Atmospheric Chemistry and Physics

Supporting Information for

Characterizing the Global Tropospheric Budget of NO_y

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Contents of this file

Introduction

This document includes text, figures, and tables that provide additional details about the GEOS-Chem model configuration, and a speciated model-observation comparison of NO_y.

Text S1: Correction to reactive nitrogen mass balance in GEOS-Chem

We add the following three species to KPP to better account for reactive nitrogen mass in GEOS-Chem:

- ALKONITA: Alkyl nitrate organic aerosol
- IDNITA: Lumped isoprene dinitrate-derived organic aerosol
- INDIOLN: Aerosol-phase IDNITA hydrolysis product

We replace IONITA as the product of the following reactions, which are the only sources of ALKONITA and IDNITA:

$$R4N2 \longrightarrow ALKONITA$$

$$IDN \longrightarrow IDNITA$$

The losses of these two species are also modeled after IONITA as follows:

$$ALKONITA \longrightarrow INDIOL + HNO_3$$

$$IDNITA \longrightarrow INDIOLN + HNO_3$$

Here, the hydrolysis of IDNITA produces a nitrogen-containing INDIOLN to conserve reactive nitrogen mass. There is no other production pathway for INDIOLN, and it is given the same properties as INDIOL.

Text S2: Species included in GEOS-Chem planeflight diagnostics

The GEOS-Chem planeflight diagnostic used to sample the model at ATom sampling times uses the following definitions for NO_y and RO_2:

- NOy = NO + NO2 + NO3 + HNO2 + HNO4 + HNO3 + PAN + PYPAN* + MPAN + PPN + N2O5
- RO2 = HO2 + MO2 + A3O2 + ATO2 + B3O2 + ETO2 + HPALD1OO + HPALD2OO + ICHOO + GCO3* + IAO2* + KO2 + MCO3 + PO2 + ACO3* + EO2* + ENCO3* + ENO2* + GLCO3* + ICNOO + IDHNBOO + IDHNDOO1 + IDNOO + IDHNDOO2 + IEPOXAOO + IEPOXBOO + IHOO1 + IHOO4 + IHPNBOO + IHPNDOO + IHPOO1 + IHPOO2 + IHPOO3 + INO2B + INO2D + ISOPNOO1 + ISOPNOO2 + LIMO2 + MACR1OO + MACRNO2 + MCROHOO + PIO2 + MVKOHOO + R4O2 + R4N1 + C4HVP1 + C4HVP2 + BRO2 + TRO2 + XRO2 + NRO2 + NICO3* + NIO2* + PYPO2* + RCO3

* Not present in v14.3.0 of GEOS-Chem

Text S3: Modeled NO_y families

We define the following families from the species in Table S1:

- XNOy = $BrNO_2$ + $BrNO_3$ + $ClNO_2$ + $ClNO_3$ + INO + IONO + $IONO_2$
- ΣPNs = PAN + PPN + BZPAN + MPAN + MPN
- ALKNIT = ETHN + ETNO3 + IPRNO3 + MENO3 + NPRNO3 + R4N2
- ALKNRO2 = R4N1
- ISOPNIT = ICN + 2 IDN + IHN1 + IHN2 + IHN3 + IHN4 + INPB + INPD + ITCN + ITHN + MACRNO2 + MCRHN + MCRHNB + MVKN
- ISOPNITOO = ICNOO + 2 IDNOO + IDHNBOO + IDHNDOO1 + IDHNDOO2 + IHPNBOO + IHPNDOO + INA + INO2B + INO2D + ISOPNOO1 + ISOPNOO2
- MTNIT = MONITS + MONITU + OLND + OLNN + HONIT
- C3NIT = ETHLN + PROPNN + PRPN
- C3NITOO = PRN1
- orgNIT = ALKNIT + ALKNRO2 + ISOPNIT + ISOPNITOO + MTNIT + C3NIT + C3NITOO + NPHEN
- AERNIT = ALKONITA* + AONITA + IONITA + 2 IDNITA* + MONITA + INDIOLN*

*Added to GEOS-Chem KPP to better account for nitrogen mass in organic nitrates.

