Supplements
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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S1 EMAC simulation setup

EMAC (version 2.55.2, Jöckel et al., 2016) simulations in T42L90MA (truncation 42 and 90 vertical levels) were performed. EMAC was nudged (Aalst et al., 2004; Jöckel et al., 2006; Jöckel et al., 2016) towards ERA5 data (Hersbach et al., 2020). The simulations were started on September 1st, 2013. This EMAC simulation had two goals. (1) The first was to derive reasonable tracer input data for the case study for the species which were not measured during the NASA SEAC^{4}RS field mission. MCTS was not evaluated with respect to these species, but they are required as input for the simulations. (1) was achieved by using input data for the species originating from a historical simulation performed following the CCMI phase 2 protocol (REF-D1 hindcast simulation for 1960 - 2018). For more information regarding the protocol see `https://blogs.reading.ac.uk/ccmi/ccmi-2022/` (last accesed: 10.04.2026). The used simulation data has been published by Jöckel et al. (2024b) and Jöckel et al. (2024a).

The second goal (2) was to provide the EMAC output of one convective event and the associated convective scavenging and transport tendencies to enable a comparison between MCTS and EMAC for one case. Any EMAC simulation applying SCAV with the SCM mechanism and CVTRANS could be used to fulfil this purpose.

The Tiedtke–Nordeng (Tiedtke, 1989; Nordeng, 1994) convection parameterisation was applied via the CONVECT submodel (Tost et al., 2006b), which is known to produce strong updrafts compared to other convection schemes (Tost et al., 2006b). A list of the applied submodels is given in Tables S1.

The simulations were performed using the SCM mechanism for the aqueous chemistry, see Tost et al. (2007a) and supplements of Jöckel et al. (2006). The ice phase uptake in the simulation was based on the effectives Henry coefficient. Retention is not included in SCAV. The EMAC simulations were performed without aerosol scavenging via the liquid phase, because the considered processes should be as close to MCTS as possible and MCTS does not consider aerosol scavenging.

Table S1: MESSy submodels applied for the EMAC simulations. Note, that infrastructure and not used diagnostic submodels are not explicitly listed.

Submodel	Reference	Description
TRACER	Jöckel et al. (2008)	handling of trace species
TIMER	Jöckel et al. (2010)	handling of events and clock
IMPORT	Kerkweg and Jöckel (2015)	importing input and boundary data
TENDENCY	Eichinger and Jöckel (2014)	tendency diagnostics per process
AEROPT	Dietmüller et al. (2016)	aerosol optical properties
AIRSEA	Pozzer et al. (2006)	air sea exchange
ALBEDO	Nützel et al. (2024)	ground albedo
BIOBURN	Cabrera Perez (2017)	emissions from biomass burning
CLOUD	Lohmann and Roeckner (1996)	grid scale cloud processes
CLOUDOPT	Dietmüller et al. (2016)	optical properties of clouds
CONVECT	Tost et al. (2006b)	parameterised convection
CVTRANS	Tost et al. (2010)	convective tracer transport
DDEP	Kerkweg et al. (2006a)	dry deposition at the surface
GMXE	Pringle et al. (2010)	aerosol composition and microphysics
GWAVE	Roeckner et al. (2003)	gravity wave effects on circulation
JVAL	Sander et al. (2014)	photolysis
LNOX	Tost et al. (2007b)	lightning NO_x emissions
MECCA	Sander et al. (2005) and Sander et al. (2019)	gas phase chemistry
MSBM	Jöckel et al. (2010)	polar stratospheric clouds
OFFEMIS	Kerkweg et al. (2006b)	emission data assignment
ONEMIS	Kerkweg et al. (2006b)	online emission calculations
ORBIT	Dietmüller et al. (2016)	orbital parameters for radiation
OROGW	Roeckner et al. (2003)	orographic gravity waves
QBO	Jöckel et al. (2006), Giorgetta and Bengtsson, 1999	QBO nudging
RAD	Dietmüller et al. (2016)	radiation calculations
SCAV	Tost et al. (2006a)	cloud chemistry and wet deposition
SCOUT	Jöckel et al. (2016)	single column diagnostic output
SEDI	Kerkweg et al. (2006a)	aerosol sedimentation
E5VDIFF	Roeckner et al. (2006)	boundary layer processes and mixing
SURFACE	Roeckner et al. (2006), Hagemann, 2002	surface processes
TBUDGET	Jöckel et al. (2016)	tracer budgeting
TNUDGE	Kerkweg et al. (2006b)	tracer nudging

