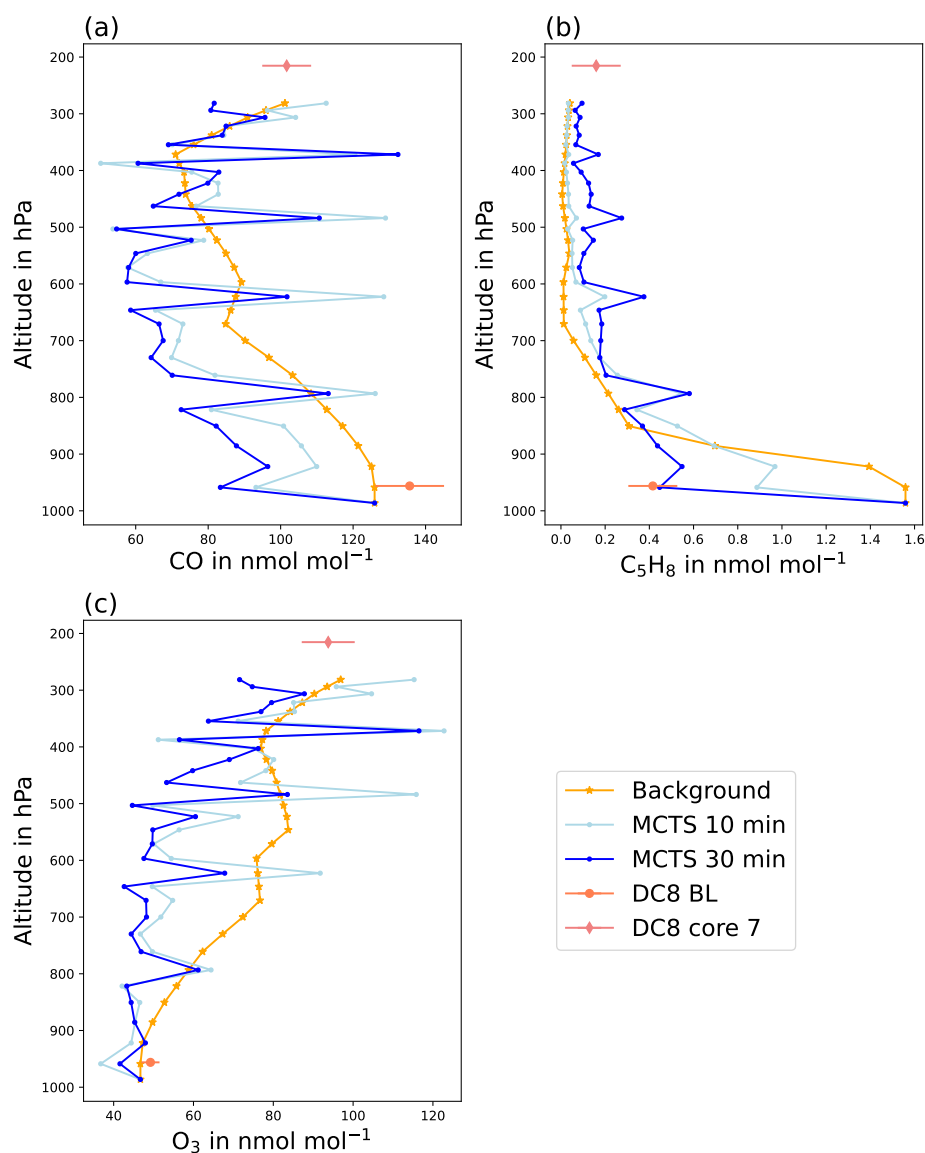


Figure 5. MCTS profiles of insoluble tracers and tracers of low solubility compared to the background profiles and inflow and outflow observations. The orange line shows the background profile/initial values for the MCTS simulation, the light blue line shows the resulting profile after 10 min, and the blue curve displays the resulting profile after 30 min of simulation with MCTS. The circles indicate the observed mean inflow mixing ratios in the boundary layer (DC8 BL) and outflow mixing ratio observed in the convective core 7 (DC-8 core 7) with their standard deviations. (a) shows the mixing ratios of CO, (b) of C₅H₈, and (c) of O₃.

the background at many levels except for two levels (at about 372 hPa and 484 hPa). The peaks are highly correlated with the
 425 inflow and outflow patterns of the multicell storm, i.e. with organised entrainment and detrainment. In the top level, the mixing



ratios are enhanced with respect to the background value after 10 min and decreased after 30 min. The observed outflow CO is similar to the background mixing ratios in the top level. The top level in MCTS and the values at the real outflow height are comparable, although the two outflow levels are not at the same height. The height difference of the convection is mainly due to the sampling criteria for the production of column values from 3D data.

430 The observed inflow mixing ratios are not equal to the applied initial values for the simulations; therefore, deviations are also expected for the comparison of the simulated and observed outflow mixing ratios in the upper troposphere. Therefore, the outflow-inflow ratios are compared, see Table 4. For that purpose, the outflow mixing ratios are divided by the inflow mixing ratios. This calculation is performed for the observations and for MCTS. 75 % of the inflow CO is measured in the outflow, which is a smaller ratio than reported by Bozem et al. (2017). Outflow-inflow-ratios unequal 100 % indicate that mixing with
 435 the environment is taking place during the upward transport. Accordingly, the inflow-outflow-ratio might indicate that in the considered multicore storm case stronger mixing is taking place than in the case observed by Bozem et al. (2017). For the calculation of the MCTS outflow-inflow ratio, the resulting mixing ratios in the model level with the lowest pressure are used as outflow values. The MCTS outflow-inflow ratios are higher after 10 min than the ratios derived based on the observations and lower after 30 min. MCTS reproduces the measured results on time scales between 10 and 30 min. However, the rather
 440 low outflow-inflow ratios after 30 min suggest that MCTS might underestimate the direct transport from the BL to the upper troposphere in this case. The latter is supported by the result for C₅H₈.

The background C₅H₈ profile has nearly its typical "L"-shape with enhanced values in the boundary layer (Fig. 5(b)). Isoprene is largely reduced in the boundary layer by the convective transport during the simulation with MCTS. The mixing ratios increases with regard to the background profile above the boundary layer. The simulated upper tropospheric mixing ratios
 445 after 30 min are smaller than the observed mean outflow value, but are within the range of the measurements. It is necessary to consider that the background values overestimate the observed inflow values. The inflow was measured in the afternoon, whereas the background profile includes all measurements during the flight, which were obtained in cloud-free air. Therefore, more material is present in the model in the boundary layer than suggested by the inflow observations, which can be transported upward via the updraft. The outflow-inflow ratio of MCTS is about an order of magnitude smaller than the observed ratio. As
 450 already indicated by the CO mixing ratios after 30 min, the upward transport is not efficient enough which points towards a non-optimal representation of the mixing.

The O₃ is reduced at most height levels with respect to the background during the simulation with MCTS, see Fig. 5(c). From a conceptual point of view, this reduction is in good agreement with the expectations as ozone-low air is transported upward from the boundary layer. After 10 min, MCTS suggests an increase of O₃ at the uppermost level compared to the
 455 background. The mixing ratios are largely reduced at this level after 30 min, which is in better agreement with the expectation. Still, the profile shows a high vertical variability.

Figure 6 shows the background profiles of the soluble species and the simulated profiles with MCTS after 10 and 30 minutes. As before, the inflow and outflow measurements are shown. The outflow measurements have been performed within the convective cloud, where it is likely that the soluble trace gases are still partially attached to the hydrometeors in the observed area.
 460 Therefore, the observed phase mixing ratios of the highly soluble species might be lower than the resulting MCTS profiles, as

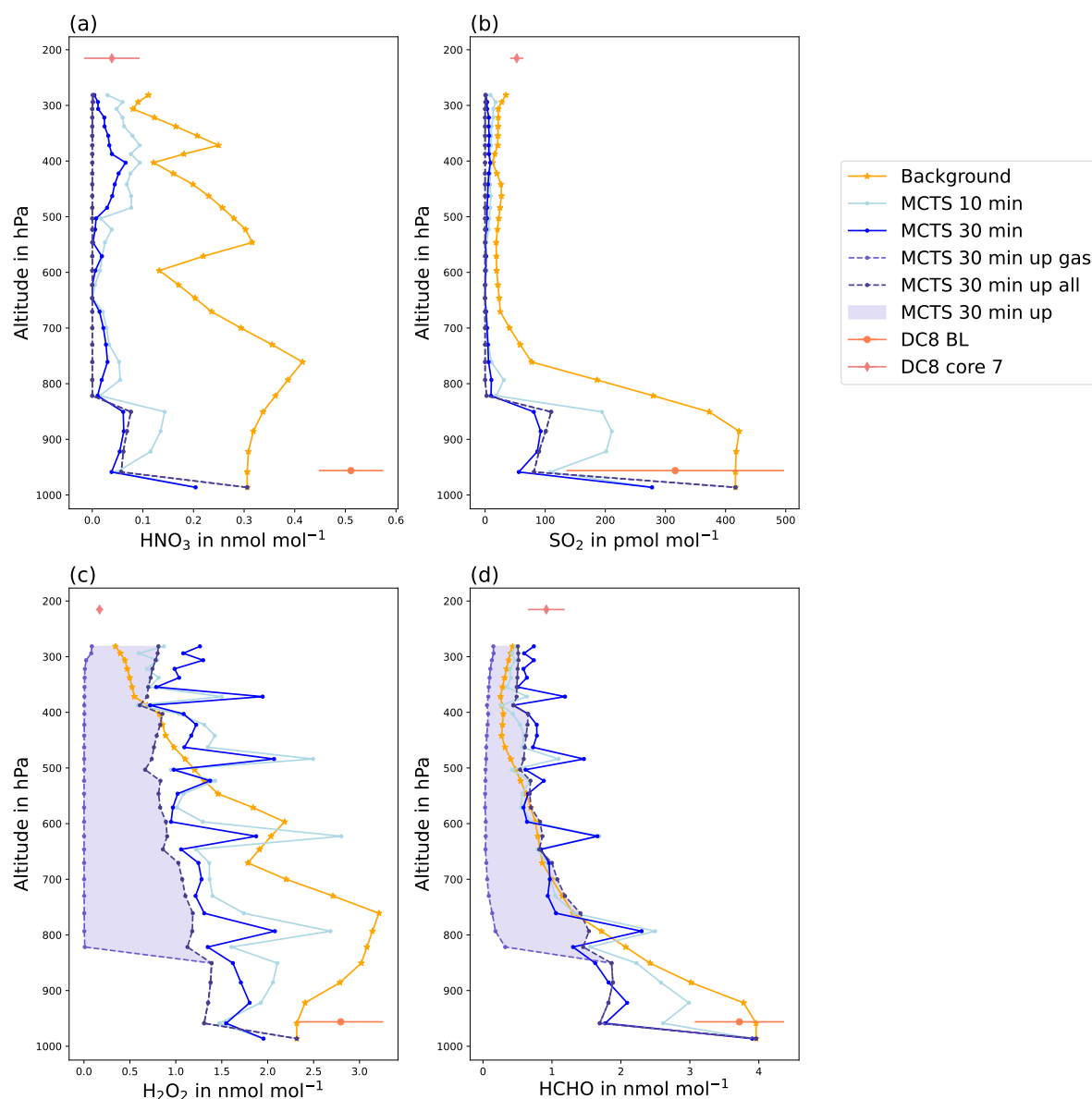


Figure 6. Comparison of soluble atmospheric tracer profiles simulated with MCTS with DC-8 observations. This Figure is as Fig. 5 but for (a) HNO_3 , (b) SO_2 , (c) H_2O_2 , and (d) HCHO . The blue shaded area shows the mixing ratios within the updraft after 30 min; the range is given between the gas-phase mixing ratios (lighter blue dashed line) and the mixing ratios in the gas-phase plus the mixing ratios in the cloud droplets plus the mixing ratios in or attached to the cloud ice crystals (darker blue dashed line). For, SO_2 , the dissociation products (SO_3^{2-} and HSO_3^-) are considered as well to constrain the multi-phase profile (darker blue dashed line) in (b).



the latter considers the molecules in all phases. To enable a fairer comparison, the simulated gas-phase updraft mixing ratios are displayed as well in Fig. 6. The updraft mixing ratios in the gas phase plus the mixing ratios in the cloud hydrometeors are given for comparison. The shaded area is the range between the two updraft mixing ratios. It can directly be seen from Fig. 6 that only very few molecules stay within the gas phase in the updraft. Most of the gaseous compounds transfer into or onto the cloud hydrometeors.

