

Documentation of **M**ainz **C**onvective **T**ransport and **S**cavenging (MCTS) version 1.0

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Contents

1	Introduction	4
2	The basics	4
2.1	MCTS is designed for the use in global models	4
2.2	Input and Output	4
2.3	The idea behind MCTS	5
2.4	Reservoirs	6
3	Species	7
3.1	Insoluble tracer	7
3.2	Soluble tracers	9
4	Chemistry and scavenging	9
4.1	Liquid phase	10
4.1.1	Gas-liquid partitioning	10
4.1.2	Aqueous chemistry	13
4.2	Ice phase	15
4.2.1	Retention	15
4.2.2	Ice surface uptake	17
4.3	Precipitation	18
5	Transport	19
5.1	The transport in the gas phase	19
5.1.1	Entrainment and detrainment	21
5.1.2	The representation of the mass balancing subsidence	21
5.1.3	Grid scale ascent	23
5.2	Multiphase-transport	23
5.3	Ion transport	24
6	Time integration	24
7	Getting started with MCTS	25
7.1	The structure of MCTS	26
7.2	Closure test	26
7.3	Remark	27
8	Final remarks	27
A	Appendix	29
A.1	An overview of all transport and phase-transition reactions included in MCTS	29
A.1.1	Gas phase transport of tracers	29

A.1.2	Liquid phase processes	30
A.1.3	Ice phase processes	30
A.1.4	Ions	31

1 Introduction

Mainz Convective Transport and Scavenging (MCTS) is a single-column model to simulate the impact of convection on vertical tracer profiles. MCTS considers the convective transport and multiphase processes quasi-simultaneously. MCTS requires information about the convective system, some meteorological quantities, i.e., the temperature profile, and the background profile of the species as input. Based on this information, MCTS calculates new vertical profiles of the trace species.

A first description of a former version of MCTS (version 0) was given by Jeske (2023) in her Master’s thesis with the title “Simulationen zu konvektivem Spurenstofftransport”¹. The thesis was submitted at the Johannes Gutenberg University in 2023. The main difference between MCTS version 0 and MCTS version 1 is that version 0 did not include any processes with respect to the ice-phase scavenging.

2 The basics

In this section, the basic idea behind MCTS is introduced. The considered processes are described in the following sections.

2.1 MCTS is designed for the use in global models

MCTS is currently a stand-alone column model, but it is designed to be applied in global chemistry climate models. Therefore, the frame for MCTS is somehow constrained by the handling of convection in these models. Convection parametrisations usually make use of one column to represent the convection in global climate models (see, e.g., Tiedtke, 1989; Emanuel and Živković-Rothman, 1999; Lin et al., 2022), which cannot interact with any other processes. The convective transport and scavenging are tailored to this: (1) The processes are considered in one column and do not know about the neighbouring grid boxes. There is no horizontal exchange of species. (2) After one time step, MCTS will pretend the convective event is over, i.e., all the precipitation falls out of the column, and all cloud hydrometeors evaporate/sublimate. The species are only transferred to the next time step as gas phase compounds. We do not claim that this treatment is realistic. However, we aim to ensure that MCTS fits in the framework of MESSy (Jöckel et al., 2005), and can be used in EMAC (Jöckel et al., 2006; Jöckel et al., 2010; Jöckel et al., 2016) or other global circulation models.

2.2 Input and Output

It is necessary to provide the background profile of the species and the convective properties as input for MCTS. All required input variables are listed in Table 1. We apply output from EMAC simulations with a Tiedtke-Nordeng convection scheme (Tiedtke,

¹Translation of the title in English: “Simulations of convective tracer transport”

1989; Nordeng, 1994). Generally, it is possible to use a different convection parameterisation, another large-scale model or even convection-permitting simulations to produce a suitable input data set. It is not trivial to use measured data due to a lack of mass flux measurements within convective systems, but it is possible to replace the background species profile with observational data.

Based on these input data, MCTS calculates the redistributed vertical profiles of the trace species, i.e., the vertical tracer profiles after the passing of the convective system. It is also possible to generate the partition of species between different media (i.e., dissolved in cloud droplets, attached to the ice crystal surface, etc.). The species and processes included in MCTS are briefly described 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
Hybrid coefficients	-
Pressure	Pa
Interface pressure	Pa
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	-

2.3 The idea behind MCTS

MCTS was developed to enable the treatment of convective transport and scavenging quasi-simultaneously, and to test the influence of this approach in comparison with procedures, where transport and scavenging are considered successively. The latter is designated as the operator splitting method.

The transport equations in MCTS are represented as pseudo-chemical reactions. This means that all transport processes correspond to a loss reaction equivalent to a chemical loss process. The transport loss reaction does not produce a new species but increases the number of molecules at the destination. Figure 1 shows the transport of a species by

the updraft into the model level located above. For this illustration, it is assumed that the upward transport is so strong that it can lift 25 % of the molecules from the lower box n to the upper box $(n-1)$ within one minute. We also assume that 100 molecules are initially in the lower box and zero in the upper box $(n-1)$. After one minute, 25 molecules were taken out of the lower box and transferred to the upper box.

In this example, the two boxes have the same volume. This is not the case for typical vertical boxes in a model. Therefore, in MCTS, the concentration is considered in $\# \text{ kg}^{-1}$ and not in $\# \text{ m}^{-3}$ or $\# \text{ cm}^{-3}$. The species in EMAC, C , are in mol mol^{-1} . In MCTS, they are transformed into $\# \text{ kg}^{-1}$ (c) via

$$c = C * \frac{N_{avo}}{M_{air}}. \quad (1)$$

N_{avo} is the Avogadro constant and M_{air} the molar mass of dry air.

The amount of water in $\# \text{ kg}^{-1}$ is calculated based on the liquid water content, LWC and the density ρ of water and air.

$$c(\text{H}_2\text{O}) = LWC * \frac{\rho_{\text{water}}}{\rho_{\text{air}}} * \frac{N_{avo}}{mw(\text{H}_2\text{O})} \quad (2)$$

The value for the molar weight, mw , was taken from Wagman (1982). ρ is the density. Water is not transported in MCTS because the underlying convection scheme takes care of water in the different phases. The MCTS output is in mol mol^{-1} .

2.4 Reservoirs

The species are contained in different reservoirs:

1. The gaseous phase is associated with
 - (a) the regime of the updraft ($_{\text{up}}$),
 - (b) the downdraft regime ($_{\text{do}}$), and
 - (c) the environment ($_{\text{env}}$). (The environment is divided into sub-reservoirs (see Subsec. 5.1.2.)
2. Two reservoirs are considered for the aqueous phase, i.e.,
 - (a) the cloud droplets ($_{\text{c}}$), and
 - (b) the rain droplets ($_{\text{r}}$).
3. The ice phase is divided into four reservoirs, two for bulk ice and two for surface ice:
 - (a) The cloud bulk ice ($_{\text{i,c}}$),
 - (b) the snow/precipitating bulk ice ($_{\text{i,p}}$),

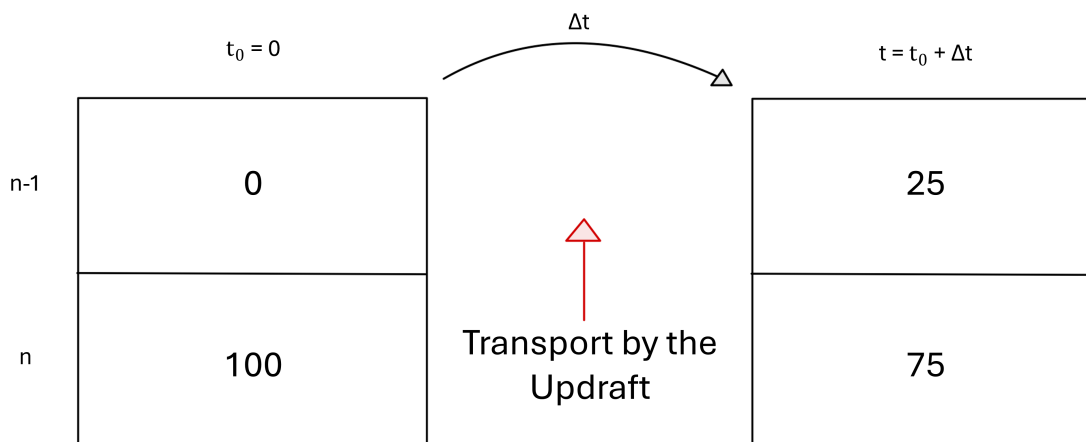


Figure 1: Simple sketch of a transport loss reaction to make the representation of the transport in MCTS clear. n is the current model level. The level above has by definition a lower model level number, i.e. is level $n-1$. 100 molecules are located in level n and 0 in level $n-1$ at the starting time. If the upward transport is transporting 0.25 molecules per minute upward. 25 molecules end up in level $n-1$, and 75 are still in level n after one minute has passed.

- (c) the cloud surface ice ($i_{c,s}$), and
- (d) the snow/precipitating surface ice ($i_{p,s}$).

Molecules can be transported/partitioned from one reservoir to another. These processes are described via a first-order loss, similar to the upward transport into the next higher level (the level with the next lower model level number and lower pressure), which is shown in Fig. 1. The processes are discussed in more detail in Sec. 4 and 5. Figure 2 illustrates most of these transitions of molecules between different reservoirs and levels (processes (1) to (23)).

3 Species

Only a limited number of species are embedded in MCTS because of the high amount of differential equations (more than 20,000) and the computational costs. Further processes can be added in the future. An overview of the considered species and processes is given in Table 2.

3.1 Insoluble tracer

Two insoluble tracers are considered to test the transport mechanism in MCTS, namely CO and C₅H₈. It is not necessary to consider these species in the multi-phase framework

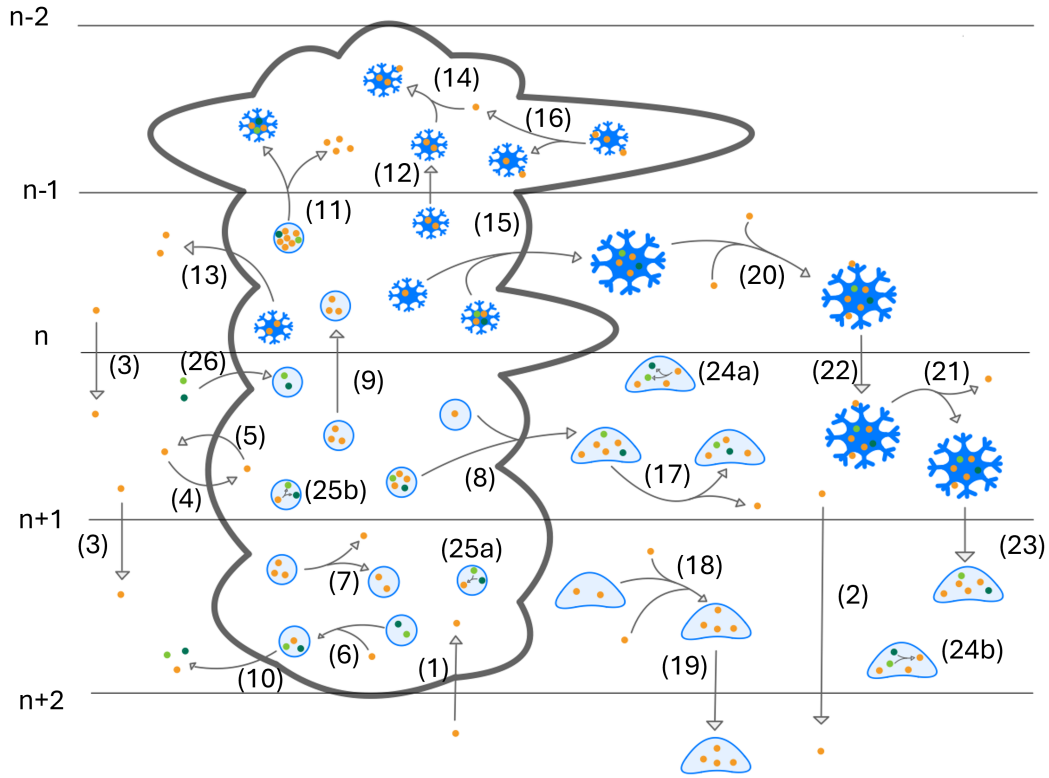


Figure 2: Sketch of most of the considered transport and transition processes in MCTS. The orange points illustrate the trace species. The different blue symbols refer to the four types of hydrometers considered in MCTS: cloud droplets, rain droplets, ice crystals/cloud ice and snow/precipitating ice. The thin black lines hint at the level structure, whereby n denotes the model level number. The processes: (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 raindrops, (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 layer, (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. The following processes for ions (green dots) are shown: (24a) and (24b) recombination and dissociation/formation of ions in rain droplets, (25a) and (25b) as (24a) (24b) but in cloud droplets and (26) entrainment of ions in the updraft in the cloud droplet reservoir.

due to their low solubility. Consequently, it could be considered to exclude them from future MCTS versions, because they introduce additional computational cost without

any benefits beyond analysis of pure vertical transport. The computational cost is especially relevant for the application of MCTS in global models.