Text S4: NO_y definition for global model output of NO_x:NO_y

The following species and families were included in the definition of NO_y to generate maps of NO_x:NO_y (see Text S3 and Table S1 for details):

NO_y = NO + NO2 + NO3 + HNO2 + HNO3 + HNO4 + NIT + NITs + 2 N2O5 + XNOy + ΣPNs + ALKNIT + ALKNRO2 + C3NIT + C3NITOO + ISOPNIT + ISOPNITOO + MTNIT + NPHEN + AERNIT

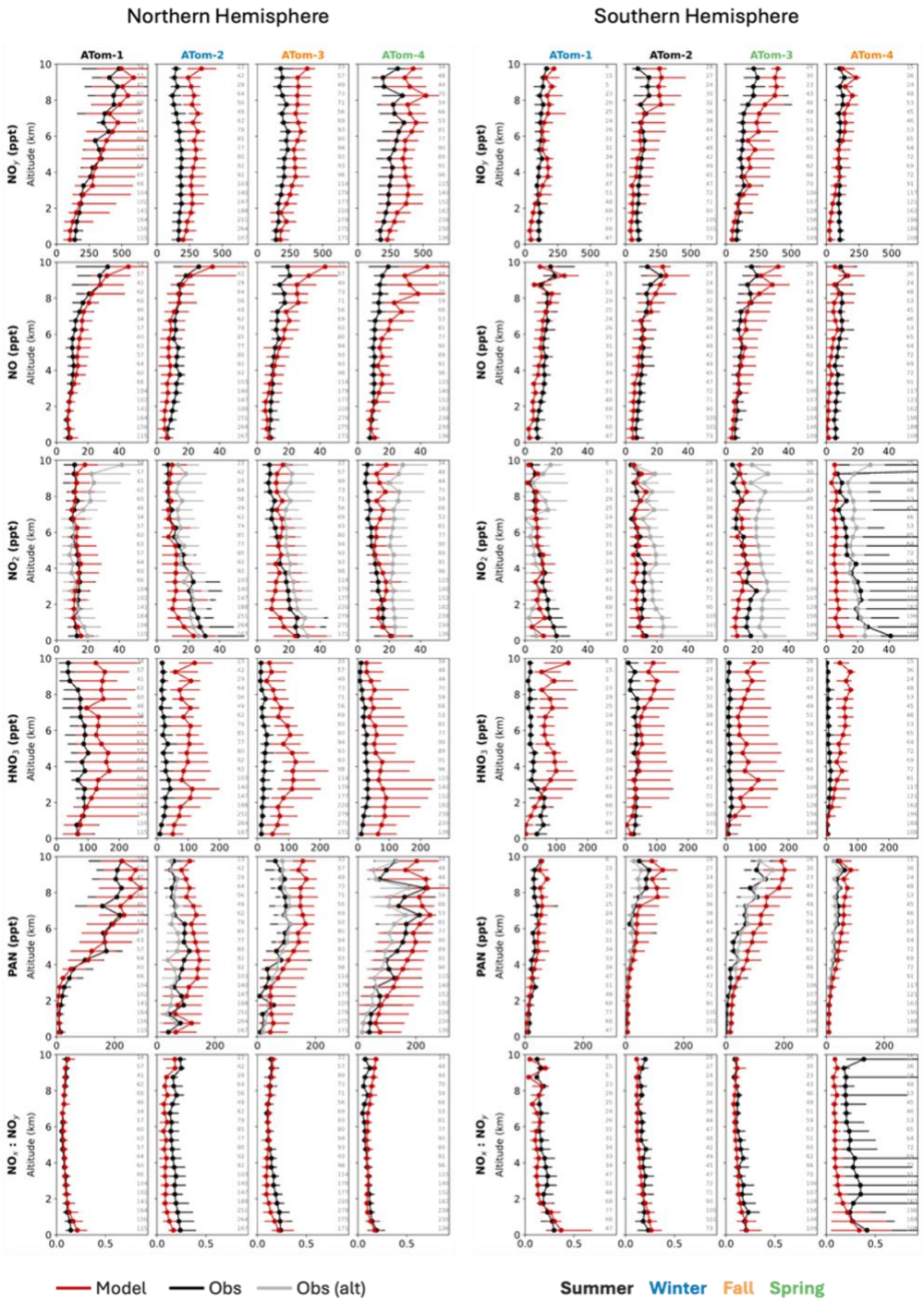

Figure S1: Modeled (red) and observed (black) median vertical profiles of NO_y species during ATom flights (from 2016-2018, see Section 2.2 for details). Horizontal bars show the interquartile range of values for each altitude bin, and values on the right side of the panels indicate the number of data points in each altitude bin. The NO_2 panel shows observations directly from the CL instrument (grey) in addition to the PSS-adjusted observations (black). The PAN panel shows additional observations taken by the GT-CIMS (grey). Campaign label colors indicate hemispheric seasons across the mission (see flight tracks in Figure 1).

