Quick Look at the NASA Atmospheric Tomography (ATom) Mission: Profiling and Model-Measurement Analysis

Michael Prather & the ATom Team

30 August 2016 Aura Science Team Meeting

NASA Atmospheric Tomography Mission:

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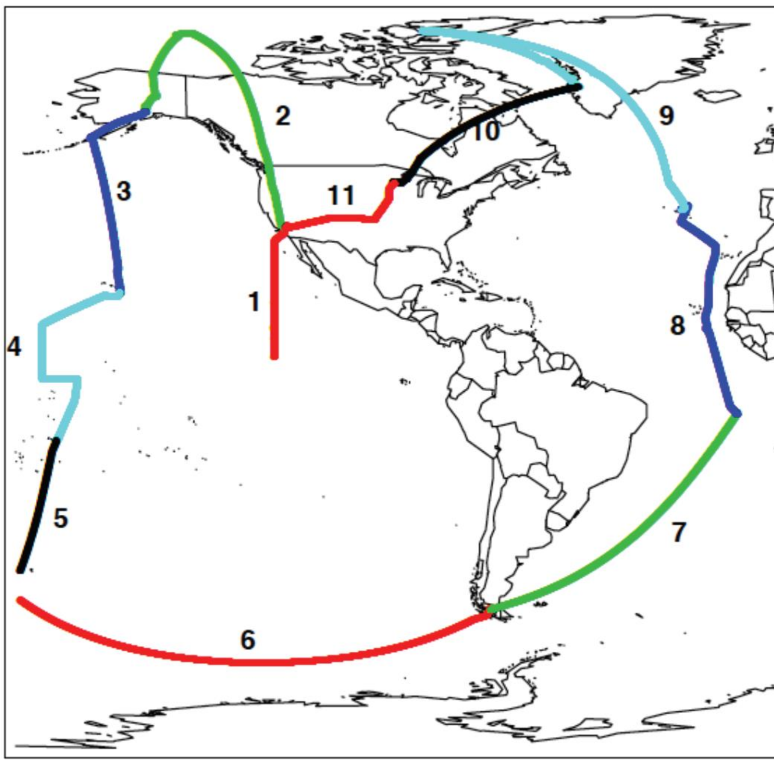
. . . cast of thousands

23 Aug 2016



The NASA EVS2 Atmospheric Tomography Mission (ATom):

A unique mission to test tropospheric chemical reactivity in chemistry-climate models.

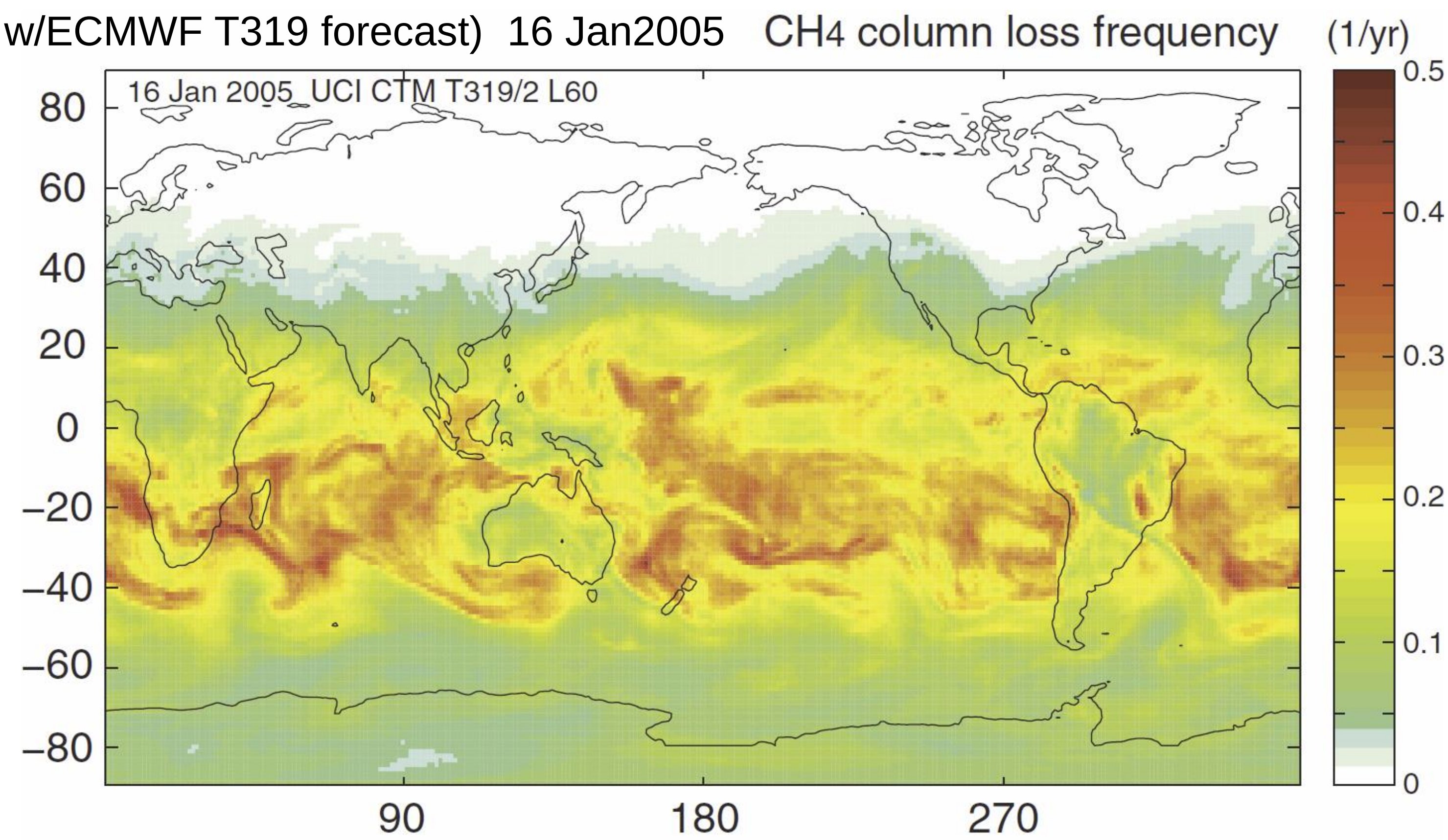
ATom establishes a single, contiguous global-scale data set that will be ***used to improve the representation of chemically reactive gases and short-lived climate forcers in global models of atmospheric chemistry and climate*.**

Statistical analysis of the air parcels in terms of key species (e.g., NOx, CH2O, H2O2) weighted by reactivity (P-O3, L-O3, L-CH4) provides a novel approach for evaluating the global chemistry-climate models.

Quantifying the heterogeneity of tropospheric chemistry

Our models predict rivers of CH_4 loss,
how can we see/measure them?