3.2 Soluble tracers

13 soluble species are taken into account to represent a simplified aqueous chemistry. The selection of soluble tracers and the considered reactions was made according to the supplementary material to Jöckel et al. (2006) and Tost et al. (2007). The chosen species were labelled with "Scm" by Jöckel et al. (2016). HBr as well as the associated reactions, are not considered in MCTS. Tost et al. (2007) analysed the effect of using this simplified aqueous chemical mechanism in comparison to a more complex one in global model simulations. They found that SCM performed similar well as the more complex mechanism compared to observations of SO_4^{2-} , NO_3^- and NH_4^+ (Tost et al., 2007).

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. Therefore, N_2O_5 is not listed within this table.

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
CO	no	no	no	no
C_5H_8	no	no	no	no

4 Chemistry and scavenging

Gas-phase chemistry and the lightning production of NO_x are not considered in MCTS. MCTS focuses on the transport and the multiphase processes. The interactions between the (convective) cloud and the species are described in this section. Hereby, the focus

lies on the influence of hydrometeors on trace substances and the chemistry within the droplets.

4.1 Liquid phase

MCTS considers the partitioning of species between droplets (liquid phase) and the air, and the chemistry inside droplets. It is assumed that the partitioning only takes place (1) between the updraft reservoir (gas phase) and the cloud droplets (liquid phase), and (2) between the downdraft (gas phase) and the rain droplets. The downdraft does not interact with the cloud droplets, and the updraft is not in a direct exchange with the rain droplet reservoir. The cloud droplets can grow due to collision-coalescence into rain droplets. Via this process, material in the cloud droplet reservoir is transferred into the rain droplet reservoir. Consistently, aqueous chemistry is considered in the cloud and rain droplet reservoir separately.

The phase transition and the included chemistry are illustrated in Fig. 3. In the following, the gas-liquid partitioning is described in more detail, and the aqueous reactions are introduced.

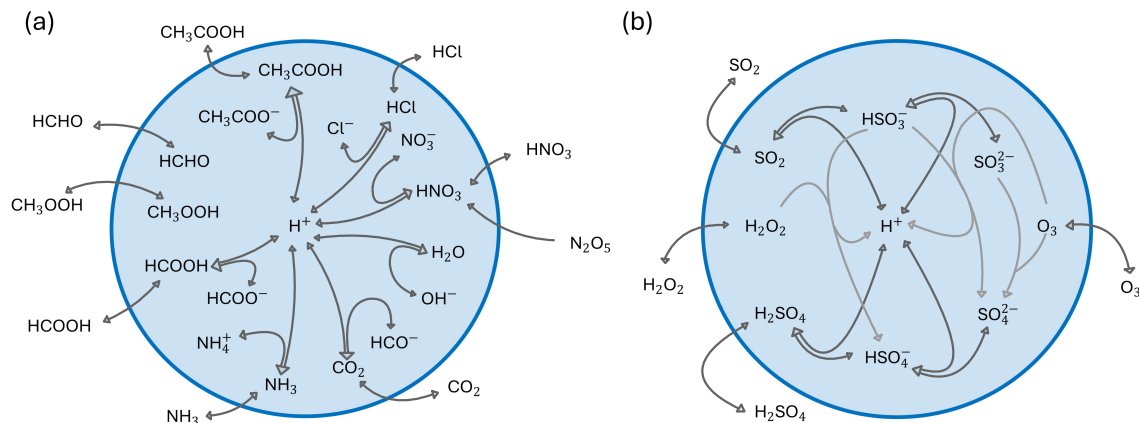


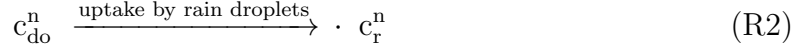
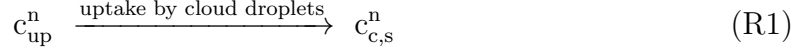
Figure 3: Sketch of the considered chemical processes and liquid-gas partitioning in MCTS. The blue circles represent droplets and the white background the surrounding air. (a) shows the partitioning and the dissociation for all species not involved in further reactions. (b) illustrates with the dark grey arrows the phase transition and the dissociation, and the light grey arrows represent the oxidations.

4.1.1 Gas-liquid partitioning

The partitioning between the droplets (cloud and rain) and the gas phase is based on SCAV developed by Tost et al. (2006). According to Sander (1999) the phase transition consists of three processes: (1) the diffusion in the gas phase (towards the droplet), (2) the transport across the droplet surface and (3) the diffusion inside the droplet. See also Schwartz (1986) for more details on the partitioning. Based on (1) and (2), the

calculation of the rates for the partition is performed in MCTS (and SCAV). As in SCAV, the last process (3) is neglected, and an instantaneous mixture in the droplets is assumed.

The uptake of the cloud and rain droplet is described by the reactions



The uptake reaction rate (k_{exf} in s^{-1}) is given by

$$k_{\text{exf},j} = k_{\text{mt},j} \times LWC_j \quad (3)$$

(Sander, 1999). Thereby, k_{mt} is the mass transfer coefficient (s^{-1}) and LWC is the liquid water content regarding the cloud water or rain water (Sander, 1999). In MCTS, the LWC is used in $\text{kg}_{\text{water}} \text{kg}_{\text{air}}^{-1}$. The suffix j can denote c for cloud droplets or r for rain droplets. The mass transfer coefficient

$$k_{\text{mt}} = \left(\frac{r^2}{3D_g} + \frac{4r}{3v\alpha} \right)^{-1} \quad (4)$$

is given by is given by via the gas-phase diffusion and the interfacial mass transfer, see eq. 69 in Sander (1999) and eq. 7.32 in Schwartz (1986). r is the droplet radius in m, D_g the gas-phase diffusivity in $\text{m}^2 \text{s}^{-1}$, v the mean molecular velocity in m s^{-1} , and α the accommodation coefficients. α is dimensionless. For further information the interested reader is referred to Schwartz (1986), Sander (1999), and Tost et al. (2006). The accommodation coefficients are given in the "Supplementary material to: Global cloud and precipitation chemistry and wet deposition: tropospheric model simulations with ECHAM5/MESSy1" (supplements to Tost et al., 2007). Most values can also be found in the mechanism used by Kerkweg et al. (2007); the values are given in the supplements called "The Chemical Equations of MECCA-AERO" by Kerkweg et al. (2007). See in both cases references therein. For CH_3COOH , the value for MCTS was taken from the mechanism Herrmann et al. (2000) used, see again also references therein. The values for N_2O_5 are estimated based on "The Chemical Equations of MECCA-AERO" by Kerkweg et al. (2007), see supplements to Kerkweg et al. (2007). A fixed radius of $20 \times 10^{-6} \text{ m}$ ($20 \mu\text{m}$) is used for the calculation of the $k_{\text{mt},c}$. For rain droplets, the calculation takes into account a droplet size spectrum. The number concentration is derived using equation (17) in Levine and Schwartz (1982), which is according to Levine and Schwartz (1982) based on the Best (1950). The mass transfer coefficient is based on Frössling (1938). Levine and Schwartz (1982) give the mass transfer coefficient $k_{\text{mt},r,j}^*$ in cm s^{-1}

$$k_{\text{mt},r,j}^* = \frac{D_g}{D_0} \left(2 + 0.6 \left(\frac{D_0 \times u}{\nu} \right)^{\frac{1}{2}} \left(\frac{\nu}{D_g} \right)^{\frac{1}{3}} \right) \quad (5)$$

with D_0 the equivalent diameter of the rain droplets, u the terminal velocity of the droplet and ν is the kinematic viscosity of the air (Levine and Schwartz, 1982). Alternatively, see also eq. 21.2-27 (p.649) by Bird et al. (1960). The Rayleigh number is used to determine the terminal velocity; it is calculated following Pruppacher and Klett (2000) (p. 417, eq. 10-145) based on Beard (1976). $k_{\text{mt},r,j}^*$ is multiplied by the number of droplets derived based on the size spectra. Afterwards, the sum is calculated over the considered radii j_r and divided by the total number of rain droplets

$$k_{\text{mt},r} = 1/N_{\text{total}} \sum_{j_r=1}^{R_r} k_{\text{mt},r,j_r}^* \times \frac{dN_{rj}}{dD_0}. \quad (6)$$

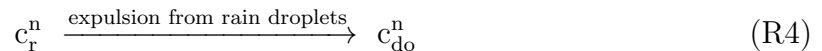
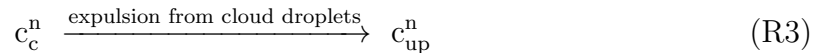
The backward reaction rate ($k_{\text{exb},j}$ in s^{-1}), i.e., for the expulsion is derived from

$$k_{\text{exb},j} = k_{\text{mt},j} \times H^{-1} \quad (7)$$

with H the (unit-less) physical Henry coefficient (Tost et al., 2006). The Henry's coefficient is derived via a van't Hoff equation

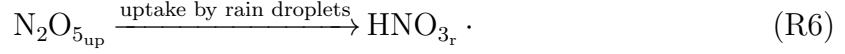
$$H = hs_0 \times \exp \left(DHT \times \left(\frac{1}{T} + \frac{1}{T_{298.15}} \right) \right) \quad (8)$$

(Sander, 1999). hs_0 is the Henry coefficient at a reference temperature of $T_{298.15} = 298.15$ K, T is the temperature in K, and DHT given by minus the enthalpy of the dissolution divided by the gas constant (Sander, 1999). The values hs_0 and DHT used in MCTS were again taken from SCAV. The values and their references are given in the "Supplementary material to: Global cloud and precipitation chemistry and wet deposition: tropospheric model simulations with ECHAM5/MESSy1", see Tost et al. (2007). They are also summarised with references in "The Chemical Equations of MECCA-AERO" by Astrid Kerkweg and Rolf Sander, 2006, which is the supplementary material by Kerkweg et al. (2007). The values for HNO_3 and HCl were taken from the supplements of Kerkweg et al. (2007). The mechanism was, at least for large parts, already used by Sander and Crutzen (1996). A comprehensive overview of literature values is given by Sander (2023). For N_2O_5 , only the forward reaction is considered, i.e. the Henry coefficient is not needed.