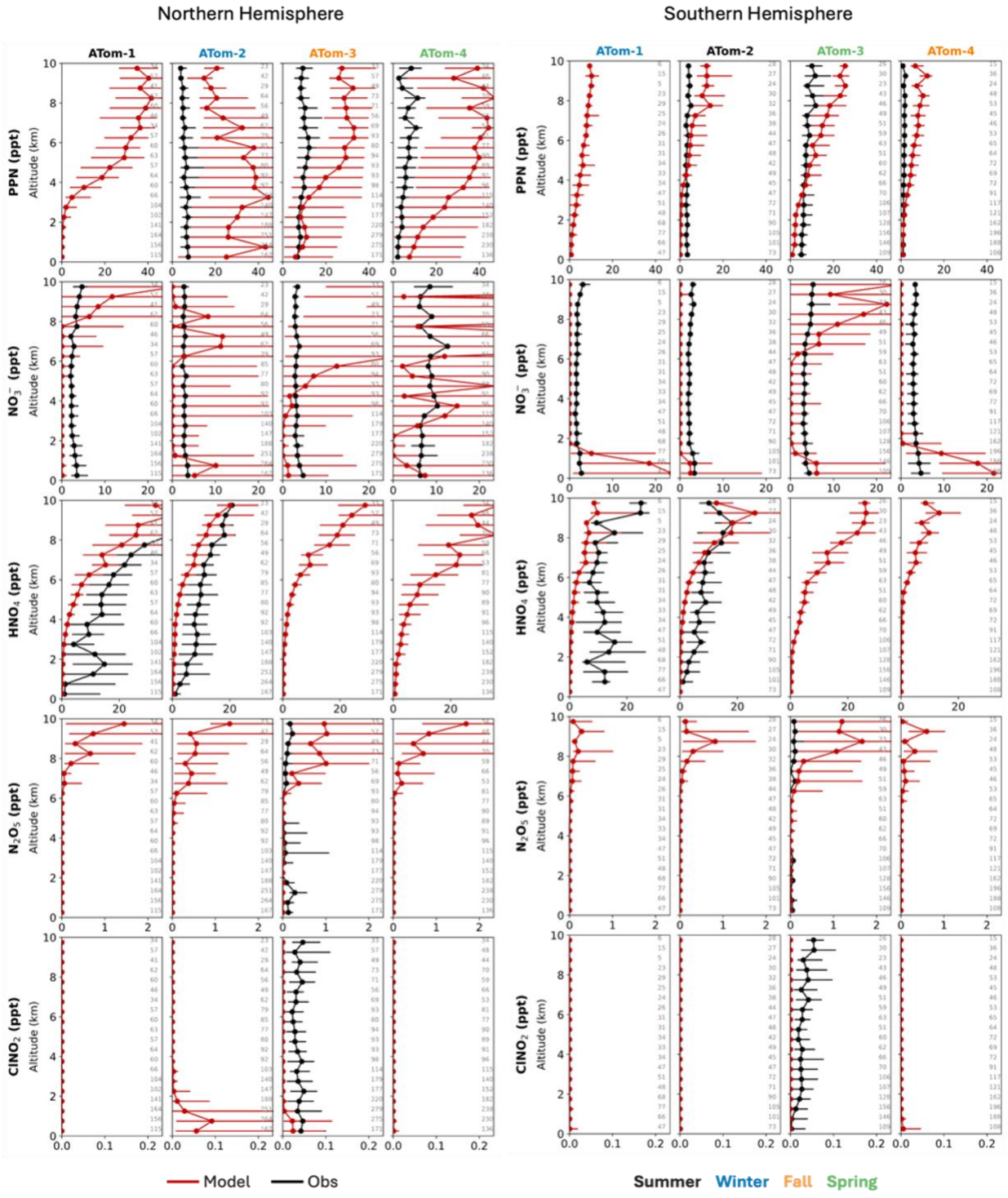

Figure S2: Modeled (red) and observed (black, where available) median vertical profiles of additional NO_y species during ATom flights (from 2016-2018, see Section 2.2 for details). Horizontal bars show the interquartile range of values for each altitude bin, and values on the right side of the panel indicate the number of data points in each altitude bin. Campaign label colors indicate hemispheric seasons across the mission (see flight tracks in Figure 1).

