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Supplement of

CESM/CAM5 improvement and application: comparison and evaluation of updated CB05_GE and MOZART-4 gas-phase mechanisms and associated impacts on global air quality and climate

J. He et al.

Correspondence to: Y. Zhang (yang_zhang@ncsu.edu)

Supplementary Material

Table S1. Geometric standard deviations (σ_g) and dry diameter size ranges for MAM7 modes

MAM7	σ_g[1]	D_g (μm)[2]	Size Range (μm)
Aitken	1.6	0.026	0.0087-0.052
Accumulation	1.8	0.11	0.0535-0.44
Primary Carbon	1.6	0.05	0.01-0.1
Fine Sea Salt	2.0	0.2	0.05-1.0
Fine Dust	1.8	0.1	0.05-0.5
Coarse Sea Salt	2.0	2.0	1.0-4.0
Coarse Dust	1.8	1.0	0.5-2.0

[1] σ_g: geometric standard deviation;

[2] D_g: initial geometric mean diameter used in this work; it varies as the number and total dry and wet volume change

Table S2 Reaction pathways and coefficients of TPAN in MOZART-4x and CB05_GE[1]

MOZART-4x[2]	CB05_GE[3]
[4]PAN + hv →→ .6*CH_3CO_3 + .6*NO_2 + .4*CH_3O_2 + .4*NO_3 + .4*CO_2	[4]PAN + hv → C_2O_3 + NO_2
[4]MPAN + hv → MCO_3 + NO_2	[4]PANX + hv → C_XO_3 + NO_2
CH_3CO_3 + NO_2 + M → PAN + M; [5]troe: $k_o = 9.70 \times 10^{-29}$ (300/T)$^{6.50}$, $k_i = 9.30 \times 10^{-12}$ (300/T), f = 0.60	C_2O_3 + NO_2 → PAN; [5]fall: $k_o = 2.7 \times 10^{-28}$ (300/T) $^{7.1}$, $k_i = 1.2 \times 10^{-11}$ (300/T) $^{0.9}$, f= 0.30
PAN + M → CH_3CO_3 + NO_2 + M; [6]k(CH_3CO_3+ NO_2+M) × 1.111×10^{28} exp(14000/T)	PAN → C_2O_3 + NO_2 ; fall: $k_o = 4.9 \times 10^{-3}$ exp(-12100/T), $k_i = 5.4 \times 10^{16}$ exp(-13830/T), f = 0.30
MCO_3 + NO_2 + M → MPAN + M; 1.1×10^{-11} 300/T/[M]	C_XO_3 + NO_2 → PANX; fall $k_o = 2.7 \times 10^{-28}$ (300/T) $^{7.1}$, $k_i = 1.2 \times 10^{-11}$ (300/T) $^{0.9}$, f = 0.30
MPAN + M → MCO_3 + NO_2 + M; [6]k(MCO_3+NO_2+M) × 1.111×10^{28}* exp(14000/T)	PANX→ C_XO_3 +NO_2 ; fall $k_o = 4.9 \times 10^{-3}$ exp(-12100/T), $k_i = 5.4 \times 10^{-16}$ exp(-13830/T), f = 0.30
MPAN + OH + M → .5 * HYAC + .5 * NO_3 + .5 * CH_2O + .5 *HO_2 + 0.5 * CO_2 + M; troe : $k_o = 8.00 \times 10^{-27}$(300/T) $^{3.50}$, ki = 3.00×10^{-11}, f = 0.50	[7]PANX + OH → ALD2 + NO_2; 3.0×10^{-13}
[7]PAN + OH → CH_2O + NO_3; 4.00×10^{-14}	

[1] PAN: peroxyacetyl nitrate; TPAN: PAN+MPAN (methacryloyl peroxynitrate) for MOZART-4x and PAN+PANX (C3 and higher peroxyacyl nitrates) for CB05_GE.

[2] CH_3CO_3: acetylperoxy radical; NO_2: nitrogen dioxide; CH_3O_2: methylperoxy radical; NO_3: nitrate radical; CO_2: carbon dioxide; MCO_3: peroxy radical derived from abstraction reaction of hydroxyl radical (OH) with methacrolein; HYAC: hydroxyacetone; CH_2O: formaldehyde; HO_2: hydroperoxyl radical.