The background HNO_3 is much lower in the boundary layer than the observed inflow HNO_3 , see Fig. 6(a). MCTS suggest an efficient reduction of HNO_3 across all height levels compared to the background. In the upper troposphere, HNO_3 after 10 and 30 min is within the range of the observed outflow mixing ratios. The MCTS updraft mixing ratios are very low within the gas phase and also within the hydrometeors, which indicates that HNO_3 rapidly dissociates within the droplets. The Scavenging Efficiency (SE) is calculated for the soluble species following eq. 7 of Fried et al. (2016), but here CO is used as an insoluble reference instead of *n*-butane,

$$\text{SE} = \frac{\frac{C_{\text{inflow}}}{\text{CO}_{\text{inflow}}} - \frac{C_{\text{outflow}}}{\text{CO}_{\text{outflow}}}}{\frac{C_{\text{inflow}}}{\text{CO}_{\text{inflow}}}}. \quad (6)$$

C can represent any soluble species, for example, HNO_3 or SO_2 . Using an insoluble reference species enables the exclusion of the transport effects on the SE (Fried et al., 2016). The SEs given in Table 5 are derived using the gas-phase updraft values, the multi-phase mixing ratios in the updraft, and the resulting mixing ratios (all reservoirs) as outflow values. MCTS leads to a HNO_3 SE between 0.89 and 1. The SE is 90 % derived from the observations. The measurements performed within the anvil cloud show a high variability. Bela et al. (2016) reported a HNO_3 SE of 75 % to 95 % based on the observations of four different storm cases which took place during the DC3 mission.

For SO_2 , the inflow observations show a high variability (Fig. 6(b)). The background SO_2 mixing ratio is within one standard deviation of the inflow observations. SO_2 decreases during the simulation with MCTS due to scavenging. The MCTS SO_2 profiles after 10 and 30 min indicate much lower mixing ratios at all height levels as the background. The rapid loss of SO_2 can result from a too efficient chemical loss of SO_2 or from too strong washout. Nearly all SO_2 is scavenged during its ascent. MCTS suggest a SE of 100 % after 30 min, but only 78 % of the inflow SO_2 is scavenged based on the observations. The SO_2 SE has high uncertainty due to the huge SO_2 mixing ratio variability in the inflow. Still, MCTS overestimates the SE of SO_2 . The SO_2 SEs simulated by Bela et al. (2016) and Bela et al. (2018) show a dependence on the chosen retention factor. Therefore, it might be that retention is too strong in MCTS. Further uncertainties might arise from the representation of the convective system. Mari et al. (2000) reported SE of 0.28 for SO_2 for their selected case which is much lower than the SE derived for the storm analysed in this study. Cuchiara et al. (2020) calculated an average SE of 58 % for the multicell storm, i.e. the storm considered here, when using different SE calculation methods than applied in this study. The SO_2 SE of the air mass storm is 81 % (Cuchiara et al., 2020).

The background H_2O_2 is at the lower edge of the observed inflow values, see Fig. 6(c). In the lower to mid troposphere, the mixing ratios are reduced during the convective event compared to the background values. H_2O_2 increases in the upper troposphere due to a sufficient upward transport by the convection in MCTS. This upward transport takes place mainly via the hydrometeor phases. Nearly no H_2O_2 remains in the gas-phase in the updraft, but the H_2O_2 in the hydrometeors exceeds the



background mixing ratios in the levels with lower pressure. The observed values are within the range of the updraft MCTS values, but much lower than the mixing ratios MCTS suggest, considering all reservoirs. Therefore, MCTS underestimates the SEs. If only the gas phase updraft H_2O_2 is considered, the SE is 0.91 close to the observed SE of 92 %. It might be that most of the H_2O_2 molecules were still attached to the ice crystals in the area where the outflow measurements took place. Also, the ice retention might not be optimally represented in MCTS as higher ice retention can lead to larger SEs (the SE is 75 % with no retention and 92 % with high retention for the multicell storm, Cuchiara et al., 2020). However, Bela et al. (2018) and Cuchiara et al. (2020) reported that the H_2O_2 SEs did not show a strong dependence on the retention. Cuchiara et al. (2023) argue that the scavenging of H_2O_2 takes place primarily in the liquid phase which could lead to the low dependence of the H_2O_2 SE on retention. The SE of 92 % based on the DC-8 observations is similar SEs obtained by Barth et al. (2016) which range between 79 % and 97 % for six different storms during DC3 and is slightly higher than the SEs derived by Cuchiara et al. (2020) for multicell storm also analysed in this study.

The background boundary layer HCHO fits well with the observed HCHO inflow mixing ratios (Fig. 6(d)). HCHO is mostly reduced during the convective event at pressures higher than 500 hPa. The mixing ratios in the outflow after the 30 min simulation are a bit lower than the observed mixing ratios. The updraft mixing ratios are too low compared to the observations. This underestimation likely results from the too weak upward transport and a too high SE. MCTS suggests a SE between 69 % and 91 % which is much higher than the SE of 67 % derived from the observations. Photochemical HCHO production could lead to an underestimation of the calculated SEs based on the observations, see Fried et al. (2016). The WRF-Chem simulations performed by Li et al. (2019) also lead to too high HCHO SEs compared to observations during the DC3 campaign. Similar results were obtained by Bela et al. (2016) especially when the retention factor larger than zero are considered in the WRF simulations. Furthermore, literature values suggest that the HCHO SEs are sensitive to the specific storms: Fried et al. (2016) found that weak convection leads to a more efficient scavenging of HCHO (81 %) than stronger convection (41 % to 58 %). Cuchiara et al. (2020) reported SEs of 50 % for HCHO for the multicell storm after correction for lightning induced chemistry effects. Borbon et al. (2012) derived HCHO SEs ranging between 4 % and 39 % for mesoscale convective systems based on observations obtained during the African Monsoon Multidisciplinary Analysis (AMMA, Redelsperger et al., 2006) mission. Borbon et al. (2012) reported that the SEs are related to the convective storm properties, i.e. the rainfall rate and the updraft strength. Mari et al. (2000) gives an SE of 23 % based on the observations and the SE derived based on the values given by Bozem et al. (2017) is 0.42.

In summary, MCTS produces tracer profiles which overall go well along with the expectations and the observations, but cannot reproduce the observed outflow mixing ratios in all cases. The upward transport in MCTS seems to be slightly too inefficient which could be related to mixing. The SEs of H_2O_2 highly depend on the considered reservoir and MCTS overestimates the SEs of SO_2 and HCHO. The SEs of different storm cases also show a significant variations (see Cuchiara et al. (2020) and compare the SEs by Mari et al. (2000) and derived from Bozem et al. (2017) in Table 5). The H_2O_2 SEs ranges between 79 % and 97 % for the storms targeted during DC3 missions (Barth et al., 2016). The difference in the reported SEs suggest that also the meteorological input and its uncertainties has a huge impact on the results. However, Cuchiara et al. (2023) reported that the SE of H_2O_2 and HCHO vary only slightly between land and marine convection. To get a better estimate of the uncertainties



530 of the MCTS results, two sensitivity studies are discussed in the following focussing on turbulent mixing and on the impact of multi-phase chemistry on the SEs.

Table 4. Mean outflow-inflow ratios for the aircraft observations, MCTS after 10 min and 30 min, and the values by Bozem et al. (2017) (see their Table 2). The values for MCTS were derived by comparing the uppermost level to the level closest to the surface.

Species	DC-8	MCTS 10 min	MCTS 30 min	Bozem et al. (2017)
CO	0.75	0.89	0.65	0.94
C ₅ H ₈	0.38	0.02	0.06	-
O ₃	1.91	2.47	1.53	1.03

Table 5. Scavenging efficiencies for the aircraft observations and the MCTS results. The table also shows the SEs from Mari et al. (2000) and the SEs derived based on the observations by Bozem et al. (2017) (see their Table 2). The values for MCTS were derived by comparing the uppermost level to the level closest to the surface after 10 and 30 min. The MCTS SEs are displayed for the updraft mixing ratios and gas-phase updraft mixing ratios after 30 min as well.

Species	DC-8	MCTS 10 min	MCTS 30 min	MCTS updraft gas	MCTS updraft all	Mari et al. (2000)	Bozem et al. (2017)
HNO ₃	0.90	0.89	0.98	1.00	0.98	0.77	-
SO ₂	0.78	0.98	1.00	1.00	1.00	0.28	-
H ₂ O ₂	0.92	0.58	0.16	0.91	0.15	0.66	0.35
HCHO	0.67	0.87	0.71	0.91	0.69	0.23	0.42

5.1.1 Sensitivity of convective transport to turbulent mixing

535 The sensitivity of the convective transport is analysed regarding the turbulent mixing, i.e. turbulent entrainment and detrainment. In Figure 7, the CO, C₅H₈, and O₃ profiles were shown using ten times the turbulent entrainment and detrainment mass fluxes of the values used for the analysis presented above. The turbulent mixing was increased for both the up- and down-draft. The difference in CO is striking when comparing Fig. 7(a) and Fig. 5(a): with enhanced turbulent mixing the resulting MCTS CO increases significantly in the upper troposphere compared to the background. The enhanced turbulence leads to a
 540 smaller enhancement of the C₅H₈ mixing ratios in the upper troposphere with regard to the background profiles (Fig. 7(b) and Fig. 5(b)), whereas the changes of the O₃ profile have a high similarity to CO. The response of isoprene profiles is different compared to the one of CO and O₃; this difference indicates that the effect of turbulence is also sensitive to the background profile; CO and isoprene undergo the same processes, but are not affected in the same way by the changes in turbulent mixing. Barth et al. (2016) also reported that the trace gas profiles in combination with mixing (mixing in general not explicitly

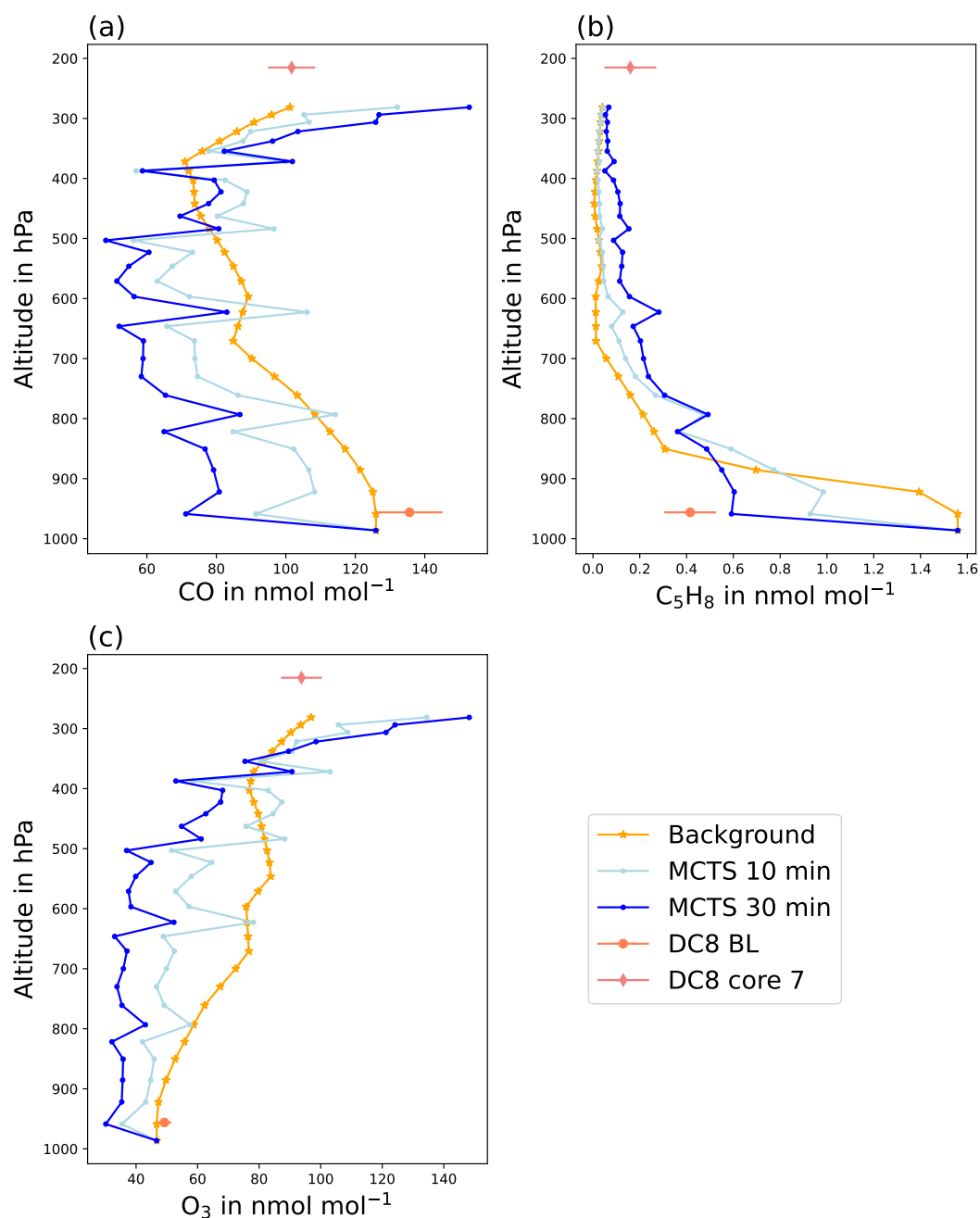


Figure 7. As Fig. 5 but with 10 times larger turbulent mixing.

