Supplementary Tables

Table S 1: Selection of effective Henry law coefficients (H*) used in TM5-MP for the MOGUNTIA chemic	al scheme.
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Trace gas	H* (M atm ⁻¹)	ΔH R ⁻¹ (K)	Reference
CH ₃ OOH, n-C ₃ H ₇ OOH, i-C ₃ H ₇ OOH, CH ₃ COCH ₂ OH, C ₄ H ₉ OO	ОН, МЕКООН, 20 т 10 ²	5200	1
ISOPOOH, MVKOOH, MACROOH	2.9 x 10-	5200	1
CH ₃ ONO ₂ ,	2.0	4700	1
CH ₃ OONO ₂	2.0	4700	1
НСНО	3.2 x 10 ³	6800	1
CH ₃ OH	$2.0 \ge 10^2$	5600	1
НСООН	8.8 x 10 ³	6100	1
CH ₃ CH ₂ OOH	3.3	6000	1
CH ₃ CH ₂ ONO ₂	1.6	5400	1
HOCH ₂ CH ₂ OOH	1.7 x 10 ⁶	9700	1
HOCH ₂ CH ₂ ONO ₂	$3.9 \ge 10^4$		1
CH ₃ CHO	13	5900	1
CH ₃ COOH	8.3 x 10 ²	5300	1
HOCH ₂ CHO	$4.1 \ge 10^4$	4600	1
СНОСНО	4.19 x 10 ⁵	7500	1
CH ₃ CH ₂ OH	190	6400	1
CH ₃ COOH	$4.0 \ge 10^3$	6200	1
n-C ₃ H ₇ ONO ₂	1.1	5500	1
<i>i</i> -C ₃ H ₇ ONO ₂	0.78	5400	1
HOC ₃ H ₆ OOH	1.7 x 10 ⁶	9700	1
CH ₃ COCH ₃	27	5500	1
CH ₃ CH ₂ CHO	9.9	4300	1
CH ₃ COCHO	3.2 x 10 ³	7500	1
CH ₃ C(O)COOH	3.1 x 10 ⁵	5100	1
C4H9ONO2	1	5800	1
MEK	18	5700	1
MEKONO ₂	0.7	5200	1
CH ₃ COCOCH ₃	73	5700	1
ISOPONO ₂ , MACRONO ₂ , MVKONO ₂	$1.7 \ge 10^4$	9200	2
IEPOX	9.1 x 10 ⁴	6600	3
HPALD	2.3		1
MVK	26	4800	1
MACR	4.8	4300	1

¹ Sander (2015) and references therein

² Ito et al. (2007) for all biogenic hydroxy nitrates

 3 Browne et al. (2014), as for $\rm H_2O_2$

Trace gas	r _{soil}	r _{wat}	r _{snow/ice}	r _{mes}	r _{cut}
O ₃	400	2000	2000	1	105
CO	5000	105	105	5000	105
NO	105	105	105	500	105
NO ₂ /NO ₃	600	3000	3000	1	105
HNO ₃ /N ₂ O ₅	1	1	1	1	1
H ₂ O ₂ , IEPOX	80	72	80	1	105
SO ₂	100	1	1	1	105
CH ₃ ONO ₂ , CH ₃ OONO ₂ , CH ₃ C(O)OONO ₂ , <i>n</i> -C ₃ H ₇ ONO ₂ ,	2004	205	2204	1	105
<i>i</i> -C ₃ H ₇ ONO ₂ , C ₄ H ₉ ONO ₂ , MEKONO ₂ , ISOPONO ₂	3994	293	3394	1	10-
CH ₃ CHO, C ₂ H ₅ CHO, CH ₃ C(O)CH ₃ , CH ₃ C(O)C(O)CH ₃ ,	105	200	105	200	105
HOCH ₂ C(O)CH ₃ , MEK, MVK, MACR, HPALD	105	300	105	200	105
HCHO, CH ₃ COCHO, CHOCHO, HOCH ₂ CHO,	1666	254	1666	1	105
CH3OOH, CH3OH, HCOOH, CH3CH2OOH, CH3CH2OH, CH3COOH, n-					
C ₃ H ₇ OOH, i-C ₃ H ₇ OOH, CH ₃ C(O)CH ₂ OOH,	2(50	202	2(50	1	105
<i>n</i> -C ₃ H ₇ OOH, <i>i</i> -C ₃ H ₇ OOH, HOC ₃ H ₆ OOH, CH ₃ C(O)COOH, C ₄ H ₉ OOH,	3030	293	3030	1	10-
MEKOOH, MVKOOH, MACROOH, CH3C(O)OOH, ISOPOOH					
NH ₃	100	1	105	1	105

Table S 2: Soil, water, snow/ice and mesophyl resistances (s m⁻¹) used in TM5-MP for the CB05 and MOGUNTIA chemical schemes.