S2 Scaling of the dissociation reactions

The scaling factors for the dissociation reactions are shown in Table S4 for the reference simulation and in Table S3 for the sensitivity study. The scaling factor choices were originally based on the scaling factors used in SCAV (Tost et al., 2006a; Tost et al., 2007a) and then adapted so that the MCTS mechanism is solvable. The scaling factors for the sensitivity simulations were chosen to take place at similar time scales as the upward transport. Future work is needed to determine realistic and computationally efficient scaling factors for the dissociation reactions.

Table S2: Scaling of the dissociation reactions used in the reference simulations.

reaction	scaling factor cloud droplet	scaling factor rain droplet
$SO_2 \rightleftharpoons HSO_3^- + H^+$	1.E2	1.E2
$HSO_3^- \rightleftharpoons SO_3^{2-} + H^+$	1.E3	1.E3
$H_2SO_4^- \rightleftharpoons HSO_4^- + H^+$	1.E4	1.E4
$HSO_4^- \rightleftharpoons SO_4^{2-} + H^+$	1.E-3	1.E-3
$HCl \rightleftharpoons HCl^- + H^+$	1.E-12 × 1.E-1	1.E-12 × 1.E-1
$HNO_3 \rightleftharpoons NO_3^- + H^+$	1.E-3	1.E-3
$H_2O \rightleftharpoons OH^- + H^+$	1.E8	1.E8
$CO_2 \rightleftharpoons HCO_3^- + H^+$	1.E4	1.E4
$HCOOH \rightleftharpoons HCOO^- + H^+$	1.	1.
$CH_3COOH \rightleftharpoons CH_3COO^- + H^+$	1.	1.
$NH_3 + H^+ \rightleftharpoons NH_4^+$	1.E3	1.E3

Table S3: Scaling of the dissociation reactions applied in the sensitivity simulations.

reaction	scaling factor cloud droplet	scaling factor rain droplet
$SO_2 \rightleftharpoons HSO_3^- + H^+$	1.E-6 × 1.E3	1.E-6 × 1.E3
$HSO_3^- \rightleftharpoons SO_3^{2-} + H^+$	1.E-2 × 1.E6	1.E-2 × 1.E6
$H_2SO_4^- \rightleftharpoons HSO_4^- + H^+$	1.E-9 × 1.E4	1.E-9 × 1.E4
$HSO_4^- \rightleftharpoons SO_4^{2-} + H^+$	1.E1 × 1.E-5	1.E1 × 1.E-5
$HCl \rightleftharpoons HCl^- + H^+$	1.E-19 × 1.E-1	1.E-18 × 1.E-1
$HNO_3 \rightleftharpoons NO_3^- + H^+$	1.E-15 × 1.E-3	1.E-14 × 1.E-3
$H_2O \rightleftharpoons OH^- + H^+$	1.E7 × 1.E8	1.E6 × 1.E8
$CO_2 \rightleftharpoons HCO_3^- + H^+$	1.E3 × 1.E3	1.E3 × 1.E3
$HCOOH \rightleftharpoons HCOO^- + H^+$	1.E2	1.E2
$CH_3COOH \rightleftharpoons CH_3COO^- + H^+$	1.E3	1.E3
$NH_3 + H^+ \rightleftharpoons NH_4^+$	1.E8 × 1.E3	1.E8 × 1.E3

S3 Additional information regarding the comparison of MCTS and EMAC

Table S4: Scavenging efficiencies based on MCTS and EMAC. The values are given using 997 hPa as inflow level and 140 hPa as outflow level.

species	EMAC	MCTS
HNO_3	0.5970	0.5684
SO_2	0.9647	0.9654
H_2O_2	0.9696	0.9828
HCHO	0.9797	0.9828