545 turbulent mixing) might be relevant for the upward transport. Barth et al. (2016) use the example that the dilution of upward transported CH_3OOH is higher, when the background profile rapidly decreases with height, which is the case in this study for



C_5H_8 in Fig. 7(b) than in the case of a background profile with a less steep gradient with height as for CO in Fig. 7(a) in this study.

5.2 Sensitivity regarding the dissociation rate

550 The dissociation reactions are equilibrium reactions within the droplets. In MCTS, we applied scaling factors to these equilibrium reactions, which influence how fast or slow the equilibrium is reached¹. This scaling is important to reduce the stiffness of the ordinary differential equation system. Sensitivity studies were performed with different scaling factors. Figure 8 shows the resulting profiles when it is assumed that the faster reaction of the equilibrium reactions has about the same order of magnitude as the convective updraft rate. The scaling factors for the reference simulation and the sensitivity simulation are listed in the

555 supplements. The differences between the two simulations are striking for HNO_3 and SO_2 compared to Fig. 6. More HNO_3 survives in the upper troposphere when the dissociation is slower. SO_2 increases within the upper troposphere during the convective event compared to the background. The upper tropospheric SO_2 values are in better agreement with the observations in Fig. 8 than in Fig. 6. Also, the scavenging efficiency is in better agreement with the observations, i.e. the SE for SO_2 is 76 % within the updraft after 30 min. $HCHO$ and H_2O_2 do not dissociate. Therefore, the differences are smaller and originate only

560 from indirect effects, e.g. H_2O_2 could be influenced indirectly by the amount of HSO_3^- . However, the results for H_2O_2 are not sensitive to the choice of scaling factor for the dissociation reactions.

This sensitivity study highlights the importance of representing the competition between dissociation and transport, which cannot be done when operator splitting is applied. It is not possible to tell which scaling factors are the right ones. Considering SO_2 , the comparison with the observations suggests that the dissociation reactions are not much faster than the upward

565 transport. For other species, the dissociation might be faster than the transport time scale, for example, HCl.

Table 6. As Table 5 only for HNO_3 and SO_2 with different dissociation scaling factors.

Species	DC-8	MCTS 10 min	MCTS 30 min	MCTS updraft gas	MCTS updraft all
HNO_3	0.90	0.70	0.67	0.99	0.69
SO_2	0.78	0.92	0.79	0.76	0.76

5.3 Performance of MCTS vs. EMAC

MCTS is compared to the EMAC submodels CVTRANS and SCAV. An EMAC simulation at T42L90 was performed to (1) derive the input data for MCTS and (2) to get the effect of the convective transport and scavenging on the tracer profiles. It is

570 not possible to simply use the tracer profile simulated by EMAC after one time step as EMAC takes several other processes, i.e. advection, gas-phase chemistry and others. The tendency submodel was used to extract the tendency of CVTRANS and

¹The equilibrium will not be reached, when other processes have an impact on the species and their dissociation products.

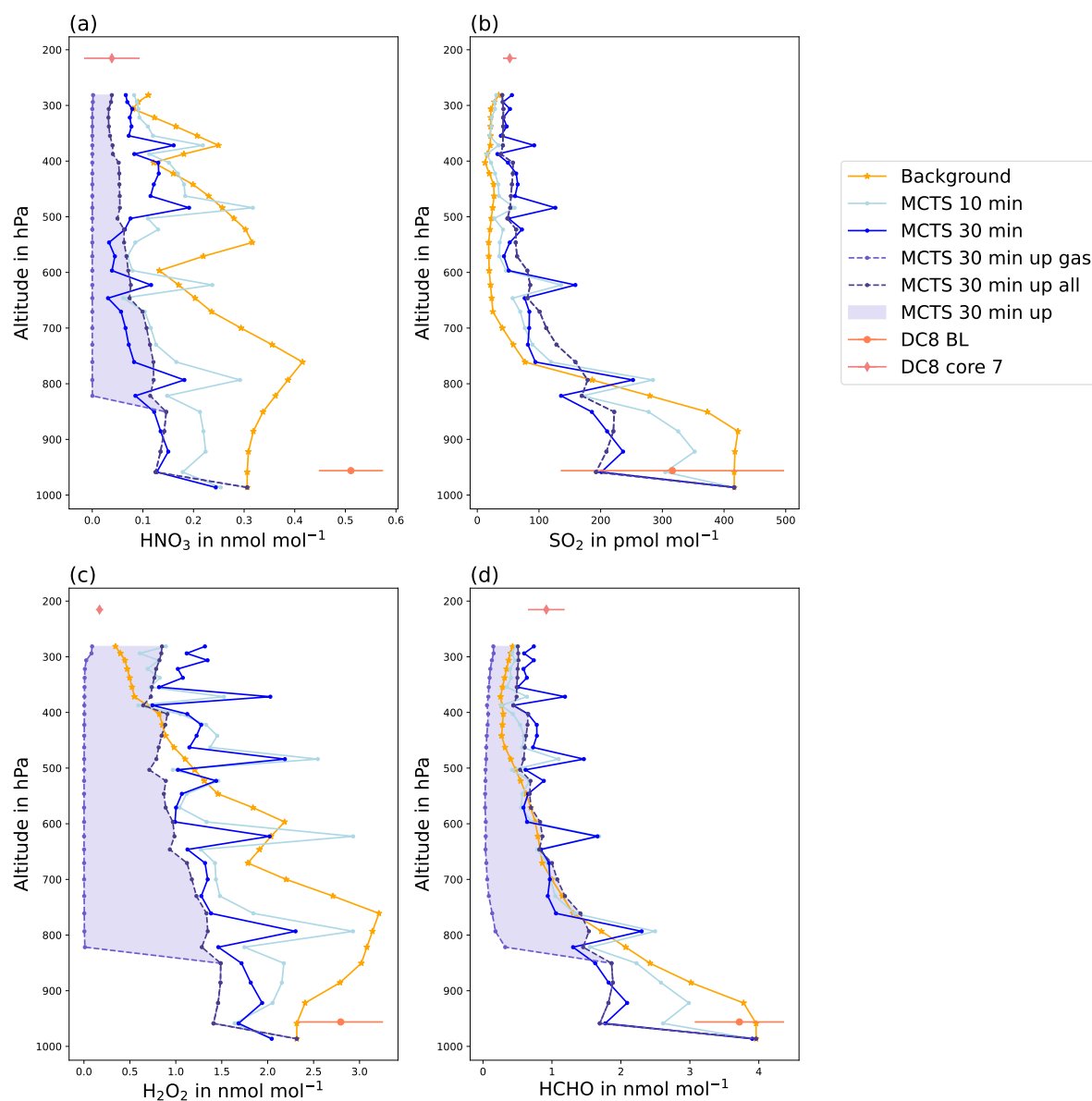


Figure 8. As Figure 6 but with different dissociation scaling factors.

SCAV (convective scavenging) which were added to the tracer profile from the time step before. The derived tracer profiles only take into account the convective impact and are compared to MCTS. The comparison was done for 10 min which is corresponding to the EMAC time step. Comparing the results after longer periods is not possible in a meaningful way as the non-convective processes would affect the EMAC results. The MCTS simulations was set up in such a manner that the 31 vertical levels corresponded exactly to the 31 levels closest to the surface of the EMAC simulations. The convection took place



only within these levels and did not reach lower pressures. The considered area for this comparison is the whole EMAC grid box.

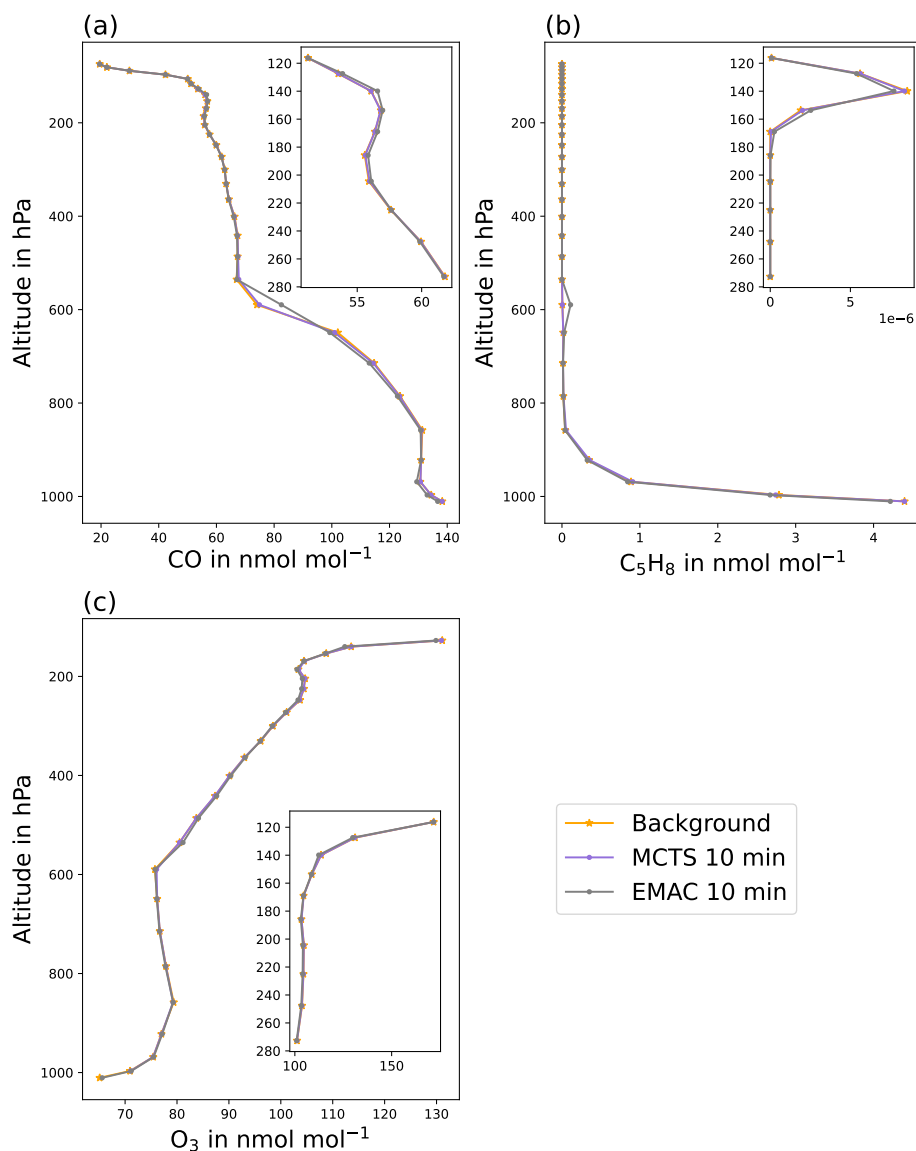


Figure 9. As Fig. 5 but for a whole grid box and for simulations with EMAC input at the respective EMAC scales. The MCTS profile is shown after 10 min in purple. The grey curve shows the tracer profiles based on the impact of the convection in EMAC. The small plots within each panel show the upper tropospheric mixing ratios in more detail. The chosen case tool place September 2nd, 2013 at 23:40 UTC in the area for the SEAC⁴RS campaign.