(UCI CTM run w/ECMWF T319 forecast) 16 Jan2005

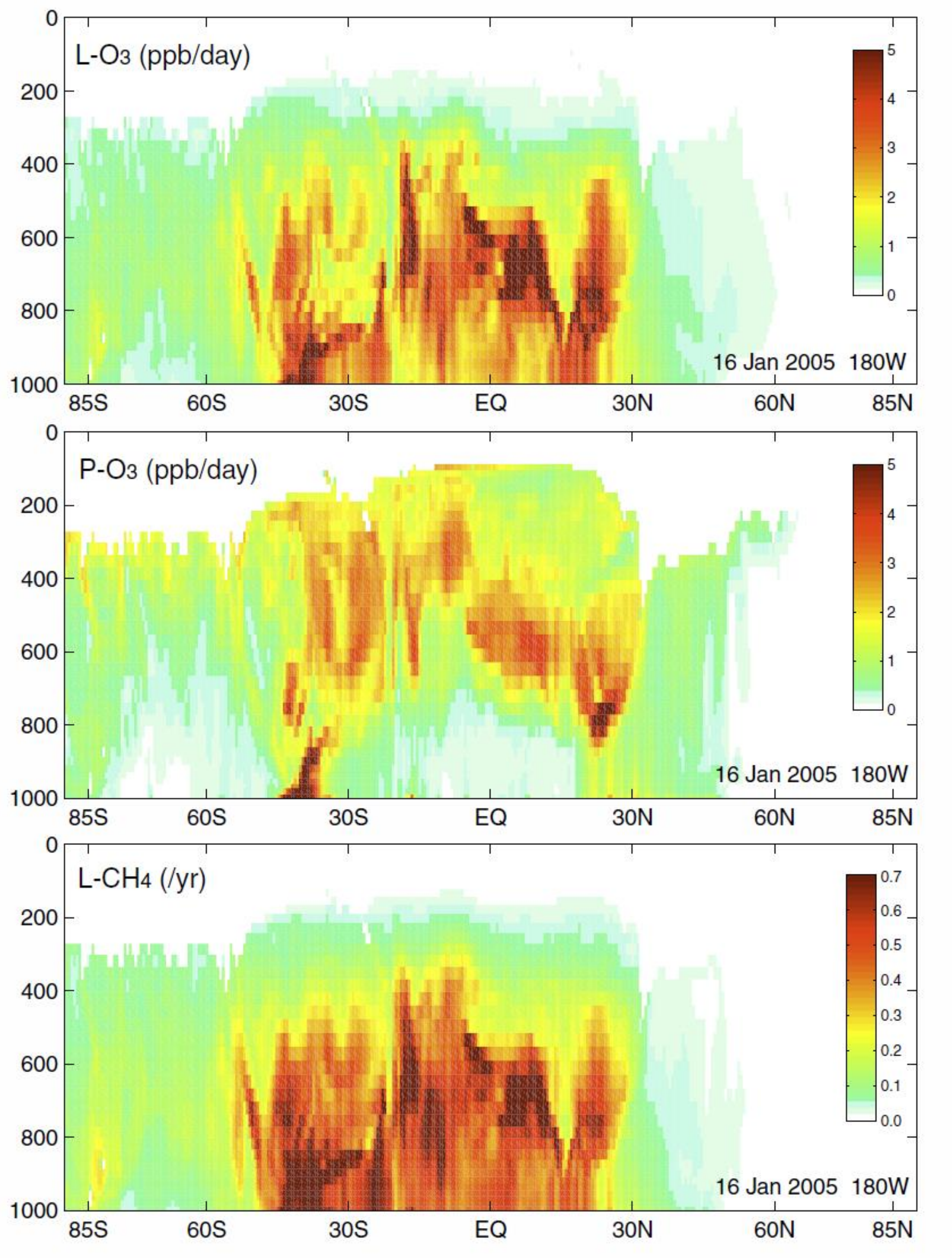


A Tomographic slice down the dateline shows large (daily) variability in UCI CTM modeled rates for

L-O$_3$

P-O$_3$

L-CH$_4$



When averaged over lat.-height bins, the slice is representative of the Pacific basin within ~15%

ATom measurements quantify *chemical reactivity*, and *identify and attribute the controlling species*:

- **Definitions**
  - ***Reactivity: rates of chemical reactions that transform trace gases and aerosols in the atmosphere, primarily the OH radical.***
  - ***Removal of CH_4*** *(+ many others): via* ***OH radical***
    - ***OH*** *+ CH_4 → CH_3 + H_2O*
  - ***Removal of tropospheric O_3: HO_2 and OH*** *radicals*
    - ***OH*** *+ O_3 → O_2 + HO_2* ***HO_2*** *+ O_3 → HO + O_2 +O_2* ***$O(^1D)$*** *+ H_2O → OH + OH*
  - ***Production of tropospheric O_3: NOx radicals (NO, NO_2)***
    - ***HO_2*** *+* ***NO*** *→ NO_2 + OH* ***RO_2*** *+* ***NO*** *→ NO_2 + RO* *➔ NO_2 +hv → NO + O → O_3*
  - ***<u>Chemical tendency</u> of tropospheric O_3:*** *extremely sensitive to tiny amounts of* ***HOx and NOx radical <u>precursors</u> (PAN, VOCs) ⇔ the big lever for highly dilute pollutants in the remote atmosphere.***

ATom strategy to Measure Reactivity –

- ***Radical precursors, sinks, and sunlight*** *control global reactivity:* ***CH_4, CO, H_2CO, HOOH, CH_3OOH, NOx*** *($NO+NO_2$),* ***HNO_4, PAN, O_3***.
  ➔***Priority*** *species for the core focus for ATom measurements.* 🡐

- ***ATom*** *applies its core measurements to generate* ***data-constrained models*** *of chemistry, clouds, etc., to compute:*
  - *the* ***24-hour mean reactivity at each point in the flight path***
  - *the* ***statistical distributions*** *of* ***reactive intermediates****.*

- ***Radical species*** *(****OH, HO_2, CH_3OO, NO, NO_2, O(^{1}D)****) individually fluctuate, instantaneously responding to sun angle, albedo, precursors, overhead O_3, clouds. ATom measures most of these*

➔ *checks on ATom-derived reactivity* 🡐.

- ***Tracers*** *(****CO, VOCs, S & N species, GHGs, ODSs****) fingerprint pollution influences.*

ATom approach to measurements, modeling, and analysis is now being tested with the global chemistry models used by the ATom modeling PIs:

Sarah Strode (Susan Strahan, Jose Rodriguez & others)
*(NASA GSFC **GMI**)*
Arlene Fiore & Lee Murray
*(**GEOS-Chem** & **GFDL AM3** & **GISS**)*
Jean-Francois Lamarque
*(NCAR CESM/**CAM5**)*
Michael Prather
*(**UC Irvine CTM**)*

Comparing the statistics of the 3D model grid cells (bigger than ATom air parcels) for both frequency of occurrence and reactivity in the way that ATom data will be used.

For the pre-ATom paper we are analyzing grid cells from the model as we would ATom air parcels. We all took Aug 16 (different years) as our reference data set.

Named 3-D (I,j,k) data sets.

Basic cell data (mixed)

1) AIR, Air in each cell (moles)
2) T, temperature (K), from either model C or Atom
3) q, water vapor (g/kg-air), ditto
4) p, mid-level pressure of cell (hPa), from model C
5) ATom-AIR, the size of the ATom air parcel used here (moles), not initialized with ATom data. Note that this is used only for w
6) STT, strat-trop tracer (e90, O3, or PV or something to split stra explain in metadata)

<u>Species (mole fraction)</u> Initial Values (or ATom Measurements)

7) O3
8) NOx = NO+NO2
9) HONO2
10) HO2NO2
11) C2H3NO5 = PAN
12) RONO2 (if any)
13) H2O2
14) CH3OOH
15) HCHO
16) C2H5OOH
17) CH3CHO = acetaldehyde
18) C3H6O = acetone
19) CO
20) C2H6
21) Alkanes (>C2)
22) Alkenes
23) Aromatics (benzene + …)
24) C5H8 = Isoprene

Derived / Integrated products (either ppb/day, /day, …)

25) L-CH4 (OH+CH4, but scale to 1800 ppb CH4, so get

26) P-O3 (HO2/RO2 + NO only)

27) L-O3 (O1d+H2O, OH+O3, HO2+O3 only)

28) dO3/dt = O3(24h) - O3(00h) as checksum for missin

29) J-O1D (/day)

30) J-NO2 (/day)

31) P-SO4 sulfate formation = OH+SO2, OH+DMS, …. (

32) P-SOA SOA formation = OH + VOCs (with potential

(ppt C /day)

ATom approach to measurements, modeling, and analysis is different from most chemistry missions.

Two Types of CCM runs: **C-runs** & A-runs

When calculating the reactivity within a grid cell of the standard (Eulerian) model – it includes air flowing through the box over 24 hours, mixing with parcels around it, emissions, vertical mixing through convection and precip scavenging, dry deposition.

All the normal processes a Chemistry-Climate or Chemistry-Transport Model (CCM/CTM).

We refer to this result from initialization and a free running CCM/CTM as the **C-runs**.

ATom approach to measurements, modeling, and analysis is different from most chemistry missions.