Table S1: List of relevant reactive nitrogen-containing species in GEOS-Chem

GC Name	Formula	FullName	MW
NO	NO	Nitrogen oxide	30.01
NO2	NO_2	Nitrogen dioxide	46.01
NO3	NO_3	Nitrate radical	62.01
N2O5	N_2O_5	Dinitrogen pentoxide	108.02
HNO2	HNO_2	Nitrous acid	47.01
HNO3	HNO_3	Nitric acid	63.01
HNO4	HNO_4	Peroxynitric acid	79.01
NIT	NO_3	Inorganic nitrates	62.01
NITs	NO_3^-	Inorganic nitrates on surface of sea salt aerosol	31.4
BrNO2	$BrNO_2$	Nitryl bromide	125.91
BrNO3	$BrNO_3$	Bromine nitrate	141.91
ClNO2	$ClNO_2$	Nitryl chloride	81.45
ClNO3	$ClNO_3$	Chlorine nitrate	97.45
INO	INO	Nitrosyl iodide	156.91
IONO	IONO	Nitryl iodide	172.91
IONO2	$IONO_2$	Iodine nitrate	188.91
PAN	$CH_3C(O)OONO_2$	Peroxyacetyl nitrate	121.06
PPN	$CH_3CH_2C(O)OONO_2$	Lumped peroxypropionyl nitrate	135.08
MPAN	$CH_2=C(CH_3)C(O)OONO_2$	Peroxymethacroyl nitrate (PMN)	147.1
MPN	$CH_3O_2NO_2$	Methyl peroxy nitrate	93.05
BZPAN	$C_7H_5O_5N$	Peroxybenzoylnitrate	183.12
ETHN	$HOCH_2CH_2ONO_2$	hydroxy-nitrooxy-ethane	107.07
ETNO3	$C_2H_5ONO_2$	Ethyl nitrate	91.08
IPRNO3	$C_3H_7ONO_2$	Isopropyl nitrate	105.11
MENO3	CH_3ONO_2	Methyl nitrate	77.05
NPRNO3	$C_3H_7ONO_2$	n-propyl nitrate	105.11
R4N2	RO_2NO	Lumped alkyl nitrate	119.1
R4N1	$C_4H_8NO_5$	Peroxy radical from R4N2	150.13
ETHLN	$CHOCH_2ONO_2$	Ethanal nitrate	105.06
PROPNN	$CH_3C(=O)CH_2ONO_2$	Propanone nitrate	119.08
PRPN	$O_2NOCH_2CH(OOH)CH_3$	Peroxide from PRN1	137.11
PRN1	$O_2NOCH_2CH(OO)CH_3$	Peroxy radical from propene + NO3	136.09
ICN	$C_5H_7NO_4$	Lumped isoprene carbonyl-nitrates	145.13
IDN	$C_5H_8N_2O_6$	Lumped isoprene dinitrates	192.15
IHN1	$C_5H_9NO_4$	Isoprene-d-4,1-hydroxynitrate	147.15
IHN2	$C_5H_9NO_4$	Isoprene-b-1,2-hydroxynitrate	147.15
IHN3	$C_5H_9NO_4$	Isoprene-b-4,3-hydroxynitrate	147.15
IHN4	$C_5H_9NO_4$	Isoprene-d-4,1-hydroxynitrate	147.15

INPB	$C_5H_9NO_5$	Lumped b-hydroperoxy isoprene nitrates	163.15
INPD	$C_5H_9NO_5$	Lumped d-hydroperoxy isoprene nitrates	163.15
ITCN	$C_5H_9NO_7$	lumped isoprene tetrafunctional carbonylnitrates	195.15
ITHN	$C_5H_{11}NO_7$	Lumped isoprene tetrafunctional hydroxynitrates	197.17
MACRNO2	$C_4H_6NO_7$	Product of MCRHN + OH	180.1
MCRHN	$HOCH_2C(ONO_2)(CH_3)CHO$	Nitrate from MACR	149.11
MCRHNB	$O_2NOCH_2C(OH)(CH_3)CHO$	Nitrate from MACR	149.11
MVKN	$HOCH_2CH(ONO_2)C(=O)CH_3$	Nitrate from MVK	149.12
ICNOO	$C_5H_8NO_7$	Peroxy radicals from ICN	194.14
IDHNBOO	$C_5H_{10}NO_7$	Peroxy radicals from INPB	196.16
IDHNDOO1	$C_5H_{10}NO_7$	Peroxy radicals from INPD	196.16
IDHNDOO2	$C_5H_{10}NO_7$	Peroxy radicals from INPD	196.16
IDNOO	$C_5H_9N_2O_6$	IDNOO	241.14
IHPNBOO	$C_5H_{10}NO_8$	Peroxy radicals from INPB	212.16
IHPNDOO	$C_5H_{10}NO_8$	Peroxy radicals from INPD	212.16
INA	$C_5H_8NO_4$	Alkoxy radical from INO2D	146.14
INO2B	$C_5H_8NO_5$	beta-peroxy radicals from isoprene + NO3	162.14
INO2D	$C_5H_8NO_5$	delta-peroxy radicals from isoprene + NO3	162.14
ISOPNOO1	$C_5H_{10}NO_7$	Peroxy radicals from IHN2	196.16
ISOPNOO2	$C_5H_{10}NO_7$	Peroxy radicals from IHN3	196.16
HONIT		2nd gen monoterpene organic nitrate	215
MONITS	$C_{10}H_{17}NO_4$	Saturated 1st gen monoterpene organic nitrate	215.28
MONITU	$C_{10}H_{17}NO_4$	Unsaturated 1st gen monoterpene organic nitrate	215.28
OLND	$C_{10}H_{16}NO_5$	Monoterpene-derived NO3-alkene adduct	230.27
OLNN	$C_{10}H_{16}NO_5$	Monoterpene-derived NO3 adduct	230.27
NPHEN	$C_6H_5NO_3$	Nitrophenols	139.11
ALKONITA		Aer-phase ALK4 organic nitrate from R4N2 uptake	119.1
IONITA		Aer-phase organic nitrate from isoprene precursors	14.01
IDNITA		Aer-phase organic nitrate from IDN	192.15
MONITA		Aer-phase organic nitrate from monoterpene precursors	14.01
AONITA	$C_6H_6O_6N$	Aerosol-phase organonitrates from aromatics	189.12
INDIOLN		Aerosol-phase IDN (IDNITA) hydrolysis product	147