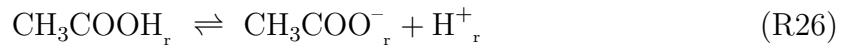
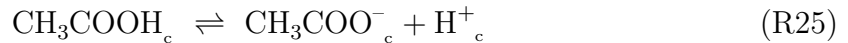
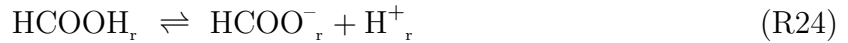
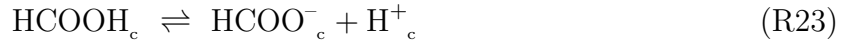
are the reaction for the backward transfer from the cloud/rain droplets to the air. Detailed information about the calculation of the partitioning rates can be found in Tost et al. (2006) and Sander (1999).

N_2O_5 is a special case. It reacts rapidly (nearly instantaneous) to HNO_3 once dissolved in water (see the SCAV mechanism supplementary to Jöckel et al., 2006). Therefore, the rates for the phase transfer are considered for the following reactions



4.1.2 Aqueous chemistry

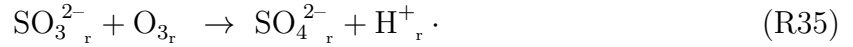
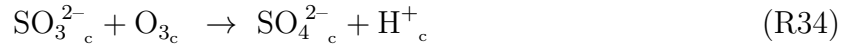
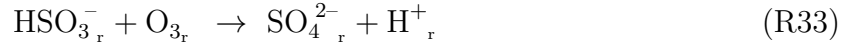
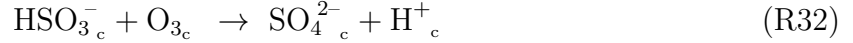
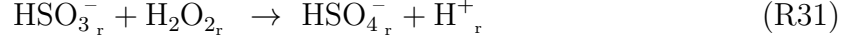
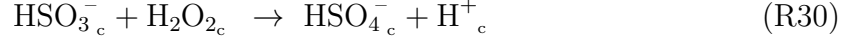
The considered aqueous chemistry is rather limited due to computational constraints. The reactions in the supplement of Jöckel et al. (2006) are implemented in MCTS except reactions including bromine. The included reactions are either dissociations and recombination of acids inside the cloud and rain droplets



(indicated by the processes (24a), (24b), (25a) and (25b) in Fig. 2), protolysis



or oxidations



The reaction rates (k) are temperature-dependent and are calculated in MCTS for nearly all reactions with the Arrhenius equation

$$k(T) = k_0 \times \exp\left(\frac{-E_a}{RT}\right) \quad (9)$$

(see for the Arrhenius equation, for example, Logan, 1982). Thereby, k_0 is the reaction rate at the reference temperature and E_a the activation energy. The in MCTS used k_0 and $\frac{-E_a}{R}$ values are given in Table 2 and 3 in "The Chemical Mechanism of SCAV" which is published supplementary to Jöckel et al., 2006.

For R 30 and 31, the ph value is considered when the reaction rate is calculated. The reaction rates are again computed with the same $k_{0,\text{HSO}_3^-+\text{H}_2\text{O}_2}$ and E_a values as in SCAV (supplements to Tost et al., 2007) applying

$$k_{\text{HSO}_3^-+\text{H}_2\text{O}_2}(T) = k_{0,\text{HSO}_3^-+\text{H}_2\text{O}_2} \times \exp\left(\frac{-E_a}{R} \left(\frac{1}{T} - 3.3540 \times 10^{-3}\right)\right) \times \frac{C_{\text{H}^+}}{C_{\text{H}^+} + 0.1} \quad (10)$$

based on Robbin Martin and Damschen (1981). C_{H^+} is the concentration of H^+ .

Using the given formalism all second order reaction rates (k) are given in $\text{cm}^3_{\text{water}} \text{mol}^{-1} \text{s}^{-1}$. A unit conversion is done for all second order reactions using

$$\tilde{k}_i = \frac{k}{N_{\text{avo}} \widetilde{LWC}_i}. \quad (11)$$

$\tilde{k}_i$ is the reaction rate in $\text{kg} \#^{-1} \text{s}^{-1}$, N_{avo} the Avogadro constant and $\widetilde{LWC}_i$ the cloud or rain water content in $\text{m}^3_{\text{water}} \text{kg}_{\text{air}}^{-1}$. The liquid water content of the rain is not an

input variable. It is calculated following eq. (17) in Kumar (1985) which is based on Mason (1957)²

A unit conversion would also be necessary for the reactions with higher orders than two; however, no such reactions are included in MCTS (yet).

4.2 Ice phase

MCTS distinguishes between bulk and surface ice. It is assumed in MCTS that the bulk ice species are locked inside the ice crystals. They do not play a role in chemical reactions and cannot leave the ice as long as the ice crystal does not melt or sublimate. The surface ice substances are located at the surface of the ice crystal or in the ice layers near the crystal’s surface. They can desorb from the surface in MCTS. In MCTS, no transfer between the surface ice and the bulk ice takes place. Therefore, the bulk ice and the surface ice are completely independent of each other and do not interact with each other. We do not claim that this is the “right” way to do it. First, the processes relevant for the species in the bulk ice are described. Afterwards, the processes affecting the surface layer take the centre stage.

4.2.1 Retention

Retention is the only process in MCTS, which can trap species in the bulk ice. The retention efficiency (RC with values between 0 and 1) describes how large the portion of material is which is contained in a freezing droplet (see among others Jost et al., 2017; Li et al., 2019). Accordingly, $1 - RC$ is the portion which is expelled out into the gas phase during the freezing process. This is illustrated by Fig. 4 and by process (11) in Fig. 2.

The following parameterisation was used for the retention coefficient

$$RC = (1 + (a/H)^b)^{-1} \quad (12)$$

with $a = 1.69 \times 10^5$ and $b = 0.26$ derived by Jost et al. (2017). This parameterisation was derived for freezing due to riming (Jost et al., 2017). MCTS itself does not distinguish between different freezing processes. Fixed retention values are used for HCl, NH₃, SO₂ and HCHO based on table 4 by Jost et al. (2017). The retention is coupled at the upward transport of cloud droplets to lower temperatures, where the droplets start freezing.

To calculate the actual retention, it is necessary to make sure that there are freezing droplets. Accordingly, two conditions must be fulfilled when the droplet is transported upward with the rate r_{up} :

²Mason (1957) refers to Best (1950) (see p.431 by Mason (1957)). The constant values to obtain the liquid water content of rain ($LWC_r = 72 \times I_r^{0.88}$) based on the rain intensity (I_r) by Kumar (1985) are the values given in Table B.1 (p.432) by Mason (1957), which were originally determined from observations by Marshall et al. (1947). The constant values can also be found in the publication by Marshall and Palmer (1948).

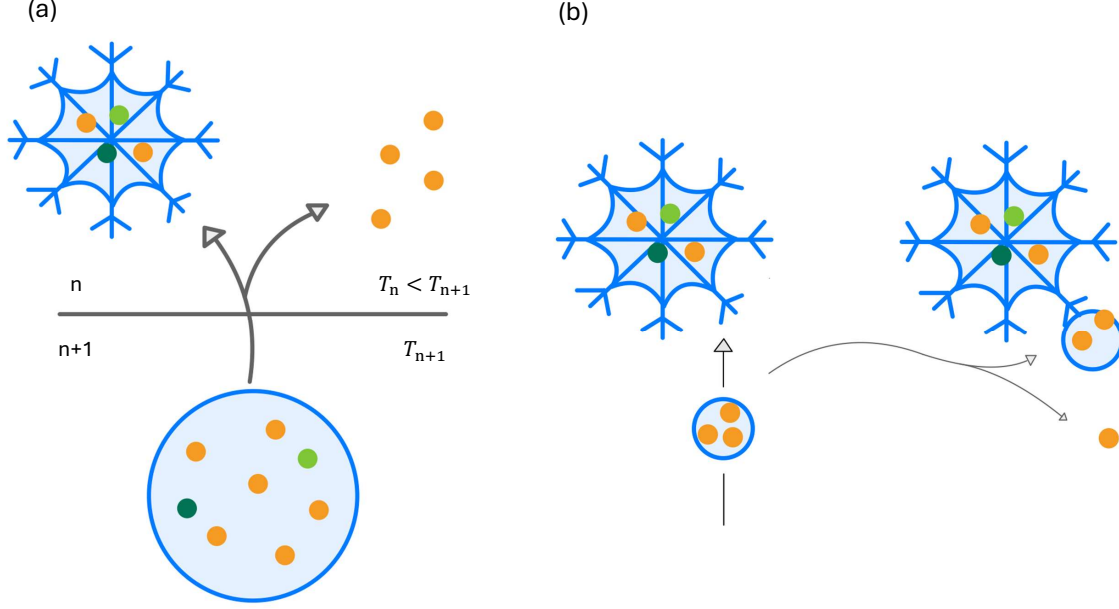


Figure 4: Retention for (a) a directly freezing cloud droplet and (b) a cloud droplet freezing via riming. The tracer molecules in the droplet either stay in the freezing droplet and are then contained in the bulk ice or are expelled in the gas phase during the freezing.

- There is ice in the level ($IWC > 0$, $SF_{\text{freezing}}^{n+1} = 1$) and
- the liquid water content needs to be reduced.

The rate for the retention ($r_{\text{up,freezing}}^{n+1}$) is then given by

$$r_{\text{up,freezing}}^{n+1} = SF_{\text{freezing}}^{n+1} \times \left(1 - \frac{LWC_c^n}{LWC_c^{n+1}}\right) \times RC^n \times r_{\text{up}}^{n+1} \quad (13)$$

Thereby, it is assumed that the cloud droplets do not evaporate when transported upward.

The rate for the expulsion is derived by

$$r_{\text{up,no retention}}^{n+1} = SF_{\text{freezing}}^{n+1} \times \left(1 - \frac{LWC_c^n}{LWC_c^{n+1}}\right) \times (1 - RC^n) \times r_{\text{up}}^{n+1}. \quad (14)$$

Retention of rain droplets is not considered in MCTS. For simplicity, it is assumed that the rain droplets are too heavy to be transported upward. For this reason, we do not

consider the adaptations of the retention coefficient parameterisations by Gautam et al. (2025) at this point.

The retention concerning cloud droplets is connected to the transport of the cloud hydrometeors, because the cloud droplets start freezing when they reach cold enough temperatures. Therefore, the reaction combines the upward transport and the retention and is mentioned after the transport itself is introduced (Subsec. 5.2).

4.2.2 Ice surface uptake

The surface adsorption is shown in Fig. 5 and Fig. 2 (14) and (20) and the desorption is illustrated by (16) and (21).