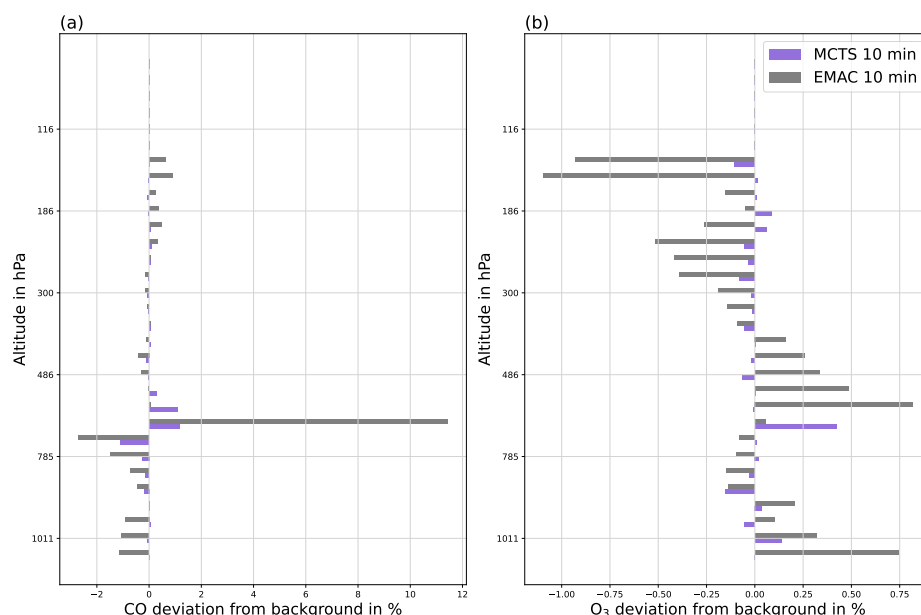


Figure 10. Deviations in % of the MCTS profiles from the background profiles (purple) and of EMAC from the background profile (gray) for (a) CO and (b) O₃. C₅H₈ is not shown because the very small background values lead to extremely high relative differences. The convective case is the same as in Fig. 9.

The convective transport has only little effect on the vertical profiles of the insoluble species and the species with low solubility due to the grid box size and the rather short time step (Fig. 9). The deviations of the modelled mixing ratios from the background mixing ratios are shown in Fig. 10. The convective transport in EMAC has a slightly larger impact on the CO profile than the transport with MCTS. The CO mixing ratios from the EMAC simulation are a bit smaller than the background mixing ratios between 1010 hPa and 649 hPa and larger than the background values at 590 hPa. At 590 hPa is the level located with the lowest pressure, where the cloud is purely liquid. During the EMAC simulations, CVTRANS is called twice within one model time step. First, the transport is calculated up to the uppermost level where rain production takes place. Then, the scavenging submodel is called, which does not affect CO. Third, the convective transport of CO is calculated from the uppermost level of rain production to the top. Splitting the transport this way can lead to enhanced mixing at 590 hPa, which could explain the positive difference of the EMAC CO from the background at 590 hPa. Considering the upper tropospheric CO, EMAC calculates a small increase after 10 min compared to the background. The MCTS mixing ratios differ little from the background after 10 min.

For isoprene, the two models behave rather similar again and do not alter the vertical profiles substantially. CVTRANS predicts a distinct increase of isoprene at 590 hPa, which is not present in the MCTS profiles. MCTS indicates a very small increase at about 969 hPa with regard to the background. In contrast, CVTRANS predicts a slight decrease of isoprene at the same height. At 140 hPa, the isoprene of the EMAC simulation is a bit lower as the MCTS and background isoprene. The



relative differences are partially very large, because the background isoprene mixing ratios is extremely low at certain levels. Therefore large relative differences can be produced by the transport of a small isoprene fraction from the boundary layer into the free troposphere. The O_3 profiles based on the two different models are also very similar (Fig. 9(c)) and lead only to small changes (up to $\sim 1\%$) in the vertical profile and Fig. 10(b)). In summary, MCTS transports the insoluble species in a similar manner than CVTRANS. The similar transport effects fit with the expectations, because the representation of the convective transport in MCTS is derived from the same assumptions as in CVTRANS.

The profiles of the soluble species show stronger variations from the background than the profiles of the insoluble species. The deviations are especially at the pressure levels associated with the liquid and mixed phase of the convective cloud (pressures larger than ~ 280 hPa), see Fig. 11(a)–(d). The deviations between the different profiles are shown in the supplements. Both models predict a reduction of the mixing ratios compared to the background for most of these pressure levels. The reduction of HNO_3 is larger for the EMAC simulations than for MCTS for nearly all level. This reduction can result either from (1) a more effective washout and dissociation of HNO_3 in EMAC-SCAV than in MCTS, (2) more HNO_3 production from N_2O_5 in MCTS, or a combination of both. Between 140 hPa and 225 hPa, MCTS even suggest a slight increase of the mixing ratios compared to the background, whereas the EMAC HNO_3 is reduced (see Fig. S1).

The upper tropospheric SO_2 does not indicate a clear trend. At about 140 hPa, the EMAC SO_2 is marginally higher than the background values. MCTS does not alter the mixing ratios at this altitude as much as EMAC. At ~ 220 hPa, the MCTS SO_2 is higher than the EMAC SO_2 . Between 273 hPa and 435 hPa, both models simulated a reduction of SO_2 relative to the background. EMAC predicts an increase and MCTS a decrease at 590 hPa compared to the background. At 590 hPa is the model level with the lowest pressure, which is purely liquid, i.e. freezing starts directly above that level (at lower pressures). Therefore, the different behaviour of EMAC and MCTS at 590 hPa might be related to the missing representation of retention in EMAC or to the enhanced mixing occurring at this level within EMAC. At higher pressures than 590 hPa, both models agree that the mixing ratios are reduced during the convective event.

According to SCAV and CVTRANS, H_2O_2 would increase compared to the background close to the surface. MCTS simulates a reduction at the same pressure levels. Between 922 hPa and 300 hPa, both models agree that the convective system leads to a reduction of the mixing ratios. At most heights, EMAC suggests a greater reduction of the mixing ratios than MCTS when comparing to the background. In the upper troposphere, the MCTS mixing ratios closely follow the background values. EMAC suggest higher mixing ratios than MCTS. A distinct increase in the EMAC mixing ratios takes place at 140 hPa.

HCHO is more efficiently scavenged in the boundary layer by MCTS than by EMAC. Both models predict a small reduction of the mixing ratios at the most levels between 1011 hPa and 273 hPa. EMAC HCHO is about 1.5 times higher than the background HCHO at 590 hPa, i.e. the level with the lowest pressure where the cloud is purely liquid. MCTS suggests at this pressure height still a decrease of HCHO with respect to the background. In the outflow region, the simulated mixing ratios are mostly slightly higher than the background profile for both models. However, this enhancement compared to the background is more pronounced for EMAC than for MCTS. The MCTS values follow again nearly the background profile as it is the case for H_2O_2 .

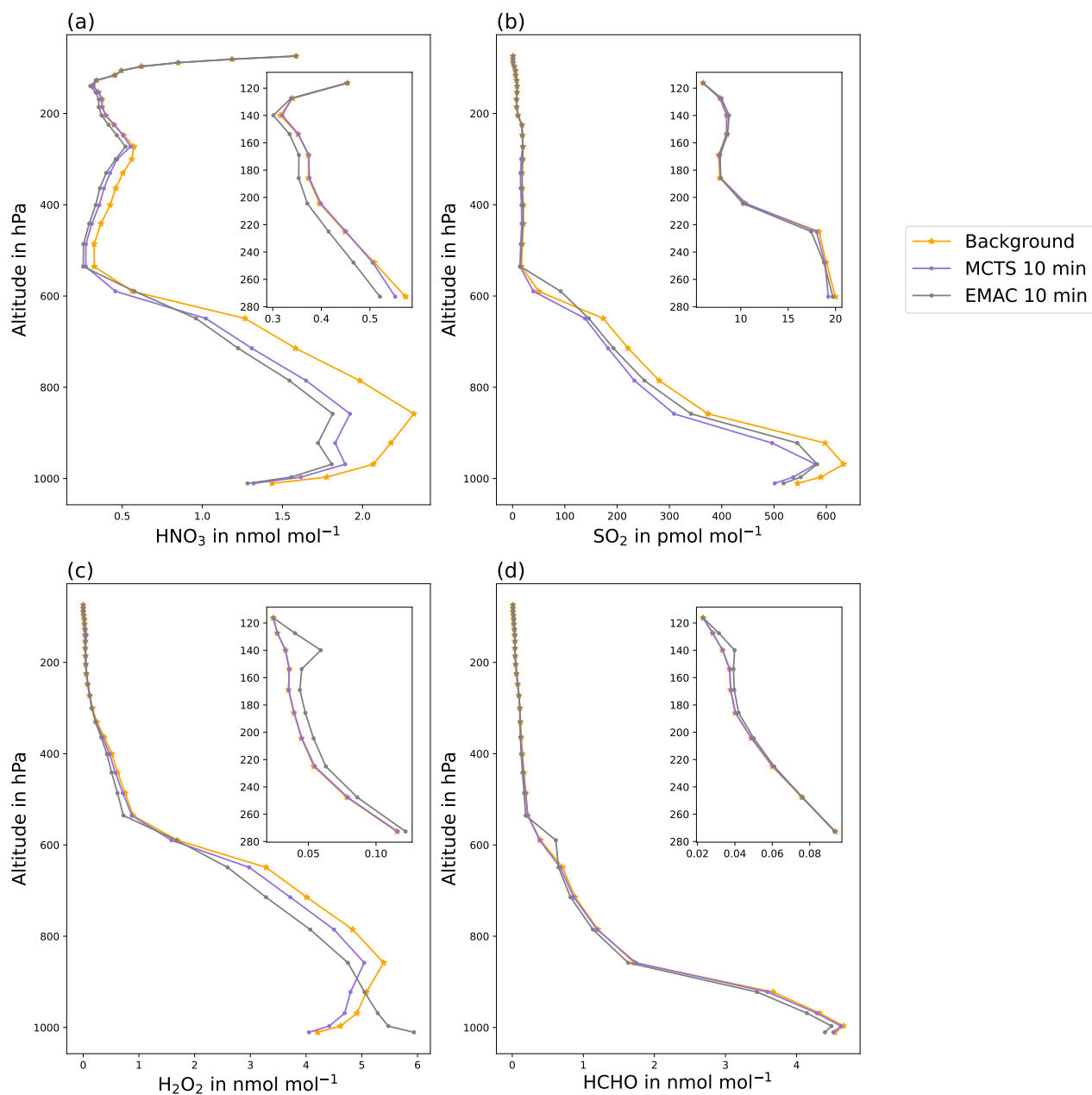


Figure 11. As Fig. 9 but for HNO_3 (a), SO_2 (b), H_2O_2 (c) and HCHO (d).