***Table S1**: List of relevant reactive nitrogen-containing species in GEOS-Chem.*

Table S2: Full list of tracers added to KPP for NO_y chemistry

Tracer	Description	Source	Sink	Flux
PNO2O3	Dummy species to track production of NO2 from O3 + NO	NO	NO2	6106.36
LNO2NOz	Dummy species to track formation of NOz from NO2	NO2	NOz	1655.73
PNO2HO2	Dummy species to track production of NO2 from HO2 + NO	NO	NO2	1087.26
PMPNt	Dummy species to track thermal formation of MPN from NO2	NO2	PANs	654.85
LMPNt	Dummy species to track thermal loss of MPN to NO2	PANs	NO2	654.22
PN2O5t	Dummy species to track production of N2O5 from NO3 + NO2	NO2	N2O5	518.74
PN2O5t	Dummy species to track production of N2O5 from NO3 + NO2	NO3	N2O5	518.74
LN2O5t	Dummy species to track loss of N2O5 to NO3 + NO2	N2O5	NO2	511.86
LN2O5t	Dummy species to track loss of N2O5 to NO3 + NO2	N2O5	NO3	511.86
PHO2NO2	Dummy species to track production of HO2NO2	NO2	HNO4	276.79
LHNO4m	Dummy species to track loss of HNO4 bimolecular	HNO4	NO2	267.13
PNO2XO	Dummy species to track production of NO2 from XO + NO	NO	NO2	197.14
PPANt	Dummy species to track thermal formation of PAN	NO2	PANs	132.45
LPANt	Dummy species to track thermal loss of PAN	PANs	NO2	129.55
PNO3NO2	Dummy species to track production of NO3 from O3 + NO2	NO2	NO3	52.19
LNO3pNO2	Dummy species to track loss of NO3 by photolysis to form NO2 + O	NO3	NO2	46.24
PXNOyNO2	Dummy species to track production of XNOy from NO2	NO2	XNOy	41.38
LNO2HNO3	Dummy species to track production of HNO3 from NO2 + OH	NO2	HNO3	35.63
LHNO2p	Dummy species to track loss of HONO by photolysis	HNO2	NO	28.32
LNONOz	Dummy species to track formation of NOz from NO	NO	NOz	26.97
LXNOyNO3p	Dummy species to track loss of XNOy by photolysis to NO3	XNOy	NO3	25.05
PHNO2OH	Dummy species to track production of HONO from NO + OH	NO	HNO2	20.29
PPPNt	Dummy species to track thermal formation of PPN	NO2	PANs	19.02
LPPNt	Dummy species to track thermal loss of PPN	PANs	NO2	18.79
LNO3NO2	Dummy species to track loss of NO3 to NO2 by NOx cycling	NO3	NO2	14.54