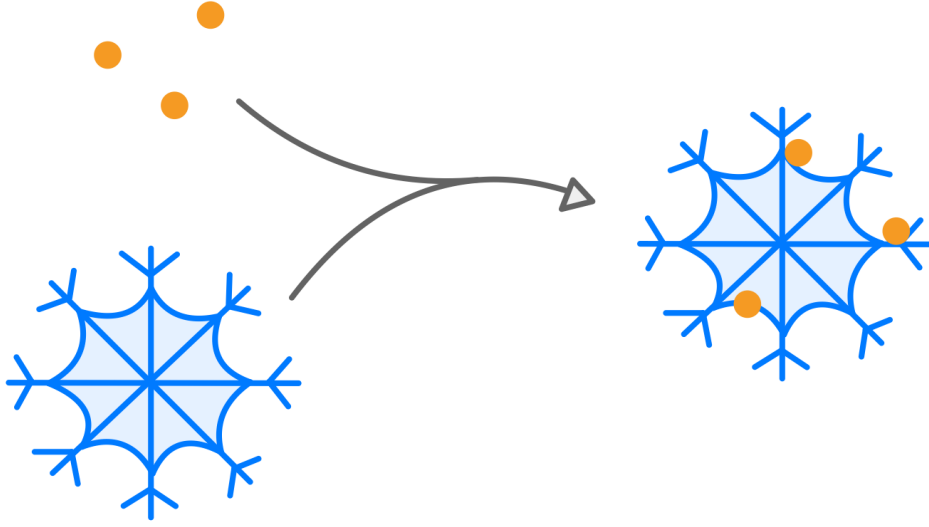
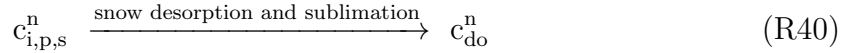


Figure 5: Sketch of the surface uptake. Molecules of some tracers can stick to the surface of ice crystals.

The uptake of species at the ice surface is often described with the Langmuir adsorption (see, for example, Crowley et al., 2010). Kuhlmann et al. (2003) calculated the ice uptake based on the Henry value, which is suggested by the measurements of Conklin et al. (1993). Recent measurements by Seymore et al. (2025) point towards a bulk-like or burial uptake. Also, Conklin et al. (1993) reported that besides the surface adsorption also bulk uptake of H_2O_2 takes place. Furthermore, Seymore et al. (2025) found an indication for the existence of a quasi-liquid layer. Therefore, the ice uptake in MCTS is derived based on Henry’s law, equivalent to the liquid uptake described in Subsubsec. 4.1.1, but for a different temperature range. Only the surface ice layer

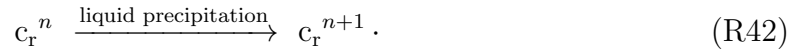
reservoir is affected by the uptake in MCTS. It is common approach for model applications. von Kuhlmann and Lawrence (2006) tested different uptake mechanisms in their model study, one is based on the Henry values. von Kuhlmann and Lawrence (2006) argue that this approach takes quasi-bulk uptake into account. Also, Bardakov et al. (2020) treats the condensation and evaporation at the ice hydrometeors in the same way as for droplets. The Henry-based uptake can be applied in SCAV nowadays. However, different α values are used to calculate the mass transfer coefficient for the cloud ice crystal uptake $k_{mt,ic}$. The values were taken from the proffered values given in Crowley et al. (2010)³. For the cloud ice a diameter of 30 μm was assumed which is well within the size range found by Krämer et al. (2020). As for rain, a discretised size spectra was used for the precipitating ice hydrometeors. The hail size spectra is calculated following eq. 11 and 12 by Balakrishnan and Zrnica (1990), whereby the size spectra formula is based on eq. 12 by Cheng and English (1983). For the size distribution calculation, the size parameter is needed, which is derived based on eq. (14) by Torlaschi et al. (1984).

The reactions for the uptake and the desorption are given by

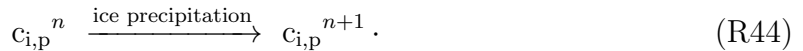
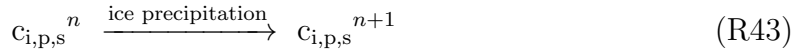


4.3 Precipitation

In MCTS, two types of precipitation are considered: rain and snow/ice precipitation (processes (19) and (22) in Fig.2). The rain can be represented by



For the snow, two equations need to be taken into account, one for the surface ice and one for the bulk ice:



³For H_2SO_4 no α value is given by Crowley et al. (2010). Therefore, a value of 0.1 was assumed. Crowley et al. (2010) do not mention a proffered value for H_2O_2 ; they give the values based on Conklin et al. (1993). The preferred value for HNO_3 given by Crowley et al. (2010) is larger 0.2. In MCTS, exactly 0.2 is used as a first approach. No temperature dependence of the α values for ice was taken into account in MCTS.

The rates for these two precipitation rates are calculated based on the precipitation fluxes, which are obtained from the input.

The mass fluxes (MF) are reformulated as first-order reactions (r) with

$$r^n = \text{MF}^n \times \frac{g}{\Delta p}. \quad (15)$$

Thereby, g is the gravitational acceleration and Δp is the pressure difference between the model level interfaces.

It is considered that snow flakes can melt (process (23) in Fig. 2). Also, the sublimation of snow flakes and the evaporation of rain droplets are taken into account if they fall into (highly) undersaturated regions (not shown in Fig. 2). These processes are described by the following equations

$$c_{i,p,s}^n \xrightarrow{\text{ice precipitation melting}} c_r^{n+1} \quad (R45)$$

$$c_{i,p,s}^n \xrightarrow{\text{snow desorption and sublimation}} c_{do}^n \quad (R46)$$

$$c_{i,p}^n \xrightarrow{\text{ice precipitation melting}} c_p^{n+1} \quad (R47)$$

$$c_{i,p}^n \xrightarrow{\text{precipitation sublimation}} c_{do}^n \quad (R48)$$

$$c_r^n \xrightarrow{\text{rain evaporation}} c_{do}^{n+1}. \quad (R49)$$

To reduce the number of equations, desorption from the ice surface and sublimation are summarised in one equation for the species at the snow surface.

5 Transport

MCTS makes use of a bulk approach (Yanai et al., 1973) to describe the convective transport (Lawrence and Rasch, 2005; Tost et al., 2010). The representation of the transport in MCTS is based on and to a large part consistent with CVTRANS (Tost et al., 2010; Ouwersloot et al., 2015; Jeske and Tost, 2025). In the following, the convective transport is described in more detail.

5.1 The transport in the gas phase

Figure 6 sketches these basic transport mechanisms.

The convective transport is driven by the updraft and downdraft mass fluxes. These fluxes are taken from the input. The upward and downward transport must balance each other in one column, see Bjerknes (1938)⁴. Otherwise, a major fraction of the material might be in the upper model levels (lower model level numbers and at lower

⁴The publication by Bjerknes (1938) can be found in the “Proceedings at the meetings of the society. January 19, 1938” (1938)

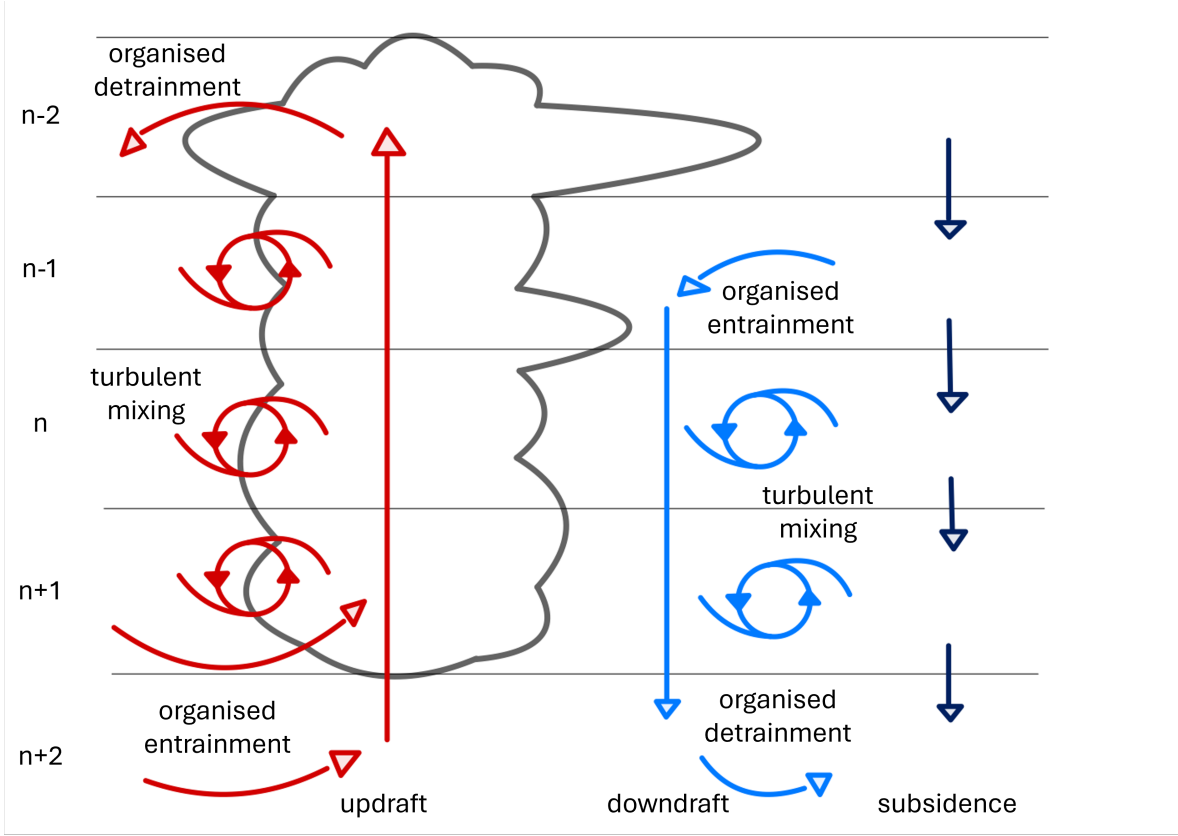


Figure 6: Simple sketch of the convective transport processes. Similar illustrations are given for example by Yanai et al. (1973), Mari et al. (2000), Bozem et al. (2017), and Jeske and Tost (2025). n denotes the model level. Level $n+1$ has higher pressure than level n .

pressures). This is avoided by introducing the sub-grid mass-balancing subsidence. The subsidence (MF_{sub}^n) is calculated by subtracting the downdraft mass flux (MF_{do}^n) from the updraft mass flux, (MF_{up}^n)

$$MF_{sub}^n = MF_{up}^n - MF_{do}^n, \quad (16)$$

as the updraft is usually much stronger than the downdraft mass flux. (Remark: All mass fluxes are positively defined.)

The mass fluxes in $\text{kg m}^{-2} \text{s}^{-1}$ are reformulated as first-order reaction rates (r) in s^{-1} to represent the transport as loss reactions (illustrated in Fig. 1) with equation (15)

The associated reactions are



5.1.1 Entrainment and detrainment

As can be seen in Fig. 6, the updraft and downdraft are connected to the environment via entrainment and detrainment. Entrainment and detrainment can either be organised or turbulent. The entrainment and detrainment mass fluxes are taken from the input for the updraft and the downdraft. However, it is important to make sure that they do not lead to a mass imbalance: If a tracer is homogeneously distributed in the column, this homogeneous tracer field must stay homogeneous as long as only transport is considered. In MCTS, this is realised as in Tost et al., 2010. The following equations must be full filled

$$MF_{up}^n = MF_{up}^{n+1} + ME_u^n - MD_u^n \quad (17)$$

$$MF_{do}^{n+1} = MF_{do}^n + ME_{do}^n - MD_{do}^n \quad (18)$$

as already applied by Lawrence and Rasch (2005) and also used in CVTRANS (Tost et al., 2010). The representation of this closure in CVTRANS was adapted by Jeske and Tost (2025). The adaptations described in the supplements to Jeske and Tost (2025) are also used in MCTS. The same calculation is done analogously in MCTS for the downdraft.