[3] C_2O_3: acetylperoxy radical; C_XO_3: C3 and higher acylperoxy radicals; ALD2: acetaldehyde.

[4] The photolysis rate constants are same for the four photolysis reactions, and based on the photolysis of PAN. The calculation of photolysis reaction rate is based on Lamarque et al. (2012).

[5] The rate constant k is based on

$$k = \left(\frac{k_o[M]}{1+k_o[M]/k_i}\right) f^G \quad G = [1 + (log\{k_0[M]/k_i)^{-2}]^{-1}$$

[6] The rate constants for this reaction are calculated online.

[7] The rate constants are constant, independent of temperature or pressure.

Table S3. Definitions of NO_y species in MOZART-4x and CB05_GE

	NO_y species[1]
MOZART-4x	N, NO, NO_2, NO_3, N_2O_5, HNO_3, HO_2NO_2, $CLONO_2$, $BRONO_2$, PAN, MPAN, $ISOPNO_3$, ONITR, aerosol nitrate
CB05_GE	NO, NO_2, NO_3, N_2O_5, HNO_3, PNA, $CLONO_2$, $BRONO_2$, HONO, PAN, PANX, NTR, aerosol nitrate

[1] NO: nitrogen monoxide; NO_2: nitrogen dioxide; NO_3: nitrate radical; N_2O_5: nitrogen pentoxide; HNO_3: nitric acid; HO_2NO_2: peroxynitric acid; $ClONO_2$: chlorine nitrate; $BrONO_2$: bromine nitrate; PAN: peroxyacetyl nitrate; ONIT: organic nitrate; MPAN: methacryloyl peroxynitrate; ISOPNO3: peroxy radical from the reaction of NO_3 with ISOP; ONITR: lumped isoprene nitrate; PNA: peroxynitric acid (HO_2NO_2); HONO: nitrous acid; PANX: higher peroxyacyl nitrates; NTR: organic nitrate.