LN2O5HNO3w	Dummy species to track loss of N2O5 from N2O5 + H2O = 2HNO3	N2O5	HNO3	9.31
PNO3NO2R	Dummy species to track production of NO3 from NO2 + R	NO2	NO3	7.25
LNO3pNO	Dummy species to track loss of NO3 by photolysis to form NO + O2	NO3	NO	5.95
PHNO3HALNOy	Dummy species to track production HNO3 from XNO3	XNOy	HNO3	5.60
PHNO3AERNIT	Dummy species to track production of HNO3 from IONITA, IDNITA, MONITA, and ALKONITA hydrolysis to INDIOL	AERNIT	HNO3	5.41
LXNOyNO2p	Dummy species to track loss of XNOy by photolysis to NO2	XNOy	NO2	5.33
LHNO4pNO2	Dummy species to track loss of HNO4 by photolysis to NO2	HNO4	NO2	4.88
PMPANt	Dummy species to track thermal formation of MPAN	NO2	PANs	4.86
LNITpHONO	Dummy species to track loss of NIT by photolysis to HONO	NIT	HNO2	4.81
LHNO4OH	Dummy species to track loss of HNO4 from oxidation by OH	HNO4	NO2	4.50
PHNO3NO3R	Dummy species to track production of HNO3 from R + NO3	NO3	HNO3	4.37
LXNOyNO2	Dummy species to track loss of XNOy to NO2	XNOy	NO2	4.20
PISOPNITNO	Dummy species to track production of ISOPNIT from NO	NO	ISOPNIT	4.08
LHNO3OH	Dummy species to track loss of HNO3 from HNO3 + OH = H2O + NO3	HNO3	NO3	3.85
LMPANt	Dummy species to track thermal loss of MPAN	PANs	NO2	3.76
LNO3NO2R	Dummy species to track loss of NO3 to NO2 by R + NO3	NO3	NO2	3.73
LNITspHONO	Dummy species to track loss of NITs by photolysis to HONO	NIT	HNO2	3.23
PIONITAup	Dummy species to track production of IONITA from ISOPNIT uptake	ISOPNIT	IONITA	3.16
PHNO3NO3up	Dummy species to track production of HNO3 from NO3 uptake	NO3	HNO3	2.99
LNO3INRO2	Dummy species to track loss of NO3 to form ISOPNRO2	NO3	ISOPNRO2	2.96
PISOPNITNRO2	Dummy species to track production of ISOPNIT from NRO2	ISOPNRO2	ISOPNIT	2.87
LNITpNO2	Dummy species to track loss of NIT by photolysis to NO2	NIT	NO2	2.41
LHNO3p	Dummy species to track loss of HNO3 by photolysis	HNO3	NO2	2.20
LN2O5HNO3c	Dummy species to track loss of N2O5 from N2O5 = 2HNO3 in cloud	N2O5	HNO3	2.17
PMTNITNO3	Dummy species to track production of MTNIT from MTP + NO3	NO3	MTNIT	2.12

PALKNITNO	Dummy species to track production of ALKNIT from RO2 + NO	NO	ALKNIT	1.98
LNO3HOx	Dummy species to track loss of NO3 to NO2 by HOx cycling	NO3	NO2	1.63
LNITspNO2	Dummy species to track loss of NITs by photolysis to NO2	NIT	NO2	1.62
LISOPNITNRO2	Dummy species to track loss of ISOPNIT to NRO2	ISOPNIT	ISOPNRO2	1.53
LXNOyNO3	Dummy species to track loss of XNOy to NO3	XNOy	NO3	1.42
PNO2NRO2ISOP	Dummy species to track production of NO2 from isoprene-NRO2	ISOPNRO2	NO2	1.27
PMONITAup	Dummy species to track production of MONITA from MTNIT uptake	MTNIT	MONITA	1.18
LPANp	Dummy species to track loss of PAN by photolysis	PANs	NO2	1.16
PALKONITAup	Dummy species to track production of ALKONITA from >= C4 alkyl nitrate uptake	ALKNIT	ALKONITA	1.10
LMPANOH	Dummy species to track loss of MPAN by OH to NO3	PANs	NO3	1.09
LISOPNITNO2p	Dummy species to track loss of ISOPNIT to NO2 by photolysis	ISOPNIT	NO2	1.02
LMTNITNO2	Dummy species to track loss of MTNIT to NO2	MTNIT	NO2	0.93
LMPNNO2p	Dummy species to track photolytic loss of MPN to NO2	PANs	NO2	0.74
LHNO2OH	Dummy species to track loss of HONO from oxidation by OH	HNO2	NO2	0.66
LN2O5p	Dummy species to track loss of N2O5 by photolysis	N2O5	NO2	0.56
LN2O5p	Dummy species to track loss of N2O5 by photolysis	N2O5	NO3	0.56
LNO2up	Dummy species to track production of HNO3 and HONO from NO2 uptake	NO2	HNO2	0.54
LNO2up	Dummy species to track production of HNO3 and HONO from NO2 uptake	NO2	HNO3	0.54
LPANp	Dummy species to track loss of PAN by photolysis	PANs	NO3	0.50
LISOPNITNO2	Dummy species to track loss of ISOPNIT to NO2	ISOPNIT	NO2	0.49
LC3NITNO2p	Dummy species to track loss of C3NIT to NO2 by photolysis	C3NIT	NO2	0.45
LALKNITNO2p	Dummy species to track loss of ALKNIT to NO2 by photolysis	ALKNIT	NO2	0.38
PHNO3N2O5s	Dummy species to track production of HNO3 from N2O5 + SALACL/SALCCL	N2O5	HNO3	0.37
PHNO3N2O5s	Dummy species to track production of HNO3 from N2O5 + SALACL/SALCCL	N2O5	XNOy	0.37
PC3NITINRO2	Dummy species to track production of C3NIT from ISOPNRO2	ISOPNRO2	C3NIT	0.36
PMTNITNO	Dummy species to track production of MTNIT from RO2 + NO	NO	MTNIT	0.36