MCTS is build upon CVTRANS and SCAV; therefore, the differences between convectively induced changes of the tracer
 630 profiles are overall similar, especially for the insoluble species. The relative deviations from the model run and the background
 are huge for C_5H_8 , but the absolute changes are small and the modelled profiles are similar to the background profile. The



absolute differences in the two model results are larger for the soluble species than for insoluble trace gases. MCTS considers multi-phase transport and scavenging and treats all processes quasi-simultaneous in contrast to SCAV and CVTRANS which should first and foremost affect the soluble trace gases. Fig. 11 suggests that the two models lead to the largest absolute differences of the considered species at pressures of about 600 hPa and higher pressures. Especially at 590 hPa, the differences between the two models are large. MCTS predicts a decrease of CO, SO₂ and HCHO at 590 hPa, whereas EMAC predicts an increase of up to 80 % compared to the background. The differences in the results of the two models are correlated to the freezing level. This correlation might be caused by the fact that retention is considered in MCTS and not considered in EMAC. The upper tropospheric mixing ratios are affected by the choice of the model as well. However, the SEs based on MCTS and EMAC are similar (Table S4). MCTS suggest slightly higher SE for H₂O₂ than EMAC using the original scaling factors for the dissociation (Table S2). The difference between the SEs of MCTS and EMAC are smaller than 1 % for SO₂ and HCHO. For HNO₃, EMAC leads to a more sufficient scavenging than MCTS, which might be related to the chemical production of HNO₃ from N₂O₅. MCTS produces a SE about 3 % smaller than the SE based on EMAC. In the following, the results will be discussed further.

6 Discussion

The comparison of MCTS with observations is accompanied by rather large uncertainties:

- MCTS considers fixed meteorological data, i.e. the convective system does not change within the time frame of 10 to 30 minutes. Assuming that the convective system does not change with time is a simplification which is typical for convection parametrisations embedded in global models.
- Sampling the cloud-resolving WRF-Chem data to produce the required column input data leads to further inaccuracies.
- For some species, EMAC output (originating from relatively coarse resolution) was used as input for MCTS due to a lack of observational data. Considering these species is important to create a sufficient H_(aq)⁺ concentrations.
- Also the measured profiles introduce uncertainty due to measurement errors and the horizontal variability of the mixing ratios.

In general, MCTS is still highly idealised and simplified, even though it is more comprehensive than current parametrisations in global chemistry climate models. Changing the meteorological input can have a huge effect on the resulting tracer profiles. On the one hand, the dependence of the MCTS results on the meteorological input is unpleasant because it makes the comparison with the measurements difficult due to the rather large uncertainty with respect to the input data. On the other hand, it shows that MCTS is sensitive to the individual features of a convective storm. The latter seems to be rather realistic, because also the SEs differ significantly for different convective cases, e.g. compare the different SEs based on DC-8 and based on Bozem et al. (2017) as well as from Mari et al. (2000), which are displayed in Table 5 and also from Borbon et al. (2012). Further, the chemical mechanism considered in MCTS is rather simple and gas-phase chemistry is not considered at



all. Chemical reactions which are not considered in MCTS can have a huge impact on the vertical tracer profiles as well. A well known example is the production of ozone from convectively redistributed pre-cursors, for example, see the results by Lawrence et al. (2003) and Apel et al. (2012). The changes in the MCTS SO_2 look similar to the results by Tost et al. (2010), compare Fig. 6(c) of Tost et al. (2010) with Fig. 6(b). The model simulations by Tost et al. (2010) underestimated the upper and mid tropospheric SO_2 mixing ratios. MCTS leads to too much scavenging of SO_2 , because the dissociation equilibrium is reached too fast. If these equilibrium reactions take place slower (e.g. due to the consideration of ventilation effects or higher viscosity in the droplets), MCTS can reproduce the observed upper tropospheric SO_2 mixing ratios and the predicted SE is in good agreement with the observed SE, see Fig. 8 and Table 6. Further investigations are necessary to obtain the ideal reaction rates for these processes. However, these results already indicate the importance of representing the competition of convective scavenging and convective tracer transport within models.

MCTS was developed based on CVTRANS and SCAV, therefore it is good in terms of consistency that MCTS and these two EMAC submodels lead to similar results for the considered case. Significant differences occur for the soluble species. Here, further investigations are needed whether these differences arise from operator splitting or from the fact that MCTS considers more processes than the two EMAC submodels. It is not clear whether MCTS is superior to EMAC for the predictions of SO_2 profiles, because both models behave rather similar in the analysed case. Neither of them suggests a large decrease of the mid to upper tropospheric SO_2 as was found by Tost et al. (2010) for EMAC simulations. It is not possible to conclude whether MCTS performs better than EMAC based on the presented comparison of the two models, but MCTS is physically more consistent and the comparison of MCTS with the measurements is promising.

The goal of MCTS is to provide a quasi-simultaneous model setup for convective transport and scavenging to improve chemistry-climate models in the future. This setup has the potential to produce more realistic vertical profiles of soluble trace gases. However, MCTS has a major weak point: It takes MCTS roughly 10 s to calculate the redistributed tracer profiles after 30 min (without any meteorological calculations). Roughly 10 s seems to be a little computational effort compared to cloud resolving simulations, but not in terms of computing time for the application in global model simulations. For this reason, it is not yet feasible to run a global chemistry-climate model with MCTS for several decades. MCTS consists of an enormous ODE system, which is responsible for the high computational cost. The large number of ODEs derives from the fact that all processes need to be considered at 31 vertical levels and for all species separately. To reduce the number of equations, insoluble trace gases could be excluded from MCTS, since MCTS primarily benefits the prediction of soluble trace gases. However, MCTS can be used for several process studies and forecast on regional scales and for periods shorter than typical climate simulations, i.e. air quality applications.

7 Conclusions

Mainz Convective Transport and Scavenging (MCTS) is a novel column model which can treat convective transport and scavenging quasi-simultaneously. Thereby, a wide range of processes are taken into account: transport in the gas and in the



695 hydrometeors, uptake by liquid droplets, aqueous phase chemistry, retention, uptake at ice hydrometeor surfaces, and washout by precipitation.

The evaluation of MCTS builds upon the work of Cuchiara et al. (2020), who performed high-resolution WRF-Chem simulations to investigate convective transport and scavenging of a multi-cell storm. This storm took place on September 2nd, 2013. The WRF-Chem simulations were performed by Cuchiara et al. (2020) in such a way that the resulting convective system
 700 matched with the storm, which occurred during the NASA SEAC⁴RS field mission. The MCTS simulations were performed using the output from WRF-Chem simulations by Cuchiara et al. (2020) as input to capture the meteorological state. The observed clear air profiles were used as initial profiles. The resulting MCTS profiles were compared to the aircraft observations during the DC-8 core 7 intercept flights, see Cuchiara et al. (2020) for more details regarding the convective cores. MCTS tends to underestimate the upward transport. The underestimation might result from uncertainty associated with the turbulent
 705 entrainment and detrainment. The performed sensitivity study revealed that the convective upward transport is highly sensitive to large portions of turbulent mixing. The effect of the turbulence itself also depends on the initial profile. Further, the profiles of the acids and bases is sensitive to the speed of the dissociation reactions. The simulated SO₂ profiles agree better with observations if the dissociation reactions take place within a similar time frame as the upward transport. The sensitivity study with different scaling factors for the dissociation highlights the importance of considering convective transport and convective
 710 scavenging simultaneously. The simultaneous treatment of these processes can largely improve the representation of soluble trace gases profiles in models.

MCTS is also compared to the EMAC submodels CVTRANS and SCAV, which are used to calculate the convective transport and the scavenging effects on trace species on the global scale. MCTS produces similar results than EMAC for the insoluble gases and tracers with low solubility. The transport is largely consistent between the two models. Differences arise when
 715 multi-phase processes come into play which is in accordance with the expectations as MCTS includes a more comprehensive representation of these processes and does not suffer from operator splitting effects. It is highly desirable to improve the convective transport and scavenging representation in global models because the changes in the trace gas distribution induced by convection have a wide range of impacts especially in the upper troposphere, e.g. on the photo-chemistry (Prather and Jacob, 1997), and on the new particle formation (Curtius et al., 2024).

720 MCTS opens the pathway for a wide range of future studies, for example:

- testing the sensitivity of the tracer profiles regarding ice phase processes, i.e. retention and surface adsorption,
- analysing the errors operator splitting might introduce,
- estimating the effect of different convective systems on the tracers distribution,
- including background aerosol to investigate its effects on the convective scavenging, and
- 725 – extending MCTS for biomass burning events or volcanic plumes.

MCTS is computationally too expensive to be used for simulations with a global chemistry-climate model covering long time scales, but it is much cheaper than cloud resolving simulations. Future work is needed to overcome this issue. It would



be an option to improve or to exchange the integrator in KPP or to use a different software to generate the code for the time integration. Up to now, we are not aware of any software that would perform better for a system of more than 20,000 ordinary differential equations than KPP. There might also be some GPU based approaches (Sophocleous et al., 2026) which can be applied in the future. Furthermore, there is room for improvement regarding the automatic step size control within KPP (see Dreger et al., 2025).

For now, MCTS could be used to create benchmarks to estimate the errors deriving from the representation of convection-chemistry-interactions. We plan to include MCTS in EMAC to investigate the uncertainties arising from operator splitting in global chemistry simulations in the future. MCTS is a step towards more accurate chemistry-climate simulations as the representation of convective transport and scavenging is improved and to gain a better process understanding. Furthermore, MCTS could also be extended for the application in weather and composition forecast models.

Code and data availability. The code of MCTS is available under <https://doi.org/10.5281/zenodo.21872890> (Jeske et al., 2026b) and <https://github.com/a-jeske/MCTS> (Commit 5a68b63, last accessed: 10.08.2026). The input data and the MCTS output can be found here <https://doi.org/10.5281/zenodo.21869008> (Jeske et al., 2026a). The SEAC⁴RS data is published under <https://www-air.larc.nasa.gov/cgi-bin/ArcView/seac4rs> (last accessed: 18.05.2026) and <https://doi.org/10.5067/AIRCRAFT/SEAC4RS/AEROSOL-TRACEGAS-CLOUD> (Toon et al., 2014). For the WRF-Chem output, please see Cuchiara et al. (2020).

The Modular Earth Submodel System (MESSy) is being continuously further developed and applied by a consortium of institutions. The usage of MESSy and access to the source code is licenced to all affiliates of institutions who are members of the MESSy Consortium. Institutions can become a member of the MESSy Consortium by signing the MESSy Memorandum of Understanding. More information can be found on the MESSy Consortium website (<http://www.messy-interface.org>, last accessed: 10.08.2026).

Author contributions. AJ and HT designed the study with contributions from MCB. AJ and HT developed MCTS and HR contributed to achieving a better computational performance and smaller compilation times. MCB and GC provided the WRF-Chem and DC-8 data. JMM and HT contributed to the EMAC simulations performed by AJ. AJ carried out the MCTS simulations in consultation with HT. With contributions from all authors, AJ analysed and wrote the manuscripts.

Competing interests. At least one of the (co-)authors is a member of the editorial board of Geoscientific Model Development.