Table S 3: TM5-MP performance calculations of the mCB05(EB1), mCB05(KPP) and MOGUNTIA configurations for the different components, i.e. transport (advection in the x-, y- and z-directions along with the vertical transport), the chemistry as well as all other procedures contribution simulated years per day (SYPD), and the core-hours per simulated years (CHPSY) using a) 360 cores, and b) 450 cores. Timings are in seconds changes are in %. In parentheses, the runtime and the SYPD without the meteorology reading are also presented. All simulations have been perfor in the ECMWF CRAY XC40 high-performance computer facility.

360 cores			Transpor	t		Chamistry	Other	Runtime	SVPD	C
Configuration	Advx	Advy	Advz	Vertical	Total	Circuinstry	Other	Kuntinie	5110	C
CB05(EBI)	1322	948	165	364	2799	3338	3925	10062 (6723)	0.73 (1.10)	1
CB05(KPP)	1312	934	165	362	2773	5301	4222	12296 (9105)	0.60 (0.81)	1
MOGUNTIA	1892	1303	233	527	3955	8230	4680	16865 (13556)	0.44 (0.54)	2
% solver changes	-1%	-1%	0%	-1%	-1%	-1%	59%	8% (35%)	-18% (-26%)	
% chemistry scheme changes	44%	40%	41%	46%	43%	43%	55%	11% (49%)	-27% (-33%)	

b)

a)

450 cores			Transpor	t		Chomistry	Other	Duntimo	SVBD	
Configuration	Advx	Advy	Advz	Vertical	Total	Chemistry	Other	Kuntinie	5110	C
CB05(EBI)	1268	860	138	292	2558	2639	3687	8884 (5696)	0.83 (1.30)	1
CB05(KPP)	1292	853	133	300	2578	4320	4079	10977 (7733)	0.67 (0.95)	1
MOGUNTIA	1806	1126	193	423	3548	6526	4376	14450 (11211)	0.51 (0.65)	2
% solver changes	2%	-1%	-4%	3%	1%	64%	11%	24% (36%)	-19% (-27%)	
% chemistry scheme changes	40%	32%	45%	41%	38%	51%	7%	32% (45%)	-24% (-32%)	

Supplementary Equations

Statistics Formulas: Correlation coefficient (R; Eq. S1), mean normalized bias (MNB; Eq. S2), root mean square error (RMSE;
Eq. S3), mean normalized error (MNE; Eq. S4) and standard error (STD; Eq. S5) values have been calculated to compare the model calculations, where O_i and P_i stand for observations and predictions respectively and N is the number of pairs (observations, predictions) that are compared.

$$R = \begin{bmatrix} \frac{1}{N} \sum_{i=1}^{N} (O_i - \overline{O})(P_i - \overline{P}) \\ \overline{\sigma_o \sigma_P} \end{bmatrix}$$
(Eq. S1)

$$10 \quad NMB = \frac{\sum_{i=1}^{N} (M_i - O_i)}{\sum_{i=1}^{N} O_i} \times 100$$
(Eq. S2)

$$RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (P_i - O_i)^2}$$
(Eq. S3)

$$NME = \frac{\sum_{i=1}^{N} |M_i - O_i|}{\sum_{i=1}^{N} O_i} \times 100$$
(Eq. S4)

$$STD = \frac{\sqrt{\frac{1}{N} \sum_{i=1}^{N} (O_i - \overline{O})^2}}{\sqrt{N}}$$
(Eq. S5)

Supplementary Figures



a)

5

Figure S1: Comparison of simulated a) tropospheric NO₂ columns with OMI retrievals from the QA4ECV dataset and b) simulated total CO columns with MOPITT retrievals (vers. MOP02J V008) for the year 2006. Green, orange, and blue bars show the comparison of OMI with the MOGUNTIA, mCB05(KPP), and mCB05(EBI) chemistry mechanisms, respectively: Pearson correlation coefficient (top left), root mean square error (top right), mean bias (measurement minus model, bottom left), and

normalized mean bias (measurement minus model, bottom right) are given for both daily (D) and yearly (Y) averages per model

10

grid cell.

