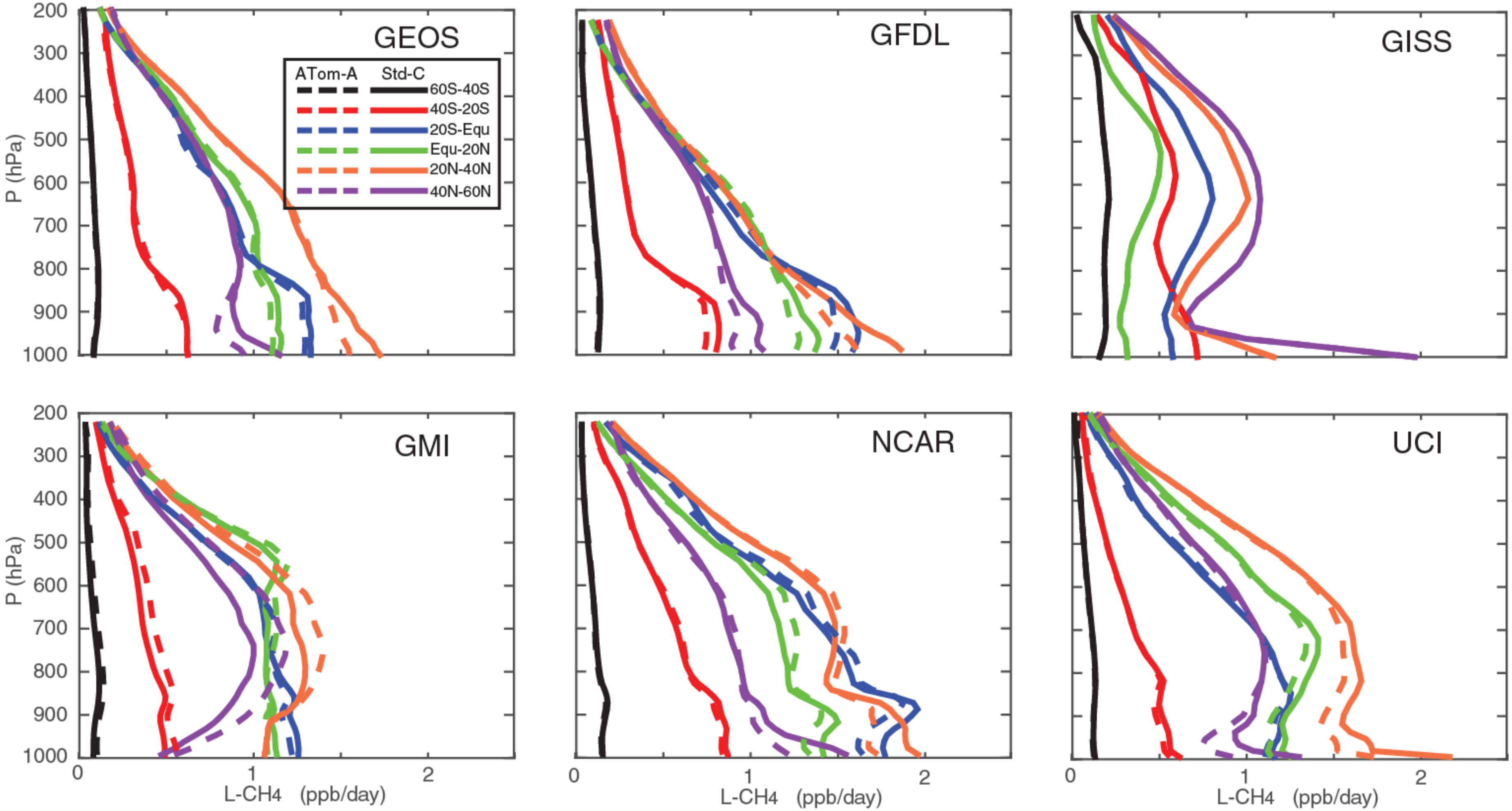
Two Types of CCM runs: C-runs & **A-runs**

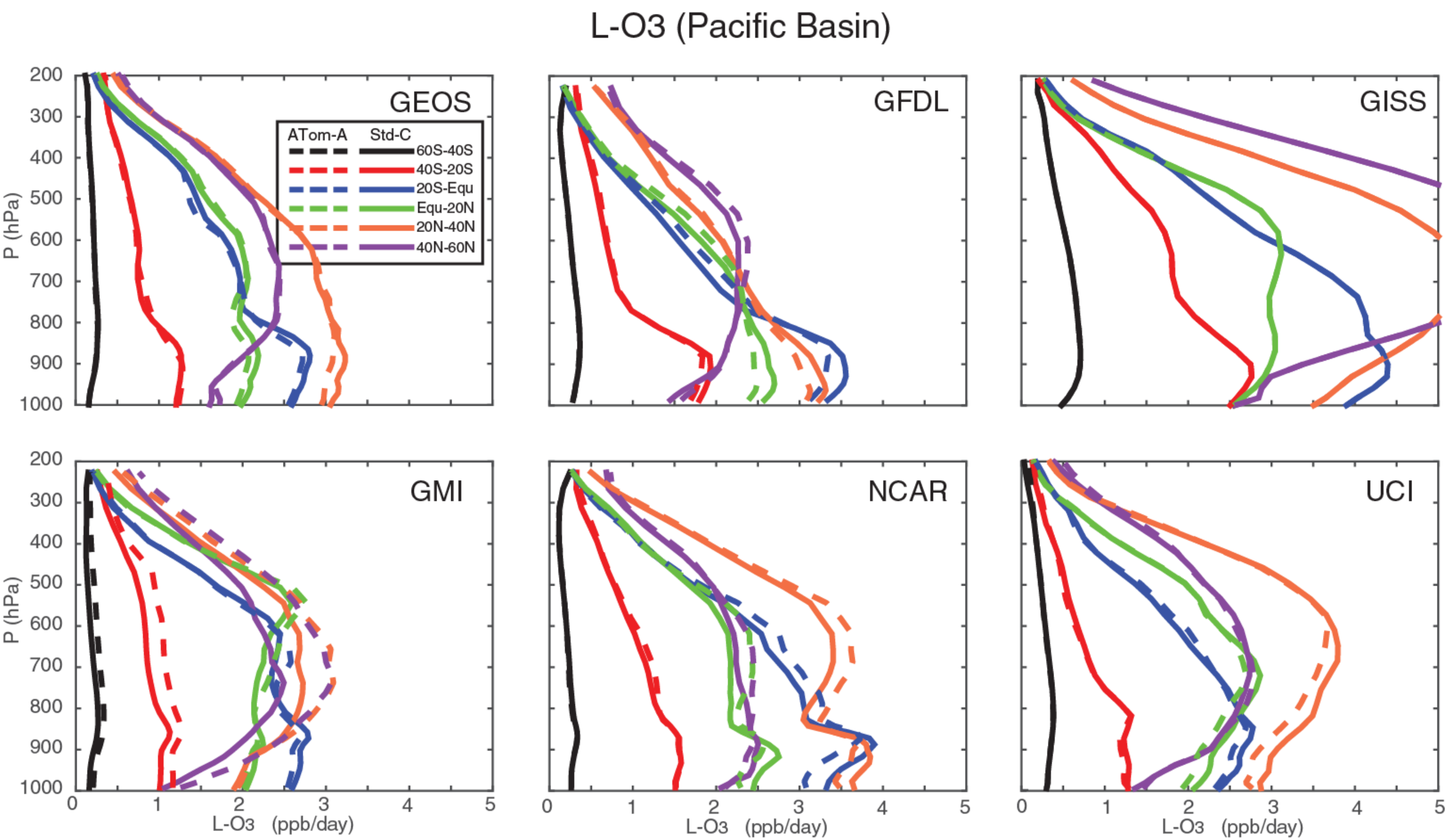
With an ***ATom initialization*** for some model grid cells, we need to ensure that the model's background tropospheric species (those cells not initialized by ATom) do not influence the results (except for overhead O_3).

Thus we must run in Lagrangian mode (no transport, no convection, no vertical mixing by precip or other) without emissions.

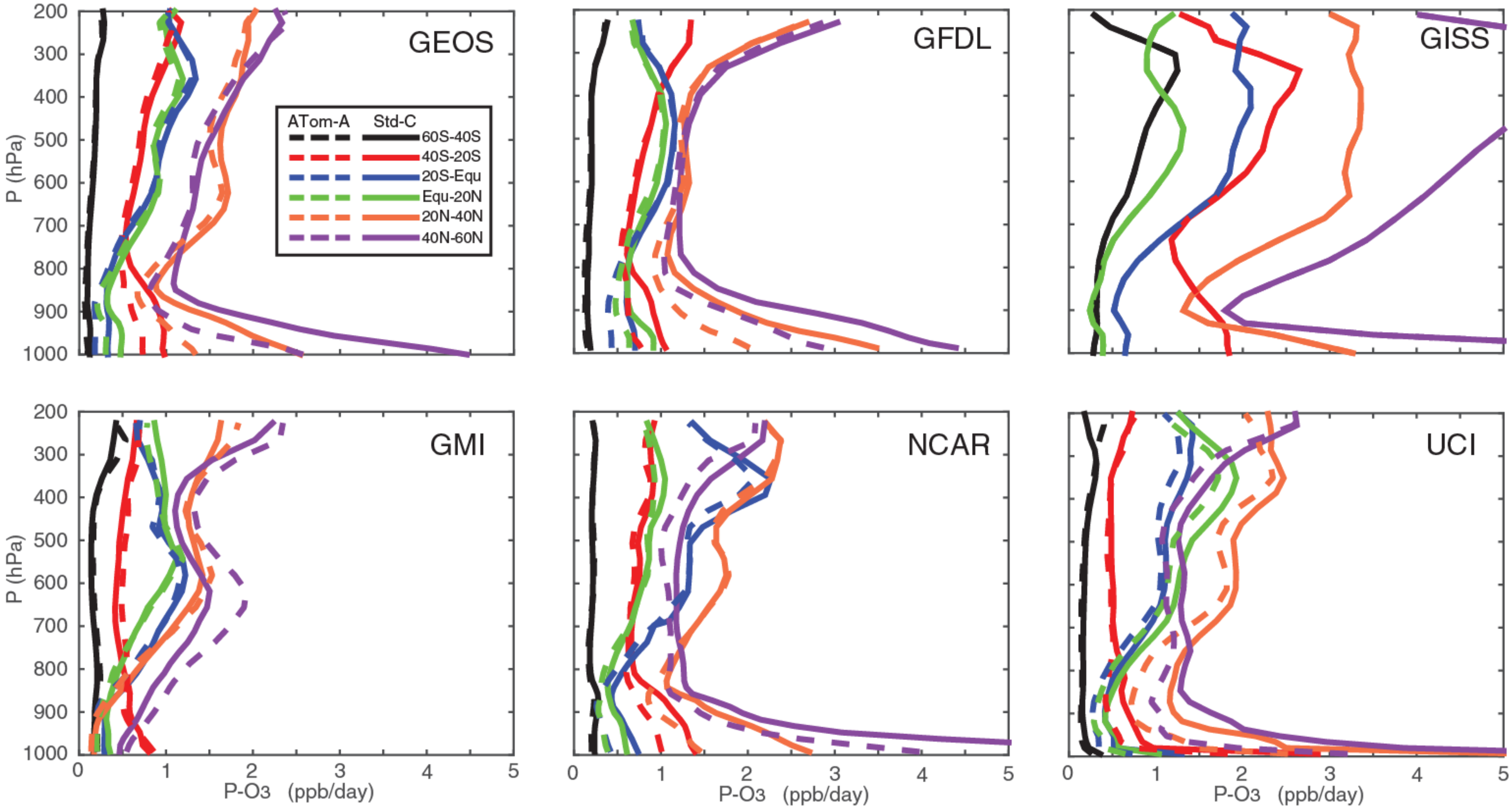
We refer to this result designed for eventual ATom initialization as the **A-runs**.