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770 References

- Apel, E. C., Olson, J. R., Crawford, J. H., Hornbrook, R. S., Hills, A. J., Cantrell, C. A., Emmons, L. K., Knapp, D. J., Hall, S., Mauldin III, R. L., Weinheimer, A. J., Fried, A., Blake, D. R., Crounse, J. D., Clair, J. M. S., Wennberg, P. O., Diskin, G. S., Fuelberg, H. E., Wisthaler, A., Mikoviny, T., Brune, W., and Riener, D. D.: Impact of the deep convection of isoprene and other reactive trace species on radicals and ozone in the upper troposphere, *Atmospheric Chemistry and Physics*, 12, 1135–1150, <https://doi.org/10.5194/acp-12-1135-2012>, 2012.
- 775 Baboolal, L. B., Pruppacher, H. R., and Topalian, J. H.: A Sensitivity Study of a Theoretical Model Of SO₂ Scavenging by Water Drops in Air, *Journal of Atmospheric Sciences*, 38, 856 – 870, [https://doi.org/10.1175/1520-0469\(1981\)038<0856:ASSOAT>2.0.CO;2](https://doi.org/10.1175/1520-0469(1981)038<0856:ASSOAT>2.0.CO;2), 1981.
- Bardakov, R., Riipinen, I., Krejci, R., Savre, J., Thornton, J. A., and Ekman, A. M. L.: A Novel Framework to Study Trace Gas Transport in Deep Convective Clouds, *Journal of Advances in Modeling Earth Systems*, 12, e2019MS001 931, <https://doi.org/10.1029/2019MS001931>, 2020.
- 780 Bardakov, R., Thornton, J. A., Riipinen, I., Krejci, R., and Ekman, A. M. L.: Transport and chemistry of isoprene and its oxidation products in deep convective clouds, *Tellus B: Chemical and Physical Meteorology*, 73, 1–21, <https://doi.org/10.1080/16000889.2021.1979856>, 2021.
- Bardakov, R., Krejci, R., Riipinen, I., and Ekman, A. M. L.: The Role of Convective Up- and Downdrafts in the Transport of Trace Gases in the Amazon, *Journal of Geophysical Research: Atmospheres*, 127, e2022JD037 265, <https://doi.org/10.1029/2022JD037265>, 2022.
- Bardakov, R., Thornton, J. A., Ekman, A. M. L., Krejci, R., Pöhlker, M. L., Curtius, J., Williams, J., Lelieveld, J., and Riipinen, I.: High Con-
 785 centrations of Nanoparticles From Isoprene Nitrates Predicted in Convective Outflow Over the Amazon, *Geophysical Research Letters*, 51, e2024GL109 919, <https://doi.org/10.1029/2024GL109919>, 2024.
- Barth, M. C., Kim, S.-W., Wang, C., Pickering, K. E., Ott, L. E., Stenchikov, G., Leriche, M., Cautenet, S., Pinty, J.-P., Barthe, C., Mari, C., Helsdon, J. H., Farley, R. D., Fridlind, A. M., Ackerman, A. S., Spiridonov, V., and Telenta, B.: Cloud-scale model intercomparison of chemical constituent transport in deep convection, *Atmospheric Chemistry and Physics*, 7, 4709–4731, <https://doi.org/10.5194/acp-7-4709-2007>, 2007.
- 790 Barth, M. C., Cantrell, C. A., Brune, W. H., Rutledge, S. A., Crawford, J. H., Huntrieser, H., Carey, L. D., MacGorman, D., Weisman, M., Pickering, K. E., Bruning, E., Anderson, B., Apel, E., Biggerstaff, M., Campos, T., Campuzano-Jost, P., Cohen, R., Crounse, J., Day, D. A., Diskin, G., Flocke, F., Fried, A., Garland, C., Heikes, B., Honomichl, S., Hornbrook, R., Huey, L. G., Jimenez, J. L., Lang, T., Lichtenstern, M., Mikoviny, T., Nault, B., O’Sullivan, D., Pan, L. L., Peischl, J., Pollack, I., Richter, D., Riener, D., Ryerson, T.,
 795 Schlager, H., Clair, J. S., Walega, J., Weibring, P., Weinheimer, A., Wennberg, P., Wisthaler, A., Wooldridge, P. J., and Ziegler, C.: The Deep Convective Clouds and Chemistry (DC3) Field Campaign, *Bulletin of the American Meteorological Society*, 96, 1281 – 1309, <https://doi.org/10.1175/BAMS-D-13-00290.1>, 2015.
- Barth, M. C., Bela, M. M., Fried, A., Wennberg, P. O., Crounse, J. D., St. Clair, J. M., Blake, N. J., Blake, D. R., Homeyer, C. R., Brune, W. H., Zhang, L., Mao, J., Ren, X., Ryerson, T. B., Pollack, I. B., Peischl, J., Cohen, R. C., Nault, B. A., Huey, L. G., Liu, X., and
 800 Cantrell, C. A.: Convective transport and scavenging of peroxides by thunderstorms observed over the central U.S. during DC3, *Journal of Geophysical Research: Atmospheres*, 121, 4272–4295, <https://doi.org/https://doi.org/10.1002/2015JD024570>, 2016.
- Barth, M. C., Ervens, B., Herrmann, H., Tilgner, A., McNeill, V. F., Tsui, W. G., Deguillaume, L., Chaumerliac, N., Carlton, A., and Lance, S. M.: Box Model Intercomparison of Cloud Chemistry, *Journal of Geophysical Research: Atmospheres*, 126, e2021JD035 486, <https://doi.org/10.1029/2021JD035486>, 2021.



- 805 Barth, M. C., Campuzano-Jost, P., Cuchiara, G., Parottil, A., Jimenez, J. L., Hilario, M. R. A., Lorenzo, G. R., and Sorooshian, A.: Aerosol Scavenging in DC3 and SEAC⁴RS Deep Convective Storms, *EGUsphere*, 2026, 1–32, <https://doi.org/10.5194/egusphere-2025-6552>, preprint, 2026.
- Bechara, J., Borbon, A., Jambert, C., Colomb, A., and Perros, P. E.: Evidence of the impact of deep convection on reactive Volatile Organic Compounds in the upper tropical troposphere during the AMMA experiment in West Africa, *Atmospheric Chemistry and Physics*, 10, 10 321–10 334, <https://doi.org/10.5194/acp-10-10321-2010>, 2010.
- 810 Bela, M. M., Barth, M. C., Toon, O. B., Fried, A., Homeyer, C. R., Morrison, H., Cummings, K. A., Li, Y., Pickering, K. E., Allen, D. J., Yang, Q., Wennberg, P. O., Crounse, J. D., St. Clair, J. M., Teng, A. P., O’Sullivan, D., Huey, L. G., Chen, D., Liu, X., Blake, D. R., Blake, N. J., Apel, E. C., Hornbrook, R. S., Flocke, F., Campos, T., and Diskin, G.: Wet scavenging of soluble gases in DC3 deep convective storms using WRF-Chem simulations and aircraft observations, *Journal of Geophysical Research: Atmospheres*, 121, 4233–4257, <https://doi.org/10.1002/2015JD024623>, 2016.
- 815 Bela, M. M., Barth, M. C., Toon, O. B., Fried, A., Ziegler, C., Cummings, K. A., Li, Y., Pickering, K. E., Homeyer, C. R., Morrison, H., Yang, Q., Mecikalski, R. M., Carey, L., Biggerstaff, M. I., Betten, D. P., and Alford, A. A.: Effects of Scavenging, Entrainment, and Aqueous Chemistry on Peroxides and Formaldehyde in Deep Convective Outflow Over the Central and Southeast United States, *Journal of Geophysical Research: Atmospheres*, 123, 7594–7614, <https://doi.org/10.1029/2018JD028271>, 2018.
- 820 Borbon, A., Ruiz, M., Bechara, J., Aumont, B., Chong, M., Huntrieser, H., Mari, C., Reeves, C. E., Scialom, G., Hamburger, T., Stark, H., Afif, C., Jambert, C., Mills, G., Schlager, H., and Perros, P. E.: Transport and chemistry of formaldehyde by mesoscale convective systems in West Africa during AMMA 2006, *Journal of Geophysical Research: Atmospheres*, 117, <https://doi.org/https://doi.org/10.1029/2011JD017121>, 2012.
- Borchers, C., Seymore, J., Gautam, M., Dörholt, K., Müller, Y., Arndt, A., Gömmers, L., Ungeheuer, F., Szakáll, M., Borrmann, S., Theis, A., Vogel, A. L., and Hoffmann, T.: Retention of α -pinene oxidation products and nitro-aromatic compounds during riming, *Atmospheric Chemistry and Physics*, 24, 13 961–13 974, <https://doi.org/10.5194/acp-24-13961-2024>, 2024.
- 825 Bozem, H., Pozzer, A., Harder, H., Martinez, M., Williams, J., Lelieveld, J., and Fischer, H.: The influence of deep convection on HCHO and H₂O₂ in the upper troposphere over Europe, *Atmospheric Chemistry and Physics*, 17, 11 835–11 848, <https://doi.org/10.5194/acp-17-11835-2017>, 2017.
- 830 Bozem, H., Joppe, P., Li, Y., Emig, N., Afchine, A., Breuninger, A., Curtius, J., Hofmann, S., Ismayil, S., Kandler, K., Kunkel, D., Kutschka, A., Lachnitt, H.-C., Petzold, A., Richter, S., Rösenthaller, T., Rolf, C., Schneider, L., Schneider, J., Vogel, A., and Hoor, P.: The TropoPause Composition TOWed Sensor Shuttle (TPC-TOSS): a new airborne dual platform approach for atmospheric composition measurements at the tropopause, *Atmospheric Measurement Techniques*, 18, 6545–6568, <https://doi.org/10.5194/amt-18-6545-2025>, 2025.
- Brinkop, S. and Jöckel, P.: ATTILA 4.0: Lagrangian advective and convective transport of passive tracers within the ECHAM5/MESSy (2.53.0) chemistry–climate model, *Geoscientific Model Development*, 12, 1991–2008, <https://doi.org/10.5194/gmd-12-1991-2019>, 2019.
- 835 Cho, H. R., Niewiadomski, M., Iribarne, J. V., and Melo, O.: A model of the effect of cumulus clouds on the re-distribution and transformation of pollutants, *Journal of Geophysical Research: Atmospheres*, 94, 12 895–12 910, <https://doi.org/https://doi.org/10.1029/JD094iD10p12895>, 1989.
- 840 Croft, B., Pierce, J. R., Martin, R. V., Hoose, C., and Lohmann, U.: Uncertainty associated with convective wet removal of entrained aerosols in a global climate model, *Atmospheric Chemistry and Physics*, 12, 10 725–10 748, <https://doi.org/10.5194/acp-12-10725-2012>, 2012.



- Cuchiara, G. C., Fried, A., Barth, M. C., Bela, M., Homeyer, C. R., Gaubert, B., Walega, J., Weibring, P., Richter, D., Wennberg, P., Crounse, J., Kim, M., Diskin, G., Hanisco, T. F., Wolfe, G. M., Beyersdorf, A., Peischl, J., Pollack, I. B., St. Clair, J. M., Woods, S., Tanelli, S., Bui, T. V., Dean-Day, J., Huey, L. G., and Heath, N.: Vertical Transport, Entrainment, and Scavenging Processes Affecting Trace Gases in a Modeled and Observed SEAC4RS Case Study, *Journal of Geophysical Research: Atmospheres*, 125, e2019JD031957, <https://doi.org/10.1029/2019JD031957>, 2020.
- Cuchiara, G. C., Fried, A., Barth, M. C., Bela, M. M., Homeyer, C. R., Walega, J., Weibring, P., Richter, D., Woods, S., Beyersdorf, A., Bui, T. V., and Dean-Day, J.: Effect of Marine and Land Convection on Wet Scavenging of Ozone Precursors Observed During a SEAC4RS Case Study, *Journal of Geophysical Research: Atmospheres*, 128, e2022JD037107, <https://doi.org/10.1029/2022JD037107>, 2023.
- Curtius, J., Heinritzi, M., Beck, L. J., Pöhlker, M. L., Tripathi, N., Krumm, B. E., Holzbeck, P., Nussbaumer, C. M., Hernández Pardo, L., Klimach, T., et al.: Isoprene nitrates drive new particle formation in Amazon's upper troposphere, *Nature*, 636, 124–130, <https://doi.org/10.1038/s41586-024-08192-4>, 2024.
- Daescu, D. N., Sandu, A., and Carmichael, G. R.: Direct and adjoint sensitivity analysis of chemical kinetic systems with KPP: II—numerical validation and applications, *Atmospheric Environment*, 37, 5097–5114, <https://doi.org/10.1016/j.atmosenv.2003.08.020>, 2003.
- Damian, V., Sandu, A., Damian, M., Potra, F., and Carmichael, G. R.: The kinetic preprocessor KPP—a software environment for solving chemical kinetics, *Computers & Chemical Engineering*, 26, 1567–1579, [https://doi.org/10.1016/S0098-1354\(02\)00128-X](https://doi.org/10.1016/S0098-1354(02)00128-X), 2002.
- Desouza, N. D.: Trace Gas Pollutants Led to New Particle Formation and a Strong Convective System Over Telangana, India, *National Academy Science Letters*, 46, 239–243, <https://doi.org/10.1007/s40009-023-01221-2>, 2023.
- Dickerson, R. R., Huffman, G. J., Luke, W. T., Nunnermacker, L. J., Pickering, K. E., Leslie, A. C. D., Lindsey, C. G., Slinn, W. G. N., Kelly, T. J., Daum, P. H., Delany, A. C., Greenberg, J. P., Zimmerman, P. R., Boatman, J. F., Ray, J. D., and Stedman, D. H.: Thunderstorms: An Important Mechanism in the Transport of Air Pollutants, *Science*, 235, 460–465, <https://doi.org/10.1126/science.235.4787.460>, 1987.
- Doherty, R. M., Stevenson, D. S., Collins, W. J., and Sanderson, M. G.: Influence of convective transport on tropospheric ozone and its precursors in a chemistry-climate model, *Atmospheric Chemistry and Physics*, 5, 3205–3218, <https://doi.org/10.5194/acp-5-3205-2005>, 2005.
- Dreger, R., Kirfel, T., Pozzer, A., Rosanka, S., Sander, R., and Taraborrelli, D.: Optimized step size control within the Rosenbrock solvers for stiff chemical ordinary differential equation systems in KPP version 2.2.3_rs4, *Geoscientific Model Development*, 18, 4273–4291, <https://doi.org/10.5194/gmd-18-4273-2025>, 2025.
- Fast, J. D., Gustafson Jr., W. I., Easter, R. C., Zaveri, R. A., Barnard, J. C., Chapman, E. G., Grell, G. A., and Peckham, S. E.: Evolution of ozone, particulates, and aerosol direct radiative forcing in the vicinity of Houston using a fully coupled meteorology-chemistry-aerosol model, *Journal of Geophysical Research: Atmospheres*, 111, <https://doi.org/https://doi.org/10.1029/2005JD006721>, 2006.
- Feichter, J. and Crutzen, P. J.: Parameterization of vertical tracer transport due to deep cumulus convection in a global transport model and its evaluation with 222Radon measurements, *Tellus B*, 42, 100–117, <https://doi.org/10.1034/j.1600-0889.1990.00011.x>, 1990.
- Frey, W., Schofield, R., Hoor, P., Kunkel, D., Ravegnani, F., Ulanovsky, A., Viciani, S., D'Amato, F., and Lane, T. P.: The impact of overshooting deep convection on local transport and mixing in the tropical upper troposphere/lower stratosphere (UTLS), *Atmospheric Chemistry and Physics*, 15, 6467–6486, <https://doi.org/10.5194/acp-15-6467-2015>, 2015.
- Fried, A., Barth, M., Bela, M., Weibring, P., Richter, D., Walega, J., Li, Y., Pickering, K., Apel, E., Hornbrook, R., Hills, A., Riemer, D. D., Blake, N., Blake, D., Schroeder, J. R., Luo, Z. J., Crawford, J. H., Olson, J., Rutledge, S., Betten, D., Biggerstaff, M. I., Diskin, G., Sachse, G., Campos, T., Flocke, F., Weinheimer, A., Cantrell, C., Pollack, I., Peischl, J., Froyd, K., Wisthaler, A., Mikoviny, T., and Woods, S.: Convective transport of formaldehyde to the upper troposphere and lower stratosphere and associated scavenging in