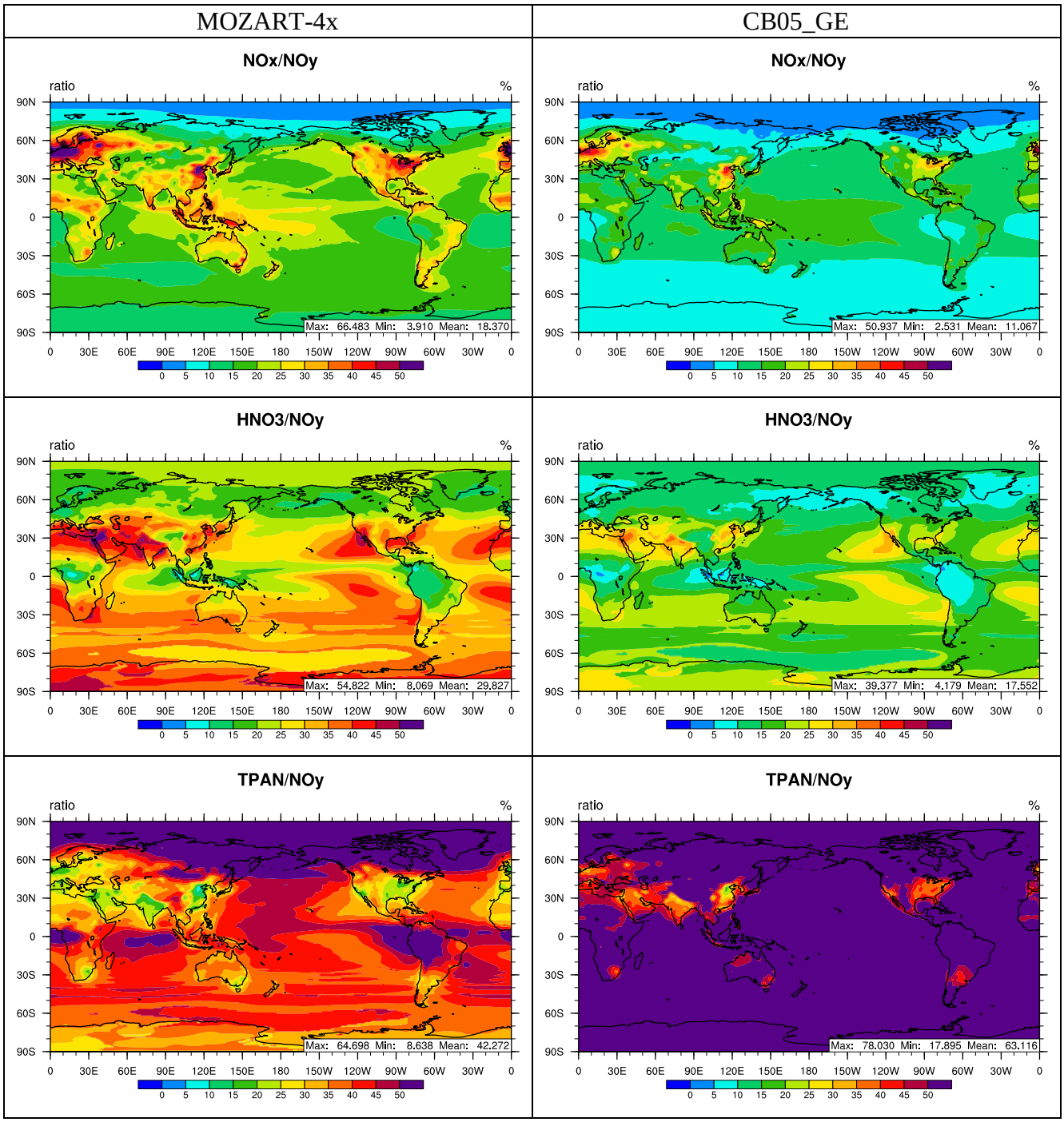

Figure S1. The dominant species in NO_y. For MOZART-4x, TPAN = PAN + MPAN; for CB05_GE, TPAN = PAN + PANX.