The reactions for the entrainment and detrainment are the following

$$c_{up}^n \xrightarrow{\text{updraft detrainment}} c_{env}^n \quad (R53)$$

$$c_{env}^n \xrightarrow{\text{updraft entrainment}} c_{up}^n \quad (R54)$$

$$c_{do}^n \xrightarrow{\text{downdraft detrainment}} c_{env}^n \quad (R55)$$

$$c_{env}^n \xrightarrow{\text{downdraft entrainment}} c_{do}^n \quad (R56)$$

The reaction rates are again derived via equation (15). The turbulent mixing is calculated according to Tiedtke (1989) and references therein for **MCTS_SEAC4RS_advect**, i.e. the MCTS version which is compared to the observations. The different versions of MCTS are described in Sec. 7.

5.1.2 The representation of the mass balancing subsidence

As in CVTRANS, the transport by the mass-balancing subsidence in MCTS should be slow; the mass is only allowed to subside one level within one model time step (see Fig. 6 for illustration). This restriction for the mass-balancing subsidence has a drawback within the chemical setup used within MCTS. It is not straightforward to implement a mass-balancing subsidence, which is only allowed to transport material exclusively to the next level without violating the homogeneous tracer field closure. We came up with a rather complicated workaround. A schematic of the process is provided in Fig. 7. This might not be the most elegant option to deal with this problem. The workaround is discussed in further detail below.

The subsidence reservoir is split into four sub-reservoirs:

1. env: the reservoir interacting with the downdraft and updraft reservoir,
2. sub: the reservoir where the subsiding material from one level above arrives to,
3. res: a constant reservoir from which the material flows in to env to make up for the material loss due to the subsidence, and
4. diag: a reservoir where the same amount of material as to env from res flows into.

The mixing ratios in the environment ($c_{\text{env,total}}$) after one time step are added together for the reservoirs env (c_{env}), sub (c_{sub}) and res (c_{res}). From which are deducted the diag reservoir (c_{diag}), the start values of the sub ($c_{\text{sub,start}}$) and res reservoirs. As res is constant, it cancels out. The equation to calculate the subsidence mixing ratios after the time integration is

$$c_{\text{env,total}} = c_{\text{env}} + c_{\text{sub}} - c_{\text{diag}} - c_{\text{sub,start}} \quad (19)$$

The environment is assumed to be large compared to the convective cloud and only a part of the environment is directly influenced by mixing with the convective system.

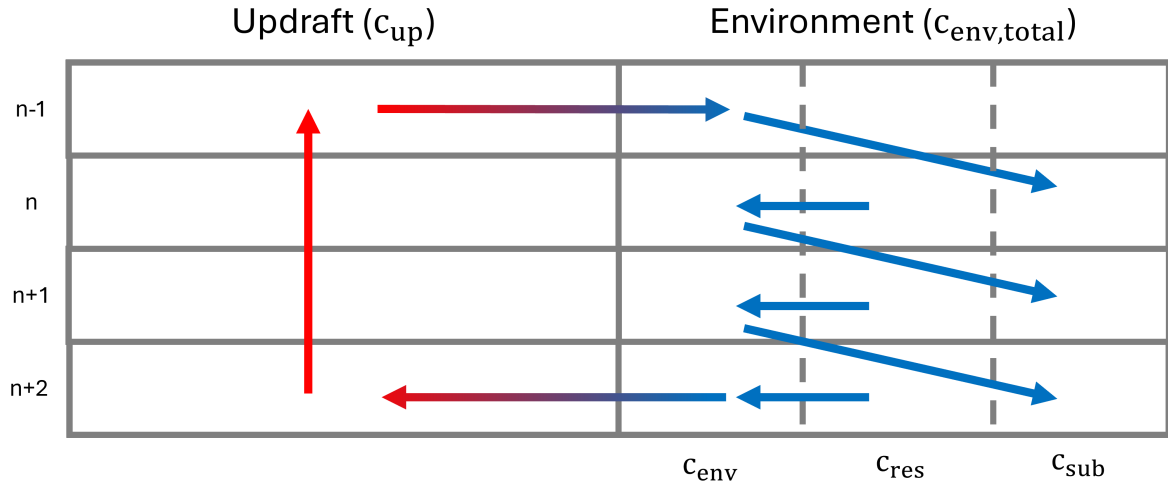


Figure 7: Illustration of the mass-balancing subsidence in MCTS. For simplicity, it is assumed that the downdraft is zero and the subsidence in the environment completely balances the upward motion due to the updraft. Further, no mixing processes in the levels in between the inflow and outflow levels are considered, and only four vertical levels are taken into account. The environment is subdivided into four reservoirs: the reservoir which interacts with the updraft reservoir (and the downdraft reservoir which is not shown here), c_{env} , the constant reservoir, c_{res} and the reservoir where the molecules are subsiding to, c_{sub} . There is a fourth reservoir to track the molecule transfer (c_{diag}), which is not shown here. The red arrows denote the updraft, the blue the subsidence and the red-blue ones the exchange between the environment and the updraft reservoir.

The subsidence (reaction (R52)) is reformulated

$$c_{\text{env}}^n \xrightarrow{\text{subsidence}} c_{\text{sub}}^{n+1} \quad (\text{R57})$$

$$c_{\text{res}}^n \xrightarrow{\text{subsidence}} c_{\text{env}}^n + c_{\text{res}}^n + c_{\text{diag}}^n. \quad (\text{R58})$$

5.1.3 Grid scale ascent

If the mass flux for the downdraft is stronger than the updraft, the grid-scale ascent mass flux is derived via

$$\text{MF}_{\text{asc}}^n = \text{MF}_{\text{do}}^n - \text{MF}_{\text{up}}^n. \quad (20)$$

Stronger downdrafts as updrafts are aconsidered in MCST to avoid mass impalance problems.

$$c_{\text{env}}^n \xrightarrow{\text{subsidence}} c_{\text{sub}}^{n+1} \quad (\text{R59})$$

5.2 Multiphase-transport

The up- and downward can redistribute and transport hydrometeors, which was already taken into account by Gidel (1983). Furthermore, the transport of hydrometeors might also impact trace gas or aerosol particle concentrations. Solid and liquid hydrometeors are considered in MCTS. In the following, the transport processes of the species within these hydrometeors are discussed.

The cloud droplets can be redistributed by the updraft, and with them also the species dissolved in these droplets (process (9) in Fig. 2). This is described by

$$c_c^{n+1} \xrightarrow{\text{updraft without freezing}} c_c^n. \quad (\text{R60})$$

$$c_c^n \xrightarrow{\text{updraft detrainment}} c_{\text{env}}^n \quad (\text{R61})$$

point out that the small cloud droplets can be detrained from the updraft (process (10) in Fig. 2). It is assumed that the air is undersaturated in the environment; the droplets are forced to evaporate. The species is therefore released in the gas phase (into the environment reservoir).

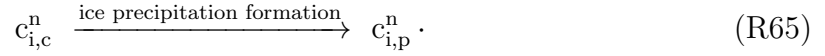
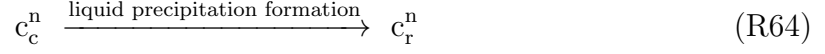
If the droplet is transported upward, it might reach temperatures where it freezes. Then comes the retention (process (11) in Fig. 2) into play as some molecules stay within the freezing droplet

$$c_c^{n+1} \xrightarrow{\text{updraft freezing}} c_{i,c}^n \quad (\text{R62})$$

and some are expelled into gas-phase

$$c_c^{n+1} \xrightarrow{\text{expulsion during freezing}} c_{\text{up}}^n. \quad (\text{R63})$$

Rain droplets can form from cloud droplets (process (8) in Fig. 2) and snow crystals from cloud ice (process (15) in Fig. 2). The impact of this process is represented by



Also, the cloud ice can be transported upward and be detrained from the updraft reservoir. These processes are given by (12) and (13) in Fig. 2). The associated reactions are



5.3 Ion transport

Ions form in the droplets as described in Sec. 4. They are transported within the droplets in the same way as the soluble species. They can be transitioned into the “aerosol phase” when they are, i.e., in a cloud droplet which gets detrained. Species in the “aerosol phase” can undergo the transport processes discussed in Subsec. 5.1. However, there are two differences:

1. Ions within a cloud droplet always stay within the droplet if the droplet freezes (compare (11) in Fig. 2), and
2. if a ion is entrained into the updraft (area), it will directly transit into the cloud droplet reservoir (process (26) in Fig. 2), because it is assumed that the ions are part of aerosols forming cloud nucleation particles.

6 Time integration

More than 20,000 ordinary differential equations are needed to describe all processes considered in MCTS considered processes. All these equations are formulated as chemical reactions. Describing the transport as reactions enables the use of a software designed to solve chemical systems to integrate the system which is a combination of chemical reactions and transport reactions. KPP (Damian et al., 2002; Sandu et al., 2003; Daescu et al., 2003) is the standard software for these kind of applications within the MESSy community. It is also used by Sander et al., 2019 and Tost et al., 2006. KPP version 2 (Sandu and Sander, 2006) is applied to produce a Fortran code for the time integration of the equation system. This code is then embedded in MCTS. Within MCTS the type of the integrator, the tolerances and the start step size are set for the time integration with KPP.

A Rodas integrator (Rosenbrock type method, see Harier and Wanner, 1991, p. 450–452 for further information) of order 4 is applied and adaptive time stepping is used.

The reader is referred to Damian et al. (2002), Sandu et al. (2003), Daescu et al. (2003), and Sandu and Sander (2006) for further information about KPP.

7 Getting started with MCTS

Two versions of MCTS are currently available: (1) the column model for applications on typical grid box scales of a GCM (**MCTS_with_EMAC**) and (2) the column model for a single convective storm (**MCTS_SEAC4RS_advect**). Please make sure to use (1) for applications with input from global models! (2) can be used to compare MCTS with observations for a single event.

Before using MCTS, you need to adapt the file paths to the output directories within **rates_all.f90**. Otherwise you end up with an error message because the directories do not exist. MCTS makes use of gfortran and needs netCDF. If these are installed on your machine, you can go to one of the two MCTS folders and simply type

gmake

The compilation of the kpp generated code for the time integration will take some time. Afterwards, type

./mcts.exe

Now, you are good to go. Within **rates_all.f90**, several user choices can be made. The choices in **MCTS_SEAC4RS_advect** are

- the integration time: `num_h_str` is a two digit character which indicates the integration time. `time_u` gives the unit which is either m for minutes or h for hours. These two characters are only relevant for the name of the output file. The real `t_end` gives the time in seconds MCTS uses for the time integration. It is the total time step, not the KPP time step. If the time step is too long, MCTS will tell you the following "ERROR: You need to reduce the time step!". Please follow these instruction and do not use the results!
- `sensi`: If `sensi = .False.`, the meteorological input is used as is. If `sensi = .True.`, the hydrometeors are purely ice in the uppermost niceonly levels, i.e. in level 1 to a user set prescribed level, which is given by the integer called `niceonly`.
- `sensi_trac`: If `sensi_trac = .False.` the original tracer input file is used. If `sensi_trac = .True.`, the values plus one standard deviation are used.
- `aqchem`: If `aqchem = .True.`, the aqueous chemistry is calculated. If `aqchem = .False.`, the rates for the aqueous chemistry are set to zero.
- `sensi_turb`: If `sensi_turb = .False.` the turbulence is calculated following the treatment in the convection scheme by Tiedtke, 1989 (see also references therein). If `sensi_turb = .True.`, the turbulence is scaled with the factor `turb_fac`. `turb_fac` can be chosen as well.

- **d_fac**: **d_fac** is an integer with values between zero and one. It decides, which scaling factors are used for the equilibrium reactions within the droplets. If **disso** = 4, no scaling is used. If **disso** = 6, the same scaling is used as in **MCTS_with_EMAC**. If **disso** = 0, the equilibrium reactions are about the order of magnitude as the updraft rates. Please see the code for the other options. This scaling is important to reduce the stiffness of the ordinary differential equation system and can influence the resulting tracer profiles..