Figure S 1: Comparison of monthly mean surface O₃ observations (black dots) in ppb with model results (red-line for mCB05(EBI), green-line for mCB05(KPP) and blue-line for MOGUNTIA) at various stations around the globe, as obtained from the European Monitoring and Evaluation Programme (EMEP; <u>http://www.emep.int</u>) and the World Data Centre for Greenhouse Gases (WDCGG; <u>http://ds.data.jma.go.jp/gmd/wdcgg/introduction.html</u>), for the year 2006.









Figure S 2: Comparison of monthly mean ozone sonde observations (black line) in ppb with model results (red-line for mCB05 configuration using the EBI solver, green-line for mCB05 configuration using the solver as generated by the KPP software and blue-line for MOGUNTIA configuration) at various stations around the globe, as obtained from the World Data Centre for Greenhouse Gases (WDCGG; https://gaw.kishou.go.jp), for the year 2006.



5 Figure S 3: Monthly mean comparisons of TM5-MP UTLS O₃ (top) and CO (bottom) mixing ratios (ppb) for the two chemistry schemes; mCB05(KPP) (blue line) and MOGUNTIA (red line), sampled at the measurement place and time against MOZAIC flight data (black line) between Frankfurt (50.0° N, 8.6° E) and Windhoek (22.5° S, 17.7° E) for April (left column) and October 2006 (right column). Data at pressures (P) lower than 300 hPa has been filtered out.















•	•	OBS	••	mCB05(EBI)	++	mCB05(KPP)		MOGUNTIA
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Figure S 4: Comparison of monthly mean surface CO flask measurements (black dots) in ppb with model results (red-line for mCB05(EBI), green-line for mCB05(KPP) and blue-line for MOGUNTIA) at various stations around the globe, as obtained from NOAA database, for the year 2006.











Figure S 5: Comparison of monthly mean surface C_2H_6 flask measurements (black dots) in ppb with model results (red-line for mCB05(EBI), green-line for mCB05(KPP) and blue-line for MOGUNTIA) at various stations around the globe, as obtained from NOAA database, for the year 2006.









• • OBS --- mCB05(EBI) +-- mCB05(KPP) - - MOGUNTIA

Figure S 6: Comparison of monthly mean surface propane flask measurements (black dots) in ppb with model results (red-line for mCB05(EBI), green-line for mCB05(KPP) and blue-line for MOGUNTIA) at various stations around the globe, as obtained from NOAA database, for the year 2006.











OBS mCB05(EBI) mCB05(KPP) MOGUNTIA •---• +---+ - -

Figure S 7: Comparison of TM5-MP vertical profiles (in km) of C₂H₆ against aircraft observations (black line) in ppt with model results (red-line for mCB05(EBI), green-line for mCB05(KPP) and blue-line for MOGUNTIA), using co-located model output for 2006 sampled at the measurement times; error bars indicate the standard deviation. The numbers on the right vertical axis indicate the number of available measurements.











Figure S 8: Comparison of TM5-MP vertical profiles (in km) of C₃H₈ against aircraft observations (black line) in ppt, with model results (red-line for mCB05(EBI), green-line for mCB05(KPP) and blue-line for MOGUNTIA), using co-located model output for 2006 sampled at the measurement times; error bars indicate the standard deviation. The numbers on the right vertical axis indicate the number of available measurements.









Figure S 9: Comparison of TM5-MP vertical profiles (in km) of C₂H₄ against aircraft observations (black line) in ppt, with model results (red-line for mCB05(EBI), green-line for mCB05(KPP) and blue-line for MOGUNTIA), using co-located model output for 2006 sampled at the measurement times; error bars indicate the standard deviation. The numbers on the right vertical axis indicate the number of available measurements.









\rightarrow OBS \rightarrow mCB05(EBI) \rightarrow mCB05(KPP) $-$ MOGUNT	↔ obs	← mCB05(EBI)	← mCB05(KPP)		MOGUNTIA
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Figure S 10: Comparison of TM5-MP vertical profiles (in km) of C₃H₆ against aircraft observations (black line) in ppt, with model results (red-line for mCB05(EBI), green-line for mCB05(KPP) and blue-line for MOGUNTIA), using co-located model output for 2006 sampled at the measurement times; error bars indicate the standard deviation. The numbers on the right vertical axis

5 indicate the number of available measurements.

Supplementary References

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