L-CH4 (Pacific Basin)




L-O3 (Pacific Basin)
GEOS
GFDL
GISS
GMI
NCAR
UCI
ATom-A
Std-C
60S-40S
40S-20S
20S-Equ
Equ-20N
20N-40N
40N-60N
P (hPa)
L-O3 (ppb/day)

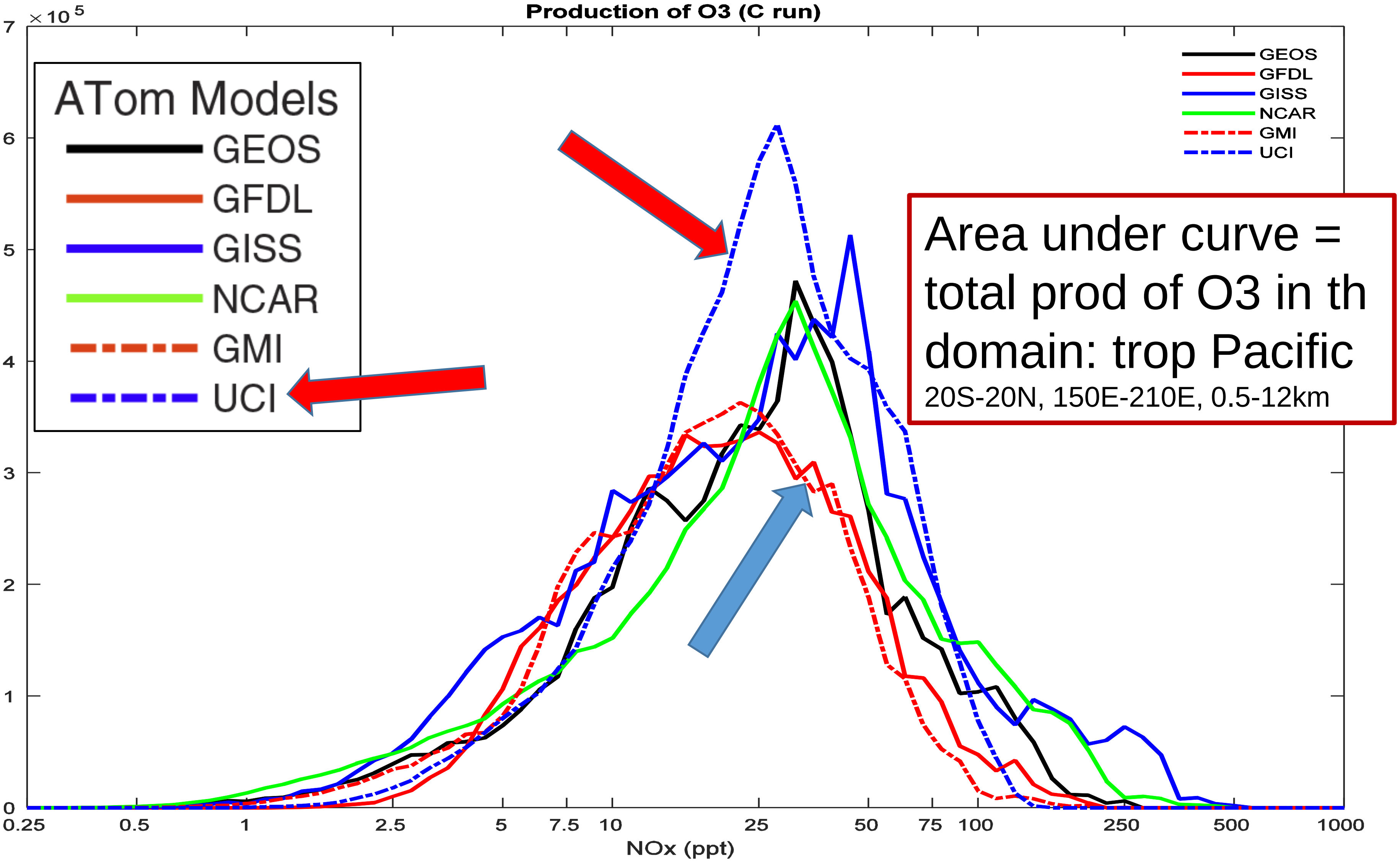
P-O3 (Pacific Basin)