PNPHENNO2	Dummy species to track production of NPHEN from BENZO + NO2	NO2	NPHEN	0.36
PHONITOx	Dummy species to track production of HONIT from MTNIT + OH or O3	MTNIT	MTNIT	0.36
PNO2ALKNRO2	Dummy species to track production of NO2 from ALKNRO2	ALKNRO2	NO2	0.31
LALKNITNRO2	Dummy species to track loss of R4N2 NIT to R4N1 RO2 by OH	ALKNIT	ALKNRO2	0.31
PNPHENNO3R	Dummy species to track production of NPHEN from R + NO3	NO3	NPHEN	0.30
PAONITAup	Dummy species to track production of AONITA from NPHEN uptake	NPHEN	AONITA	0.30
LHNO3NITs	Dummy species to track uptake of HNO3 on sea salt to NITs	HNO3	NIT	0.29
LNO3C3NRO2	Dummy species to track loss of NO3 to form C3NRO2	NO3	C3NRO2	0.29
LXNOyNOp	Dummy species to track loss of XNOy by photolysis to NO	XNOy	NO	0.26
PXNOyNO	Dummy species to track production of XNOy from NO	NO	XNOy	0.26
LHNO4pNO3	Dummy species to track loss of HNO4 by photolysis to NO3	HNO4	NO3	0.26
PISOPNITNO2	Dummy species to track production of ISOPNIT from NO2	NO2	ISOPNIT	0.23
PNO2C3NRO2	Dummy species to track production of NO2 from C3NRO2	C3NRO2	NO2	0.21
LALKNITNO2	Dummy species to track loss of ALKNIT to NO2 by OH	ALKNIT	NO2	0.20
LNO3NO	Dummy species to track loss of NO3 to NO by NOx cycling	NO3	NO	0.18
PBZPANt	Dummy species to track thermal formation of BZPAN	NO2	PANs	0.16
LBZPANt	Dummy species to track thermal loss of BZPAN	PANs	NO2	0.15
LNPHENNO2	Dummy species to track loss of NPHEN to NO2 by OH or NO3	NPHEN	NO2	0.15
LNPHENR4N1	Dummy species to track production of R4N1 from NPHEN	NPHEN	ALKNRO2	0.15
PALKNITNRO2	Dummy species to track production of R4N2 NIT from R4N1 RO2 by HO2	ALKNRO2	ALKNIT	0.14
PIDNITAup	Dummy species to track production of IDNITA from IDN uptake	IDN	IDNITA	0.11
LISOPNITC3NITp	Dummy species to track loss to ISOPNIT to C3NIT by photolysis	ISOPNIT	C3NIT	0.10
PC3NITNRO2	Dummy species to track production of C3NIT from C3NRO2	C3NRO2	C3NIT	0.10
PHONITNO3	Dummy species to track production of HONIT from MTNIT + NO3	NO3	MTNIT	0.08
LISOPNITNO3	Dummy species to track loss of ISOPNIT to NO3	ISOPNIT	NO3	0.08
PHNO2NPHENp	Dummy species to track production of HONO from NPHEN photolysis	NPHEN	HNO2	0.05