The choices in **MCTS_with_EMAC** are

- the integration time: as above.
- **scal_trans**: If **scal_trans** = **.False.**, the grid box mean values are used. If **scal_trans** = **.True.**, the values are scaled with the updraft cloud cover.

If you want to use your one netCDF input files, make sure that they include the needed variables with the same dimensions as the provided input files. Otherwise, you need to change the dimensions of the variables within MCTS.

7.1 The structure of MCTS

The program structure is illustrated in Fig. 8. It shows all MCTS modules except one file, called **idx_names.f90**. Within **idx_names.f90**, different indice were defined. They are than used across the other modules.

The heart of MCTS is **rates_all.f90**. It is the main code program within MCTS. Within this code section, the user can choose the simulation time. Further, the user has the option to enable several sensitivity studies. Please, be aware that some sensitivity studies require additional input. **rates_all.f90** calls **read_tracer_profiles.f90** to read (additional) input data. All input data are given in NetCDF format. The rates for the convective processes are calculated and the output files are generated within **rates_all.f90**.

cvt_vertical_loop.f90 calls the scripts to calculate all multiphase rates and the rates of the aqueous chemistry reactions, see the yellow box in Fig. 8. Than it calls **messy_cvt_inp_all_kpp.f90**, which connects the reaction rate between MCTS and the KPP generated code, **messy_all_int_cvt_kpp.f90**. This file was produced with an adapted version of **xscav** which is based **xmecca**. **xmecca** is part of MECCA, see supplements to Sander et al. (2019).

The input data of version (2) can be found in the directory **input_wrf_dc8** and of version (1) in **input_emac/**.

7.2 Closure test

If changes in the **MCTS_with_EMAC** code are made, developers should check whether the closure is still fulfilled after the code was adapted. Therefore, use a constant tracer

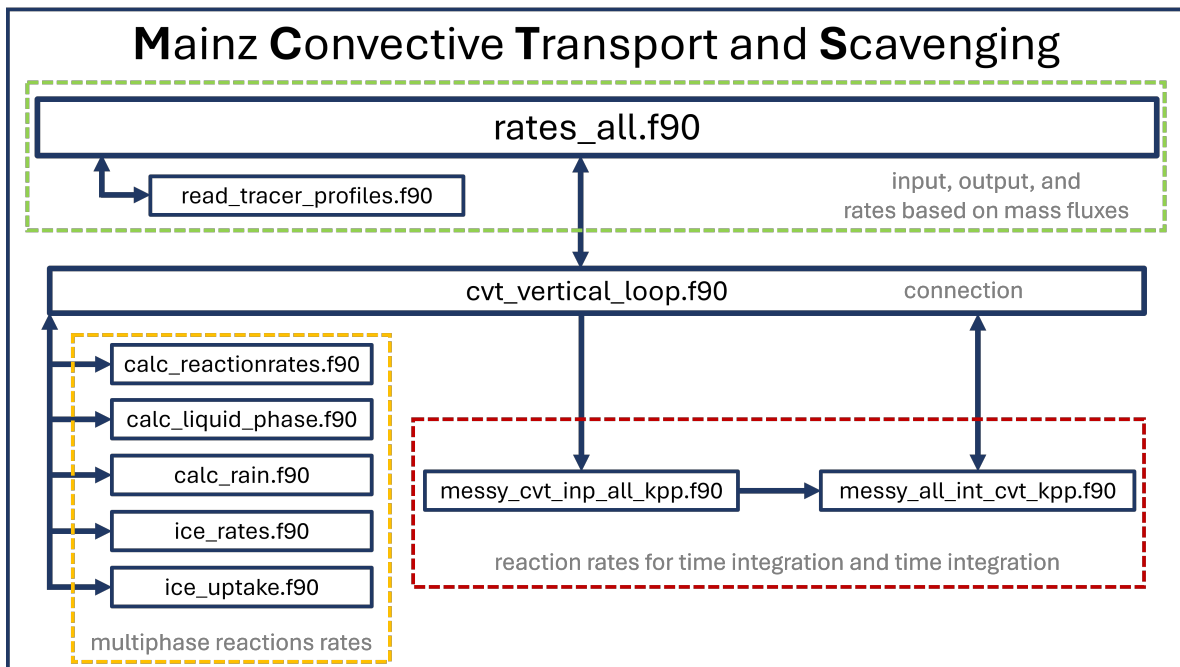


Figure 8: Program structure of MCTS. The modules of MCTS with their names are given in the dark blue frames. The errors denote between which modules and in which directions informations are exchanged. The light green, orange and dark red dashed boxes show which modules can be considered as some kind of a unit. The gray words shortly introduce the jobs of the different modules / module units.

profile as CO background profile input or set them manually within **rates_all.f90**. Check that the output field is still a homogeneous field. For **MCTS_SEAC4RS_advect**, this test cannot be performed as **MCTS_SEAC4RS_advect** is not closed due to the consideration of advection.

7.3 Remark

Oxygen and water are not conserved in MCTS, because there are so many oxygen and water molecules in the atmosphere that it is reasonable to assume that the number is anyway constant.

8 Final remarks

We want to acknowledge the developers and providers of the "pillars" on which MCTS stands:

- Damian et al., 2002; Sandu et al., 2003; Daescu et al., 2003; Sandu and Sander, 2006 for KPP,

- Tost et al., 2006 for SCAV,
- Sander et al., 2019 for CAABA/MECCA,
- Tost et al., 2010 for CVTRANS, and
- University Corporation for Atmospheric Research/Unidata for providing NetCDF and example code for reading the NetCDF data , which was developed by Hartnett (2006), and is provided within the GitHub repository *netcdf-fortran* (<https://github.com/Unidata/netcdf-fortran>) (NSF Unidata, 2026) and among other code examples under <https://archive.unidata.ucar.edu/software/netcdf/examples/programs/> (NSF Unidata, 2014).

A Appendix

A.1 An overview of all transport and phase-transition reactions included in MCTS

Below are listed all transport and phase transition reactions included in MCTS. First, the equations for the tracers and afterwards the equations for the ions are given.

A.1.1 Gas phase transport of tracers

The gas phase reaction for the global MCTS configuration are given by

$$c_{\text{up}}^{n+1} \xrightarrow{\text{updraft}} c_{\text{up}}^n \quad (\text{R68})$$

$$c_{\text{do}}^n \xrightarrow{\text{downdraft}} c_{\text{do}}^{n+1} \quad (\text{R69})$$

$$c_{\text{env}}^n \xrightarrow{\text{subsidence}} c_{\text{sub}}^{n+1} \quad (\text{R70})$$

$$c_{\text{up}}^n \xrightarrow{\text{updraft detrainment}} c_{\text{env}}^n \quad (\text{R71})$$

$$c_{\text{env}}^n \xrightarrow{\text{updraft entrainment}} c_{\text{up}}^n \quad (\text{R72})$$

$$c_{\text{do}}^n \xrightarrow{\text{downdraft detrainment}} c_{\text{env}}^n \quad (\text{R73})$$

$$c_{\text{env}}^n \xrightarrow{\text{downdraft entrainment}} c_{\text{do}}^n \quad (\text{R74})$$

$$c_{\text{env}}^{n+1} \xrightarrow{\text{ascent}} c_{\text{env}}^n \quad (\text{R75})$$

$$c_{\text{Sres}}^n \xrightarrow{\text{subsidence}} c_{\text{Senv}}^n + c_{\text{Sres}}^n + c_{\text{Sdiag}}^n. \quad (\text{R76})$$

The transport reactions for the single storm case are slightly different. There is no grid scale subsidence included, but the advection is considered. The advection is described by the following reactions

$$c_{\text{env}}^n \xrightarrow{\text{advect out}} c_{\text{env2}}^n \quad (\text{R77})$$

$$c_{\text{env2}}^n \xrightarrow{\text{advect in}} c_{\text{env2}}^n + c_{\text{env}}^n \quad (\text{R78})$$

$$(\text{R79})$$

Thereby, two different environments are considered. c_{env} is the direct environment of the cloud and c_{env2} the environmental air further away from the cloud. It is expected that the later one does not suffer from any material loss as c_{env2} is very large compared to the convective cloud area. The reaction rates for advect in and advect out are determined by the gradients of the updraft and downdraft mass fluxes.

A.1.2 Liquid phase processes

$$C_{\text{up}}^n \xrightarrow{\text{uptake by cloud droplets}} C_{\text{c,s}}^n \quad (21)$$

$$C_{\text{c}}^n \xrightarrow{\text{expulsion from cloud droplets}} C_{\text{up}}^n \quad (22)$$

$$C_{\text{c}}^{n+1} \xrightarrow{\text{expulsion during freezing}} C_{\text{up}}^n \quad (23)$$

$$C_{\text{c}}^{n+1} \xrightarrow{\text{updraft without freezing}} C_{\text{c}}^n \quad (24)$$

$$C_{\text{c}}^n \xrightarrow{\text{updraft detrainment}} C_{\text{env}}^n \quad (25)$$

$$C_{\text{do}}^n \xrightarrow{\text{uptake by rain droplets}} C_{\text{r}}^n \quad (26)$$

$$C_{\text{r}}^n \xrightarrow{\text{expulsion from rain droplets}} C_{\text{do}}^n \quad (27)$$

$$C_{\text{c}}^n \xrightarrow{\text{liquid precipitation formation}} C_{\text{r}}^n \quad (28)$$

$$C_{\text{r}}^n \xrightarrow{\text{liquid precipitation}} C_{\text{r}}^{n+1} \quad (29)$$

$$C_{\text{r}}^n \xrightarrow{\text{rain evaporation}} C_{\text{do}}^{n+1} \quad (30)$$

A.1.3 Ice phase processes

$$C_{\text{up}}^n \xrightarrow{\text{ice uptake}} C_{\text{i,c,s}}^n \quad (31)$$

$$C_{\text{i,c,s}}^n \xrightarrow{\text{ice desorption}} C_{\text{up}}^n \quad (32)$$

$$C_{\text{i,c,s}}^{n+1} \xrightarrow{\text{(ice) updraft}} C_{\text{i,c,s}}^n \quad (33)$$

$$C_{\text{i,c,s}}^n \xrightarrow{\text{(ice) updraft detrainment}} C_{\text{env}}^n \quad (34)$$

$$C_{\text{i,c,s}}^n \xrightarrow{\text{ice precipitation formation}} C_{\text{i,p,s}}^n \quad (35)$$

$$C_{\text{do}}^n \xrightarrow{\text{snow uptake}} C_{\text{i,p,s}}^n \quad (36)$$

$$C_{\text{i,p,s}}^n \xrightarrow{\text{snow desorption and sublimation}} C_{\text{do}}^n \quad (37)$$

$$C_{\text{i,p,s}}^n \xrightarrow{\text{ice precipitation}} C_{\text{i,p,s}}^{n+1} \quad (38)$$

$$C_{\text{i,p,s}}^n \xrightarrow{\text{ice precipitation melting}} C_{\text{r}}^{n+1} \quad (39)$$

$$c_c^{n+1} \xrightarrow{\text{updraft freezing}} c_{i,c}^n \quad (40)$$

$$c_{i,c}^n \xrightarrow{\text{ice precipitation formation}} c_{i,p}^n \quad (41)$$

$$c_{i,p}^n \xrightarrow{\text{ice precipitation}} c_{i,p}^{n+1} \quad (42)$$

$$c_{i,p}^n \xrightarrow{\text{ice precipitation melting}} c_p^{n+1} \quad (43)$$

$$c_{i,c}^n \xrightarrow{(\text{ice}) \text{ updraft detrainment}} c_{\text{env}}^n \quad (44)$$

$$c_{i,p}^n \xrightarrow{\text{precipitation sublimation}} c_{\text{do}}^n \quad (45)$$

$$c_{i,c}^{n+1} \xrightarrow{(\text{ice}) \text{ updraft}} c_{i,c}^n \quad (46)$$