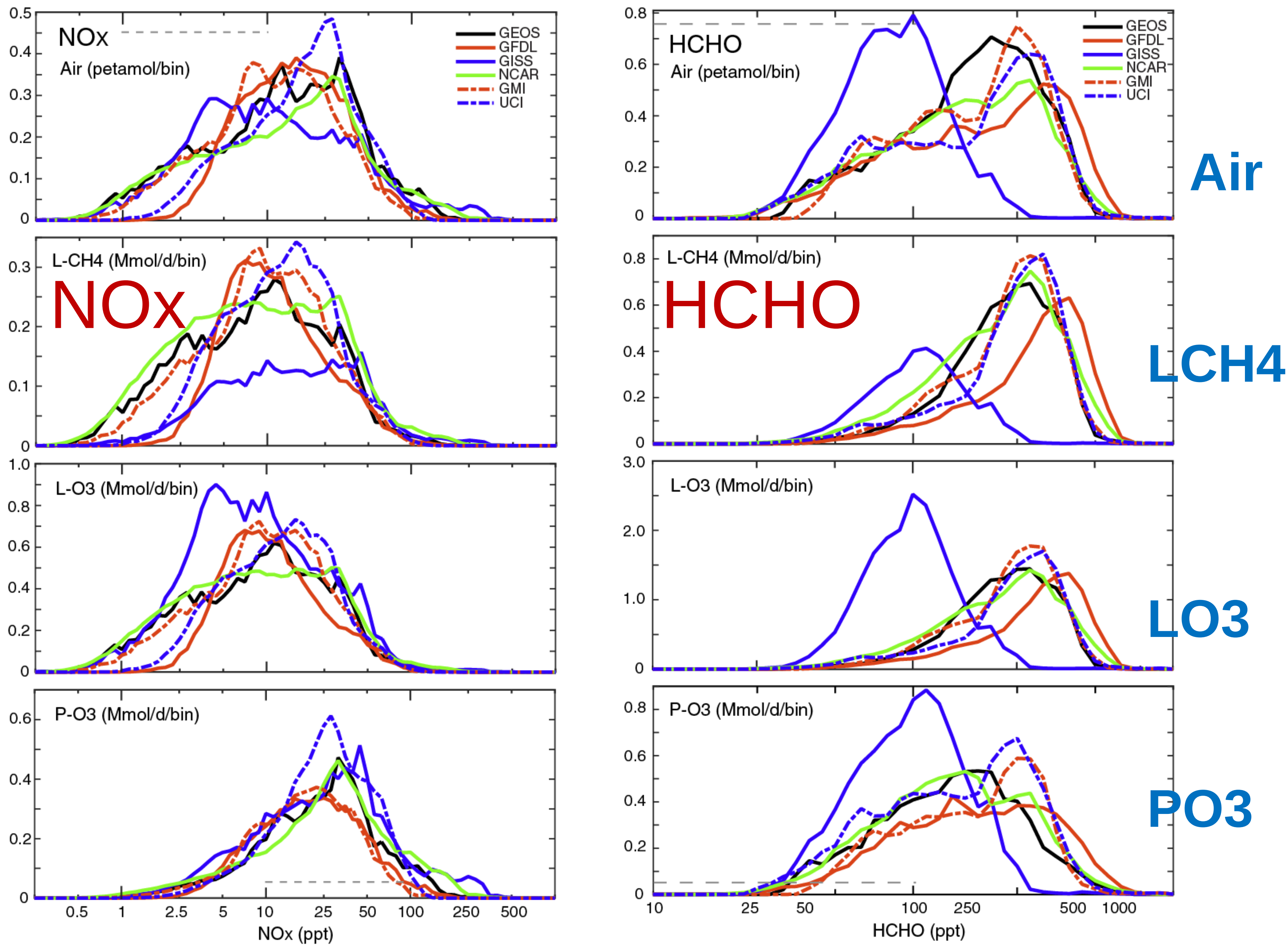


NOx prob distrib **0.25 to 1000 ppt**

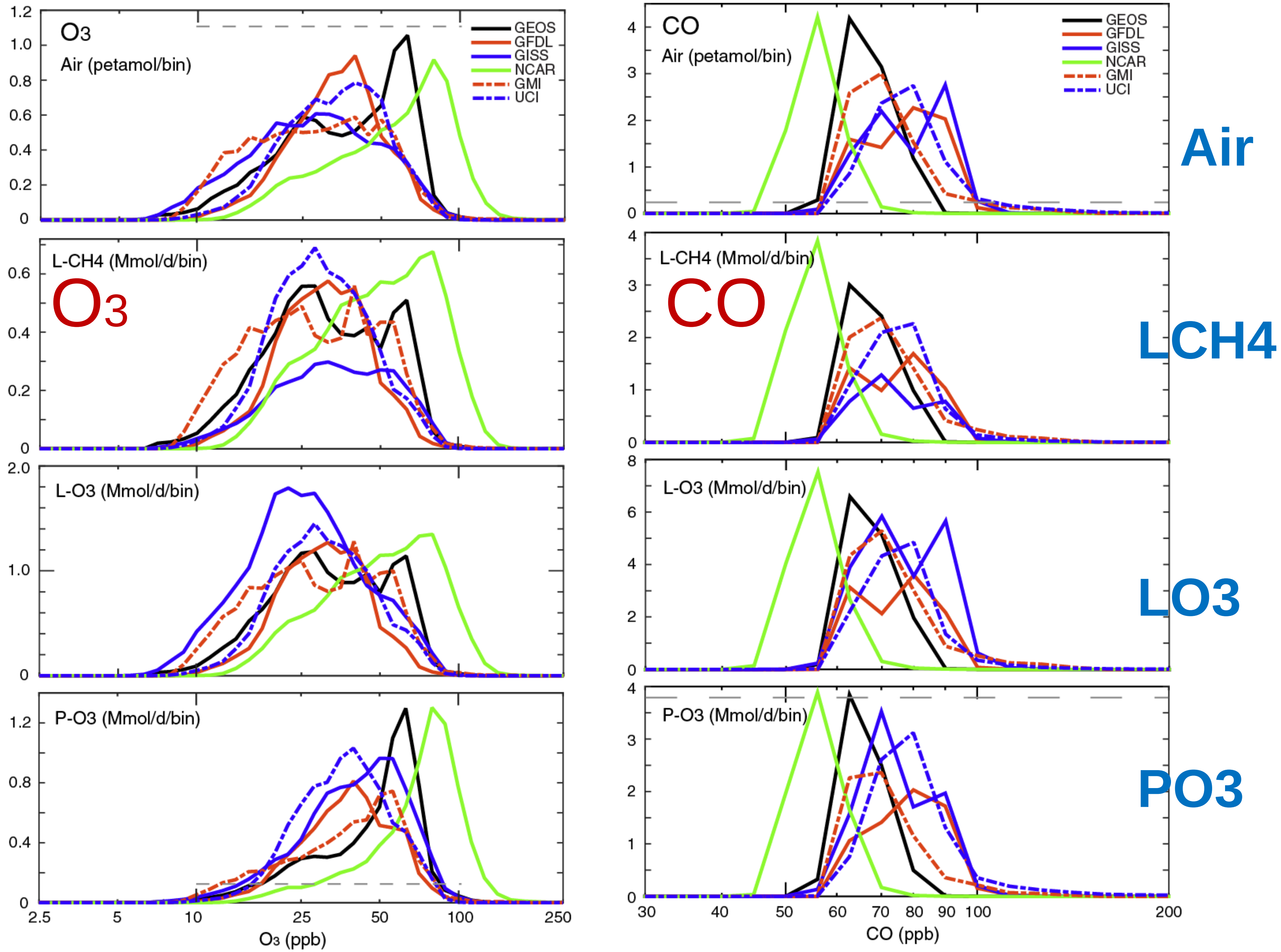
Trop Pac: 20S-20N, 150E-210E, 0.5-12km

P O3



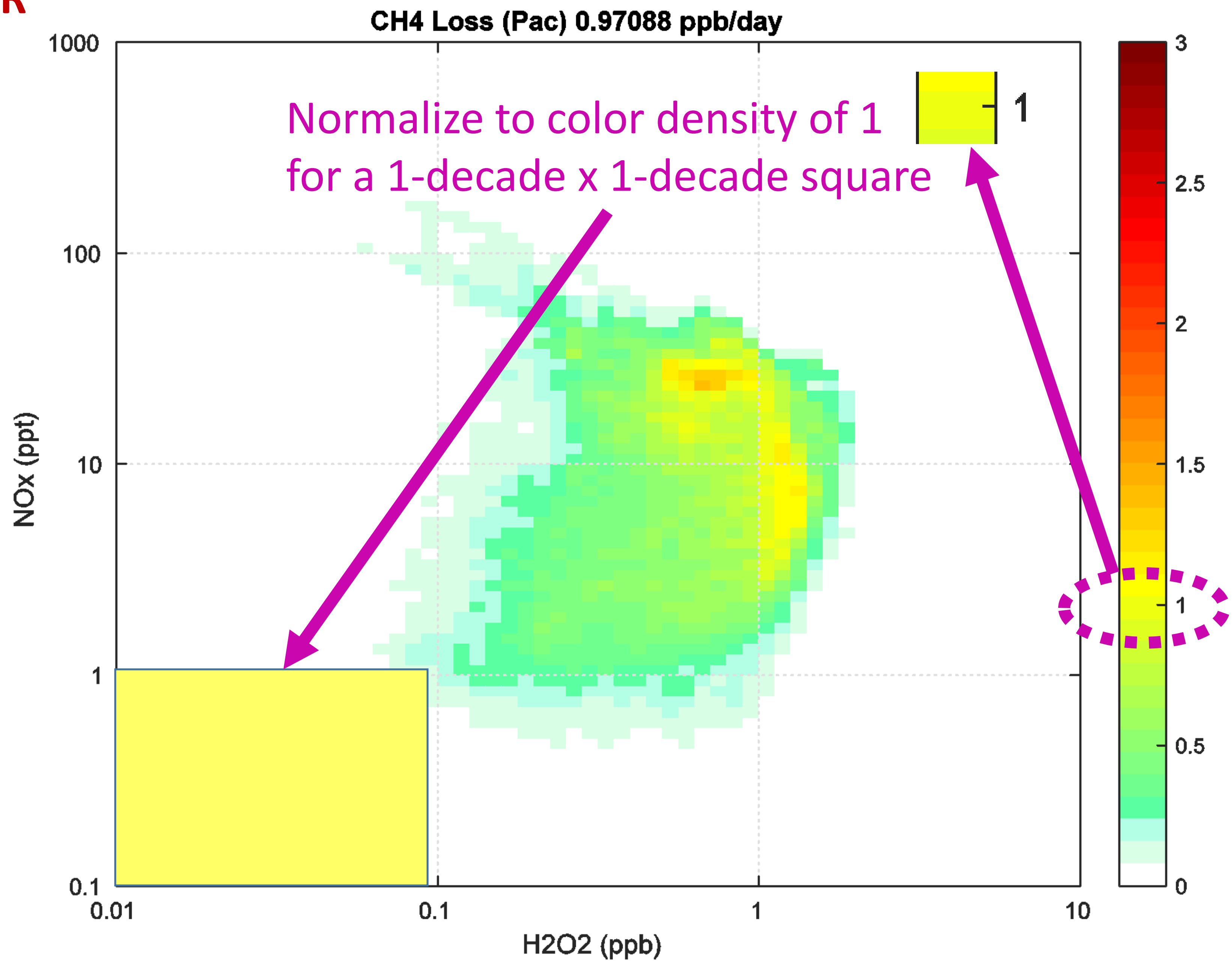


NOx
Air (petamol/bin)
GEOS
GFDL
GISS
NCAR
GMI
UCI
L-CH4 (Mmol/d/bin)
NOx
L-O3 (Mmol/d/bin)
P-O3 (Mmol/d/bin)
NOx (ppt)
HCHO
Air (petamol/bin)
L-CH4 (Mmol/d/bin)
HCHO
L-O3 (Mmol/d/bin)
P-O3 (Mmol/d/bin)
HCHO (ppt)
Air
LCH4
LO3
PO3



O3
Air (petamol/bin)
GEOS
GFDL
GISS
NCAR
GMI
UCI
L-CH4 (Mmol/d/bin)
L-O3 (Mmol/d/bin)
P-O3 (Mmol/d/bin)
O3 (ppb)
CO
CO (ppb)
Air
LCH4
LO3
PO3