- 880 thunderstorms over the central United States during the 2012 DC3 study, *Journal of Geophysical Research: Atmospheres*, 121, 7430–7460, <https://doi.org/10.1002/2015JD024477>, 2016.
- Gautam, M., Theis, A., Seymore, J., Hey, M., Borrmann, S., Diehl, K., Mitra, S. K., and Szakáll, M.: Retention during freezing of raindrops – Part 1: Investigation of single and binary mixtures of nitric, formic, and acetic acids and 2-nitrophenol, *Atmospheric Chemistry and Physics*, 25, 11 813–11 828, <https://doi.org/10.5194/acp-25-11813-2025>, 2025.
- 885 Gidel, L. T.: Cumulus cloud transport of transient tracers, *Journal of Geophysical Research: Oceans*, 88, 6587–6599, <https://doi.org/10.1029/JC088iC11p06587>, 1983.
- Grell, G. A., Peckham, S. E., Schmitz, R., McKeen, S. A., Frost, G., Skamarock, W. C., and Eder, B.: Fully coupled “online” chemistry within the WRF model, *Atmospheric Environment*, 39, 6957–6975, <https://doi.org/10.1016/j.atmosenv.2005.04.027>, 2005.
- Harier, E. and Wanner, G.: Solving ordinary differential equations II: stiff and differential algebraic problems, Springer Verlag, Berlin, Heidelberg, 1 edn., 1991.
- 890 Hegglin, M. I., Brunner, D., Wernli, H., Schwierz, C., Martius, O., Hoor, P., Fischer, H., Parchatka, U., Spelten, N., Schiller, C., Krebsbach, M., Weers, U., Staehelin, J., and Peter, T.: Tracing troposphere-to-stratosphere transport above a mid-latitude deep convective system, *Atmospheric Chemistry and Physics*, 4, 741–756, <https://doi.org/10.5194/acp-4-741-2004>, 2004.
- Hobbs, P. V.: Field Studies of Cloud Chemistry and the Relative Importance of Various Mechanisms of the Incorporation of Sulfate and Nitrate into Cloud Water, in: *Chemistry of Multiphase Atmospheric Systems*, edited by Jaeschke, W., pp. 191–211, Springer Berlin Heidelberg, Berlin, Heidelberg, https://doi.org/10.1007/978-3-642-70627-1_7, 1986.
- 895 Homeyer, C. R., Pan, L. L., Dorsi, S. W., Avallone, L. M., Weinheimer, A. J., O’Brien, A. S., DiGangi, J. P., Zondlo, M. A., Ryerson, T. B., Diskin, G. S., and Campos, T. L.: Convective transport of water vapor into the lower stratosphere observed during double-tropopause events, *Journal of Geophysical Research: Atmospheres*, 119, 10,941–10,958, <https://doi.org/10.1002/2014JD021485>, 2014.
- 900 Jain, S., Jain, A. R., and Mandal, T. K.: Role of convection in hydration of tropical UTLS: implication of AURA MLS long-term observations, *Annales Geophysicae*, 31, 967–981, <https://doi.org/10.5194/angeo-31-967-2013>, 2013.
- Jeske, A. and Tost, H.: The historical climate trend resulted in changed vertical transport patterns in climate model simulations, *Atmospheric Chemistry and Physics*, 25, 14 435–14 448, <https://doi.org/10.5194/acp-25-14435-2025>, 2025.
- Jeske, A., Barth, M. C., and Cuchiara, G. C.: Input and Output data MCTS (Mainz Convective Transport and Scavenging (MCTS version 1.0) – Introduction and Evaluation of the new Column Model for Convection-Chemistry-Interactions), <https://doi.org/10.5281/zenodo.21869008>, [data set], 2026a.
- 905 Jeske, A., Tost, H., and Ranocha, H.: Mainz Convective Transport and Scavenging model code, <https://doi.org/10.5281/zenodo.21872890>, [code], 2026b.
- Jöckel, P., Sander, R., Kerkweg, A., Tost, H., and Lelieveld, J.: Technical Note: The Modular Earth Submodel System (MESSy) - a new approach towards Earth System Modeling, *Atmospheric Chemistry and Physics*, 5, 433–444, <https://doi.org/10.5194/acp-5-433-2005>, 2005.
- 910 Jöckel, P., Tost, H., Pozzer, A., Brühl, C., Buchholz, J., Ganzeveld, L., Hoor, P., Kerkweg, A., Lawrence, M. G., Sander, R., Steil, B., Stiller, G., Tanarhte, M., Taraborrelli, D., van Aardenne, J., and Lelieveld, J.: The atmospheric chemistry general circulation model ECHAM5/MESSy1: consistent simulation of ozone from the surface to the mesosphere, *Atmospheric Chemistry and Physics*, 6, 5067–5104, <https://doi.org/10.5194/acp-6-5067-2006>, 2006.



- Jöckel, P., Kerkweg, A., Pozzer, A., Sander, R., Tost, H., Riede, H., Baumgaertner, A., Gromov, S., and Kern, B.: Development cycle 2 of the Modular Earth Submodel System (MESSy2), *Geoscientific Model Development*, 3, 717–752, <https://doi.org/10.5194/gmd-3-717-2010>, 2010.
- Jöckel, P., Tost, H., Pozzer, A., Kunze, M., Kirner, O., Brenninkmeijer, C. A. M., Brinkop, S., Cai, D. S., Dyroff, C., Eckstein, J., Frank, F., Garny, H., Gottschaldt, K.-D., Graf, P., Grewe, V., Kerkweg, A., Kern, B., Matthes, S., Mertens, M., Meul, S., Neumaier, M., Nützel, M., Oberländer-Hayn, S., Ruhnke, R., Runde, T., Sander, R., Scharffe, D., and Zahn, A.: Earth System Chemistry integrated Modelling (ESCiMo) with the Modular Earth Submodel System (MESSy) version 2.51, *Geoscientific Model Development*, 9, 1153–1200, <https://doi.org/10.5194/gmd-9-1153-2016>, 2016.
- Jost, A., Szakáll, M., Diehl, K., Mitra, S. K., and Borrmann, S.: Chemistry of riming: the retention of organic and inorganic atmospheric trace constituents, *Atmospheric Chemistry and Physics*, 17, 9717–9732, <https://doi.org/10.5194/acp-17-9717-2017>, 2017.
- Konjari, P., Rolf, C., Krämer, M., Afchine, A., Spelten, N., Bartolome Garcia, I., Miltenberger, A., Emig, N., Joppe, P., Schneider, J., Li, Y., Petzold, A., Bozem, H., and Hoor, P.: Stratospheric hydration and ice microphysics of a convective overshoot observed during the TPEx campaign over Sweden, *Atmospheric Chemistry and Physics*, 25, 18 031–18 050, <https://doi.org/10.5194/acp-25-18031-2025>, 2025.
- Lawrence, M. G. and Rasch, P. J.: Tracer Transport in Deep Convective Updrafts: Plume Ensemble versus Bulk Formulations, *Journal of the Atmospheric Sciences*, 62, 2880 – 2894, <https://doi.org/10.1175/JAS3505.1>, 2005.
- Lawrence, M. G., von Kuhlmann, R., Salzmann, M., and Rasch, P. J.: The balance of effects of deep convective mixing on tropospheric ozone, *Geophysical Research Letters*, 30, <https://doi.org/10.1029/2003GL017644>, 2003.
- Lebo, Z. J. and Seinfeld, J. H.: Theoretical basis for convective invigoration due to increased aerosol concentration, *Atmospheric Chemistry and Physics*, 11, 5407–5429, <https://doi.org/10.5194/acp-11-5407-2011>, 2011.
- Leriche, M., Voisin, D., Chaumerliac, N., Monod, A., and Aumont, B.: A model for tropospheric multiphase chemistry: application to one cloudy event during the CIME experiment, *Atmospheric Environment*, 34, 5015–5036, [https://doi.org/10.1016/S1352-2310\(00\)00329-0](https://doi.org/10.1016/S1352-2310(00)00329-0), sixth Scientific Conference of the International Global Atmospheric, 2000.
- Leriche, M., Pinty, J.-P., Mari, C., and Gazen, D.: A cloud chemistry module for the 3-D cloud-resolving mesoscale model Meso-NH with application to idealized cases, *Geoscientific Model Development*, 6, 1275–1298, <https://doi.org/10.5194/gmd-6-1275-2013>, 2013.
- Li, Y., Pickering, K. E., Allen, D. J., Barth, M. C., Bela, M. M., Cummings, K. A., Carey, L. D., Mecikalski, R. M., Fierro, A. O., Campos, T. L., Weinheimer, A. J., Diskin, G. S., and Biggerstaff, M. I.: Evaluation of deep convective transport in storms from different convective regimes during the DC3 field campaign using WRF-Chem with lightning data assimilation, *Journal of Geophysical Research: Atmospheres*, 122, 7140–7163, <https://doi.org/10.1002/2017JD026461>, 2017.
- Li, Y., Pickering, K. E., Barth, M. C., Bela, M. M., Cummings, K. A., and Allen, D. J.: Evaluation of Parameterized Convective Transport of Trace Gases in Simulation of Storms Observed During the DC3 Field Campaign, *Journal of Geophysical Research: Atmospheres*, 123, 11,238–11,261, <https://doi.org/10.1029/2018JD028779>, 2018.
- Li, Y., Pickering, K. E., Barth, M. C., Bela, M. M., Cummings, K. A., and Allen, D. J.: Wet Scavenging in WRF-Chem Simulations of Parameterized Convection for a Severe Storm During the DC3 Field Campaign, *Journal of Geophysical Research: Atmospheres*, 124, 7413–7428, <https://doi.org/10.1029/2019JD030484>, 2019.
- Lohmann, U.: Global anthropogenic aerosol effects on convective clouds in ECHAM5-HAM, *Atmospheric Chemistry and Physics*, 8, 2115–2131, <https://doi.org/10.5194/acp-8-2115-2008>, 2008.