A.1.4 Ions

$$c_{\text{up}}^{n+1} \xrightarrow{\text{updraft (no LWC}_c)} c_{\text{up}}^n \quad (47)$$

$$c_{\text{do}}^n \xrightarrow{\text{downdraft}} c_{\text{do}}^{n+1} \quad (48)$$

$$c_{\text{env}}^n \xrightarrow{\text{subsidence}} c_{\text{sub}}^{n+1} \quad (49)$$

$$c_{\text{env}}^{n+1} \xrightarrow{\text{ascent}} c_{\text{env}}^n \quad (50)$$

$$c_{\text{up}}^n \xrightarrow{\text{updraft detrainment}} c_{\text{env}}^n \quad (51)$$

$$c_{\text{env}}^n \xrightarrow{\text{updraft entrainment (no LWC}_c)} c_{\text{up}}^n \quad (52)$$

$$c_{\text{do}}^n \xrightarrow{\text{downdraft detrainment}} c_{\text{env}}^n \quad (53)$$

$$c_{\text{env}}^n \xrightarrow{\text{downdraft entrainment}} c_{\text{do}}^n \quad (54)$$

Again, for the ions, the subsidence is replaced by advection for the single storm case.

$$c_{\text{env}}^n \xrightarrow{\text{updraft entrainment (LWC}_c)} c_c^n \quad (55)$$

$$c_{\text{up}}^{n+1} \xrightarrow{\text{updraft (LWC}_c)} c_c^n \quad (56)$$

$$c_c^{n+1} \xrightarrow{\text{updraft no freezing}} c_c^n \quad (57)$$

$$c_r^n \xrightarrow{\text{rain evaporation}} c_{\text{do}}^n \quad (58)$$

$$c_c^n \xrightarrow{\text{updraft detrainment}} c_{\text{env}}^n \quad (59)$$

$$c_r^n \xrightarrow{\text{liquid precipitation}} c_r^{n+1} \quad (60)$$

$$c_c^n \xrightarrow{\text{liquid precipitation formation}} c_r^n \quad (61)$$

$$c_c^{n+1} \xrightarrow{\text{updraft freezing}} c_{i,c}^n \quad (62)$$

$$c_{i,c}^n \xrightarrow{\text{ice precipitation formation}} c_{i,p}^n \quad (63)$$

$$c_{i,p}^n \xrightarrow{\text{ice precipitation}} c_{i,p}^{n+1} \quad (64)$$

$$c_{i,p}^n \xrightarrow{\text{ice precipitation melting}} c_p^{n+1} \quad (65)$$

$$c_{i,c}^n \xrightarrow{\text{updraft detrainment}} c_{\text{env}}^n \quad (66)$$

$$c_{i,p}^n \xrightarrow{\text{precipitation sublimation}} c_{\text{do}}^n \quad (67)$$

$$c_{i,c}^{n+1} \xrightarrow{(\text{ice}) \text{ updraft}} c_{i,c}^n \quad (68)$$

References

- Balakrishnan, N. and D. S. Zrnic (1990). “Use of Polarization to Characterize Precipitation and Discriminate Large Hail”. In: *Journal of Atmospheric Sciences* 47.13, pp. 1525–1540. DOI: 10.1175/1520-0469(1990)047<1525:UOPTCP>2.0.CO;2.
- Bardakov, R., I. Riipinen, R. Krejci, J. Savre, J. A. Thornton, and A. M. L. Ekman (2020). “A Novel Framework to Study Trace Gas Transport in Deep Convective Clouds”. In: *Journal of Advances in Modeling Earth Systems* 12.5, e2019MS001931. DOI: 10.1029/2019MS001931.
- Beard, K. V. (1976). “Terminal Velocity and Shape of Cloud and Precipitation Drops Aloft”. In: *Journal of Atmospheric Sciences* 33.5, pp. 851–864. DOI: 10.1175/1520-0469(1976)033<0851:TVASOC>2.0.CO;2.
- Best, A. C. (1950). “The size distribution of raindrops”. In: *Quarterly Journal of the Royal Meteorological Society* 76.327, pp. 16–36. DOI: <https://doi.org/10.1002/qj.49707632704>.
- Bird, R. B., W. E. Stewart, and E. N. Lightfoot (1960). *Transport phenomena*. John Wiley & Sons, Inc., 780 pp.
- Bjerknes, J. (1938). “Saturated-adiabatic ascent of air through dry-adiabatically descending environment”. In: *Quarterly Journal of the Royal Meteorological Society* 64.275, pp. 325–330.
- Bozem, H., A. Pozzer, H. Harder, M. Martinez, J. Williams, J. Lelieveld, and H. Fischer (2017). “The influence of deep convection on HCHO and H₂O₂ in the upper troposphere over Europe”. In: *Atmospheric Chemistry and Physics* 17.19, pp. 11835–11848. DOI: 10.5194/acp-17-11835-2017.
- Cheng, L. and M. English (1983). “A Relationship Between Hailstone Concentration and Size”. In: *Journal of Atmospheric Sciences* 40.1, pp. 204–213. DOI: 10.1175/1520-0469(1983)040<0204:ARBHCA>2.0.CO;2.
- Conklin, M. H., A. Sigg, A. Neftel, and R. C. Bales (1993). “Atmosphere-snow transfer function for H₂O₂: Microphysical considerations”. In: *Journal of Geophysical Research: Atmospheres* 98.D10, pp. 18367–18376. DOI: <https://doi.org/10.1029/93JD01194>.
- Crowley, J. N., M. Ammann, R. A. Cox, R. G. Hynes, M. E. Jenkin, A. Mellouki, M. J. Rossi, J. Troe, and T. J. Wallington (2010). “Evaluated kinetic and photochemical data for atmospheric chemistry: Volume V – heterogeneous reactions on solid substrates”. In: *Atmospheric Chemistry and Physics* 10, pp. 9059–9223. DOI: 10.5194/acp-10-9059-2010.
- Daescu, D. N., A. Sandu, and G. R. Carmichael (2003). “Direct and adjoint sensitivity analysis of chemical kinetic systems with KPP: II—numerical validation and applications”. In: *Atmospheric Environment* 37.36, pp. 5097–5114. DOI: <https://doi.org/10.1016/j.atmosenv.2003.08.020>.
- Damian, V., A. Sandu, M. Damian, F. Potra, and G. R. Carmichael (2002). “The kinetic preprocessor KPP—a software environment for solving chemical kinetics”. In:

- Computers & Chemical Engineering* 26.11, pp. 1567–1579. DOI: [https://doi.org/10.1016/S0098-1354\(02\)00128-X](https://doi.org/10.1016/S0098-1354(02)00128-X).
- Emanuel, K. A. and M. Živković-Rothman (1999). “Development and Evaluation of a Convection Scheme for Use in Climate Models”. In: *Journal of the Atmospheric Sciences* 56.11, pp. 1766–1782. DOI: 10.1175/1520-0469(1999)056<1766:DAEQAC>2.0.CO;2.
- Frössling, N. (1938). “Über die Verdunstung fallender Tropfen”. In: *Gerlands Beiträge zur Geophysik* 52, pp. 170–216.
- Gautam, M., A. Theis, J. Seymore, M. Hey, S. Borrmann, K. Diehl, S. K. Mitra, and M. Szakáll (2025). “Retention during freezing of raindrops – Part 1: Investigation of single and binary mixtures of nitric, formic, and acetic acids and 2-nitrophenol”. In: *Atmospheric Chemistry and Physics* 25.19, pp. 11813–11828. DOI: 10.5194/acp-25-11813-2025.
- Gidel, L. T. (1983). “Cumulus cloud transport of transient tracers”. In: *Journal of Geophysical Research: Oceans* 88.C11, pp. 6587–6599. DOI: <https://doi.org/10.1029/JC088iC11p06587>.
- Harier, E. and G. Wanner (1991). *Solving ordinary differential equations II: stiff and differential algebraic problems*. 1st ed. Springer Verlag.
- Hartnett, E. (2006). *simple_xy_rd.F90*. https://github.com/Unidata/netcdf-fortran/blob/main/examples/F90/simple_xy_rd.F90, last accessed: 17.04.2026. [code], GitHub, commit 749b86c9abec212aaa6a9023da6f654107e86b23.
- Herrmann, H., B. Ervens, H. Jacobi, R. Wolke, P. Nowacki, and Z. R. (2000). “CAPRAM2.3: A Chemical Aqueous Phase Radical Mechanism for Tropospheric Chemistry”. In: *Journal of Atmospheric Chemistry* 36, pp. 231–284. DOI: <https://doi.org/10.1023/A:1006318622743>.
- Jeske, A. (2023). “Simulationen zu konvektivem Spurenstofftransport”. MA thesis. Johannes Gutenberg University Mainz.
- Jeske, A. and H. Tost (2025). “The historical climate trend resulted in changed vertical transport patterns in climate model simulations”. In: *Atmospheric Chemistry and Physics* 25.21, pp. 14435–14448. DOI: 10.5194/acp-25-14435-2025.
- Jöckel, P., A. Kerkweg, A. Pozzer, R. Sander, H. Tost, H. Riede, A. Baumgaertner, S. Gromov, and B. Kern (2010). “Development cycle 2 of the Modular Earth Submodel System (MESSy2)”. In: *Geoscientific Model Development* 3.2, pp. 717–752. DOI: 10.5194/gmd-3-717-2010.
- Jöckel, P., R. Sander, A. Kerkweg, H. Tost, and J. Lelieveld (2005). “Technical Note: The Modular Earth Submodel System (MESSy) - a new approach towards Earth System Modeling”. In: *Atmospheric Chemistry and Physics* 5.2, pp. 433–444. DOI: 10.5194/acp-5-433-2005.
- Jöckel, P., H. Tost, A. Pozzer, C. Brühl, J. Buchholz, L. Ganzeveld, P. Hoor, A. Kerkweg, M. G. Lawrence, R. Sander, B. Steil, G. Stiller, M. Tanarhte, D. Taraborrelli, J. van Aardenne, and J. Lelieveld (2006). “The atmospheric chemistry general circulation model ECHAM5/MESSy1: consistent simulation of ozone from the surface