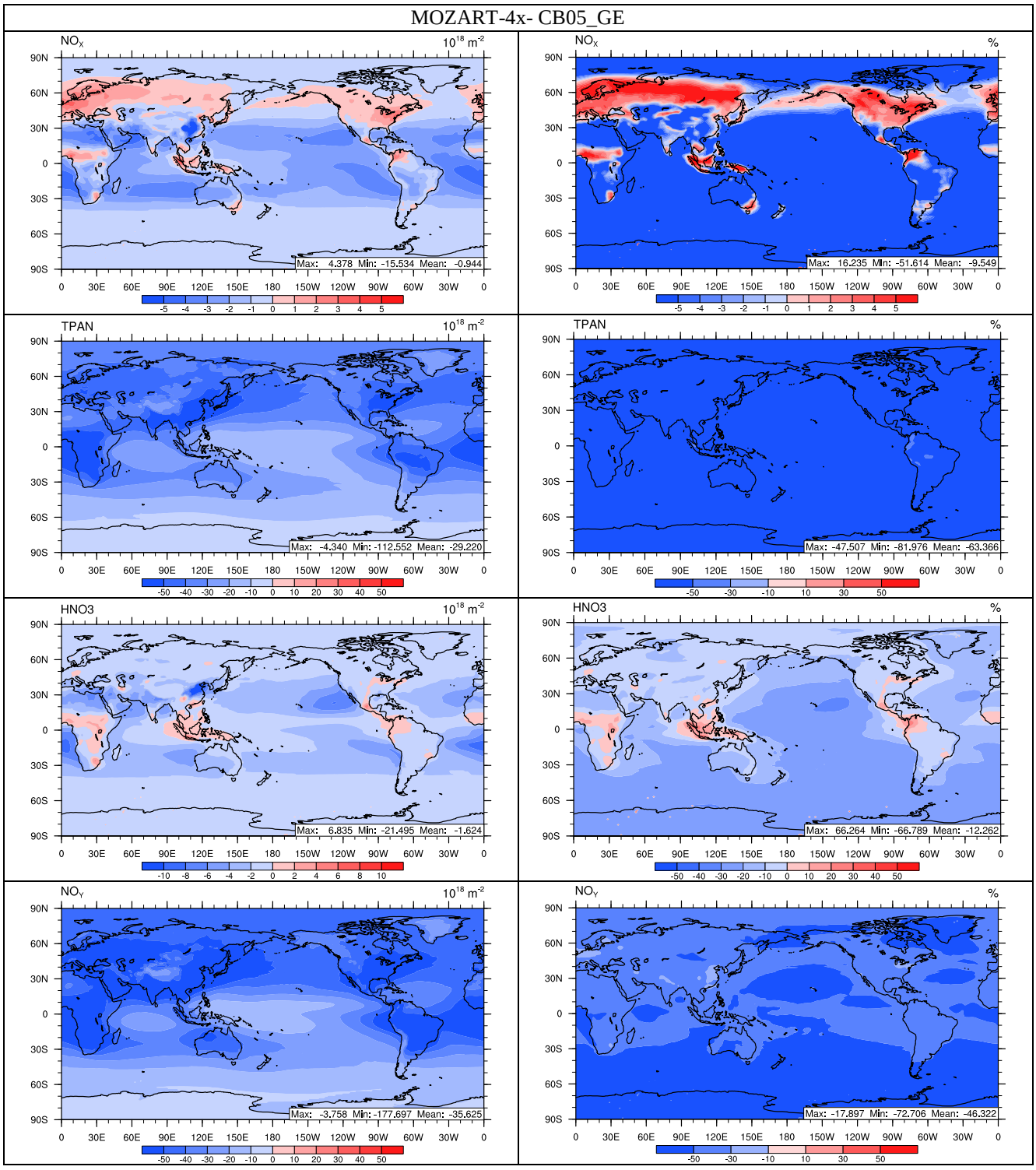

Figure S2. The absolute (left column) and relative (right column) differences for dominant NO_y species (in column concentration) between MOZART-4x and CB05_GE. For MOZART-4x, TPAN = PAN + MPAN; for CB05_GE, TPAN = PAN + PANX.

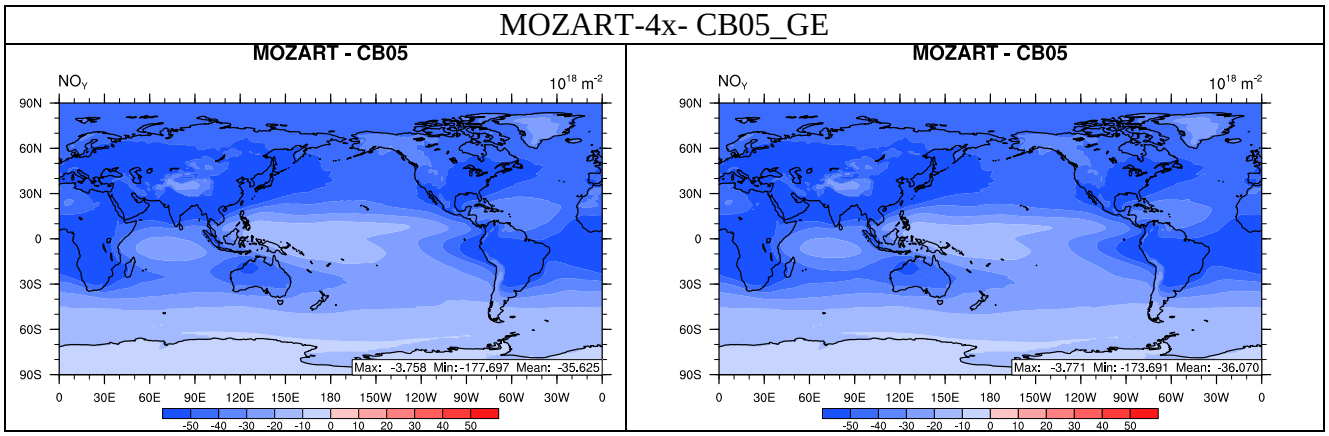

Figure S3. The absolute differences in NO_y column concentrations (left column: aerosol nitrate is not included; right column: aerosol nitrate is included) between MOZART-4x and CB05_GE.