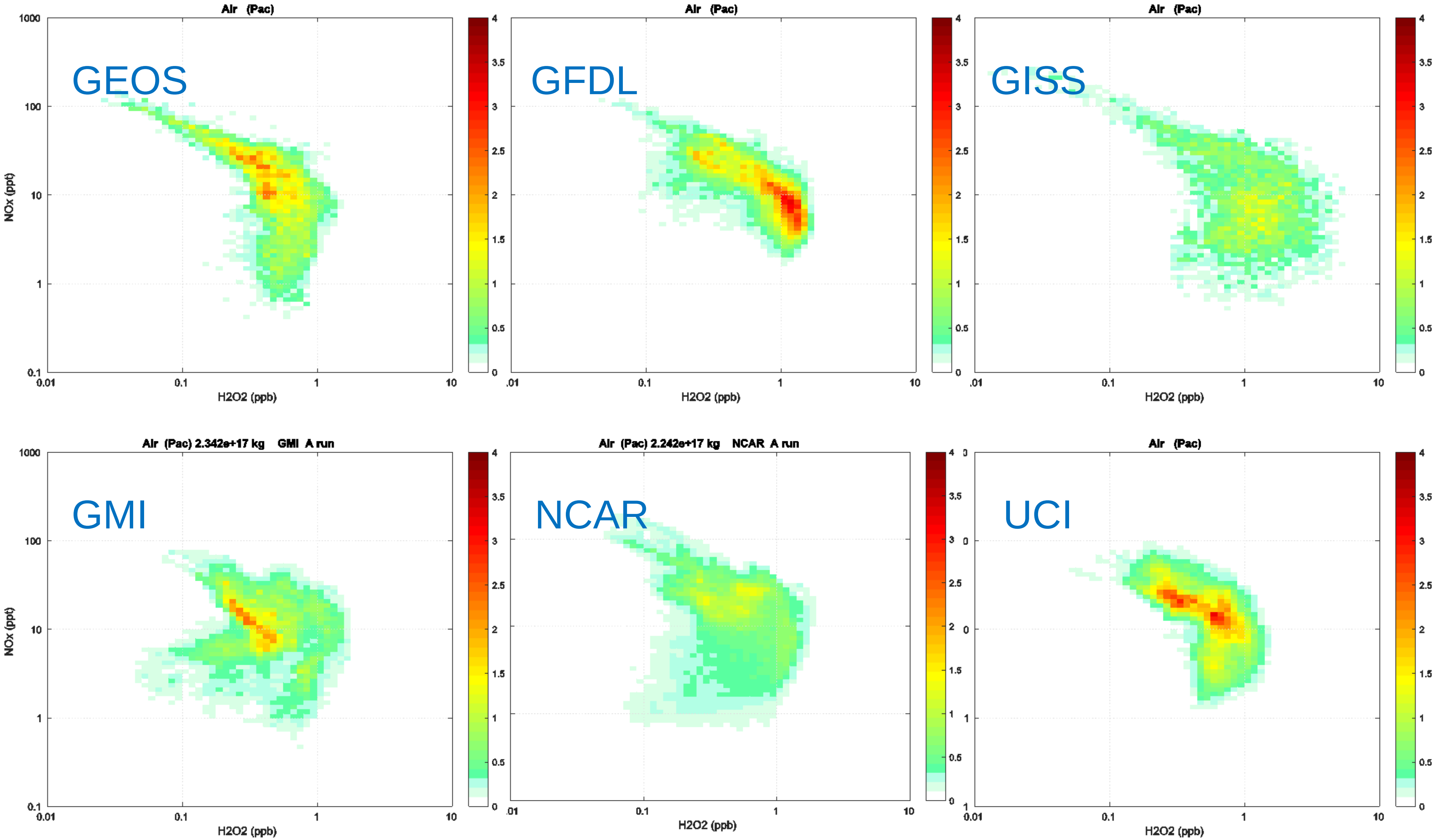
NCAR



CH4 Loss (Pac) 0.97088 ppb/day
Normalize to color density of 1
for a 1-decade x 1-decade square
1
1000
100
10
1
0.1
NOx (ppt)
0.01
0.1
1
10
H2O2 (ppb)
3
2.5
2
1.5
1
0.5
0

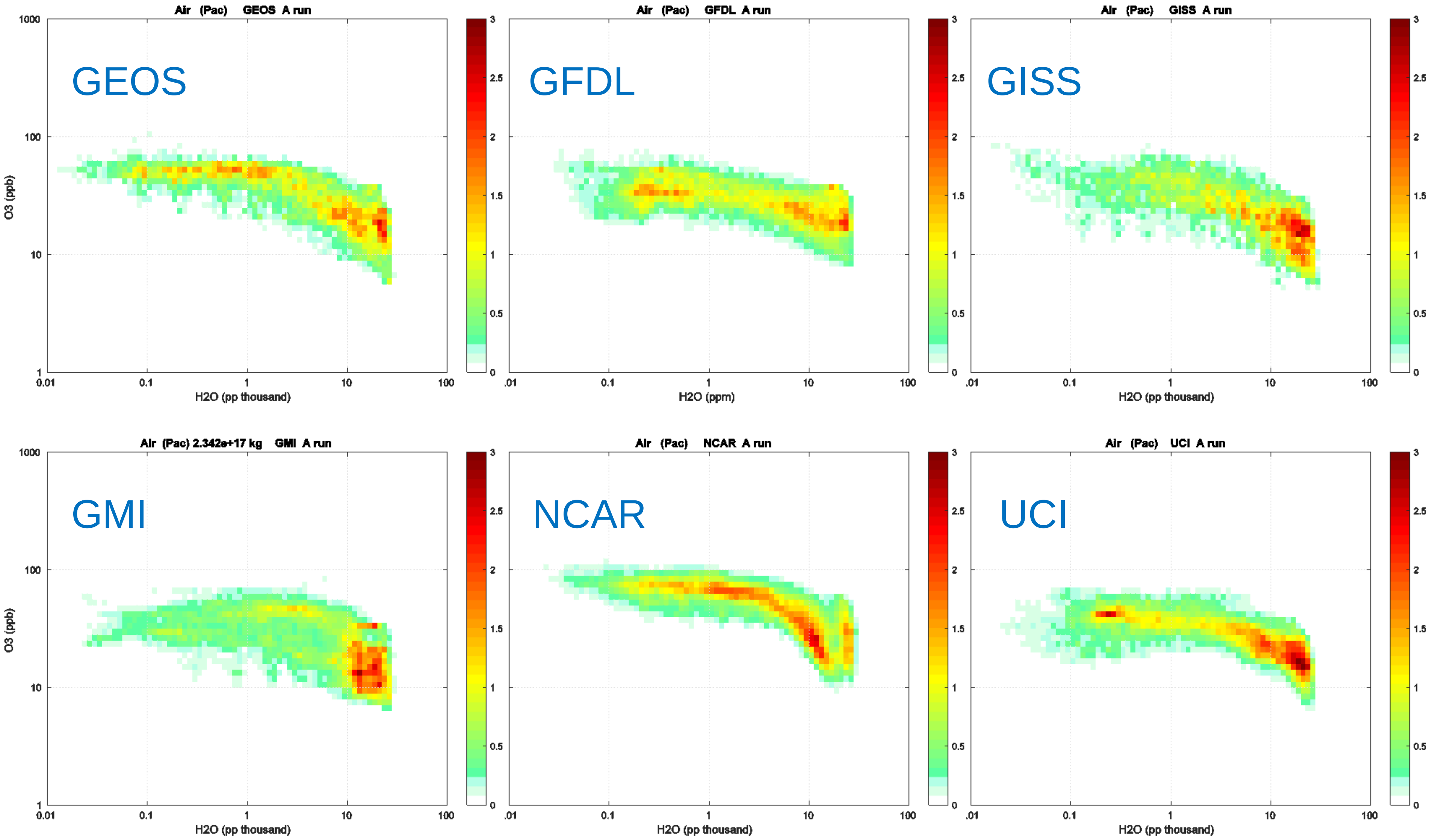
2D Prob Plots: **NOx x H2O2** wt'd by **Air**

A-runs,tropical Pacific sampling (20S-20N, 150E-150W, ½-12 km)



2D Prob Plots: **O3 x H2O** wt'd by **Air**

A-runs,tropical Pacific sampling (20S-20N, 150E-150W, ½-12 km)



Planned Deployment Schedules			
Deployment	**Upload**	**Flights**	**Download**
ATom-1, 2016	June 21-July 27	July 28-August 22	August 23-26
ATom-2, 2017	January 9-25	Jan 26-Feb 20	Feb 21-24
ATom-3, 2017	Sept 11-27	Sept 28- Oct 23	Oct 24-27
ATom-4, 2018	April 9-25	April 26-May 21	May 22-25