- to the mesosphere”. In: *Atmospheric Chemistry and Physics* 6.12, pp. 5067–5104. DOI: 10.5194/acp-6-5067-2006.
- Jöckel, P., H. Tost, A. Pozzer, M. Kunze, O. Kirner, C. A. M. Brenninkmeijer, S. Brinkop, D. S. Cai, C. Dyroff, J. Eckstein, F. Frank, H. Garny, K.-D. Gottschaldt, P. Graf, V. Grewe, A. Kerkweg, B. Kern, S. Matthes, M. Mertens, S. Meul, M. Neumaier, M. Nützel, S. Oberländer-Hayn, R. Ruhnke, T. Runde, R. Sander, D. Scharffe, and A. Zahn (2016). “Earth System Chemistry integrated Modelling (ES-CiMo) with the Modular Earth Submodel System (MESSy) version 2.51”. In: *Geoscientific Model Development* 9.3, pp. 1153–1200. DOI: 10.5194/gmd-9-1153-2016.
- Jost, A., M. Szakáll, K. Diehl, S. K. Mitra, and S. Borrmann (2017). “Chemistry of riming: the retention of organic and inorganic atmospheric trace constituents”. In: *Atmospheric Chemistry and Physics* 17.16, pp. 9717–9732. DOI: 10.5194/acp-17-9717-2017.
- Kerkweg, A., R. Sander, H. Tost, P. Jöckel, and J. Lelieveld (2007). “Technical Note: Simulation of detailed aerosol chemistry on the global scale using MECCA-AERO”. In: *Atmospheric Chemistry and Physics* 7.11, pp. 2973–2985. DOI: 10.5194/acp-7-2973-2007.
- Krämer, M., C. Rolf, N. Spelten, A. Afchine, D. Fahey, E. Jensen, S. Khaykin, T. Kuhn, P. Lawson, A. Lykov, L. L. Pan, M. Riese, A. Rollins, F. Stroh, T. Thornberry, V. Wolf, S. Woods, P. Spichtinger, J. Quaas, and O. Sourdeval (2020). “A microphysics guide to cirrus – Part 2: Climatologies of clouds and humidity from observations”. In: *Atmospheric Chemistry and Physics* 20.21, pp. 12569–12608. DOI: 10.5194/acp-20-12569-2020.
- Kuhlmann, R. von, M. G. Lawrence, P. J. Crutzen, and P. J. Rasch (2003). “A model for studies of tropospheric ozone and nonmethane hydrocarbons: Model description and ozone results”. In: *Journal of Geophysical Research: Atmospheres* 108.D9, 4294, ACH 17-1 –ACH 17-22. DOI: <https://doi.org/10.1029/2002JD002893>.
- Kumar, S. (1985). “An Eulerian model for scavenging of pollutants by raindrops”. In: *Atmospheric Environment (1967)* 19.5, pp. 769–778. DOI: [https://doi.org/10.1016/0004-6981\(85\)90065-4](https://doi.org/10.1016/0004-6981(85)90065-4).
- Lawrence, M. G. and P. J. Rasch (2005). “Tracer Transport in Deep Convective Updrafts: Plume Ensemble versus Bulk Formulations”. In: *Journal of the Atmospheric Sciences* 62.8, pp. 2880–2894. DOI: <https://doi.org/10.1175/JAS3505.1>.
- Levine, S. and S. Schwartz (1982). “In-cloud and below-cloud scavenging of Nitric acid vapor”. In: *Atmospheric Environment* 16.7. Precipitation chemistry, pp. 1725–1734. DOI: [https://doi.org/10.1016/0004-6981\(82\)90266-9](https://doi.org/10.1016/0004-6981(82)90266-9).
- Li, Y., K. E. Pickering, M. C. Barth, M. M. Bela, K. A. Cummings, and D. J. Allen (2019). “Wet Scavenging in WRF-Chem Simulations of Parameterized Convection for a Severe Storm During the DC3 Field Campaign”. In: *Journal of Geophysical Research: Atmospheres* 124.13, pp. 7413–7428. DOI: 10.1029/2019JD030484.
- Lin, J., T. Qian, P. Bechtold, G. Grell, G. J. Zhang, P. Zhu, S. R. Freitas, H. Barnes, and J. Han (2022). “Atmospheric Convection”. In: *Atmosphere-Ocean* 60.3-4, pp. 422–476. DOI: 10.1080/07055900.2022.2082915.

- Logan, S. R. (1982). “The origin and status of the Arrhenius equation”. In: *Journal of Chemical Education* 59.4, pp. 279–281. DOI: 10.1021/ed059p279.
- Mari, C., D. J. Jacob, and P. Bechtold (2000). “Transport and scavenging of soluble gases in a deep convective cloud”. In: *Journal of Geophysical Research: Atmospheres* 105.D17, pp. 22255–22267. DOI: 10.1029/2000JD900211.
- Marshall, J. S., R. C. Langille, and W. M. K. Palmer (1947). “MEASUREMENT OF RAINFALL BY RADAR”. In: *Journal of Atmospheric Sciences* 4.6, pp. 186–192. DOI: 10.1175/1520-0469(1947)004<0186:MORBR>2.0.CO;2.
- Marshall, J. S. and W. M. K. Palmer (1948). “THE DISTRIBUTION OF RAINDROPS WITH SIZE”. In: *Journal of Atmospheric Sciences* 5.4, pp. 165–166. DOI: 10.1175/1520-0469(1948)005<0165:TDORWS>2.0.CO;2.
- Mason, B. J. (1957). *The physics of clouds*. Ed. by P. A. Sheppard. Oxford University Press.
- Nordeng, T.-E. (1994). “Extended versions of the convective parametrization scheme at ECMWF and their impact on the mean and transient activity of the model in the tropics”. In: *ECMWF Technical Memoranda* 206, pp. 1–41. DOI: 10.21957/e34xwhysw.
- NSF Unidata (2014). *Example netCDF programs*. <https://archive.unidata.ucar.edu/software/netcdf/examples/programs/>, last accessed: 17.04.2026.
- NSF Unidata (2026). *netcdf-fortran*. <https://github.com/Unidata/netcdf-fortran>, last accessed: 17.04.2026. [code], GitHub, commit d0ebd7a0ceed6fc85e82c18991c4c2bedbf7b654.
- Ouwensloot, H. G., A. Pozzer, B. Steil, H. Tost, and J. Lelieveld (2015). “Revision of the convective transport module CVTRANS 2.4 in the EMAC atmospheric chemistry–climate model”. In: *Geoscientific Model Development* 8.8, pp. 2435–2445. DOI: 10.5194/gmd-8-2435-2015.
- “Proceedings at the meetings of the society. January 19, 1938” (1938). In: *Quarterly Journal of the Royal Meteorological Society* 64.275, pp. 317–330. DOI: <https://doi.org/10.1002/qj.49706427509>.
- Pruppacher, H. R. and J. D. Klett (2000). *Microphysics of clouds and precipitation*. Second Revised and Enlarged Edition. Kluwer Acad. Publ. ISBN: 0-7923-4211-9.
- Robbin Martin, L. and D. E. Damschen (1981). “Aqueous oxidation of sulfur dioxide by hydrogen peroxide at low pH”. In: *Atmospheric Environment (1967)* 15.9, pp. 1615–1621. DOI: [https://doi.org/10.1016/0004-6981\(81\)90146-3](https://doi.org/10.1016/0004-6981(81)90146-3).
- Sander, R. (2023). “Compilation of Henry’s law constants (version 5.0.0) for water as solvent”. In: *Atmospheric Chemistry and Physics* 23.19, pp. 10901–12440. DOI: 10.5194/acp-23-10901-2023.
- Sander, R., A. Baumgaertner, D. Cabrera-Perez, F. Frank, S. Gromov, J.-U. Groöß, H. Harder, V. Huijnen, P. Jöckel, V. A. Karydis, K. E. Niemeyer, A. Pozzer, H. Riede, M. G. Schultz, D. Taraborrelli, and S. Tauer (2019). “The community atmospheric chemistry box model CAABA/MECCA-4.0”. In: *Geoscientific Model Development* 12.4, pp. 1365–1385. DOI: 10.5194/gmd-12-1365-2019.

- Sander, R. (1999). “Modeling atmospheric chemistry: Interactions between gas-phase species and liquid cloud/aerosol particles”. In: *Surveys in Geophysics* 20, pp. 1–31. DOI: <https://doi.org/10.1023/A:1006501706704>.
- Sander, R. and P. J. Crutzen (1996). “Model study indicating halogen activation and ozone destruction in polluted air masses transported to the sea”. In: *Journal of Geophysical Research: Atmospheres* 101.D4, pp. 9121–9138. DOI: <https://doi.org/10.1029/95JD03793>.
- Sandu, A. and R. Sander (2006). “Technical note: Simulating chemical systems in Fortran90 and Matlab with the Kinetic PreProcessor KPP-2.1”. In: *Atmospheric Chemistry and Physics* 6.1, pp. 187–195. DOI: 10.5194/acp-6-187-2006.
- Sandu, A., D. N. Daescu, and G. R. Carmichael (2003). “Direct and adjoint sensitivity analysis of chemical kinetic systems with KPP: Part I—theory and software tools”. In: *Atmospheric Environment* 37.36, pp. 5083–5096. DOI: <https://doi.org/10.1016/j.atmosenv.2003.08.019>.
- Schwartz, S. E. (1986). “Mass-Transport Considerations Pertinent to Aqueous Phase Reactions of Gases in Liquid-Water Clouds”. In: *Chemistry of Multiphase Atmospheric Systems*. Ed. by W. Jaeschke. Berlin, Heidelberg: Springer Berlin Heidelberg, pp. 415–471. ISBN: 978-3-642-70627-1. DOI: https://doi.org/10.1007/978-3-642-70627-1_16.
- Seymore, J., M. Szakáll, A. Theis, S. K. Mitra, C. Borchers, and T. Hoffmann (2025). “Volume uptake of carbonyls during diffusional ice crystal growth”. In: *Atmospheric Chemistry and Physics* 25.23, pp. 18249–18265. DOI: 10.5194/acp-25-18249-2025.
- Tiedtke, M. (1989). “A Comprehensive Mass Flux Scheme for Cumulus Parameterization in Large-Scale Models”. In: *Monthly Weather Review* 117.8, pp. 1779–1800. DOI: 10.1175/1520-0493(1989)117<1779:ACMFSF>2.0.CO;2.
- Torlaschi, E., R. G. Humphries, and B. L. Barge (1984). “Circular polarization for precipitation measurement”. In: *Radio Science* 19.1, pp. 193–200. DOI: <https://doi.org/10.1029/RS019i001p00193>.
- Tost, H., P. Jöckel, A. Kerkweg, A. Pozzer, R. Sander, and J. Lelieveld (2007). “Global cloud and precipitation chemistry and wet deposition: tropospheric model simulations with ECHAM5/MESSy1”. In: *Atmospheric Chemistry and Physics* 7.10, pp. 2733–2757. DOI: 10.5194/acp-7-2733-2007.
- Tost, H., P. Jöckel, A. Kerkweg, R. Sander, and J. Lelieveld (2006). “Technical note: A new comprehensive SCAVenging submodel for global atmospheric chemistry modelling”. In: *Atmospheric Chemistry and Physics* 6.3, pp. 565–574. DOI: 10.5194/acp-6-565-2006.
- Tost, H., M. G. Lawrence, C. Brühl, P. Jöckel, and The GABRIEL Team and The SCOUT-O3-DARWIN/ACTIVE Team (2010). “Uncertainties in atmospheric chemistry modelling due to convection parameterisations and subsequent scavenging”. In: *Atmospheric Chemistry and Physics* 10.4, pp. 1931–1951. DOI: 10.5194/acp-10-1931-2010.

- von Kuhlmann, R. and M. G. Lawrence (2006). “The impact of ice uptake of nitric acid on atmospheric chemistry”. In: *Atmospheric Chemistry and Physics* 6.1, pp. 225–235. DOI: 10.5194/acp-6-225-2006.
- Wagman, D. D. (1982). “The NBS tables of chemical thermodynamic properties Selected values for inorganic and C1 and C2 organic substances in SI units”. In: *J. Phys. Chem. Ref. Data* 11.2. supplement No. 2.
- Yanai, M., S. Esbensen, and J.-H. Chu (1973). “Determination of Bulk Properties of Tropical Cloud Clusters from Large-Scale Heat and Moisture Budgets”. In: *Journal of Atmospheric Sciences* 30, pp. 611–627. DOI: 10.1175/1520-0469(1973)030<0611:DOBPOT>2.0.CO;2.