- Luo, Z., Kley, D., Johnson, R. H., and Smit, H.: Ten Years of Measurements of Tropical Upper-Tropospheric Water Vapor by MOZAIC. Part I: Climatology, Variability, Transport, and Relation to Deep Convection, *Journal of Climate*, 20, 418 – 435, <https://doi.org/10.1175/JCLI3997.1>, 2007.
- 955 Mahowald, N. M., Rasch, P. J., and Prinn, R. G.: Cumulus parameterizations in chemical transport models, *Journal of Geophysical Research: Atmospheres*, 100, 26 173–26 189, <https://doi.org/10.1029/95JD02606>, 1995.
- Mahowald, N. M., Rasch, P. J., Eaton, B. E., Whittlestone, S., and Prinn, R. G.: Transport of 222radon to the remote troposphere using the Model of Atmospheric Transport and Chemistry and assimilated winds from ECMWF and the National Center for Environmental Prediction/NCAR, *Journal of Geophysical Research: Atmospheres*, 102, 28 139–28 151, <https://doi.org/10.1029/97JD02084>, 1997.
- 960 Mari, C., Jacob, D. J., and Bechtold, P.: Transport and scavenging of soluble gases in a deep convective cloud, *Journal of Geophysical Research: Atmospheres*, 105, 22 255–22 267, <https://doi.org/10.1029/2000JD900211>, 2000.
- Nordeng, T.-E.: Extended versions of the convective parametrization scheme at ECMWF and their impact on the mean and transient activity of the model in the tropics, *ECMWF Technical Memoranda*, pp. 1–41, <https://doi.org/10.21957/e34xwhysw>, 1994.
- Ouwensloot, H. G., Pozzer, A., Steil, B., Tost, H., and Lelieveld, J.: Revision of the convective transport module CVTRANS 2.4 in the EMAC atmospheric chemistry–climate model, *Geoscientific Model Development*, 8, 2435–2445, <https://doi.org/10.5194/gmd-8-2435-2015>, 2015.
- 965 Prather, M. J. and Jacob, D. J.: A persistent imbalance in HO_x and NO_x photochemistry of the upper troposphere driven by deep tropical convection, *Geophysical Research Letters*, 24, 3189–3192, <https://doi.org/10.1029/97GL03027>, 1997.
- Ray, E. A., Rosenlof, K. H., Richard, E. C., Hudson, P. K., Cziczo, D. J., Loewenstein, M., Jost, H.-J., Lopez, J., Ridley, B., Weinheimer, A., Montzka, D., Knapp, D., Wofsy, S. C., Daube, B. C., Gerbig, C., Xueref, I., and Herman, R. L.: Evidence of the effect of summer-time midlatitude convection on the subtropical lower stratosphere from CRYSTAL-FACE tracer measurements, *Journal of Geophysical Research: Atmospheres*, 109, <https://doi.org/10.1029/2004JD004655>, 2004.
- 970 Redelsperger, J.-L., Thorncroft, C. D., Diedhiou, A., Lebel, T., Parker, D. J., and Polcher, J.: African Monsoon Multidisciplinary Analysis: An International Research Project and Field Campaign, *Bulletin of the American Meteorological Society*, 87, 1739 – 1746, <https://doi.org/10.1175/BAMS-87-12-1739>, 2006.
- 975 Riese, M., Ploeger, F., Rap, A., Vogel, B., Konopka, P., Dameris, M., and Forster, P.: Impact of uncertainties in atmospheric mixing on simulated UTLS composition and related radiative effects, *Journal of Geophysical Research: Atmospheres*, 117, D16 305, <https://doi.org/10.1029/2012JD017751>, 2012.
- Roeckner, E., Brokopf, R., Esch, M., Giorgetta, M., Hagemann, S., Kornbluh, L., Manzini, E., Schlese, U., and Schulzweida, U.: Sensitivity of Simulated Climate to Horizontal and Vertical Resolution in the ECHAM5 Atmosphere Model, *Journal of Climate*, 19, 3771 – 3791, <https://doi.org/10.1175/JCLI3824.1>, 2006.
- 980 Sander, R.: Modeling atmospheric chemistry: Interactions between gas-phase species and liquid cloud/aerosol particles, *Surveys in Geophysics*, 20, 1–31, <https://doi.org/10.1023/A:1006501706704>, 1999.
- Sander, R., Baumgaertner, A., Cabrera-Perez, D., Frank, F., Gromov, S., Grooß, J.-U., Harder, H., Huijnen, V., Jöckel, P., Karydis, V. A., Niemeyer, K. E., Pozzer, A., Riede, H., Schultz, M. G., Taraborrelli, D., and Tauer, S.: The community atmospheric chemistry box model CAABA/MECCA-4.0, *Geoscientific Model Development*, 12, 1365–1385, <https://doi.org/10.5194/gmd-12-1365-2019>, 2019.
- 985 Sandu, A., Daescu, D. N., and Carmichael, G. R.: Direct and adjoint sensitivity analysis of chemical kinetic systems with KPP: Part I—theory and software tools, *Atmospheric Environment*, 37, 5083–5096, <https://doi.org/10.1016/j.atmosenv.2003.08.019>, 2003.



- Sassi, F., Salby, M., and Read, W. G.: Relationship between upper tropospheric humidity and deep convection, *Journal of Geophysical Research: Atmospheres*, 106, 17 133–17 146, <https://doi.org/10.1029/2001JD900121>, 2001.
- Schwartz, S. E.: Mass-Transport Considerations Pertinent to Aqueous Phase Reactions of Gases in Liquid-Water Clouds, in: *Chemistry of Multiphase Atmospheric Systems*, edited by Jaeschke, W., pp. 415–471, Springer Berlin Heidelberg, Berlin, Heidelberg, https://doi.org/https://doi.org/10.1007/978-3-642-70627-1_16, 1986.
- Seymore, J., Szakáll, M., Theis, A., Mitra, S. K., Borchers, C., and Hoffmann, T.: Volume uptake of carbonyls during diffusional ice crystal growth, *Atmospheric Chemistry and Physics*, 25, 18 249–18 265, <https://doi.org/10.5194/acp-25-18249-2025>, 2025.
- Singh, P. and Ahrens, B.: Lightning-intense deep convective transport of water vapour into the UTLS over the Third Pole region, *Atmospheric Chemistry and Physics*, 25, 17 869–17 888, <https://doi.org/10.5194/acp-25-17869-2025>, 2025.
- Sophocleous, K., Kirfel, T., Taraborrelli, D., and Christoudias, T.: GPU-accelerated atmospheric chemical kinetics using single precision in the ECHAM/MESSy (EMAC) model v2.55 with MEDINA v2.0, *EGUsphere [preprint]*, 2026, 1–19, <https://doi.org/10.5194/egusphere-2026-2389>, 2026.
- Strand, A. and Hov, Ø.: A two-dimensional zonally averaged transport model including convective motions and a new strategy for the numerical solution, *Journal of Geophysical Research: Atmospheres*, 98, 9023–9037, <https://doi.org/10.1029/93JD00201>, 1993.
- Tiedtke, M.: A Comprehensive Mass Flux Scheme for Cumulus Parameterization in Large-Scale Models, *Monthly Weather Review*, 117, 1779 – 1800, [https://doi.org/10.1175/1520-0493\(1989\)117<1779:ACMFSF>2.0.CO;2](https://doi.org/10.1175/1520-0493(1989)117<1779:ACMFSF>2.0.CO;2), 1989.
- Tilgner, A., Schaefer, T., Alexander, B., Barth, M., Collett Jr., J. L., Fahey, K. M., Nenes, A., Pye, H. O. T., Herrmann, H., and McNeill, V. F.: Acidity and the multiphase chemistry of atmospheric aqueous particles and clouds, *Atmospheric Chemistry and Physics*, 21, 13 483–13 536, <https://doi.org/10.5194/acp-21-13483-2021>, 2021.
- Tinney, E. N. and Homeyer, C. R.: A 13-year Trajectory-Based Analysis of Convection-Driven Changes in Upper Troposphere Lower Stratosphere Composition Over the United States, *Journal of Geophysical Research: Atmospheres*, 126, e2020JD033 657, <https://doi.org/10.1029/2020JD033657>, 2021.
- Toon, B., Jensen, E., Ferrare, R. A., Singh, H., Dibb, J., Anderson, B., Anderson, J. G., Atlas, E., Bedka, K., Beyersdorf, A., Blake, D., Brock, C., Bucholtz, A., Bui, T. P., Cairns, B., Christensen, L., Cohen, R., da Silva, A., Diskin, G. S., ..., and Yang, M.: SEAC4RS Field Campaign Data - W [Dataset], <https://doi.org/10.5067/AIRCRAFT/SEAC4RS/AEROSOL-TRACEGAS-CLOUD>, 2014.
- Toon, O. B., Maring, H., Dibb, J., Ferrare, R., Jacob, D. J., Jensen, E. J., Luo, Z. J., Mace, G. G., Pan, L. L., Pfister, L., Rosenlof, K. H., Redemann, J., Reid, J. S., Singh, H. B., Thompson, A. M., Yokelson, R., Minnis, P., Chen, G., Jucks, K. W., and Pszenny, A.: Planning, implementation, and scientific goals of the Studies of Emissions and Atmospheric Composition, Clouds and Climate Coupling by Regional Surveys (SEAC4RS) field mission, *Journal of Geophysical Research: Atmospheres*, 121, 4967–5009, <https://doi.org/10.1002/2015JD024297>, 2016.
- Tost, H., Jöckel, P., Kerkweg, A., Sander, R., and Lelieveld, J.: Technical note: A new comprehensive SCAVenging submodel for global atmospheric chemistry modelling, *Atmospheric Chemistry and Physics*, 6, 565–574, <https://doi.org/10.5194/acp-6-565-2006>, 2006a.
- Tost, H., Jöckel, P., and Lelieveld, J.: Influence of different convection parameterisations in a GCM, *Atmospheric Chemistry and Physics*, 6, 5475–5493, <https://doi.org/10.5194/acp-6-5475-2006>, 2006b.
- Tost, H., Jöckel, P., Kerkweg, A., Pozzer, A., Sander, R., and Lelieveld, J.: Global cloud and precipitation chemistry and wet deposition: tropospheric model simulations with ECHAM5/MESSy1, *Atmospheric Chemistry and Physics*, 7, 2733–2757, <https://doi.org/10.5194/acp-7-2733-2007>, 2007.



- Tost, H., Lawrence, M. G., Brühl, C., Jöckel, P., Team, T. G., and Team, T. S.-O.-D.: Uncertainties in atmospheric chemistry modelling due to convection parameterisations and subsequent scavenging, *Atmospheric Chemistry and Physics*, 10, 1931–1951, <https://doi.org/10.5194/acp-10-1931-2010>, 2010.
- Tripathi, N., Krumm, B. E., Edtbauer, A., Ringsdorf, A., Wang, N., Kohl, M., Vella, R., Machado, L. A., Pozzer, A., Lelieveld, J., et al.:
1030 Impacts of convection, chemistry, and forest clearing on biogenic volatile organic compounds over the Amazon, *Nature Communications*, 16, 4692, <https://doi.org/10.1038/s41467-025-59953-2>, 2025.
- von Kuhlmann, R. and Lawrence, M. G.: The impact of ice uptake of nitric acid on atmospheric chemistry, *Atmospheric Chemistry and Physics*, 6, 225–235, <https://doi.org/10.5194/acp-6-225-2006>, 2006.
- von Kuhlmann, R., Lawrence, M. G., Crutzen, P. J., and Rasch, P. J.: A model for studies of tropospheric ozone and nonmethane hydrocar-
1035 bons: Model description and ozone results, *Journal of Geophysical Research: Atmospheres*, 108, <https://doi.org/10.1029/2002JD002893>, 2003.
- Wang, C.: A modeling study of the response of tropical deep convection to the increase of cloud condensation nuclei concentration: 1. Dynamics and microphysics, *Journal of Geophysical Research: Atmospheres*, 110, <https://doi.org/10.1029/2004JD005720>, 2005.