An overview of the NASA Atmospheric Tomography mission (ATom)

in-situ observations to constrain global-scale models

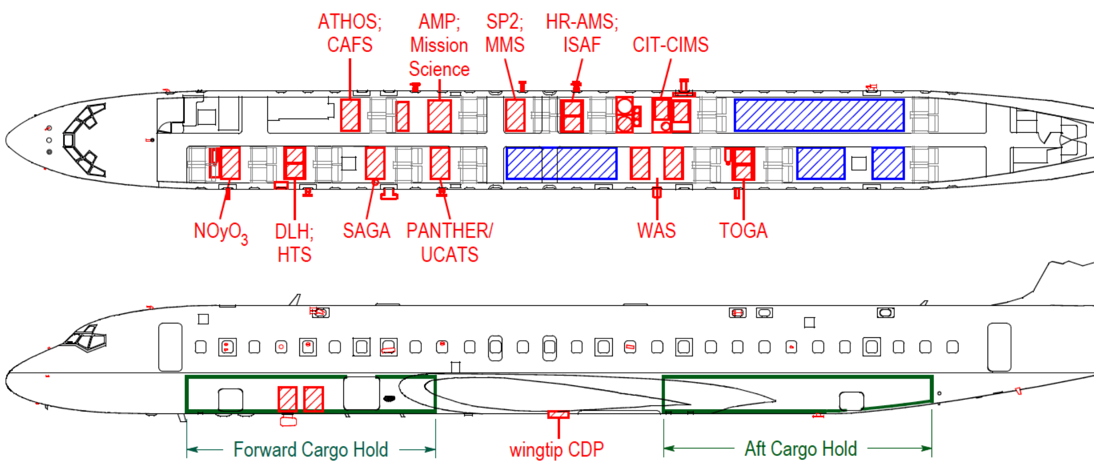
(1 of 4)

Table 4.2-1. ATom measurements, instruments, sample interval, and data quality exceed mission requirements. Core measurements for Tier 1 objectivesare shown in *italics*.

Reactive nitrogen

Species	Instrument(s)	Sampling interval	Data quality†
Reactive nitrogen			
Nitric oxide (NO)	NO_yO_3	1 s	10 ppt + 3%
Nitrogen dioxide (NO_2)	NO_yO_3	1 s	[illegible]
Nitric acid (HNO_3)	SAGA	1.5	
Nitric acid (HNO_3)	CIT-CIMS	1 s	
Pernitric acid (HNO_4)	CIT-CIMS	1 s	
Peroxyacetyl nitrate (PAN)	PANTHER	3 s ev	
C_1–C_6 alkyl nitrates ($RONO_2$)	WAS; TOGA	15-90	
Total reactive nitrogen (NO_y)	NO_yO_3	1 s	
VOCs			
C_2–C_{10} alkanes	WAS; TOGA	15-9	
C_2–C_5 alkenes	WAS; TOGA	15-9	
C_6–C_9 aromatics	WAS; TOGA	15-9	

VOCs



9 July 2016 – a packed DC8

An overview of the NASA Atmospheric Tomography mission (ATom)

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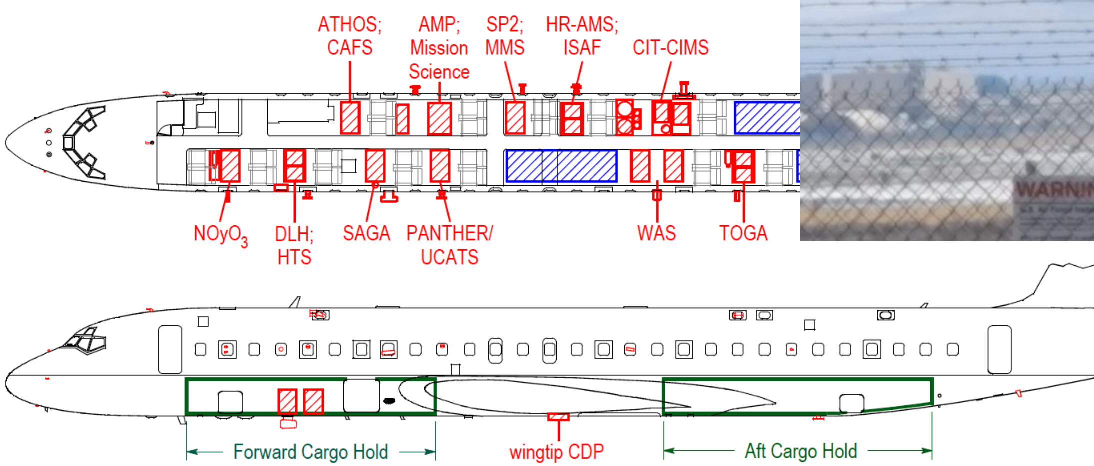
Photoproducts & Oxygenates

Photoproducts and oxygenates			
Ozone (O_3)	NO_yO_3; UCATS	1 s; 10 s	0.02 ppb + 2%
Formaldehyde (HCHO)	ISAF	1 s	10 ppt + 10%
C_2–C_5 aldehydes (RCHO)	TOGA	30 s every 2 min	3 ppt + 20%
Acetone ($CH_3C(O)CH_3$)	TOGA	30 s every 2 min	3 ppt + 20%
Methyl ethyl ketone ($CH_3C(O)C_2H_5$)	TOGA	30 s every 2 min	1 ppt + 20%
Methyl vinyl ketone ($CH_3C(O)C_2H_3$)	TOGA		
Methacrolein ($CH_2C(CH_3)CHO$)	TOGA		
Hydrogen peroxide (HOOH)	C		
Methyl peroxide (CH_3OOH)	C		
Formic acid (HCOOH)	C		
Acetic acid (CH_3COOH)	C		
Methanol (CH_3OH)	T		
Ethanol (CH_3CH_2OH)	T		
Hydroxyl radical (OH)	A		
Hydroperoxyl radical (HO_2)	A		
OH loss rate	A		

1 Aug 2016 – off to ANC



An overview of the NASA Atmospheric Tomography mission (ATom)

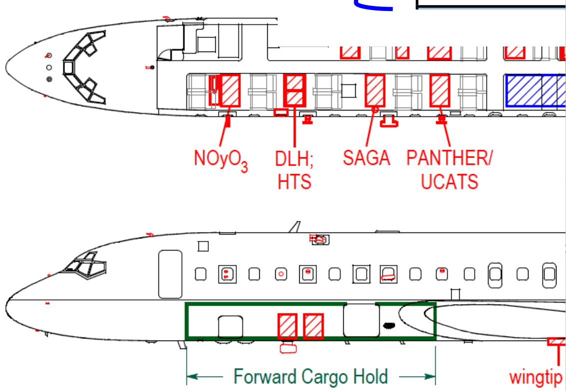
in-situ observations to constrain global-scale models

(3 of 4)

Aerosol composition and microphysics

GHGs and ODSs

Aerosol composition and microphysics			
Particle distribution (4–1000 nm)	AMP	1 s	14 cm^{-1} + 9%
Cloud drop distribution (2–50 µm)	AMP	1 s	20%
Black carbon mass and coating state	SP2	1 s	12 ng/kg + 30%
SO_4^{2-}, NO_3^-, Cl^-, NH_4^+	HR-AMS	1 s	0.1 µg/m^3 + 35%
Organic aerosol	HR-AMS		
Particle O/C, H/C, and OM/OC	HR-AMS		
Cl^-, Na^+, Ca^{2+}			
SO_4^{2-}, NO_3^-, Br^-,			
^7Be			
^{210}Pb			
Greenhouse ga			
Carbon dioxide (			
Methane (CH_4)			
Nitrous oxide (N			
Sulfur hexafluor			
CFCs, HCFCs, anc			
C_1–C_2 halides			



23 Aug 2016 – ATom-1 returns

An overview of the NASA Atmospheric Tomography mission (ATom)

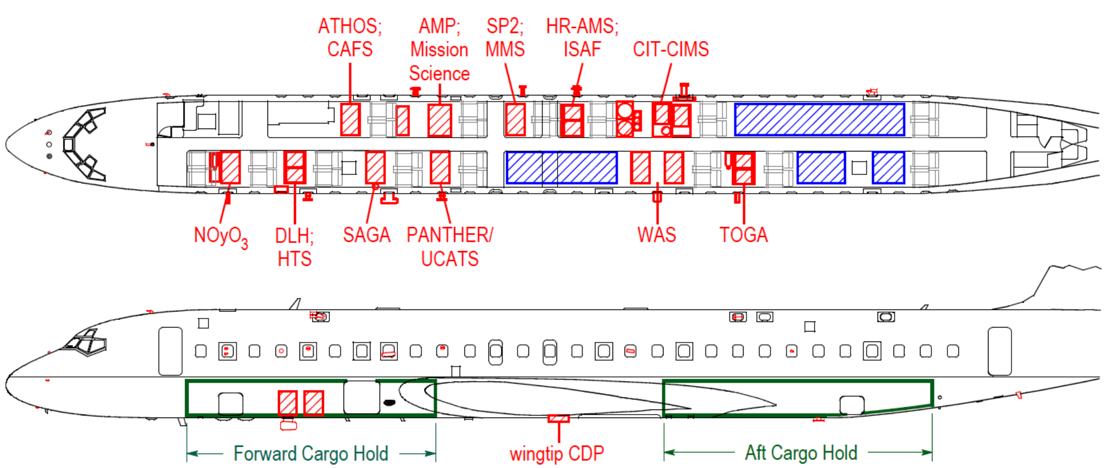
in-situ observations to constrain global-scale models