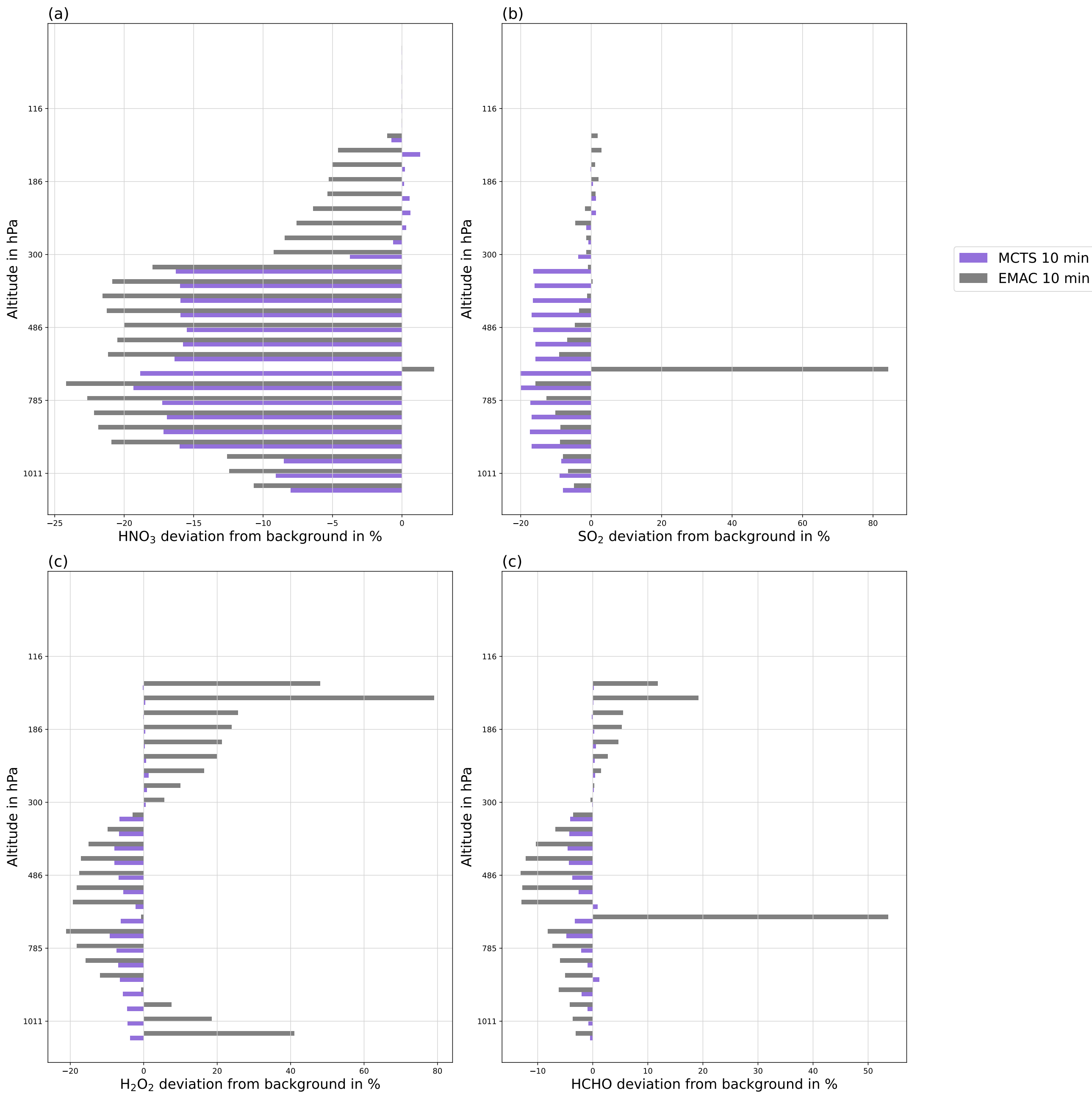

Figure S1: Deviations of MCTS and EMAC from the background for the soluble species. The differences from the background are shown for the MCTS simulation (purple) and for the convective tendencies in EMAC (grey) for HNO_3 (a), SO_2 (b), H_2O_2 (c) and HCHO (d).

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