PINDIOLNh	Dummy species to track production of INDIOL from IDNITA hydrolysis	IDNITA	HNO3	0.05
PINDIOLNh	Dummy species to track production of INDIOL from IDNITA hydrolysis	IDNITA	INDIOLN	0.05
LC3NITNO2	Dummy species to track loss of C3NIT to NO2	C3NIT	NO2	0.05
PC3NITNO3	Dummy species to track production of C3NIT from NO3	NO3	C3NIT	0.04
LMPNNO3p	Dummy species to track photolytic loss of MPN to NO3	PANs	NO3	0.04
PNO3NO2O	Dummy species to track production of NO3 by NO2 + O	NO2	NO3	0.04
PHNO2HALNOy	Dummy species to track production of HONO from XNO2	XNOy	HNO2	0.04
PMPANMACRNO2	Dummy species to track production of MPAN from MACRNO2 + NO2	ISOPNIT	PANs	0.03
LISOPNITC3NIT	Dummy species to track loss to ISOPNIT to C3NIT	ISOPNIT	C3NIT	0.03
LMTNITNO2p	Dummy species to track loss of MTNIT to NO2 by photolysis	MTNIT	NO2	0.02
LC3NITNRO2	Dummy species to track loss of C3NIT to C3NRO2	C3NIT	C3NRO2	0.02
PNO2NO3	Dummy species to track production of NO2 from NO3 + NO3	NO3	NO2	0.01
LHNO3NIT	Dummy species to track uptake of HNO3 on sea salt to NIT	HNO3	NIT	0.01
LBZPANOH	Dummy species to track loss of BZPAN by OH to NO2	PANs	NO2	0.01
LHONITNO3	Dummy species to track loss of HONIT to NO3 by OH	MTNIT	NO3	0.01
LNO3NO2Br	Dummy species to track loss of NO3 + Br to NO2	NO3	NO2	0.00
LISOPNITNRO2p	Dummy species to track loss of ISOPNIT to NRO2 by photolysis	ISOPNIT	ISOPNRO2	0.00
PXNOyNO3	Dummy species to track production of XNOy from NO3	NO3	XNOy	0.00
PNITNO3up	Dummy species to track production of NIT by NO3 uptake	NO3	NIT	0.00
PNITsNO3up	Dummy species to track production of NITs by NO3 uptake	NO3	NIT	0.00
LNO3NO2O	Dummy species to track loss of NO3 to NO2 by NO3 + O	NO3	NO2	0.00
LXNOyNO	Dummy species to track loss of XNOy to NO	XNOy	NO	0.00
PHNO3N2O5	Dummy species to track production of HNO3 from N2O5 + HCl = ClNO2 + HNO3	N2O5	HNO3	0.00
PHNO3N2O5	Dummy species to track production of HNO3 from N2O5 + HCl = ClNO2 + HNO3	N2O5	XNOy	0.00

***Table S2**: Full list of tracers added to KPP for NO_y chemistry*

Table S3: Modeled tropospheric NO_y budget

Family	Species	Burden (Gg N)	Wet Dep (Tg N yr^{-1})	Dry Dep (Tg N yr^{-1})
NO_x	NO	30.38		
	NO2	103.46		1.86
	HNO3	303.22	18.80	19.77
pNO_3^-	NIT	89.97	5.57	0.66
	NITs	10.89	2.90	4.18
	HNO4	13.99		
	N2O5	8.30		0.40
	NO3	2.68		
	HNO2	1.26		
PANs	PAN	205.04	0.05	1.14
	PPN	37.59	0.00	0.23
	BZPAN	0.21	0.00	0.00
	MPAN	0.84	0.00	0.03
	MPN	9.92	0.00	
XNO_y	BrNO2	0.03		
	BrNO3	1.55		0.07
	ClNO2	0.45		0.00
	ClNO3	0.48		0.02
	INO	0.00		
	IONO	0.01	0.00	0.00
	IONO2	0.22	0.02	0.03
	NPHEN	0.13	0.00	0.01
ALKNIT	ETHN	0.35	0.02	0.01
	ETNO3	3.60		0.03
	IPRNO3	7.86		0.04
	MENO3	10.41		0.14
	NPRNO3	1.62		0.01
	R4N2	3.67	0.00	0.06
	R4N1	0.03		
C3NIT	ETHLN	0.08	0.01	0.01
	PROPNN	0.80	0.03	0.06
	PRPN	0.11	0.00	0.01
	PRN1	0.03		
ISOPNIT	ICN	0.50	0.05	0.04
	IHN1	0.09	0.01	0.01
	IHN2	0.29	0.02	0.07
	IHN3	0.20	0.02	0.04
	IHN4	0.03	0.00	0.00
	INPB	0.16	0.01	0.01
	INPD	0.19	0.02	0.01
	ITCN	0.23	0.02	0.05
	ITHN	0.53	0.04	0.06
	MACRNO2	0.00		
	MCRHN	0.03	0.00	0.01

	MCRHNB	0.05	0.00	0.01
	MVKN	0.30	0.02	0.04
	ICNOO	0.00		
	IDHNBOO	0.06		
	IDHNDOO1	0.00		
	IDHNDOO2	0.00		
	IHPNBOO	0.00		
	IHPNDOO	0.00		
	INA	0.00		
	INO2B	0.05		
	INO2D	0.04		
	ISOPNOO1	0.00		
	ISOPNOO2	0.00		
	IDN	0.11	0.00	0.02
	IDNOO	0.00		
MTNIT	HONIT	0.50	0.03	0.04
	MONITS	0.41	0.04	0.08
	MONITU	0.05	0.01	0.02
	OLND	0.06		
	OLNN	0.01		
AERNIT	ALKONITA	0.12	0.01	0.00
	IONITA	0.35	0.03	0.01
	IDNITA	0.01	0.00	0.00
	MONITA	0.13	0.01	0.01
	AONITA	3.93	0.27	0.03
	INDIOLN	0.64	0.05	0.01

Table S3: Global tropospheric budget of NO_y families, showing burdens, wet deposition, and dry deposition.