Tracers and other species

UV–Vis actinic flux

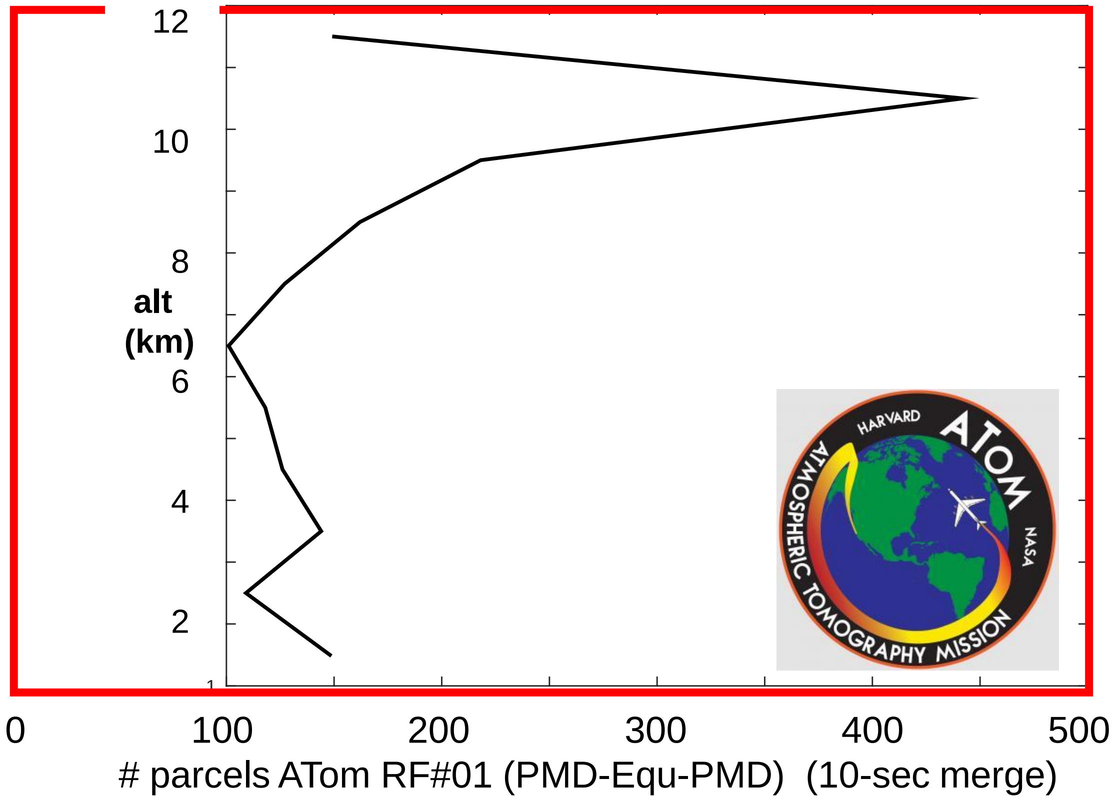
T, P, winds

Tracers and other species			
Carbon monoxide (CO)	HTS (2 sensors); PANTHER/ UCATS	1 s; 3 s every 2 min	0.1 ppb
Acetonitrile (CH_3CN)	TOGA	30 s every 2 min	5 ppt + 20%
Hydrogen cyanide (HCN)	CIT-CIMS	1 s	50 ppt + 30%
Water vapor (H_2O)	DLH; UCATS	1 s	0.2 ppm + 10%
Hydrogen (H_2)	PANTHER/UCATS	3s every 2 min	5 ppt + 2%
Sulfur dioxide (SO_2)	CIT-CIMS	1 s	
Dimethyl sulfide (CH_3SCH_3)	WAS; TOGA	15-90 s eve	
Dimethyl disulfide (CH_3SSCH_3)	WAS	15-90 s eve	
Carbonyl sulfide (OCS)	WAS; PANTHER	15-90 s eve	
Solar radiation			
spectrally-resolved actinic flux (280-650 nm)	CAFS	3 s	
Meteorological data			
Static P, static T, 3D winds; turbulence	MMS	0.05 s	



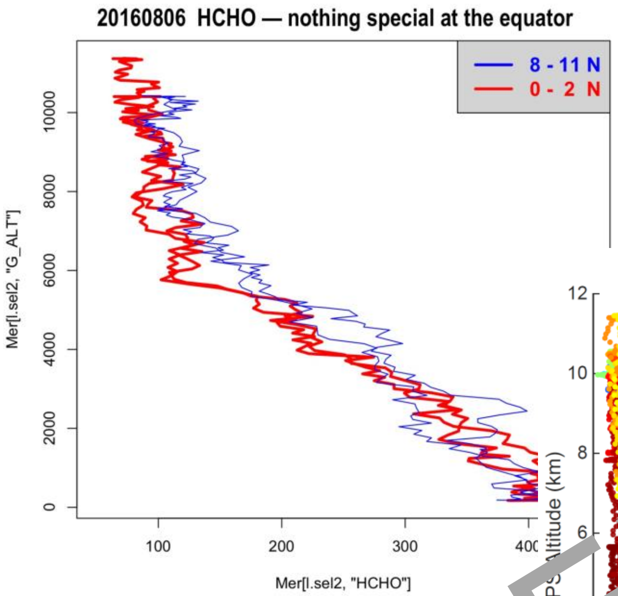
24/25 Aug 2016 – stripped

How to balance the non-uniform sampling from ATom

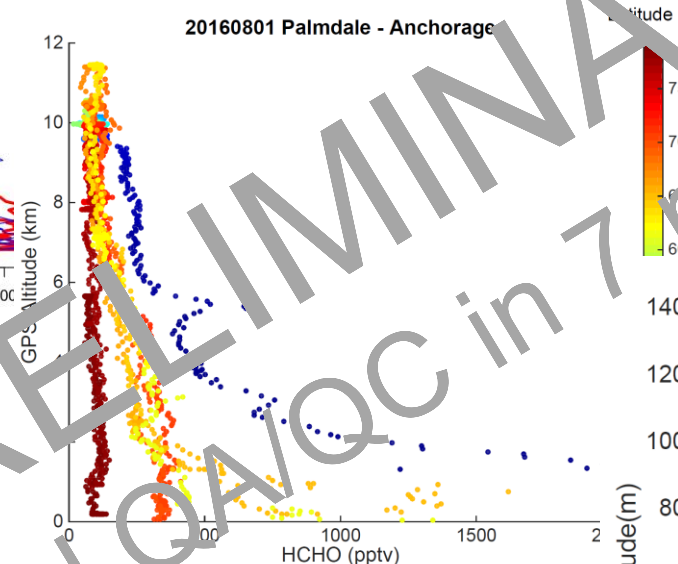


Remote profiles of HCHO for OMI/TROPOMI *a priori* …

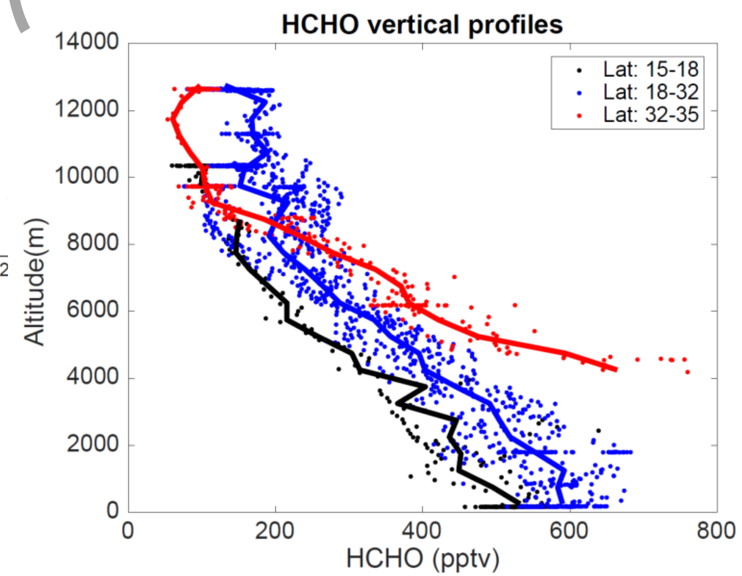
RF-04 KONA-PAGO



RF-02 PMD-ANC



TF-01 PMD-PMD



PRELIMINARY

Final QA/QC in 7 months

courtesy T. Hanisco